Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 06:03 AM EDT

PDB ID	:	4KXF
Title	:	Crystal structure of NLRC4 reveals its autoinhibition mechanism
Authors	:	Chai, J.; Hu, Z.
Deposited on	:	2013-05-25
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

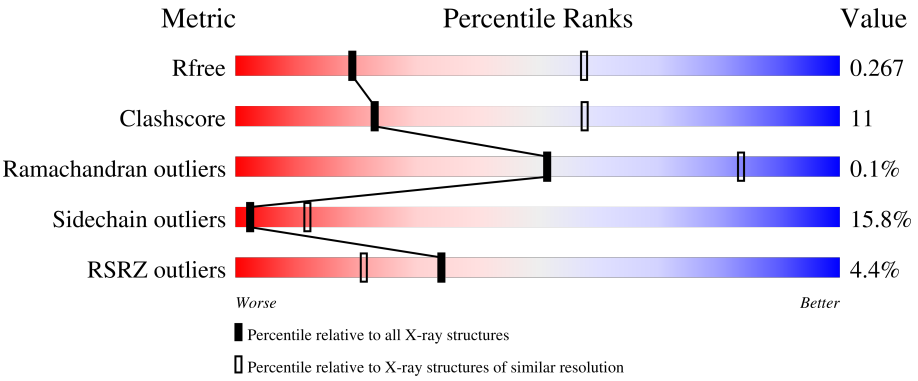
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1024	2% 57% 26% 5% 12%
1	D	1024	3% 58% 26% • 12%
1	F	1024	2% 58% 25% 5% 12%
1	H	1024	3% 57% 27% • 12%
1	K	1024	2% 56% 28% 5% 12%

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Mol	Chain	Length	Quality of chain
1	L	1024	2% 56% 26% 13%
1	N	1024	5% 52% 28% 5% 14%
1	P	1024	11% 52% 28% 15%

2 Entry composition (i)

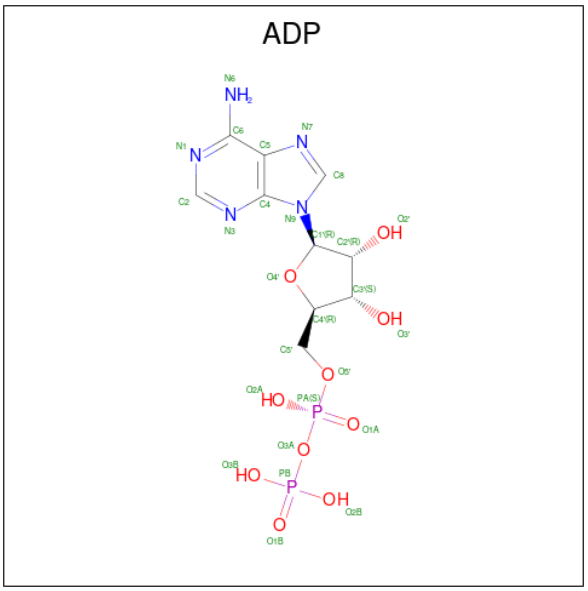
There are 3 unique types of molecules in this entry. The entry contains 57081 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NLR family CARD domain-containing protein 4.

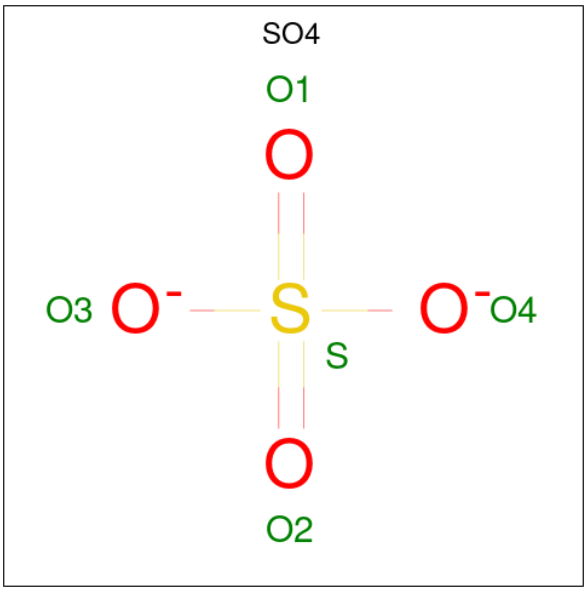
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	K	904	Total	C	N	O	P	S	0	0	0
			7208	4600	1215	1352	1	40			
1	B	903	Total	C	N	O	P	S	0	0	0
			7204	4599	1222	1342	1	40			
1	D	900	Total	C	N	O	P	S	0	0	0
			7177	4581	1208	1347	1	40			
1	F	899	Total	C	N	O	P	S	0	0	0
			7172	4577	1208	1346	1	40			
1	H	898	Total	C	N	O	P	S	0	0	0
			7135	4553	1201	1340	1	40			
1	L	893	Total	C	N	O	P	S	0	0	0
			7107	4540	1199	1327	1	40			
1	N	882	Total	C	N	O	S		0	0	0
			6996	4468	1181	1307	40				
1	P	866	Total	C	N	O	S		0	0	0
			6856	4377	1157	1282	40				

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



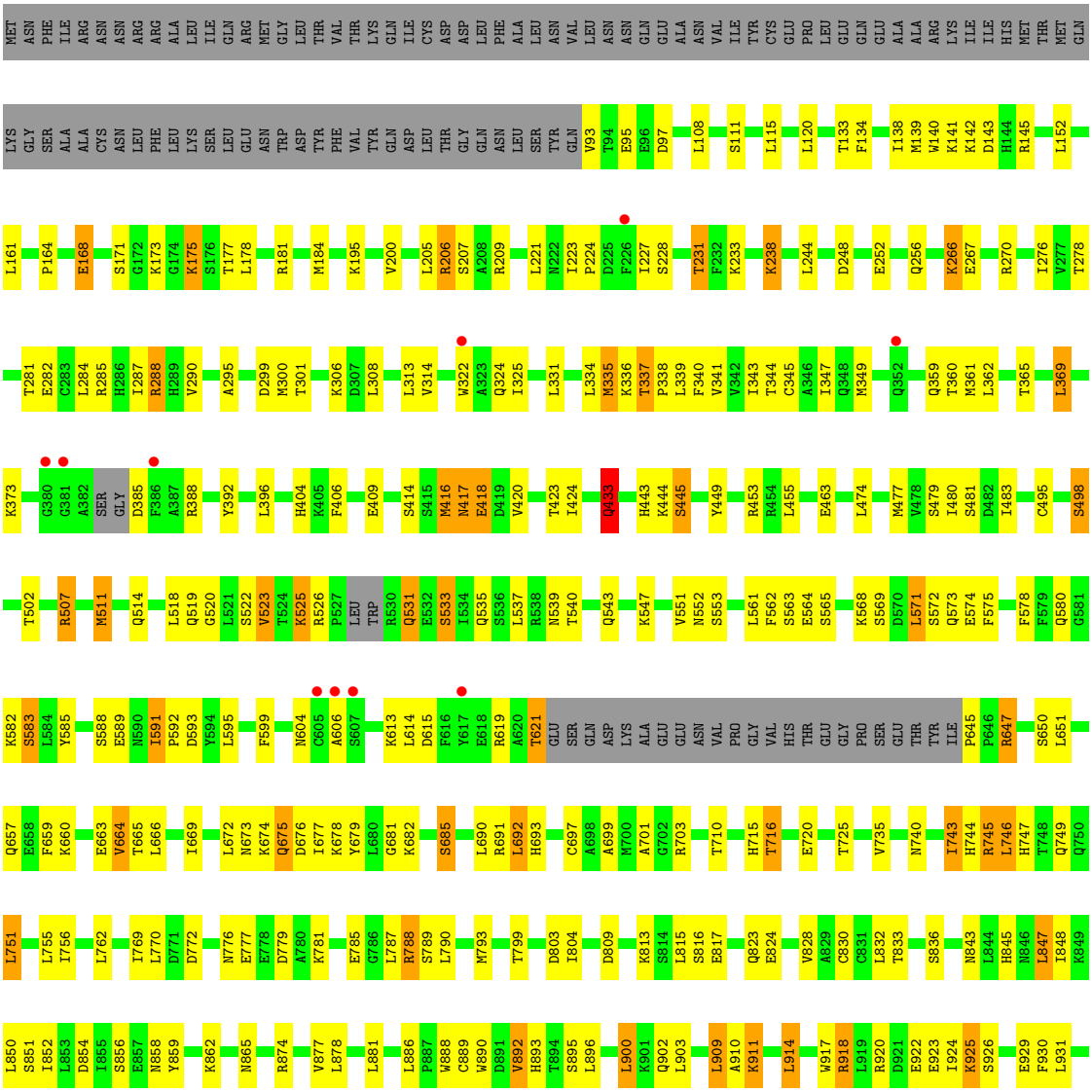
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0

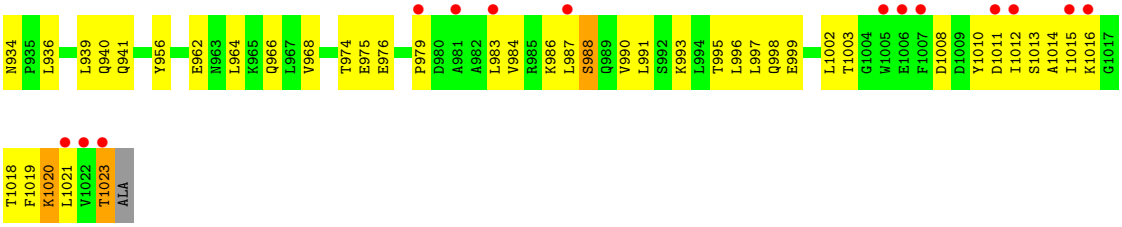
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NLR family CARD domain-containing protein 4

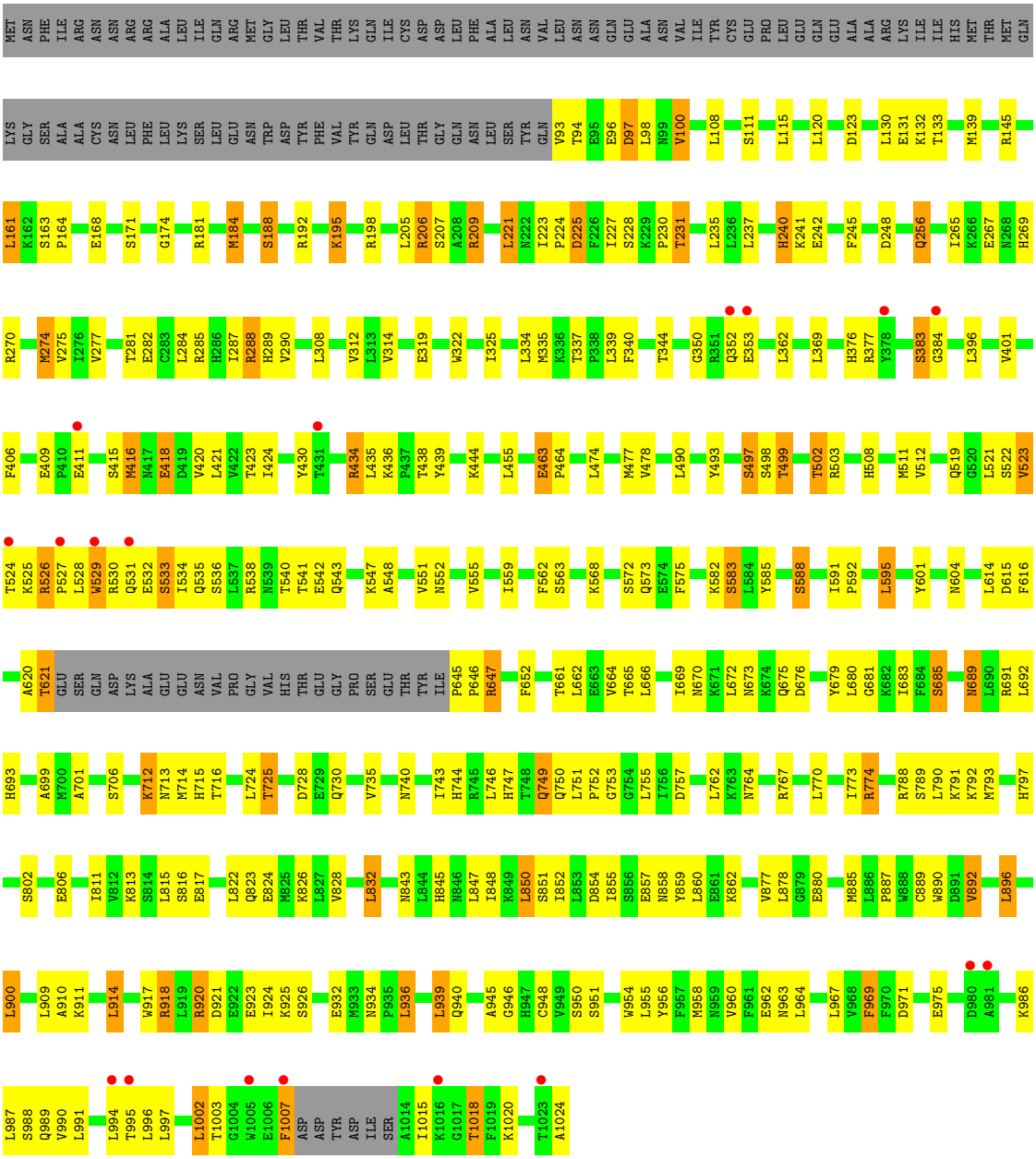
Chain K:





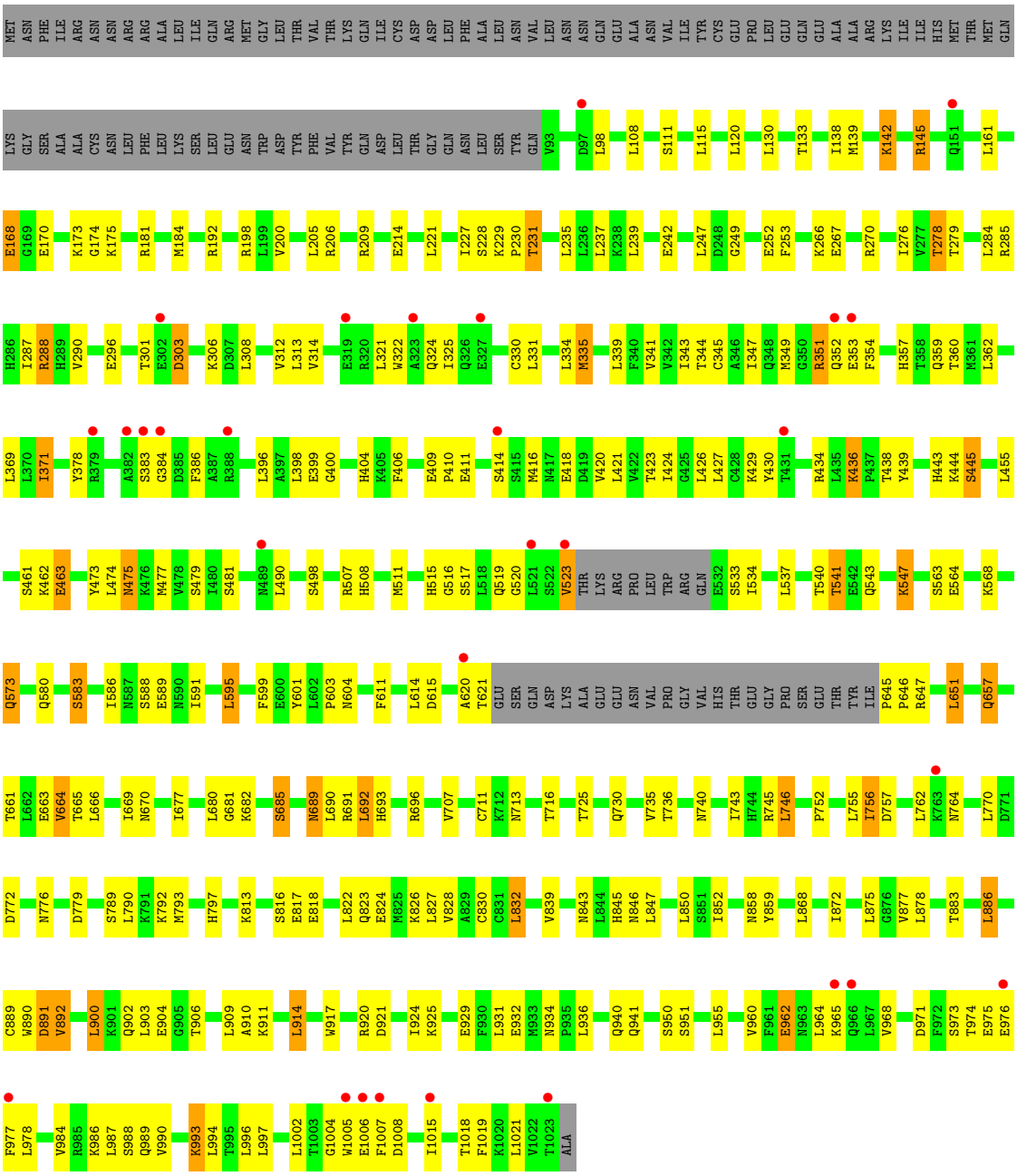
• Molecule 1: NLR family CARD domain-containing protein 4

Chain B:



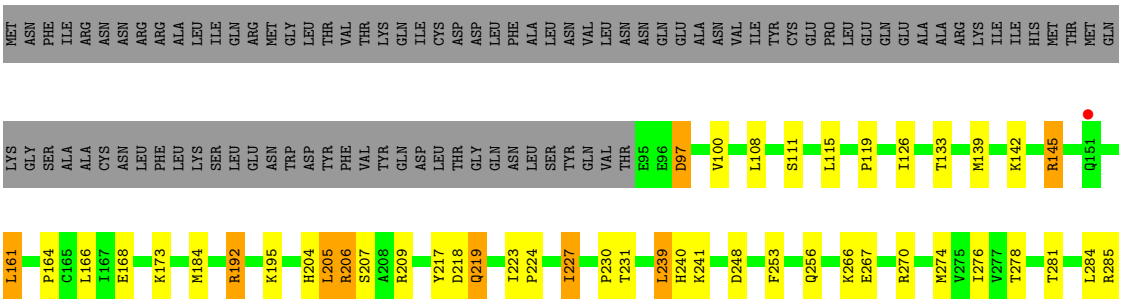
• Molecule 1: NLR family CARD domain-containing protein 4

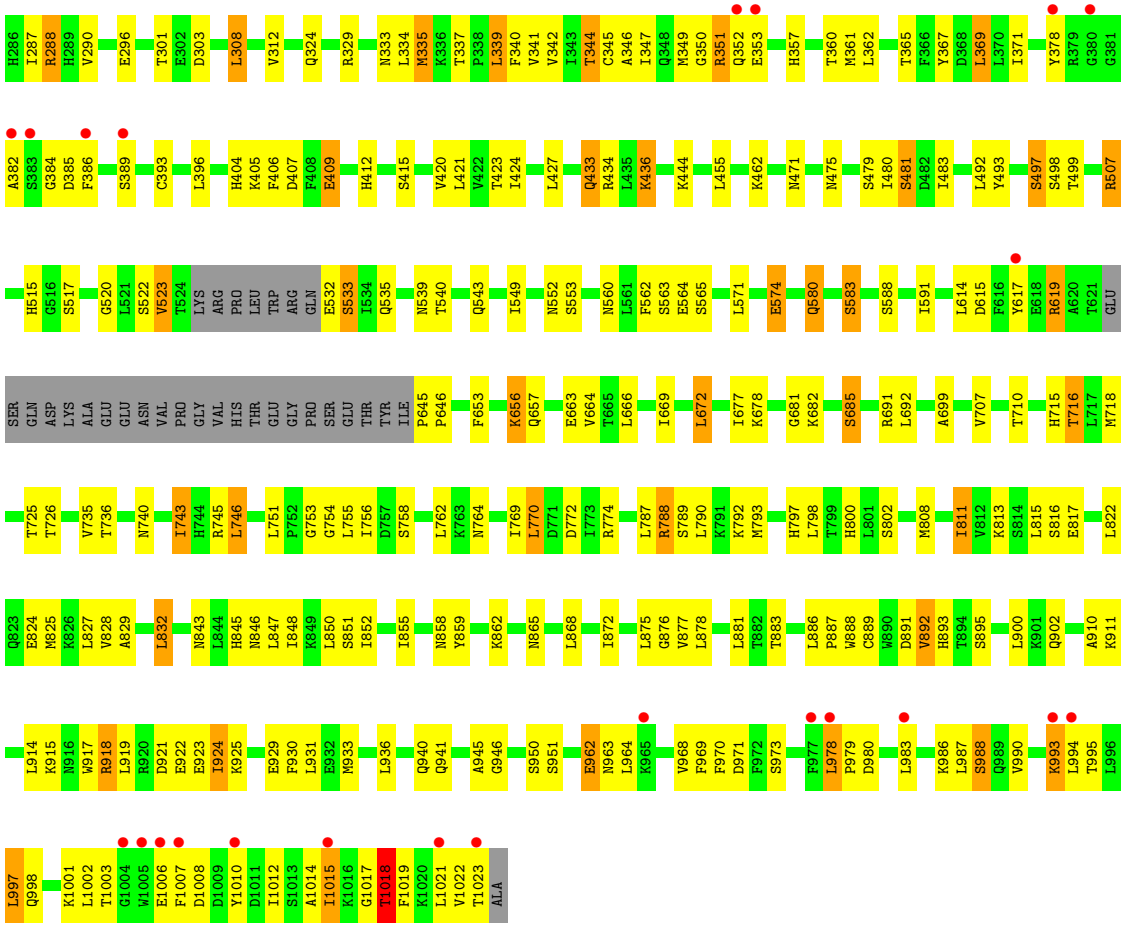
Chain D:



• Molecule 1: NLR family CARD domain-containing protein 4

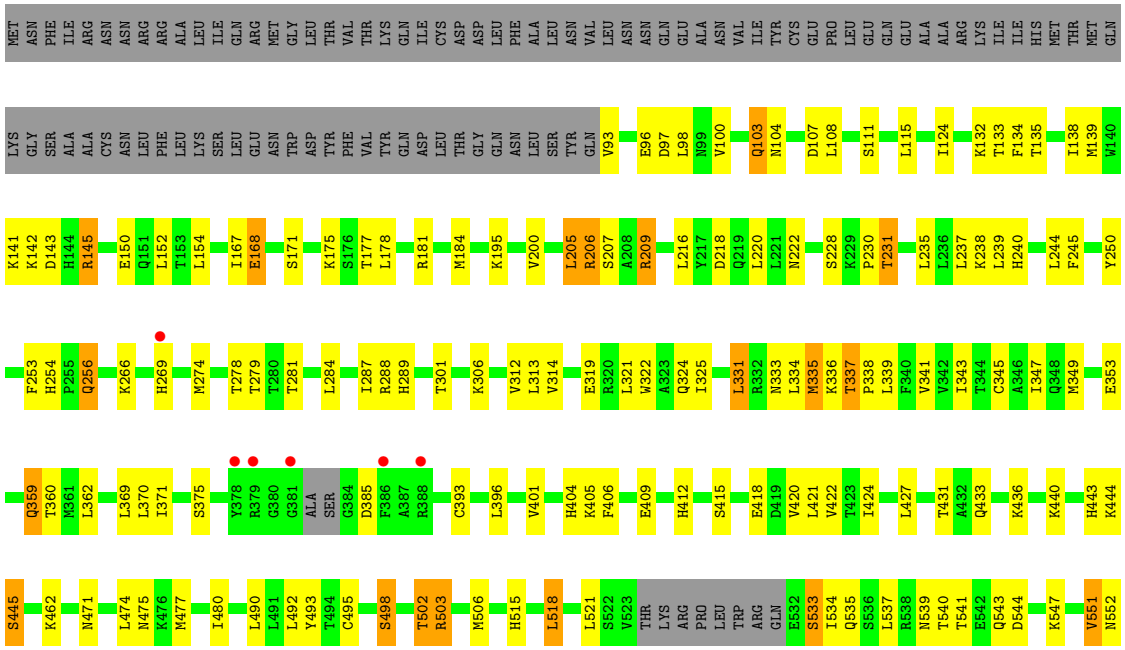
Chain F:

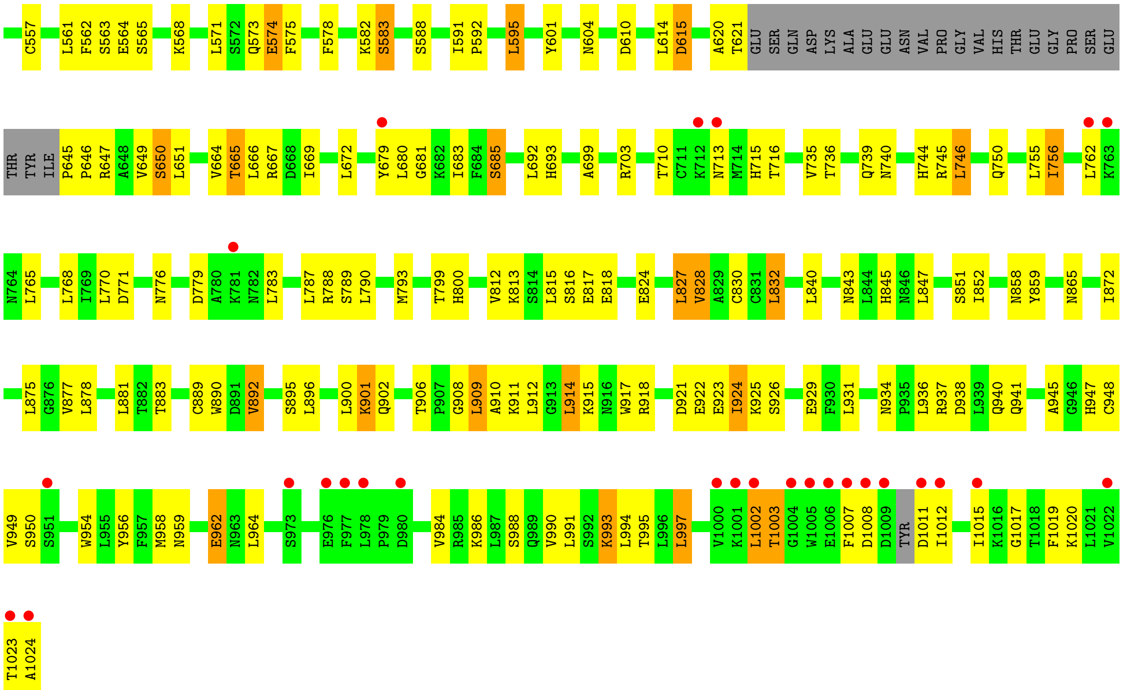




• Molecule 1: NLR family CARD domain-containing protein 4

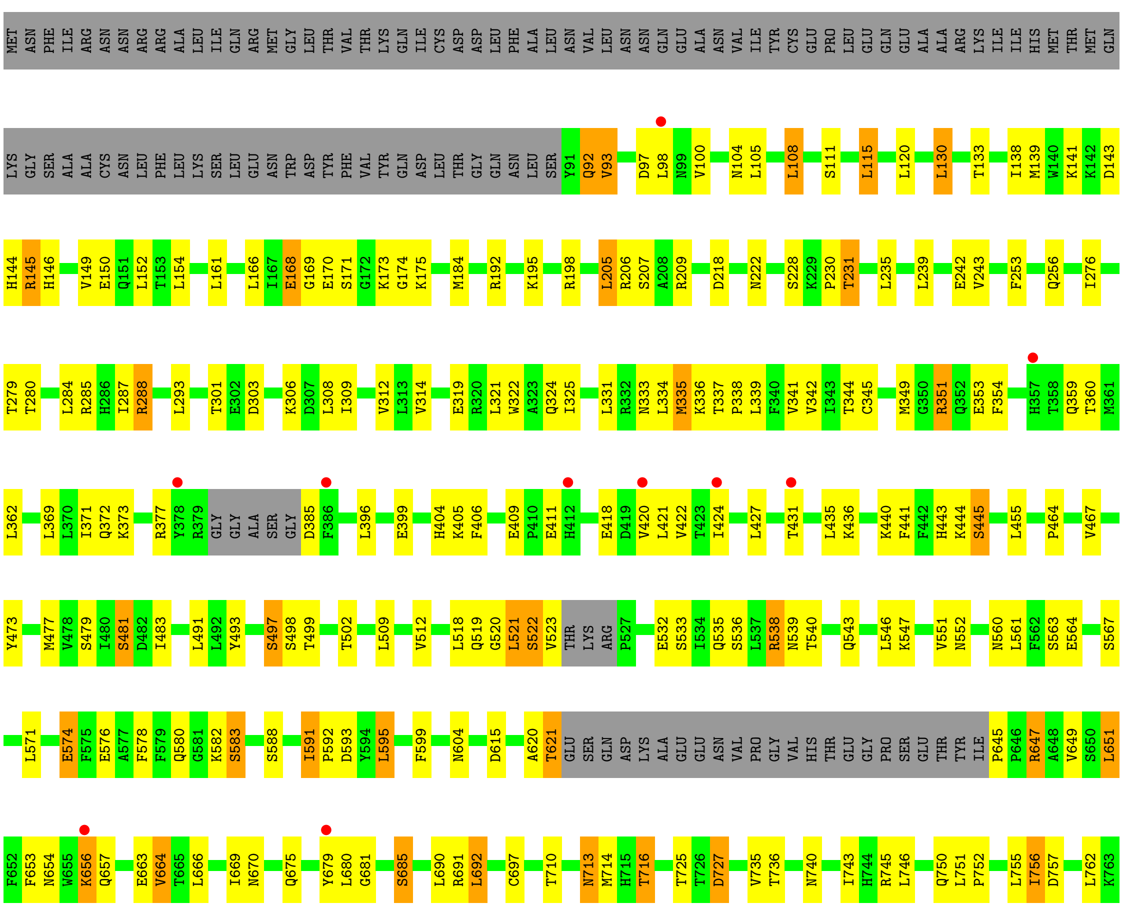
Chain H:

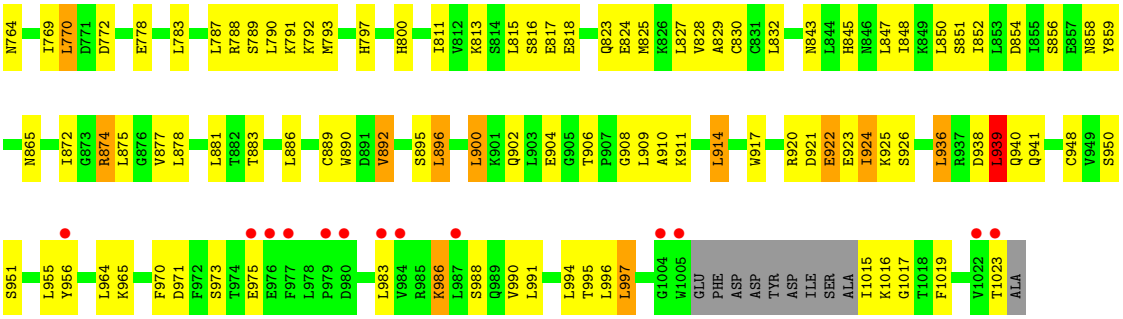




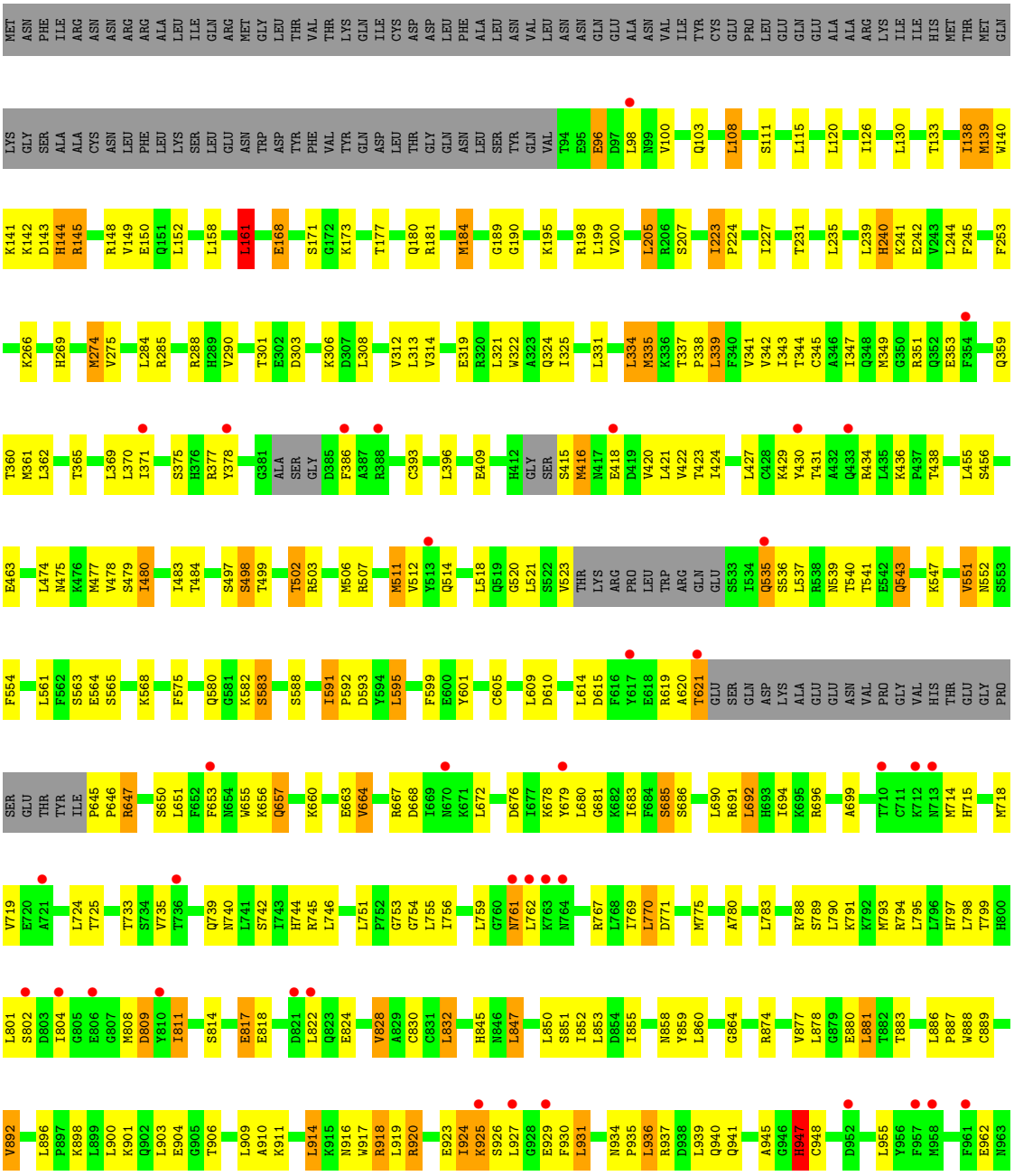
• Molecule 1: NLR family CARD domain-containing protein 4

Chain L:



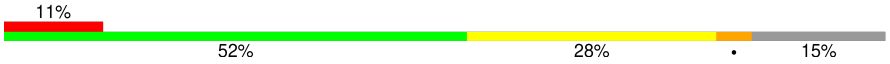


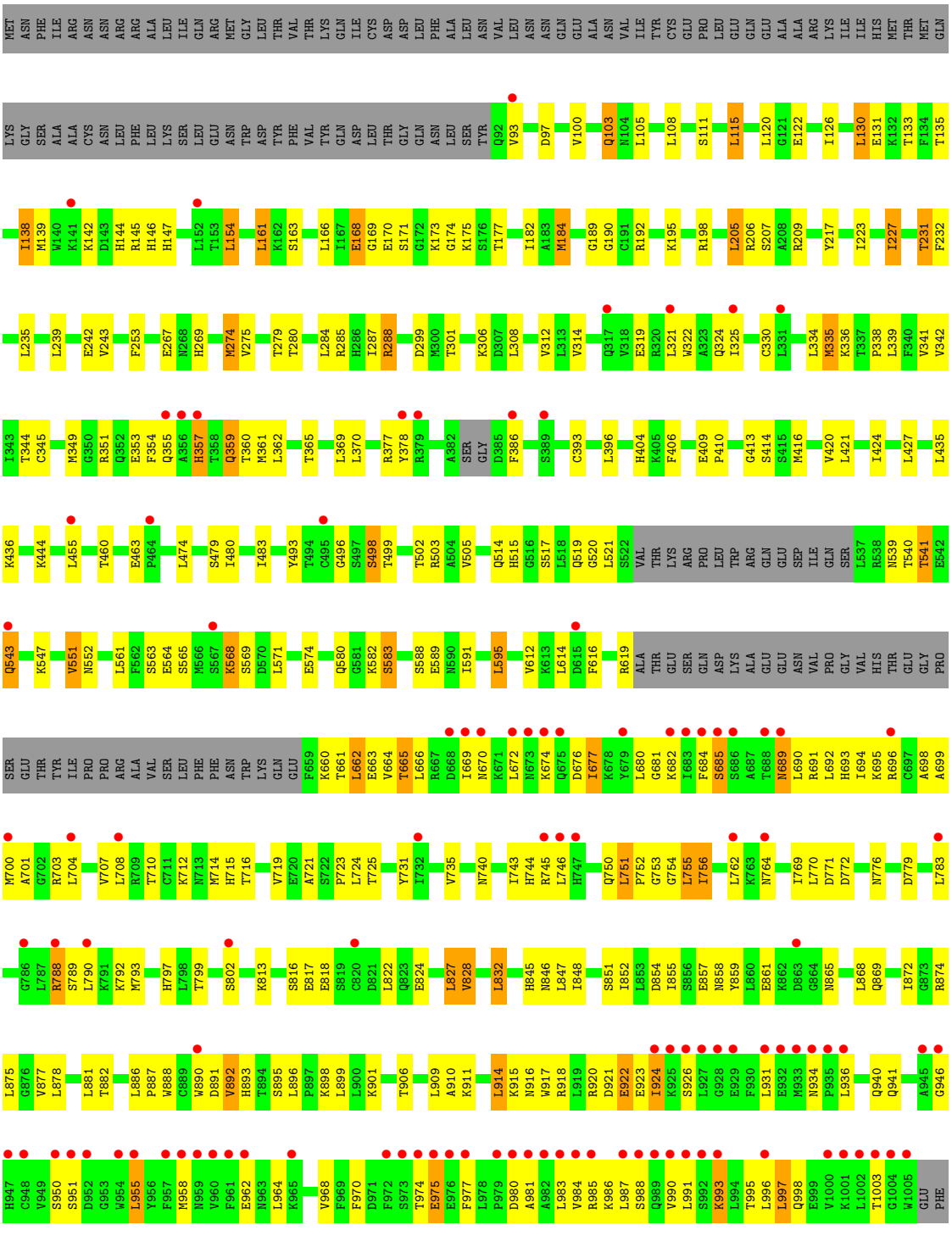
• Molecule 1: NLR family CARD domain-containing protein 4

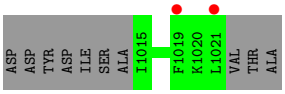


• Molecule 1: NLR family CARD domain-containing protein 4

Chain P:






ASP
ASP
TYR
ASP
ILE
SER
ALA
I1015
F1019
K1020
L1021
VAL
THR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	334.05Å 334.05Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.33 – 3.20 39.33 – 3.18	Depositor EDS
% Data completeness (in resolution range)	90.9 (39.33-3.20) 89.8 (39.33-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.226 , 0.266 0.227 , 0.267	Depositor DCC
R_{free} test set	7565 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 19.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	57081	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.28	0/7330	0.58	1/9897 (0.0%)
1	D	0.27	0/7301	0.53	0/9857
1	F	0.26	0/7296	0.52	0/9851
1	H	0.26	0/7256	0.53	0/9798
1	K	0.27	0/7332	0.57	2/9900 (0.0%)
1	L	0.28	0/7230	0.54	2/9766 (0.0%)
1	N	0.30	0/7119	0.59	2/9616 (0.0%)
1	P	0.27	0/6980	0.55	1/9426 (0.0%)
All	All	0.27	0/57844	0.55	8/78111 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
1	K	0	1
1	L	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	433	GLN	OE1-CD-NE2	-15.42	86.42	121.90
1	N	978	LEU	N-CA-C	-7.16	91.66	111.00
1	N	161	LEU	CA-CB-CG	6.39	130.01	115.30
1	B	161	LEU	CA-CB-CG	6.26	129.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	161	LEU	CA-CB-CG	5.76	128.56	115.30
1	K	751	LEU	CA-CB-CG	5.18	127.22	115.30
1	L	874	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	L	939	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	531	GLN	Peptide
1	F	412	HIS	Peptide
1	K	433	GLN	Sidechain
1	L	92	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7204	0	7237	163	0
1	D	7177	0	7190	148	0
1	F	7172	0	7186	168	0
1	H	7135	0	7126	156	0
1	K	7208	0	7216	172	2
1	L	7107	0	7104	158	0
1	N	6996	0	6969	197	0
1	P	6856	0	6838	166	0
2	B	27	0	12	1	0
2	D	27	0	12	1	0
2	F	27	0	12	1	0
2	H	27	0	12	0	0
2	K	27	0	12	2	0
2	L	27	0	12	1	0
2	N	27	0	12	0	0
2	P	27	0	12	2	0
3	B	5	0	0	0	0
3	N	5	0	0	0	0
All	All	57081	0	56962	1297	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:983:LEU:HA	1:P:986:LYS:CB	1.44	1.46
1:P:983:LEU:O	1:P:987:LEU:N	1.59	1.32
1:N:947:HIS:CE1	1:N:974:THR:OG1	1.92	1.22
1:P:983:LEU:CA	1:P:986:LYS:CB	2.32	1.06
1:L:145:ARG:HG2	1:L:523:VAL:HG11	1.39	1.01
1:L:145:ARG:HG2	1:L:523:VAL:CG1	1.89	1.00
1:P:981:ALA:HA	1:P:984:VAL:HB	1.55	0.86
1:N:916:ASN:H	1:N:945:ALA:HB3	1.39	0.85
1:N:947:HIS:ND1	1:N:974:THR:OG1	2.08	0.85
1:N:285:ARG:HH21	1:N:521:LEU:HD21	1.42	0.84
1:N:981:ALA:O	1:N:985:ARG:N	2.10	0.84
1:K:984:VAL:HG11	1:K:1011:ASP:HB3	1.60	0.82
1:N:975:GLU:OE2	1:N:975:GLU:HA	1.67	0.82
1:N:620:ALA:HB1	1:N:680:LEU:HD11	1.62	0.82
1:K:716:THR:HB	1:K:740:ASN:HB2	1.61	0.81
1:P:93:VAL:HG22	1:P:231:THR:HG22	1.62	0.81
1:H:845:HIS:HA	1:H:877:VAL:HG11	1.63	0.80
1:D:142:LYS:NZ	1:D:296:GLU:OE1	2.15	0.80
1:D:205:LEU:HD21	1:D:247:LEU:HB3	1.65	0.79
1:F:788:ARG:NH2	1:F:817:GLU:OE1	2.15	0.79
1:P:955:LEU:HD12	1:P:983:LEU:CB	2.13	0.78
1:B:591:ILE:O	1:B:647:ARG:NH1	2.15	0.78
1:P:962:GLU:HG3	1:P:990:VAL:HG13	1.66	0.78
1:K:911:LYS:HG3	1:K:941:GLN:HG2	1.66	0.78
1:N:975:GLU:OE2	1:N:975:GLU:CA	2.29	0.78
1:H:908:GLY:HA2	1:H:938:ASP:HB2	1.67	0.77
1:H:788:ARG:NH2	1:H:817:GLU:OE1	2.18	0.77
1:L:145:ARG:CG	1:L:523:VAL:HG11	2.14	0.76
1:N:808:MET:HA	1:N:811:ILE:HG23	1.67	0.76
1:P:983:LEU:O	1:P:986:LYS:CA	2.33	0.76
1:B:522:SER:HB3	1:B:525:LYS:HG3	1.65	0.75
1:L:921:ASP:OD1	1:L:950:SER:OG	2.04	0.75
1:K:344:THR:HG22	1:K:362:LEU:HD11	1.66	0.75
1:K:591:ILE:O	1:K:647:ARG:NH1	2.19	0.75
1:N:830:CYS:O	1:N:858:ASN:ND2	2.18	0.75
1:P:745:ARG:HA	1:P:772:ASP:HB3	1.69	0.75
1:H:962:GLU:HG2	1:H:993:LYS:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:874:ARG:HG3	1:L:874:ARG:HH11	1.52	0.73
1:N:783:LEU:HD21	1:N:798:LEU:HD22	1.70	0.73
1:N:975:GLU:O	1:N:976:GLU:CB	2.29	0.73
1:D:205:LEU:HB3	1:D:253:PHE:HB2	1.68	0.73
1:F:285:ARG:NH1	1:F:517:SER:O	2.22	0.73
1:P:719:VAL:HB	1:P:743:ILE:HG22	1.71	0.73
1:P:788:ARG:NH1	1:P:817:GLU:OE2	2.22	0.73
1:D:620:ALA:HB1	1:D:680:LEU:HD11	1.71	0.73
1:N:756:ILE:HD11	1:N:783:LEU:HB2	1.71	0.73
1:K:531:GLN:HG2	1:K:769:ILE:HD13	1.70	0.73
1:H:672:LEU:HB2	1:H:699:ALA:HB1	1.71	0.73
1:L:591:ILE:O	1:L:647:ARG:NH1	2.21	0.72
1:P:921:ASP:OD1	1:P:950:SER:OG	2.07	0.72
1:L:716:THR:HB	1:L:740:ASN:HB2	1.71	0.72
1:P:816:SER:O	1:P:846:ASN:ND2	2.22	0.72
1:P:845:HIS:HA	1:P:877:VAL:HG11	1.69	0.72
1:B:288:ARG:NH2	1:B:522:SER:O	2.23	0.72
1:F:816:SER:O	1:F:846:ASN:ND2	2.22	0.72
1:K:621:THR:OG1	1:K:676:ASP:OD1	2.08	0.72
1:B:816:SER:HB2	1:B:843:ASN:HB2	1.71	0.72
1:D:830:CYS:O	1:D:858:ASN:ND2	2.23	0.72
1:H:620:ALA:HB1	1:H:680:LEU:HD11	1.71	0.72
1:B:621:THR:OG1	1:B:676:ASP:OD1	2.08	0.71
1:L:908:GLY:HA2	1:L:938:ASP:HB2	1.72	0.71
1:K:284:LEU:HG	1:K:288:ARG:HG3	1.72	0.71
1:P:716:THR:HG22	1:P:740:ASN:HD22	1.54	0.71
1:F:552:ASN:OD1	1:F:583:SER:OG	2.09	0.71
1:B:701:ALA:O	1:B:725:THR:OG1	2.07	0.70
1:L:170:GLU:O	1:L:175:LYS:NZ	2.24	0.70
1:B:1002:LEU:HD23	1:B:1007:PHE:HE2	1.55	0.70
1:L:681:GLY:O	1:L:685:SER:OG	2.09	0.70
1:N:973:SER:O	1:N:974:THR:OG1	2.09	0.70
1:B:184:MET:O	1:B:188:SER:OG	2.10	0.70
1:K:675:GLN:HA	1:K:678:LYS:HE2	1.74	0.70
1:H:592:PRO:HD2	1:H:595:LEU:HD23	1.74	0.70
1:L:552:ASN:OD1	1:L:583:SER:OG	2.11	0.69
1:L:334:LEU:HD23	1:L:362:LEU:HD22	1.75	0.69
1:P:324:GLN:HE22	1:P:354:PHE:H	1.40	0.69
1:K:526:ARG:HD2	1:K:999:GLU:HB2	1.75	0.69
1:F:344:THR:HG23	1:F:362:LEU:HD11	1.74	0.69
1:L:98:LEU:HD13	1:L:235:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:170:GLU:O	1:P:175:LYS:NZ	2.25	0.69
1:P:983:LEU:O	1:P:986:LYS:C	2.29	0.69
1:K:369:LEU:HD22	1:K:373:LYS:HD3	1.75	0.69
1:N:591:ILE:O	1:N:647:ARG:NH1	2.26	0.68
1:P:958:MET:HB3	1:P:990:VAL:HG21	1.75	0.68
1:N:974:THR:HG22	1:N:975:GLU:H	1.58	0.68
1:D:911:LYS:HG2	1:D:941:GLN:HG2	1.74	0.68
1:D:463:GLU:HG3	1:F:774:ARG:HH22	1.58	0.68
1:H:256:GLN:HG2	1:L:230:PRO:HG3	1.75	0.68
1:P:324:GLN:NE2	1:P:354:PHE:O	2.27	0.68
1:D:383:SER:OG	1:D:384:GLY:N	2.26	0.68
1:F:288:ARG:NH1	1:F:522:SER:O	2.26	0.68
1:P:93:VAL:HG21	1:P:235:LEU:HB2	1.76	0.68
1:K:845:HIS:HA	1:K:877:VAL:HG11	1.77	0.67
1:P:515:HIS:CD2	1:P:547:LYS:HD3	2.28	0.67
1:F:334:LEU:HD13	1:F:362:LEU:HD22	1.76	0.67
1:P:163:SER:HB2	1:P:274:MET:HE3	1.77	0.67
1:K:788:ARG:NH1	1:K:817:GLU:OE1	2.27	0.67
1:B:256:GLN:HG2	1:F:230:PRO:HG3	1.77	0.67
1:K:552:ASN:OD1	1:K:583:SER:OG	2.12	0.67
1:B:592:PRO:HD2	1:B:595:LEU:HD23	1.76	0.67
1:K:228:SER:HG	1:K:231:THR:HG1	1.39	0.66
1:B:681:GLY:O	1:B:685:SER:OG	2.13	0.66
1:L:920:ARG:NH2	1:L:922:GLU:OE1	2.28	0.66
1:N:552:ASN:OD1	1:N:583:SER:OG	2.13	0.66
1:N:920:ARG:HG2	1:N:923:GLU:HG2	1.77	0.66
1:F:142:LYS:NZ	1:F:296:GLU:OE1	2.29	0.66
1:B:896:LEU:HD12	1:B:923:GLU:HB3	1.77	0.66
1:D:344:THR:HG22	1:D:362:LEU:HD11	1.78	0.66
1:P:174:GLY:N	2:P:1101:ADP:O3B	2.28	0.66
1:K:681:GLY:O	1:K:685:SER:OG	2.13	0.66
1:N:224:PRO:HB2	1:N:227:ILE:HG13	1.78	0.66
1:K:824:GLU:HG2	1:K:852:ILE:HB	1.77	0.66
1:F:285:ARG:NH1	1:F:481:SER:OG	2.30	0.65
1:N:98:LEU:HD11	1:N:199:LEU:HD11	1.77	0.65
1:N:918:ARG:NH2	1:N:948:CYS:SG	2.61	0.65
1:P:983:LEU:O	1:P:986:LYS:N	2.29	0.65
1:K:417:ASN:N	1:K:417:ASN:OD1	2.29	0.65
1:D:540:THR:HG23	1:D:541:THR:HG22	1.78	0.65
1:L:166:LEU:HD22	1:L:287:ILE:HD12	1.78	0.65
1:N:416:MET:SD	1:N:416:MET:N	2.68	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:975:GLU:OE2	1:N:975:GLU:N	2.30	0.65
1:L:830:CYS:O	1:L:858:ASN:ND2	2.26	0.65
1:P:975:GLU:O	1:P:977:PHE:N	2.30	0.65
1:K:511:MET:O	1:K:511:MET:HG2	1.97	0.65
1:D:568:LYS:HD3	1:D:601:TYR:CZ	2.31	0.65
1:N:681:GLY:O	1:N:685:SER:OG	2.14	0.65
1:P:227:ILE:HD11	1:P:232:PHE:HD1	1.60	0.65
1:L:727:ASP:OD2	1:L:727:ASP:N	2.29	0.65
1:B:334:LEU:HD13	1:B:362:LEU:HD22	1.78	0.65
1:B:228:SER:OG	1:B:231:THR:OG1	2.10	0.65
1:K:968:VAL:HG13	1:K:998:GLN:HB2	1.78	0.64
1:F:754:GLY:O	1:F:758:SER:OG	2.13	0.64
1:P:981:ALA:O	1:P:984:VAL:N	2.30	0.64
1:D:325:ILE:HD11	1:D:335:MET:HE2	1.80	0.64
1:F:533:SEP:O1P	1:F:535:GLN:NE2	2.30	0.64
1:L:592:PRO:HD2	1:L:595:LEU:HD22	1.80	0.64
1:K:526:ARG:NH2	1:K:1020:LYS:HB3	2.13	0.64
1:B:963:ASN:HD21	1:F:986:LYS:HE3	1.62	0.64
1:F:350:GLY:HA3	1:F:369:LEU:HD11	1.80	0.64
1:F:808:MET:HA	1:F:811:ILE:HG23	1.78	0.64
1:K:224:PRO:HB2	1:K:227:ILE:HG13	1.79	0.63
1:H:98:LEU:HD13	1:H:235:LEU:HD11	1.80	0.63
1:N:344:THR:HG22	1:N:362:LEU:HD11	1.80	0.63
1:N:845:HIS:HA	1:N:877:VAL:HG11	1.79	0.63
1:N:718:MET:HG2	1:N:742:SER:HB3	1.80	0.63
1:B:284:LEU:HG	1:B:288:ARG:HG3	1.80	0.63
1:K:325:ILE:HG12	1:K:331:LEU:HD23	1.78	0.63
1:B:588:SER:OG	1:B:615:ASP:O	2.15	0.63
1:D:816:SER:O	1:D:846:ASN:ND2	2.31	0.63
1:B:661:THR:HG23	1:B:689:ASN:HB3	1.80	0.63
1:D:910:ALA:O	1:D:940:GLN:N	2.28	0.63
1:L:713:ASN:N	1:L:713:ASN:OD1	2.31	0.63
1:K:787:LEU:HD13	1:K:815:LEU:HD21	1.80	0.62
1:F:588:SER:HB2	1:F:645:PRO:HD2	1.80	0.62
1:L:620:ALA:HB1	1:L:680:LEU:HD11	1.81	0.62
1:N:663:GLU:OE2	1:N:691:ARG:NH1	2.31	0.62
1:D:962:GLU:HG2	1:D:993:LYS:HD2	1.80	0.62
1:H:145:ARG:NH2	1:H:533:SEP:O1P	2.33	0.62
1:H:552:ASN:OD1	1:H:583:SER:OG	2.16	0.62
1:L:851:SER:HA	1:L:881:LEU:HA	1.80	0.62
1:F:480:ILE:HG12	1:F:515:HIS:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:663:GLU:OE2	1:K:691:ARG:NH1	2.32	0.62
1:D:284:LEU:HG	1:D:288:ARG:HG3	1.80	0.62
1:P:983:LEU:C	1:P:986:LYS:H	2.02	0.62
1:B:925:LYS:HA	1:B:956:TYR:HE2	1.64	0.62
1:F:340:PHE:O	1:F:344:THR:OG1	2.17	0.62
1:H:1002:LEU:HD23	1:H:1007:PHE:HE2	1.63	0.62
1:B:289:HIS:CD2	1:B:290:VAL:HG23	2.35	0.62
1:D:852:ILE:HG12	1:D:883:THR:HB	1.82	0.62
1:F:962:GLU:HG2	1:F:993:LYS:HD2	1.82	0.62
1:F:206:ARG:HG2	1:F:207:SER:N	2.13	0.62
1:H:824:GLU:HG2	1:H:852:ILE:HB	1.81	0.62
1:F:681:GLY:O	1:F:685:SER:OG	2.17	0.62
1:L:845:HIS:HA	1:L:877:VAL:HG11	1.80	0.62
1:N:983:LEU:O	1:N:987:LEU:HB2	2.00	0.62
1:P:743:ILE:HD11	1:P:755:LEU:HD11	1.81	0.61
1:D:378:TYR:HD1	1:D:386:PHE:HD1	1.45	0.61
1:N:847:LEU:HD13	1:N:850:LEU:HD13	1.82	0.61
1:B:163:SER:HB2	1:B:274:MET:HE3	1.82	0.61
1:B:123:ASP:OD1	1:B:377:ARG:NH2	2.31	0.61
1:B:526:ARG:HB3	1:B:527:PRO:HD3	1.82	0.61
1:D:399:GLU:OE1	1:D:473:TYR:OH	2.16	0.61
1:K:809:ASP:OD1	1:K:833:THR:OG1	2.18	0.61
1:K:859:TYR:CE1	1:K:889:CYS:HA	2.36	0.61
1:D:267:GLU:OE1	1:D:270:ARG:NH1	2.33	0.61
1:L:205:LEU:HB3	1:L:253:PHE:HB2	1.80	0.61
1:H:924:ILE:HG12	1:H:949:VAL:HG21	1.82	0.61
1:K:335:MET:HE3	1:K:341:VAL:HA	1.83	0.60
1:F:672:LEU:HB2	1:F:699:ALA:HB1	1.81	0.60
1:F:161:LEU:HD11	1:F:276:ILE:HD11	1.82	0.60
1:N:621:THR:OG1	1:N:676:ASP:OD1	2.19	0.60
1:D:868:LEU:HD11	1:D:886:LEU:HD13	1.83	0.60
1:H:108:LEU:O	1:H:111:SER:OG	2.20	0.60
1:L:143:ASP:OD2	1:L:144:HIS:N	2.34	0.60
1:N:809:ASP:N	1:N:809:ASP:OD2	2.35	0.60
1:P:981:ALA:O	1:P:985:ARG:N	2.29	0.60
1:P:962:GLU:HG2	1:P:993:LYS:HD2	1.82	0.60
1:F:224:PRO:HB2	1:F:227:ILE:HG23	1.83	0.60
1:H:744:HIS:NE2	1:H:771:ASP:OD2	2.34	0.60
1:L:145:ARG:HG2	1:L:523:VAL:CB	2.31	0.60
1:P:217:TYR:HA	1:P:223:ILE:HD13	1.83	0.60
1:K:200:VAL:HG22	1:K:244:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:154:LEU:HD21	1:P:182:ILE:HG12	1.83	0.60
1:K:141:LYS:HB2	1:K:152:LEU:HD11	1.84	0.60
1:F:745:ARG:HA	1:F:772:ASP:HB3	1.84	0.60
1:H:666:LEU:HB3	1:H:669:ILE:HD12	1.84	0.60
1:N:973:SER:C	1:N:974:THR:OG1	2.39	0.60
1:D:921:ASP:OD1	1:D:950:SER:OG	2.20	0.60
1:L:971:ASP:OD1	1:L:973:SER:OG	2.18	0.60
1:D:971:ASP:OD1	1:D:973:SER:OG	2.19	0.60
1:B:614:LEU:HD11	1:B:652:PHE:HZ	1.67	0.60
1:B:749:GLN:OE1	1:B:750:GLN:N	2.34	0.60
1:P:619:ARG:H	1:P:669:ILE:HG12	1.67	0.60
1:H:250:TYR:OH	1:H:266:LYS:NZ	2.34	0.59
1:K:299:ASP:HB3	1:K:336:LYS:HB3	1.84	0.59
1:B:987:LEU:O	1:B:991:LEU:HB2	2.02	0.59
1:F:971:ASP:OD1	1:F:973:SER:OG	2.19	0.59
1:K:672:LEU:HB2	1:K:699:ALA:HB1	1.85	0.59
1:H:288:ARG:HH21	1:H:521:LEU:HA	1.66	0.59
1:N:889:CYS:SG	1:N:892:VAL:HG13	2.43	0.59
1:P:681:GLY:O	1:P:685:SER:OG	2.20	0.59
1:K:701:ALA:O	1:K:725:THR:OG1	2.18	0.59
1:H:875:LEU:HB2	1:H:902:GLN:HG2	1.83	0.59
1:B:824:GLU:HG2	1:B:852:ILE:HB	1.84	0.59
1:N:920:ARG:HA	1:N:948:CYS:O	2.03	0.59
1:K:888:TRP:HH2	1:F:507:ARG:HE	1.50	0.59
1:D:306:LYS:HD2	1:D:322:TRP:CE2	2.37	0.59
1:H:921:ASP:OD1	1:H:950:SER:OG	2.20	0.59
1:B:377:ARG:NH1	1:B:423:THR:O	2.36	0.59
1:H:925:LYS:HA	1:H:956:TYR:HE2	1.67	0.59
1:K:606:ALA:HB1	1:K:659:PHE:HE1	1.68	0.59
1:N:919:LEU:O	1:N:948:CYS:N	2.35	0.59
1:P:551:VAL:HG22	1:P:582:LYS:HG2	1.84	0.59
1:K:865:ASN:OD1	1:K:895:SER:OG	2.21	0.58
1:H:716:THR:HG22	1:H:740:ASN:HD22	1.69	0.58
1:H:914:LEU:HB3	1:H:917:TRP:CG	2.38	0.58
1:P:858:ASN:HB2	1:P:887:PRO:HB3	1.85	0.58
1:B:209:ARG:NH1	1:F:218:ASP:OD1	2.31	0.58
1:F:204:HIS:H	1:F:219:GLN:HE22	1.51	0.58
1:N:430:TYR:HA	1:N:431:THR:OG1	2.03	0.58
1:P:983:LEU:C	1:P:986:LYS:CB	2.72	0.58
1:D:588:SER:OG	1:D:615:ASP:O	2.16	0.58
1:B:845:HIS:HA	1:B:877:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:940:GLN:O	1:F:968:VAL:N	2.31	0.58
1:L:174:GLY:N	2:L:1101:ADP:O2B	2.34	0.58
1:P:146:HIS:CE1	1:P:288:ARG:HD3	2.38	0.58
1:F:378:TYR:HD2	1:F:386:PHE:HD1	1.51	0.58
1:B:533:SEP:O3P	1:B:665:THR:OG1	2.18	0.58
1:D:666:LEU:HB3	1:D:669:ILE:HD12	1.86	0.58
1:L:852:ILE:HG12	1:L:883:THR:HB	1.85	0.58
1:B:376:HIS:CD2	1:H:103:GLN:HG3	2.38	0.57
1:F:535:GLN:O	1:F:539:ASN:HB2	2.04	0.57
1:N:592:PRO:HD2	1:N:595:LEU:HD23	1.86	0.57
1:H:872:ILE:HA	1:H:875:LEU:HG	1.86	0.57
1:L:750:GLN:HG3	1:L:756:ILE:HD11	1.85	0.57
1:N:168:GLU:HB3	1:N:284:LEU:HD13	1.87	0.57
1:D:588:SER:HB2	1:D:645:PRO:HG2	1.87	0.57
1:D:603:PRO:HA	1:D:657:GLN:HE21	1.70	0.57
1:N:377:ARG:NH2	1:N:423:THR:O	2.37	0.57
1:N:920:ARG:H	1:N:923:GLU:HB2	1.68	0.57
1:K:593:ASP:OD1	1:K:647:ARG:NH2	2.36	0.57
1:P:308:LEU:O	1:P:312:VAL:HG22	2.05	0.57
1:K:745:ARG:HA	1:K:772:ASP:HB3	1.86	0.57
1:D:475:ASN:HA	1:D:508:HIS:CE1	2.40	0.57
1:N:927:LEU:O	1:N:931:LEU:HB2	2.04	0.57
1:B:376:HIS:HD2	1:H:103:GLN:HG3	1.68	0.57
1:H:200:VAL:HG22	1:H:244:LEU:HB3	1.87	0.57
1:P:704:LEU:HD22	1:P:724:LEU:HD11	1.85	0.57
1:N:141:LYS:HB2	1:N:152:LEU:HD21	1.86	0.57
1:N:733:THR:O	1:N:761:ASN:ND2	2.37	0.57
1:B:889:CYS:O	1:B:892:VAL:HG22	2.05	0.57
1:K:592:PRO:HD2	1:K:595:LEU:HD22	1.85	0.56
1:F:743:ILE:HD11	1:F:746:LEU:HB2	1.86	0.56
1:K:588:SER:OG	1:K:615:ASP:O	2.20	0.56
1:B:192:ARG:HA	1:B:195:LYS:HE3	1.86	0.56
1:B:230:PRO:HG3	1:F:256:GLN:HG2	1.86	0.56
1:D:249:GLY:H	1:D:278:THR:HG22	1.70	0.56
1:N:245:PHE:HB2	1:N:275:VAL:HG12	1.87	0.56
1:P:205:LEU:HB3	1:P:253:PHE:HB2	1.86	0.56
1:F:571:LEU:O	1:F:574:GLU:HG2	2.05	0.56
1:L:344:THR:HG22	1:L:362:LEU:HD11	1.87	0.56
1:L:875:LEU:HB2	1:L:902:GLN:HG2	1.88	0.56
1:N:308:LEU:O	1:N:312:VAL:HG22	2.05	0.56
1:P:817:GLU:HB3	1:P:818:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:940:GLN:O	1:K:968:VAL:N	2.33	0.56
1:F:339:LEU:O	1:F:342:VAL:HG22	2.06	0.56
1:N:668:ASP:OD2	1:N:696:ARG:NH1	2.38	0.56
1:N:967:LEU:HD21	1:N:970:PHE:HB3	1.86	0.56
1:D:174:GLY:N	2:D:1101:ADP:O3B	2.36	0.56
1:L:663:GLU:OE2	1:L:691:ARG:NH1	2.38	0.56
1:L:756:ILE:HG22	1:L:783:LEU:HD13	1.86	0.56
1:P:413:GLY:O	1:P:414:SER:HB2	2.05	0.56
1:P:764:ASN:HA	1:P:792:LYS:HD3	1.85	0.56
1:K:803:ASP:HB2	1:F:462:LYS:HA	1.86	0.56
1:D:308:LEU:O	1:D:312:VAL:HG22	2.05	0.56
1:F:716:THR:HB	1:F:740:ASN:HB2	1.86	0.56
1:F:868:LEU:HD11	1:F:886:LEU:HD22	1.88	0.56
1:L:567:SER:HB2	1:L:571:LEU:HD23	1.88	0.56
1:B:921:ASP:OD1	1:B:950:SER:OG	2.22	0.56
1:D:434:ARG:HD3	1:D:438:THR:HB	1.87	0.56
1:D:443:HIS:ND1	1:D:445:SER:OG	2.37	0.56
1:K:340:PHE:O	1:K:344:THR:HG23	2.06	0.56
1:K:851:SER:HA	1:K:881:LEU:HA	1.88	0.56
1:L:141:LYS:HB2	1:L:152:LEU:HD11	1.87	0.56
1:N:678:LYS:HE2	1:N:679:TYR:CE1	2.41	0.56
1:K:360:THR:OG1	1:K:564:GLU:OE1	2.17	0.56
1:N:140:TRP:HB3	1:N:148:ARG:HB3	1.88	0.56
1:P:983:LEU:C	1:P:986:LYS:N	2.58	0.56
1:K:925:LYS:O	1:K:929:GLU:HG3	2.05	0.56
1:N:920:ARG:O	1:N:924:ILE:N	2.31	0.56
1:B:532:GLU:OE2	1:B:533:SEP:N	2.39	0.55
1:H:325:ILE:HD13	1:H:331:LEU:HD13	1.86	0.55
1:H:371:ILE:O	1:H:375:SER:OG	2.13	0.55
1:L:535:GLN:O	1:L:539:ASN:HB2	2.06	0.55
1:P:344:THR:HG22	1:P:362:LEU:HD11	1.89	0.55
1:F:108:LEU:O	1:F:111:SER:OG	2.23	0.55
1:P:539:ASN:ND2	1:P:541:THR:O	2.39	0.55
1:K:678:LYS:O	1:K:682:LYS:HG2	2.06	0.55
1:D:816:SER:HB2	1:D:843:ASN:HB2	1.88	0.55
1:N:200:VAL:HG12	1:N:244:LEU:HB3	1.87	0.55
1:B:98:LEU:HD13	1:B:235:LEU:HD11	1.88	0.55
1:B:797:HIS:CD2	1:B:826:LYS:HB2	2.41	0.55
1:F:851:SER:HA	1:F:881:LEU:HA	1.89	0.55
1:K:720:GLU:HA	1:K:744:HIS:HB2	1.89	0.55
1:K:830:CYS:O	1:K:858:ASN:ND2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:421:LEU:HB2	1:P:427:LEU:HD12	1.88	0.55
1:F:192:ARG:O	1:F:195:LYS:HG2	2.07	0.55
1:L:588:SER:HB2	1:L:645:PRO:HG2	1.89	0.55
1:N:977:PHE:N	1:N:977:PHE:CD1	2.75	0.55
1:K:175:LYS:N	2:K:1101:ADP:O3B	2.40	0.55
1:P:983:LEU:O	1:P:986:LYS:CB	2.54	0.55
1:K:621:THR:HG21	1:K:679:TYR:HD2	1.72	0.55
1:K:914:LEU:HB3	1:K:917:TRP:CG	2.41	0.55
1:B:620:ALA:HB1	1:B:680:LEU:HD11	1.89	0.55
1:B:914:LEU:HB3	1:B:917:TRP:CG	2.42	0.55
1:H:681:GLY:O	1:H:685:SER:OG	2.25	0.55
1:L:169:GLY:O	1:L:280:THR:HA	2.08	0.54
1:N:418:GLU:N	1:N:418:GLU:OE2	2.40	0.54
1:N:824:GLU:HA	1:N:852:ILE:HB	1.89	0.54
1:F:588:SER:OG	1:F:615:ASP:O	2.18	0.54
1:H:889:CYS:O	1:H:892:VAL:HG22	2.08	0.54
1:F:308:LEU:O	1:F:312:VAL:HG22	2.08	0.54
1:F:872:ILE:HA	1:F:875:LEU:HG	1.88	0.54
1:H:421:LEU:HB2	1:H:427:LEU:HD12	1.90	0.54
1:H:918:ARG:HB3	1:H:948:CYS:SG	2.47	0.54
1:L:896:LEU:HD12	1:L:923:GLU:HB3	1.88	0.54
1:L:970:PHE:HE2	1:L:997:LEU:HD21	1.73	0.54
1:P:665:THR:HB	1:P:693:HIS:HB3	1.90	0.54
1:L:816:SER:HB2	1:L:843:ASN:HB2	1.90	0.54
1:K:889:CYS:O	1:K:892:VAL:HG22	2.08	0.54
1:P:851:SER:HA	1:P:881:LEU:HA	1.88	0.54
1:H:816:SER:HB2	1:H:843:ASN:HB2	1.90	0.54
1:B:548:ALA:O	1:B:552:ASN:ND2	2.41	0.53
1:D:776:ASN:H	1:D:779:ASP:HB2	1.73	0.53
1:N:535:GLN:O	1:N:539:ASN:HB2	2.09	0.53
1:B:552:ASN:ND2	1:B:583:SER:OG	2.41	0.53
1:D:463:GLU:HG3	1:F:774:ARG:NH2	2.23	0.53
1:P:666:LEU:HB3	1:P:669:ILE:HD12	1.89	0.53
1:P:769:ILE:HG12	1:P:797:HIS:HB2	1.90	0.53
1:N:351:ARG:HG2	1:N:369:LEU:HD11	1.89	0.53
1:K:892:VAL:HG21	1:K:917:TRP:HA	1.91	0.53
1:D:198:ARG:N	1:D:242:GLU:O	2.41	0.53
1:D:984:VAL:HG13	1:D:1015:ILE:HD11	1.90	0.53
1:H:991:LEU:HD12	1:H:1019:PHE:CZ	2.44	0.53
1:P:198:ARG:N	1:P:242:GLU:O	2.41	0.53
1:P:406:PHE:CZ	1:P:444:LYS:HE3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:420:VAL:O	1:N:424:ILE:HG13	2.08	0.53
1:N:981:ALA:O	1:N:984:VAL:N	2.42	0.53
1:D:595:LEU:HD12	1:D:651:LEU:HD11	1.91	0.53
1:F:677:ILE:HG23	1:F:707:VAL:HA	1.90	0.53
1:H:830:CYS:O	1:H:858:ASN:ND2	2.38	0.53
1:H:962:GLU:HG3	1:H:990:VAL:HG13	1.90	0.53
1:N:941:GLN:HA	1:N:967:LEU:HD11	1.91	0.53
1:N:997:LEU:O	1:N:1019:PHE:HB3	2.08	0.53
1:B:547:LYS:O	1:B:551:VAL:HG23	2.09	0.53
1:B:910:ALA:O	1:B:940:GLN:N	2.35	0.53
1:H:228:SER:OG	1:H:231:THR:OG1	2.24	0.53
1:L:538:ARG:HD3	1:L:691:ARG:HD3	1.90	0.53
1:N:421:LEU:HB2	1:N:427:LEU:HD12	1.91	0.53
1:N:656:LYS:C	1:N:657:GLN:HE21	2.12	0.53
1:B:816:SER:HB2	1:B:843:ASN:CB	2.39	0.53
1:H:321:LEU:O	1:H:325:ILE:HG12	2.09	0.53
1:P:173:LYS:HE3	1:P:299:ASP:HA	1.90	0.53
1:K:300:MET:N	1:K:336:LYS:O	2.36	0.53
1:H:209:ARG:NH1	1:L:218:ASP:OD1	2.33	0.53
1:L:108:LEU:O	1:L:111:SER:OG	2.26	0.53
1:N:108:LEU:O	1:N:111:SER:OG	2.27	0.53
1:H:443:HIS:ND1	1:H:445:SER:OG	2.41	0.53
1:N:321:LEU:O	1:N:325:ILE:HG13	2.09	0.53
1:B:673:ASN:H	1:B:676:ASP:HB2	1.74	0.52
1:D:845:HIS:HA	1:D:877:VAL:HG11	1.91	0.52
1:H:145:ARG:HE	1:H:667:ARG:NH2	2.07	0.52
1:P:690:LEU:HD22	1:P:714:MET:HG3	1.89	0.52
1:B:936:LEU:HB3	1:B:939:LEU:HB2	1.90	0.52
1:D:1019:PHE:HE2	1:D:1021:LEU:HD13	1.74	0.52
1:L:865:ASN:OD1	1:L:895:SER:OG	2.27	0.52
1:F:351:ARG:O	1:F:352:GLN:HB2	2.09	0.52
1:N:588:SER:OG	1:N:615:ASP:O	2.26	0.52
1:P:824:GLU:HG2	1:P:852:ILE:HB	1.92	0.52
1:K:674:LYS:O	1:K:678:LYS:HG2	2.10	0.52
1:K:910:ALA:O	1:K:940:GLN:N	2.34	0.52
1:H:333:ASN:HA	1:H:336:LYS:HZ2	1.73	0.52
1:L:493:TYR:O	1:L:497:SER:OG	2.25	0.52
1:P:108:LEU:O	1:P:111:SER:OG	2.27	0.52
1:P:351:ARG:HD3	1:P:354:PHE:HB3	1.91	0.52
1:K:987:LEU:HD22	1:K:1015:ILE:HD12	1.92	0.52
1:D:716:THR:HG23	1:D:740:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:889:CYS:O	1:L:892:VAL:HG22	2.10	0.52
1:N:335:MET:HE3	1:N:341:VAL:HA	1.91	0.52
1:D:604:ASN:OD1	1:D:604:ASN:N	2.43	0.52
1:F:970:PHE:HE2	1:F:997:LEU:HD21	1.75	0.52
1:F:1015:ILE:HG23	1:F:1021:LEU:HD11	1.91	0.52
1:H:588:SER:HB2	1:H:645:PRO:HD2	1.91	0.52
1:H:787:LEU:HD13	1:H:815:LEU:HD21	1.91	0.52
1:N:345:CYS:O	1:N:349:MET:HG3	2.10	0.52
1:B:749:GLN:HG2	1:B:774:ARG:NH2	2.24	0.52
1:D:325:ILE:HG12	1:D:331:LEU:HD23	1.90	0.52
1:F:988:SER:OG	1:F:1014:ALA:O	2.28	0.52
1:L:499:THR:HG23	1:L:571:LEU:HD21	1.92	0.52
1:L:578:PHE:O	1:L:582:LYS:NZ	2.28	0.52
1:N:977:PHE:N	1:N:977:PHE:HD1	2.06	0.52
1:P:857:GLU:HG3	1:P:915:LYS:HD3	1.90	0.52
1:F:406:PHE:CZ	1:F:444:LYS:HE3	2.44	0.52
1:H:812:VAL:HG11	1:H:840:LEU:HB2	1.91	0.52
1:H:1002:LEU:HD23	1:H:1007:PHE:CE2	2.44	0.52
1:L:443:HIS:ND1	1:L:445:SER:OG	2.42	0.52
1:L:914:LEU:HB3	1:L:917:TRP:CG	2.45	0.52
1:B:145:ARG:HA	1:B:523:VAL:HG22	1.90	0.52
1:B:350:GLY:HA3	1:B:369:LEU:HD21	1.90	0.52
1:B:749:GLN:HG2	1:B:774:ARG:CZ	2.40	0.52
1:F:855:ILE:HG13	1:F:887:PRO:HD3	1.92	0.52
1:F:889:CYS:O	1:F:892:VAL:HG22	2.10	0.52
1:F:921:ASP:OD1	1:F:950:SER:OG	2.28	0.52
1:L:143:ASP:HB2	1:L:149:VAL:HG23	1.92	0.52
1:L:228:SER:OG	1:L:231:THR:OG1	2.24	0.52
1:N:947:HIS:ND1	1:N:973:SER:O	2.42	0.52
1:P:299:ASP:HB3	1:P:336:LYS:HB3	1.92	0.52
1:K:986:LYS:O	1:K:990:VAL:HG23	2.09	0.51
1:D:986:LYS:O	1:D:990:VAL:HG23	2.10	0.51
1:F:875:LEU:HB2	1:F:902:GLN:HG2	1.91	0.51
1:H:228:SER:HG	1:H:231:THR:HG1	1.58	0.51
1:P:677:ILE:HG22	1:P:707:VAL:HG22	1.92	0.51
1:B:420:VAL:O	1:B:424:ILE:HG13	2.10	0.51
1:N:850:LEU:HD21	1:N:853:LEU:HD13	1.92	0.51
1:P:345:CYS:O	1:P:349:MET:HG3	2.11	0.51
1:P:361:MET:O	1:P:365:THR:OG1	2.23	0.51
1:H:142:LYS:HD2	1:H:168:GLU:OE2	2.11	0.51
1:D:586:ILE:HG12	1:D:595:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:LEU:HG	1:H:288:ARG:HG3	1.93	0.51
1:L:418:GLU:O	1:L:422:VAL:HG23	2.10	0.51
1:L:859:TYR:CE1	1:L:889:CYS:HA	2.45	0.51
1:N:859:TYR:CE1	1:N:889:CYS:HA	2.46	0.51
1:K:854:ASP:OD2	1:K:856:SER:OG	2.22	0.51
1:B:308:LEU:O	1:B:312:VAL:HG22	2.11	0.51
1:B:508:HIS:O	1:B:511:MET:HG2	2.11	0.51
1:B:788:ARG:NH1	1:B:817:GLU:OE2	2.44	0.51
1:D:681:GLY:O	1:D:685:SER:OG	2.28	0.51
1:B:312:VAL:O	1:H:132:LYS:NZ	2.44	0.51
1:B:604:ASN:N	1:B:604:ASN:OD1	2.44	0.51
1:D:406:PHE:CZ	1:D:444:LYS:HE3	2.45	0.51
1:L:97:ASP:HA	1:L:100:VAL:HG12	1.93	0.51
1:P:499:THR:HA	1:P:502:THR:HG22	1.93	0.51
1:P:696:ARG:HA	1:P:721:ALA:HB3	1.92	0.51
1:K:134:PHE:CZ	1:K:181:ARG:HG2	2.45	0.51
1:K:776:ASN:H	1:K:779:ASP:HB2	1.75	0.51
1:B:198:ARG:N	1:B:242:GLU:O	2.44	0.51
1:B:225:ASP:HB2	1:F:405:LYS:NZ	2.25	0.51
1:L:666:LEU:HB3	1:L:669:ILE:HD12	1.91	0.51
1:K:988:SER:OG	1:K:1014:ALA:O	2.29	0.51
1:K:1015:ILE:HG22	1:K:1021:LEU:HD11	1.93	0.51
1:L:308:LEU:O	1:L:312:VAL:HG22	2.10	0.51
1:L:518:LEU:HD23	1:L:546:LEU:HB2	1.92	0.51
1:P:131:GLU:HG3	1:P:184:MET:HE1	1.93	0.51
1:P:393:CYS:HB2	1:P:421:LEU:HD22	1.93	0.51
1:K:334:LEU:HD13	1:K:362:LEU:HD22	1.92	0.50
1:B:322:TRP:HA	1:B:325:ILE:HD12	1.93	0.50
1:N:285:ARG:NH1	1:N:484:THR:OG1	2.44	0.50
1:P:690:LEU:O	1:P:715:HIS:N	2.39	0.50
1:K:604:ASN:OD1	1:K:604:ASN:N	2.42	0.50
1:B:225:ASP:OD2	1:B:225:ASP:N	2.30	0.50
1:D:345:CYS:O	1:D:349:MET:HG3	2.11	0.50
1:H:480:ILE:HG12	1:H:515:HIS:HA	1.94	0.50
1:L:769:ILE:HG12	1:L:797:HIS:HB2	1.93	0.50
1:N:547:LYS:O	1:N:551:VAL:HG13	2.11	0.50
1:N:968:VAL:HG12	1:N:998:GLN:HB2	1.92	0.50
1:D:889:CYS:O	1:D:892:VAL:HG22	2.11	0.50
1:F:986:LYS:O	1:F:990:VAL:HG23	2.12	0.50
1:H:533:SEP:OG	1:H:534:ILE:N	2.41	0.50
1:P:135:THR:O	2:P:1101:ADP:N6	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:168:GLU:HB3	1:P:284:LEU:HD13	1.92	0.50
1:L:522:SER:O	1:L:523:VAL:O	2.30	0.50
1:N:914:LEU:HB3	1:N:917:TRP:CG	2.47	0.50
1:D:416:MET:HE3	1:N:420:VAL:HG22	1.92	0.50
1:H:578:PHE:O	1:H:582:LYS:NZ	2.26	0.50
1:H:852:ILE:HG12	1:H:883:THR:HB	1.92	0.50
1:K:535:GLN:O	1:K:539:ASN:HB2	2.11	0.50
1:K:903:LEU:HD21	1:K:909:LEU:HD12	1.93	0.50
1:D:756:ILE:HD11	1:D:779:ASP:HB3	1.92	0.50
1:D:940:GLN:O	1:D:968:VAL:N	2.34	0.50
1:H:568:LYS:HD3	1:H:601:TYR:CZ	2.46	0.50
1:L:986:LYS:O	1:L:990:VAL:HG23	2.12	0.50
1:K:862:LYS:NZ	1:F:574:GLU:OE2	2.35	0.50
1:B:206:ARG:HG2	1:B:207:SER:N	2.26	0.50
1:D:108:LEU:O	1:D:111:SER:OG	2.29	0.50
1:D:266:LYS:HG3	1:D:290:VAL:HG21	1.94	0.50
1:D:474:LEU:HD23	1:D:477:MET:HE3	1.94	0.50
1:F:911:LYS:HG2	1:F:941:GLN:HG2	1.94	0.50
1:N:582:LYS:O	1:N:610:ASP:N	2.44	0.50
1:N:672:LEU:HB2	1:N:699:ALA:HB1	1.92	0.50
1:P:661:THR:HG23	1:P:689:ASN:HB3	1.94	0.50
1:D:228:SER:OG	1:D:231:THR:OG1	2.26	0.50
1:H:503:ARG:HG3	1:H:571:LEU:HD11	1.94	0.50
1:L:146:HIS:CE1	1:L:288:ARG:HE	2.29	0.50
1:P:420:VAL:O	1:P:424:ILE:HG13	2.12	0.50
1:K:816:SER:HA	1:K:847:LEU:HD21	1.93	0.50
1:B:1003:THR:HG23	1:B:1024:ALA:HA	1.93	0.50
1:D:663:GLU:OE2	1:D:691:ARG:NH1	2.44	0.50
1:N:974:THR:C	1:N:975:GLU:OE2	2.51	0.50
1:P:103:GLN:HA	1:P:103:GLN:OE1	2.10	0.50
1:D:599:PHE:CD1	1:D:651:LEU:HD22	2.47	0.49
1:D:824:GLU:HG2	1:D:852:ILE:HB	1.93	0.49
1:F:925:LYS:O	1:F:929:GLU:HG3	2.12	0.49
1:H:269:HIS:NE2	1:H:1017:GLY:HA2	2.27	0.49
1:H:547:LYS:O	1:H:551:VAL:HG12	2.12	0.49
1:N:970:PHE:HE2	1:N:997:LEU:HD21	1.76	0.49
1:P:893:HIS:HB2	1:P:923:GLU:HG2	1.92	0.49
1:P:923:GLU:N	1:P:923:GLU:OE1	2.45	0.49
1:K:799:THR:HG22	1:K:828:VAL:HG22	1.94	0.49
1:B:406:PHE:CZ	1:B:444:LYS:HE3	2.47	0.49
1:B:474:LEU:HD23	1:B:477:MET:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:HIS:NE2	1:D:547:LYS:HD2	2.27	0.49
1:F:769:ILE:HG12	1:F:797:HIS:HB2	1.94	0.49
1:H:418:GLU:O	1:H:422:VAL:HG23	2.12	0.49
1:H:776:ASN:H	1:H:779:ASP:HB2	1.77	0.49
1:L:811:ILE:O	1:L:815:LEU:HG	2.12	0.49
1:P:355:GLN:HG2	1:P:357:HIS:CE1	2.48	0.49
1:D:661:THR:HG23	1:D:689:ASN:HB3	1.93	0.49
1:L:621:THR:HG1	1:L:645:PRO:N	2.10	0.49
1:N:306:LYS:HD2	1:N:322:TRP:CE2	2.48	0.49
1:P:335:MET:HE3	1:P:341:VAL:HA	1.94	0.49
1:K:335:MET:HG3	1:K:341:VAL:HG22	1.93	0.49
1:K:552:ASN:ND2	1:K:585:TYR:HB2	2.28	0.49
1:D:1006:GLU:O	1:D:1007:PHE:HB2	2.13	0.49
1:F:492:LEU:HG	1:F:564:GLU:HG3	1.93	0.49
1:H:518:LEU:HD21	1:H:547:LYS:HG2	1.93	0.49
1:N:474:LEU:HD23	1:N:477:MET:HE3	1.93	0.49
1:P:868:LEU:HD11	1:P:886:LEU:HG	1.95	0.49
1:D:743:ILE:HG21	1:D:746:LEU:HD22	1.93	0.49
1:F:393:CYS:HB2	1:F:421:LEU:HD22	1.93	0.49
1:H:333:ASN:OD1	1:H:336:LYS:NZ	2.37	0.49
1:H:474:LEU:HD23	1:H:477:MET:HE3	1.94	0.49
1:H:859:TYR:CE1	1:H:889:CYS:HA	2.47	0.49
1:K:900:LEU:HG	1:K:930:PHE:CG	2.48	0.49
1:B:752:PRO:HA	1:B:757:ASP:OD1	2.13	0.49
1:F:672:LEU:HD12	1:F:677:ILE:HG13	1.94	0.49
1:H:471:ASN:O	1:H:475:ASN:HB2	2.12	0.49
1:H:984:VAL:HG22	1:H:1007:PHE:HE1	1.78	0.49
1:N:653:PHE:HE2	1:N:679:TYR:CD1	2.30	0.49
1:K:673:ASN:O	1:K:677:ILE:HG13	2.12	0.49
1:B:174:GLY:N	2:B:1101:ADP:O2B	2.44	0.49
1:D:324:GLN:NE2	1:D:354:PHE:O	2.46	0.49
1:D:886:LEU:HD12	1:D:917:TRP:HZ2	1.77	0.49
1:H:335:MET:HE3	1:H:341:VAL:HA	1.94	0.49
1:P:698:ALA:HA	1:P:723:PRO:HD3	1.94	0.49
1:B:340:PHE:O	1:B:344:THR:HG22	2.11	0.49
1:B:430:TYR:HD2	1:B:438:THR:HB	1.78	0.49
1:F:405:LYS:HE3	1:F:407:ASP:O	2.13	0.49
1:H:334:LEU:HD13	1:H:362:LEU:HD22	1.95	0.49
1:H:604:ASN:OD1	1:H:604:ASN:N	2.46	0.49
1:L:420:VAL:O	1:L:424:ILE:HG13	2.12	0.49
1:P:750:GLN:HG3	1:P:756:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:916:ASN:HA	1:P:946:GLY:HA3	1.94	0.49
1:B:665:THR:HG23	1:B:693:HIS:HB3	1.95	0.49
1:H:715:HIS:CE1	1:H:739:GLN:HE21	2.30	0.49
1:N:480:ILE:HD12	1:N:554:PHE:HB2	1.93	0.49
1:P:169:GLY:O	1:P:280:THR:HA	2.13	0.49
1:P:910:ALA:O	1:P:940:GLN:N	2.35	0.49
1:B:267:GLU:OE1	1:B:270:ARG:NH1	2.46	0.48
1:B:691:ARG:HG2	1:B:715:HIS:HB3	1.95	0.48
1:N:788:ARG:NH2	1:N:817:GLU:OE1	2.45	0.48
1:K:547:LYS:O	1:K:551:VAL:HG23	2.12	0.48
1:B:529:TRP:HA	1:B:529:TRP:CE3	2.47	0.48
1:D:98:LEU:HD11	1:D:239:LEU:HD21	1.94	0.48
1:D:145:ARG:HA	1:D:523:VAL:HG22	1.94	0.48
1:D:235:LEU:HD23	1:D:239:LEU:HD23	1.95	0.48
1:D:932:GLU:HG3	1:D:960:VAL:HG13	1.95	0.48
1:H:535:GLN:O	1:H:539:ASN:HB2	2.13	0.48
1:L:900:LEU:O	1:L:904:GLU:HG3	2.13	0.48
1:K:385:ASP:HB3	1:K:388:ARG:HB2	1.94	0.48
1:F:825:MET:HG2	1:F:827:LEU:HD13	1.96	0.48
1:H:788:ARG:HH21	1:H:788:ARG:HG3	1.78	0.48
1:L:464:PRO:HA	1:L:467:VAL:HG12	1.94	0.48
1:K:339:LEU:O	1:K:343:ILE:HG13	2.14	0.48
1:B:96:GLU:O	1:B:100:VAL:HG13	2.13	0.48
1:L:588:SER:OG	1:L:615:ASP:O	2.23	0.48
1:N:918:ARG:O	1:N:920:ARG:NH1	2.47	0.48
1:N:940:GLN:O	1:N:941:GLN:HB3	2.14	0.48
1:P:306:LYS:HD2	1:P:322:TRP:CE2	2.48	0.48
1:L:92:GLN:O	1:L:93:VAL:HG13	2.14	0.48
1:K:306:LYS:HD3	1:K:322:TRP:CE2	2.49	0.48
1:K:893:HIS:HB2	1:K:923:GLU:HG2	1.95	0.48
1:F:97:ASP:HA	1:F:100:VAL:HG12	1.96	0.48
1:N:599:PHE:HB3	1:N:657:GLN:OE1	2.13	0.48
1:N:690:LEU:HD23	1:N:714:MET:SD	2.53	0.48
1:N:888:TRP:HA	1:N:892:VAL:HG11	1.94	0.48
1:N:918:ARG:HE	1:N:918:ARG:HB3	1.38	0.48
1:P:571:LEU:HD22	1:P:574:GLU:HG3	1.96	0.48
1:P:676:ASP:O	1:P:680:LEU:HD13	2.14	0.48
1:P:893:HIS:CD2	1:P:918:ARG:HB2	2.49	0.48
1:K:888:TRP:HA	1:K:892:VAL:HG11	1.95	0.48
1:F:166:LEU:HD22	1:F:287:ILE:HD12	1.96	0.48
1:F:562:PHE:O	1:F:565:SER:OG	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:VAL:O	1:H:424:ILE:HG13	2.14	0.48
1:L:198:ARG:N	1:L:242:GLU:O	2.46	0.48
1:P:163:SER:HB2	1:P:274:MET:CE	2.44	0.48
1:K:525:LYS:HB2	1:K:525:LYS:HE3	1.46	0.48
1:B:533:SEP:OG	1:B:534:ILE:N	2.47	0.48
1:F:889:CYS:SG	1:F:892:VAL:HG13	2.53	0.48
1:K:1002:LEU:O	1:K:1023:THR:HA	2.13	0.48
1:F:663:GLU:HG3	1:F:691:ARG:HB2	1.95	0.48
1:L:285:ARG:O	1:L:520:GLY:HA3	2.13	0.48
1:N:860:LEU:HB2	1:N:864:GLY:HA3	1.95	0.48
1:D:889:CYS:SG	1:D:892:VAL:HG13	2.54	0.48
1:F:360:THR:OG1	1:F:564:GLU:OE1	2.20	0.48
1:N:967:LEU:HD11	1:N:969:PHE:O	2.13	0.48
1:K:665:THR:HG23	1:K:693:HIS:HB3	1.95	0.47
1:B:925:LYS:HA	1:B:956:TYR:CE2	2.46	0.47
1:H:645:PRO:O	1:H:649:VAL:HG23	2.14	0.47
1:L:421:LEU:HB2	1:L:427:LEU:HD12	1.95	0.47
1:L:925:LYS:HE2	1:L:925:LYS:HB2	1.71	0.47
1:K:205:LEU:HB2	1:K:248:ASP:O	2.13	0.47
1:K:828:VAL:C	1:K:830:CYS:H	2.16	0.47
1:F:852:ILE:HG12	1:F:883:THR:HB	1.95	0.47
1:H:412:HIS:HE1	1:H:436:LYS:HG2	1.79	0.47
1:N:593:ASP:OD1	1:N:647:ARG:NH2	2.42	0.47
1:N:851:SER:HA	1:N:881:LEU:HA	1.97	0.47
1:P:93:VAL:HG11	1:P:235:LEU:HD13	1.96	0.47
1:P:479:SER:O	1:P:483:ILE:HG13	2.14	0.47
1:B:967:LEU:O	1:B:997:LEU:HD12	2.14	0.47
1:D:886:LEU:HD12	1:D:917:TRP:CZ2	2.50	0.47
1:F:666:LEU:HB3	1:F:669:ILE:HD12	1.97	0.47
1:H:360:THR:OG1	1:H:564:GLU:OE1	2.25	0.47
1:L:406:PHE:CZ	1:L:444:LYS:HE3	2.49	0.47
1:L:745:ARG:HA	1:L:772:ASP:HB3	1.95	0.47
1:L:824:GLU:HG2	1:L:852:ILE:HD12	1.96	0.47
1:P:888:TRP:HA	1:P:892:VAL:HG11	1.96	0.47
1:P:955:LEU:HD12	1:P:983:LEU:CA	2.43	0.47
1:F:240:HIS:CE1	1:F:241:LYS:HG3	2.49	0.47
1:H:168:GLU:HB3	1:H:284:LEU:HD13	1.96	0.47
1:L:306:LYS:HD2	1:L:322:TRP:CE2	2.48	0.47
1:L:924:ILE:HD13	1:L:924:ILE:HA	1.67	0.47
1:D:827:LEU:HD23	1:D:832:LEU:HD11	1.97	0.47
1:H:947:HIS:HD2	1:H:949:VAL:HB	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:740:ASN:HD22	1:N:767:ARG:HB2	1.79	0.47
1:D:461:SER:O	1:F:802:SER:OG	2.33	0.47
1:H:571:LEU:O	1:H:574:GLU:HG2	2.15	0.47
1:H:851:SER:HA	1:H:881:LEU:HA	1.95	0.47
1:K:962:GLU:HG3	1:K:990:VAL:HG22	1.96	0.47
1:B:889:CYS:SG	1:B:892:VAL:HG13	2.55	0.47
1:D:306:LYS:HD2	1:D:322:TRP:CD2	2.50	0.47
1:H:901:LYS:HA	1:H:901:LYS:HD3	1.67	0.47
1:H:1003:THR:HG22	1:H:1024:ALA:HB3	1.96	0.47
1:L:509:LEU:O	1:L:512:VAL:HG22	2.15	0.47
1:N:739:GLN:O	1:N:740:ASN:ND2	2.47	0.47
1:N:898:LYS:HE3	1:N:898:LYS:HB3	1.74	0.47
1:P:321:LEU:O	1:P:325:ILE:HG13	2.14	0.47
1:P:663:GLU:HG3	1:P:691:ARG:HB2	1.95	0.47
1:B:224:PRO:HB2	1:B:227:ILE:HG13	1.95	0.47
1:D:288:ARG:NH1	1:D:520:GLY:O	2.48	0.47
1:D:664:VAL:HG22	1:D:692:LEU:HD23	1.97	0.47
1:F:746:LEU:HD12	1:F:746:LEU:HA	1.76	0.47
1:H:205:LEU:HB3	1:H:253:PHE:HB2	1.96	0.47
1:N:759:LEU:HD12	1:N:759:LEU:HA	1.68	0.47
1:P:914:LEU:HD12	1:P:917:TRP:CZ2	2.50	0.47
1:B:93:VAL:HG22	1:B:231:THR:HG23	1.97	0.47
1:F:420:VAL:O	1:F:424:ILE:HG13	2.14	0.47
1:F:532:GLU:HG3	1:F:718:MET:HE1	1.97	0.47
1:L:499:THR:HA	1:L:502:THR:HG22	1.97	0.47
1:N:139:MET:HB2	1:N:152:LEU:HB2	1.96	0.47
1:N:145:ARG:HD2	1:N:667:ARG:CZ	2.45	0.47
1:N:664:VAL:HG22	1:N:692:LEU:HD23	1.96	0.47
1:P:324:GLN:NE2	1:P:354:PHE:H	2.09	0.47
1:D:214:GLU:N	1:D:214:GLU:OE1	2.46	0.47
1:L:479:SER:O	1:L:483:ILE:HG13	2.15	0.47
1:L:824:GLU:HG2	1:L:852:ILE:HB	1.97	0.47
1:N:269:HIS:CD2	1:N:1017:GLY:HA2	2.51	0.47
1:K:533:SEP:O1P	1:K:613:LYS:NZ	2.35	0.46
1:F:770:LEU:HB2	1:F:798:LEU:HD23	1.96	0.46
1:H:401:VAL:HG11	1:H:490:LEU:HD22	1.96	0.46
1:N:418:GLU:O	1:N:422:VAL:HG23	2.15	0.46
1:P:701:ALA:HB2	1:P:723:PRO:HG2	1.95	0.46
1:P:744:HIS:ND1	1:P:771:ASP:OD2	2.42	0.46
1:B:666:LEU:HB3	1:B:669:ILE:HD12	1.95	0.46
1:B:826:LYS:HG2	1:B:854:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:CYS:HB3	1:D:357:HIS:O	2.15	0.46
1:L:145:ARG:HG2	1:L:523:VAL:HB	1.96	0.46
1:L:161:LEU:HD11	1:L:276:ILE:HD11	1.98	0.46
1:L:321:LEU:O	1:L:325:ILE:HG13	2.14	0.46
1:N:655:TRP:HB2	1:N:657:GLN:HE22	1.80	0.46
1:P:931:LEU:HD23	1:P:931:LEU:HA	1.83	0.46
1:K:552:ASN:HD22	1:K:585:TYR:HB2	1.79	0.46
1:K:923:GLU:N	1:K:923:GLU:OE1	2.49	0.46
1:F:493:TYR:O	1:F:497:SER:OG	2.30	0.46
1:F:923:GLU:N	1:F:923:GLU:OE1	2.49	0.46
1:H:104:ASN:HB3	1:H:222:ASN:HB2	1.97	0.46
1:H:889:CYS:SG	1:H:892:VAL:HG13	2.54	0.46
1:H:954:TRP:O	1:H:958:MET:HG2	2.15	0.46
1:L:145:ARG:CG	1:L:523:VAL:HB	2.45	0.46
1:L:571:LEU:O	1:L:574:GLU:HG2	2.14	0.46
1:N:181:ARG:O	1:N:184:MET:HG3	2.15	0.46
1:P:670:ASN:O	1:P:699:ALA:HB2	2.15	0.46
1:P:694:ILE:HG21	1:P:700:MET:HG2	1.97	0.46
1:P:708:LEU:O	1:P:731:TYR:OH	2.33	0.46
1:K:142:LYS:HD2	1:K:168:GLU:OE2	2.15	0.46
1:K:145:ARG:HA	1:K:523:VAL:HG22	1.98	0.46
1:K:267:GLU:OE1	1:K:270:ARG:NH1	2.48	0.46
1:K:285:ARG:O	1:K:520:GLY:HA3	2.15	0.46
1:K:365:THR:O	1:K:369:LEU:HB2	2.16	0.46
1:B:532:GLU:H	1:B:536:SER:CB	2.29	0.46
1:B:538:ARG:HD3	1:B:716:THR:HG21	1.97	0.46
1:D:347:ILE:O	1:D:351:ARG:HB2	2.16	0.46
1:F:471:ASN:O	1:F:475:ASN:ND2	2.34	0.46
1:F:990:VAL:O	1:F:994:LEU:HG	2.16	0.46
1:L:664:VAL:HG22	1:L:692:LEU:HD23	1.97	0.46
1:K:406:PHE:CZ	1:K:444:LYS:HE3	2.51	0.46
1:B:860:LEU:HD11	1:B:887:PRO:HG2	1.97	0.46
1:B:954:TRP:O	1:B:958:MET:HG2	2.16	0.46
1:L:690:LEU:HD23	1:L:714:MET:HG3	1.98	0.46
1:L:991:LEU:HD23	1:L:1019:PHE:HZ	1.80	0.46
1:N:568:LYS:HD3	1:N:601:TYR:CZ	2.51	0.46
1:K:666:LEU:HB3	1:K:669:ILE:HD12	1.97	0.46
1:K:743:ILE:HD13	1:K:746:LEU:HD22	1.98	0.46
1:K:914:LEU:HB3	1:K:917:TRP:CD2	2.51	0.46
1:B:932:GLU:HG3	1:B:960:VAL:HG13	1.96	0.46
1:D:421:LEU:HB2	1:D:427:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:TYR:O	1:F:371:ILE:HG12	2.15	0.46
1:L:743:ILE:HD12	1:L:746:LEU:HD22	1.96	0.46
1:P:552:ASN:OD1	1:P:583:SER:OG	2.33	0.46
1:P:974:THR:HG23	1:P:975:GLU:N	2.30	0.46
1:D:285:ARG:NH1	1:D:517:SER:O	2.49	0.46
1:F:816:SER:HB2	1:F:843:ASN:HB2	1.96	0.46
1:H:406:PHE:CZ	1:H:444:LYS:HE3	2.51	0.46
1:N:911:LYS:HG2	1:N:941:GLN:HG2	1.96	0.46
1:B:132:LYS:NZ	1:H:312:VAL:O	2.49	0.46
1:D:823:GLN:HA	1:D:850:LEU:HA	1.97	0.46
1:D:872:ILE:O	1:D:902:GLN:HG3	2.15	0.46
1:F:787:LEU:HD13	1:F:815:LEU:HD21	1.97	0.46
1:H:990:VAL:O	1:H:994:LEU:HG	2.16	0.46
1:H:175:LYS:O	1:H:178:LEU:HB3	2.15	0.46
1:H:716:THR:CG2	1:H:740:ASN:HD22	2.28	0.46
1:L:168:GLU:HA	1:L:279:THR:O	2.16	0.46
1:L:955:LEU:HD13	1:L:983:LEU:HA	1.98	0.46
1:N:173:LYS:HA	1:N:173:LYS:HD3	1.76	0.46
1:P:166:LEU:HD22	1:P:287:ILE:HD12	1.98	0.46
1:F:284:LEU:HG	1:F:288:ARG:HG3	1.96	0.46
1:N:970:PHE:CZ	1:N:1000:VAL:HG13	2.50	0.46
1:P:378:TYR:HD1	1:P:386:PHE:HD1	1.63	0.46
1:K:588:SER:HB2	1:K:645:PRO:HD2	1.97	0.45
1:B:108:LEU:O	1:B:111:SER:OG	2.33	0.45
1:F:645:PRO:HA	1:F:646:PRO:HD3	1.87	0.45
1:L:911:LYS:HG2	1:L:941:GLN:HG2	1.98	0.45
1:N:456:SER:OG	1:N:498:SER:HB3	2.16	0.45
1:N:511:MET:HG2	1:P:891:ASP:OD2	2.16	0.45
1:N:595:LEU:HD13	1:N:595:LEU:HA	1.76	0.45
1:K:164:PRO:HG2	1:K:290:VAL:CG1	2.46	0.45
1:K:288:ARG:HH11	1:K:288:ARG:HG2	1.81	0.45
1:K:991:LEU:HD23	1:K:1019:PHE:HZ	1.81	0.45
1:B:730:GLN:HG2	1:B:753:GLY:O	2.16	0.45
1:H:206:ARG:NH2	1:H:406:PHE:O	2.48	0.45
1:H:359:GLN:NE2	1:H:493:TYR:OH	2.42	0.45
1:H:557:CYS:O	1:H:561:LEU:HD13	2.16	0.45
1:L:518:LEU:HD21	1:L:547:LYS:HG2	1.99	0.45
1:P:355:GLN:HG2	1:P:357:HIS:HE1	1.81	0.45
1:P:496:GLY:HA2	1:P:564:GLU:O	2.16	0.45
1:B:526:ARG:HD2	1:B:526:ARG:C	2.35	0.45
1:D:900:LEU:O	1:D:904:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:284:LEU:HG	1:L:288:ARG:HG3	1.98	0.45
1:L:649:VAL:O	1:L:653:PHE:HB2	2.17	0.45
1:P:502:THR:HG21	1:P:565:SER:HB2	1.97	0.45
1:D:343:ILE:O	1:D:347:ILE:HG13	2.16	0.45
1:D:752:PRO:HA	1:D:757:ASP:OD1	2.17	0.45
1:F:145:ARG:CZ	1:F:523:VAL:HG21	2.47	0.45
1:L:333:ASN:ND2	1:L:593:ASP:OD1	2.46	0.45
1:N:910:ALA:O	1:N:940:GLN:N	2.45	0.45
1:P:267:GLU:HB3	1:P:269:HIS:CE1	2.52	0.45
1:P:855:ILE:HG13	1:P:887:PRO:HD3	1.98	0.45
1:K:443:HIS:ND1	1:K:445:SER:OG	2.48	0.45
1:K:578:PHE:O	1:K:582:LYS:NZ	2.32	0.45
1:K:889:CYS:SG	1:K:892:VAL:HG13	2.57	0.45
1:D:371:ILE:HD12	1:D:426:LEU:HD21	1.98	0.45
1:D:816:SER:HB2	1:D:843:ASN:CB	2.46	0.45
1:F:240:HIS:CG	1:F:241:LYS:H	2.34	0.45
1:F:335:MET:HG3	1:F:341:VAL:HG22	1.98	0.45
1:F:924:ILE:HD12	1:F:924:ILE:HA	1.69	0.45
1:F:978:LEU:HD22	1:F:1006:GLU:HB2	1.99	0.45
1:H:141:LYS:HB2	1:H:152:LEU:HD11	1.99	0.45
1:H:337:THR:HA	1:H:338:PRO:HD3	1.76	0.45
1:N:285:ARG:O	1:N:520:GLY:HA3	2.15	0.45
1:K:804:ILE:HG13	1:K:804:ILE:O	2.17	0.45
1:B:764:ASN:HA	1:B:792:LYS:HD2	1.97	0.45
1:D:977:PHE:N	1:D:1004:GLY:O	2.47	0.45
1:F:764:ASN:HA	1:F:792:LYS:HD3	1.97	0.45
1:N:343:ILE:O	1:N:347:ILE:HG13	2.16	0.45
1:N:788:ARG:HG3	1:N:814:SER:HB3	1.99	0.45
1:K:313:LEU:HD12	1:K:313:LEU:HA	1.87	0.45
1:B:493:TYR:O	1:B:497:SER:OG	2.34	0.45
1:B:499:THR:HA	1:B:502:THR:HG23	1.98	0.45
1:B:572:SER:HB2	1:B:604:ASN:HD21	1.81	0.45
1:B:855:ILE:HG13	1:B:887:PRO:HD3	1.99	0.45
1:D:173:LYS:HD3	1:D:173:LYS:HA	1.75	0.45
1:D:436:LYS:HB3	1:D:436:LYS:HE2	1.68	0.45
1:D:591:ILE:O	1:D:647:ARG:NH2	2.45	0.45
1:F:865:ASN:OD1	1:F:895:SER:OG	2.34	0.45
1:F:969:PHE:CZ	1:F:971:ASP:HB2	2.52	0.45
1:H:145:ARG:NH1	1:H:615:ASP:OD1	2.49	0.45
1:H:393:CYS:HB2	1:H:421:LEU:HD22	1.98	0.45
1:L:675:GLN:HG2	1:L:679:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:889:CYS:SG	1:L:892:VAL:HG13	2.57	0.45
1:L:896:LEU:HD22	1:L:900:LEU:HD22	1.98	0.45
1:N:753:GLY:HA3	1:N:754:GLY:HA3	1.78	0.45
1:P:115:LEU:HA	1:P:130:LEU:HD22	1.98	0.45
1:P:360:THR:OG1	1:P:564:GLU:OE1	2.23	0.45
1:K:140:TRP:O	1:K:295:ALA:HA	2.17	0.45
1:K:420:VAL:O	1:K:424:ILE:HG13	2.17	0.45
1:B:435:LEU:HD23	1:F:433:GLN:O	2.16	0.45
1:D:205:LEU:HD12	1:D:253:PHE:CG	2.52	0.45
1:L:440:LYS:HG2	1:L:441:PHE:O	2.17	0.45
1:N:378:TYR:HD2	1:N:386:PHE:HD1	1.65	0.45
1:P:285:ARG:O	1:P:520:GLY:HA3	2.17	0.45
1:K:495:CYS:SG	1:K:561:LEU:HD13	2.56	0.45
1:K:890:TRP:CZ2	1:F:580:GLN:HG2	2.52	0.45
1:B:418:GLU:HB2	1:B:439:TYR:CE2	2.52	0.45
1:F:845:HIS:HA	1:F:877:VAL:HG11	1.99	0.45
1:F:1002:LEU:HD23	1:F:1007:PHE:HZ	1.82	0.45
1:H:345:CYS:O	1:H:349:MET:HG3	2.16	0.45
1:N:974:THR:HG22	1:N:975:GLU:N	2.30	0.45
1:B:918:ARG:HE	1:B:918:ARG:HB3	1.58	0.45
1:L:104:ASN:HB3	1:L:222:ASN:HB2	1.98	0.45
1:L:338:PRO:O	1:L:342:VAL:HG23	2.17	0.45
1:N:142:LYS:HD2	1:N:168:GLU:OE2	2.16	0.45
1:P:393:CYS:HB2	1:P:421:LEU:CD2	2.47	0.45
1:D:479:SER:HB2	1:D:516:GLY:HA3	1.98	0.44
1:D:534:ILE:HG13	1:D:693:HIS:HB2	1.99	0.44
1:F:119:PRO:HB3	2:F:1101:ADP:O3'	2.16	0.44
1:H:498:SER:O	1:H:502:THR:HG22	2.17	0.44
1:H:665:THR:HB	1:H:693:HIS:HB3	2.00	0.44
1:H:865:ASN:OD1	1:H:895:SER:OG	2.35	0.44
1:H:909:LEU:HD13	1:H:912:LEU:HB2	1.98	0.44
1:L:551:VAL:CG2	1:L:582:LYS:HG2	2.48	0.44
1:L:764:ASN:HA	1:L:792:LYS:HD3	1.99	0.44
1:B:415:SER:O	1:B:418:GLU:HG2	2.17	0.44
1:B:552:ASN:OD1	1:B:585:TYR:HB2	2.17	0.44
1:D:351:ARG:HE	1:D:369:LEU:HD13	1.82	0.44
1:D:872:ILE:HA	1:D:875:LEU:HG	1.99	0.44
1:H:97:ASP:HA	1:H:100:VAL:HG12	1.99	0.44
1:P:168:GLU:HA	1:P:279:THR:O	2.17	0.44
1:K:238:LYS:HE2	1:K:238:LYS:HB2	1.56	0.44
1:K:920:ARG:NH2	1:K:922:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:962:GLU:HA	1:K:990:VAL:HG13	1.98	0.44
1:K:979:PRO:HB3	1:K:983:LEU:HD23	1.99	0.44
1:B:896:LEU:HD22	1:B:900:LEU:HD22	2.00	0.44
1:D:420:VAL:O	1:D:424:ILE:HG13	2.17	0.44
1:D:990:VAL:O	1:D:994:LEU:HG	2.18	0.44
1:F:979:PRO:O	1:F:1010:TYR:OH	2.27	0.44
1:L:756:ILE:H	1:L:756:ILE:HG12	1.49	0.44
1:N:691:ARG:HG2	1:N:715:HIS:HB3	1.98	0.44
1:N:832:LEU:HB2	1:N:858:ASN:CG	2.38	0.44
1:N:981:ALA:O	1:N:984:VAL:HB	2.16	0.44
1:K:931:LEU:HD22	1:K:964:LEU:HD21	1.99	0.44
1:B:823:GLN:HA	1:B:850:LEU:HA	2.00	0.44
1:B:969:PHE:HE1	1:B:971:ASP:HB2	1.81	0.44
1:D:892:VAL:HG21	1:D:917:TRP:HA	1.98	0.44
1:F:788:ARG:HH22	1:F:817:GLU:CD	2.18	0.44
1:H:746:LEU:HD12	1:H:746:LEU:HA	1.87	0.44
1:H:756:ILE:H	1:H:756:ILE:HG12	1.45	0.44
1:L:285:ARG:NH1	1:L:481:SER:OG	2.50	0.44
1:L:335:MET:HE3	1:L:341:VAL:HA	1.98	0.44
1:L:997:LEU:O	1:L:1019:PHE:HB3	2.17	0.44
1:N:683:ILE:O	1:N:686:SER:OG	2.26	0.44
1:P:970:PHE:HE2	1:P:997:LEU:HD21	1.83	0.44
1:B:205:LEU:HB2	1:B:248:ASP:O	2.17	0.44
1:D:914:LEU:HB3	1:D:917:TRP:CG	2.52	0.44
1:F:267:GLU:OE1	1:F:270:ARG:NH1	2.40	0.44
1:F:382:ALA:O	1:F:384:GLY:N	2.50	0.44
1:F:825:MET:HB2	1:F:850:LEU:HD11	1.99	0.44
1:F:918:ARG:HA	1:F:946:GLY:O	2.18	0.44
1:F:1017:GLY:C	1:F:1019:PHE:H	2.21	0.44
1:H:562:PHE:O	1:H:565:SER:OG	2.34	0.44
1:N:205:LEU:HB3	1:N:253:PHE:HB2	2.00	0.44
1:N:325:ILE:HG12	1:N:331:LEU:HD23	2.00	0.44
1:N:832:LEU:HD23	1:N:832:LEU:HA	1.89	0.44
1:K:816:SER:O	1:K:843:ASN:HB3	2.18	0.44
1:D:1002:LEU:HG	1:D:1005:TRP:CE2	2.53	0.44
1:H:646:PRO:O	1:H:650:SER:OG	2.36	0.44
1:L:360:THR:OG1	1:L:564:GLU:OE1	2.27	0.44
1:K:974:THR:HG23	1:K:975:GLU:O	2.18	0.44
1:D:645:PRO:HA	1:D:646:PRO:HD3	1.90	0.44
1:F:893:HIS:HB2	1:F:923:GLU:HG2	2.00	0.44
1:F:910:ALA:O	1:F:940:GLN:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:925:LYS:O	1:H:929:GLU:HG3	2.18	0.44
1:N:780:ALA:HB2	1:N:804:ILE:HB	1.99	0.44
1:P:184:MET:HE2	1:P:184:MET:HB2	1.87	0.44
1:B:94:THR:OG1	1:B:97:ASP:HB2	2.18	0.44
1:D:515:HIS:CE1	1:D:547:LYS:HD2	2.52	0.44
1:D:911:LYS:HG2	1:D:941:GLN:CG	2.45	0.44
1:L:173:LYS:NZ	1:L:337:THR:HG22	2.33	0.44
1:N:130:LEU:HD21	1:N:180:GLN:HB3	2.00	0.44
1:P:138:ILE:O	1:P:138:ILE:HG12	2.16	0.44
1:P:588:SER:OG	1:P:616:PHE:HA	2.17	0.44
1:K:343:ILE:O	1:K:347:ILE:HG13	2.18	0.44
1:B:568:LYS:HD3	1:B:601:TYR:CZ	2.52	0.44
1:D:335:MET:HG3	1:D:341:VAL:HG22	1.98	0.44
1:D:583:SER:HB2	1:D:611:PHE:CE1	2.52	0.44
1:F:798:LEU:HD13	1:F:811:ILE:HD11	1.99	0.44
1:H:168:GLU:HA	1:H:279:THR:O	2.18	0.44
1:L:743:ILE:HG12	1:L:770:LEU:HD12	2.00	0.44
1:N:799:THR:HG22	1:N:828:VAL:HG13	2.00	0.44
1:P:474:LEU:HD21	1:P:505:VAL:HG22	2.00	0.44
1:K:663:GLU:HG3	1:K:691:ARG:HB2	1.99	0.43
1:D:515:HIS:CD2	1:D:547:LYS:HD2	2.51	0.43
1:F:365:THR:O	1:F:369:LEU:HB2	2.18	0.43
1:F:479:SER:O	1:F:483:ILE:HG13	2.18	0.43
1:H:506:MET:HG3	1:H:575:PHE:CE1	2.53	0.43
1:H:923:GLU:OE1	1:H:923:GLU:N	2.51	0.43
1:L:1015:ILE:HG23	1:L:1016:LYS:H	1.82	0.43
1:N:198:ARG:N	1:N:242:GLU:O	2.49	0.43
1:N:360:THR:OG1	1:N:564:GLU:OE1	2.21	0.43
1:N:361:MET:O	1:N:365:THR:OG1	2.30	0.43
1:P:753:GLY:HA3	1:P:754:GLY:HA3	1.73	0.43
1:P:822:LEU:HD23	1:P:822:LEU:HA	1.86	0.43
1:P:827:LEU:N	1:P:854:ASP:O	2.46	0.43
1:K:392:TYR:OH	1:K:418:GLU:OE2	2.27	0.43
1:K:747:HIS:NE2	1:K:772:ASP:OD1	2.42	0.43
1:B:463:GLU:HA	1:B:464:PRO:HD2	1.80	0.43
1:F:329:ARG:O	1:F:333:ASN:ND2	2.51	0.43
1:F:393:CYS:HB2	1:F:421:LEU:CD2	2.48	0.43
1:F:900:LEU:HD22	1:F:930:PHE:CD2	2.53	0.43
1:H:313:LEU:HD12	1:H:313:LEU:HA	1.83	0.43
1:N:240:HIS:HB3	1:N:241:LYS:H	1.52	0.43
1:N:941:GLN:HA	1:N:967:LEU:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:975:GLU:C	1:P:977:PHE:N	2.71	0.43
1:F:346:ALA:HA	1:F:349:MET:HE2	2.00	0.43
1:H:910:ALA:O	1:H:940:GLN:N	2.41	0.43
1:L:599:PHE:CD1	1:L:651:LEU:HD22	2.52	0.43
1:L:787:LEU:HD13	1:L:815:LEU:HD21	2.00	0.43
1:N:393:CYS:HB2	1:N:421:LEU:CD2	2.49	0.43
1:N:499:THR:O	1:N:502:THR:HG23	2.18	0.43
1:K:715:HIS:ND1	1:K:716:THR:HG22	2.33	0.43
1:K:833:THR:O	1:K:836:SER:OG	2.31	0.43
1:D:335:MET:HE3	1:D:341:VAL:HA	1.99	0.43
1:L:145:ARG:CG	1:L:523:VAL:CB	2.95	0.43
1:L:872:ILE:HA	1:L:875:LEU:HG	2.01	0.43
1:P:359:GLN:NE2	1:P:493:TYR:OH	2.47	0.43
1:K:337:THR:HA	1:K:338:PRO:HD3	1.79	0.43
1:D:161:LEU:HD21	1:D:276:ILE:HD11	2.00	0.43
1:D:534:ILE:CG1	1:D:693:HIS:HB2	2.49	0.43
1:H:756:ILE:HG22	1:H:783:LEU:HD13	2.01	0.43
1:L:115:LEU:HA	1:L:130:LEU:HD22	2.00	0.43
1:N:138:ILE:O	1:N:138:ILE:HG12	2.19	0.43
1:B:436:LYS:HE3	1:F:217:TYR:CZ	2.54	0.43
1:B:712:LYS:HD2	1:B:712:LYS:C	2.39	0.43
1:D:410:PRO:HG3	1:D:418:GLU:HG3	2.00	0.43
1:F:266:LYS:HA	1:F:290:VAL:HG11	1.99	0.43
1:F:980:ASP:OD2	1:F:980:ASP:N	2.51	0.43
1:N:478:VAL:O	1:N:512:VAL:HG13	2.18	0.43
1:N:568:LYS:HB3	1:N:601:TYR:CD2	2.53	0.43
1:N:931:LEU:HD21	1:N:936:LEU:HB2	2.01	0.43
1:P:322:TRP:CE3	1:P:325:ILE:HD12	2.54	0.43
1:P:968:VAL:O	1:P:998:GLN:N	2.49	0.43
1:B:245:PHE:HB2	1:B:275:VAL:HG12	2.00	0.43
1:D:817:GLU:HB3	1:D:818:GLU:HG3	2.00	0.43
1:F:240:HIS:CG	1:F:241:LYS:N	2.86	0.43
1:H:962:GLU:HA	1:H:990:VAL:HG13	2.00	0.43
1:L:371:ILE:HG13	1:L:372:GLN:N	2.33	0.43
1:N:934:ASN:HB3	1:N:935:PRO:O	2.18	0.43
1:N:962:GLU:HA	1:N:994:LEU:HD21	1.99	0.43
1:B:401:VAL:HG11	1:B:490:LEU:HD22	2.00	0.43
1:B:416:MET:H	1:B:416:MET:HG2	1.38	0.43
1:B:890:TRP:CZ3	1:B:918:ARG:HD3	2.54	0.43
1:F:285:ARG:O	1:F:520:GLY:HA3	2.19	0.43
1:H:145:ARG:HH21	1:H:667:ARG:HH21	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:823:GLN:HA	1:L:850:LEU:HA	2.00	0.43
1:N:96:GLU:CD	1:N:96:GLU:H	2.21	0.43
1:B:267:GLU:HB3	1:B:269:HIS:CE1	2.53	0.43
1:D:285:ARG:O	1:D:520:GLY:HA3	2.18	0.43
1:D:573:GLN:NE2	1:F:862:LYS:HB3	2.34	0.43
1:F:205:LEU:HB2	1:F:248:ASP:O	2.19	0.43
1:H:347:ILE:HA	1:H:369:LEU:HD21	2.01	0.43
1:L:920:ARG:HA	1:L:948:CYS:O	2.19	0.43
1:N:855:ILE:HG13	1:N:887:PRO:HD3	2.01	0.43
1:K:449:TYR:OH	1:K:453:ARG:NH1	2.41	0.43
1:B:551:VAL:CG1	1:B:582:LYS:HG2	2.49	0.43
1:B:743:ILE:HG13	1:B:773:ILE:HD11	1.99	0.43
1:F:1001:LYS:HG3	1:F:1022:VAL:HB	2.01	0.43
1:L:345:CYS:O	1:L:349:MET:HG3	2.19	0.43
1:L:522:SER:C	1:L:523:VAL:O	2.55	0.43
1:L:538:ARG:HE	1:L:538:ARG:HB3	1.51	0.43
1:L:1017:GLY:C	1:L:1019:PHE:H	2.22	0.43
1:N:502:THR:HG21	1:N:565:SER:HB2	2.01	0.43
1:N:947:HIS:CG	1:N:947:HIS:O	2.71	0.43
1:N:981:ALA:HA	1:N:984:VAL:HB	2.01	0.43
1:P:142:LYS:HD2	1:P:168:GLU:OE2	2.19	0.43
1:K:308:LEU:HD13	2:K:1101:ADP:C2	2.54	0.42
1:K:746:LEU:HD12	1:K:746:LEU:HA	1.75	0.42
1:K:816:SER:HB2	1:K:843:ASN:HB2	2.00	0.42
1:B:811:ILE:O	1:B:815:LEU:HG	2.19	0.42
1:B:859:TYR:CE1	1:B:889:CYS:HA	2.53	0.42
1:F:205:LEU:HB3	1:F:253:PHE:HB2	2.01	0.42
1:F:409:GLU:HB2	1:F:436:LYS:HD3	1.99	0.42
1:H:679:TYR:O	1:H:683:ILE:HG13	2.19	0.42
1:H:827:LEU:HD13	1:H:827:LEU:HA	1.84	0.42
1:L:746:LEU:HD12	1:L:746:LEU:HA	1.92	0.42
1:L:922:GLU:H	1:L:922:GLU:HG2	1.28	0.42
1:N:143:ASP:O	1:N:144:HIS:CG	2.72	0.42
1:N:931:LEU:HD11	1:N:964:LEU:HD21	2.01	0.42
1:K:562:PHE:HB2	1:K:575:PHE:CE1	2.54	0.42
1:D:168:GLU:HA	1:D:279:THR:O	2.18	0.42
1:D:974:THR:HG23	1:D:975:GLU:N	2.33	0.42
1:F:919:LEU:HD22	1:F:923:GLU:HB3	2.02	0.42
1:F:1001:LYS:HA	1:F:1022:VAL:HB	2.01	0.42
1:F:1012:ILE:O	1:F:1015:ILE:HG22	2.19	0.42
1:H:588:SER:OG	1:H:615:ASP:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:765:LEU:HD21	1:H:768:LEU:HD13	2.00	0.42
1:H:771:ASP:OD1	1:H:800:HIS:HB2	2.19	0.42
1:H:832:LEU:HD23	1:H:832:LEU:HA	1.87	0.42
1:L:309:ILE:HD11	1:L:335:MET:HE2	2.00	0.42
1:N:143:ASP:HB3	1:N:149:VAL:CG2	2.49	0.42
1:N:645:PRO:HA	1:N:646:PRO:HD3	1.91	0.42
1:N:791:LYS:HB3	1:N:791:LYS:HE3	1.86	0.42
1:P:911:LYS:HG2	1:P:941:GLN:HG2	2.01	0.42
1:P:920:ARG:HB2	1:P:922:GLU:HG2	2.00	0.42
1:K:480:ILE:HG23	1:K:514:GLN:O	2.20	0.42
1:B:986:LYS:NZ	1:F:963:ASN:OD1	2.42	0.42
1:D:362:LEU:HD12	1:D:362:LEU:HA	1.89	0.42
1:H:124:ILE:HD11	1:H:370:LEU:HD11	2.02	0.42
1:H:218:ASP:HA	1:L:435:LEU:HD21	2.01	0.42
1:H:911:LYS:HG2	1:H:941:GLN:HG2	2.01	0.42
1:H:986:LYS:O	1:H:990:VAL:HG23	2.18	0.42
1:L:816:SER:HB2	1:L:843:ASN:CB	2.48	0.42
1:N:313:LEU:HD12	1:N:313:LEU:HA	1.88	0.42
1:N:507:ARG:HG2	1:P:890:TRP:CE3	2.53	0.42
1:P:865:ASN:OD1	1:P:895:SER:OG	2.36	0.42
1:P:895:SER:O	1:P:899:LEU:N	2.42	0.42
1:K:498:SER:O	1:K:502:THR:HG23	2.19	0.42
1:K:518:LEU:HD11	1:K:547:LYS:HG2	2.01	0.42
1:K:572:SER:HG	1:K:604:ASN:HD21	1.57	0.42
1:K:803:ASP:OD2	1:F:462:LYS:HG2	2.19	0.42
1:F:126:ILE:HG23	1:F:312:VAL:HG11	2.02	0.42
1:H:541:THR:HG23	1:H:544:ASP:H	1.83	0.42
1:L:593:ASP:OD2	1:L:647:ARG:NH2	2.40	0.42
1:L:669:ILE:HB	1:L:697:CYS:SG	2.60	0.42
1:L:910:ALA:O	1:L:940:GLN:N	2.45	0.42
1:L:936:LEU:HB3	1:L:939:LEU:HB2	2.00	0.42
1:P:595:LEU:HD13	1:P:595:LEU:HA	1.79	0.42
1:K:252:GLU:HA	1:K:406:PHE:CE2	2.54	0.42
1:D:822:LEU:HD23	1:D:822:LEU:HA	1.91	0.42
1:H:238:LYS:O	1:H:240:HIS:ND1	2.49	0.42
1:H:393:CYS:HB2	1:H:421:LEU:CD2	2.49	0.42
1:H:915:LYS:HG2	1:H:945:ALA:HB3	2.01	0.42
1:L:205:LEU:HD12	1:L:205:LEU:HA	1.88	0.42
1:L:990:VAL:O	1:L:994:LEU:HG	2.20	0.42
1:N:537:LEU:HD21	1:N:740:ASN:HB3	2.01	0.42
1:P:189:GLY:N	1:P:190:GLY:HA3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:832:LEU:HD23	1:P:832:LEU:HA	1.85	0.42
1:K:93:VAL:HG22	1:K:231:THR:HG22	2.00	0.42
1:K:479:SER:O	1:K:483:ILE:HG13	2.20	0.42
1:B:265:ILE:HG23	1:B:277:VAL:HG21	2.02	0.42
1:B:562:PHE:HB2	1:B:575:PHE:CE1	2.53	0.42
1:B:969:PHE:CD1	1:B:969:PHE:C	2.93	0.42
1:D:170:GLU:O	1:D:175:LYS:NZ	2.53	0.42
1:D:313:LEU:HD12	1:D:313:LEU:HA	1.86	0.42
1:N:775:MET:SD	1:N:801:LEU:HD22	2.60	0.42
1:P:543:GLN:O	1:P:547:LYS:HG3	2.19	0.42
1:K:474:LEU:HD23	1:K:477:MET:HE1	2.01	0.42
1:K:599:PHE:O	1:K:657:GLN:NE2	2.52	0.42
1:K:664:VAL:HG22	1:K:692:LEU:HD23	2.01	0.42
1:B:130:LEU:O	1:B:181:ARG:NH2	2.52	0.42
1:B:285:ARG:NH1	1:B:521:LEU:HD21	2.34	0.42
1:B:524:THR:O	1:B:527:PRO:HD2	2.19	0.42
1:B:675:GLN:HG2	1:B:679:TYR:CE2	2.54	0.42
1:D:341:VAL:O	1:D:344:THR:OG1	2.35	0.42
1:F:914:LEU:HB3	1:F:917:TRP:CG	2.55	0.42
1:H:333:ASN:HA	1:H:336:LYS:NZ	2.34	0.42
1:L:874:ARG:HH11	1:L:874:ARG:CG	2.26	0.42
1:N:429:LYS:O	1:N:431:THR:HG23	2.20	0.42
1:N:852:ILE:HD13	1:N:883:THR:HB	2.02	0.42
1:N:931:LEU:CD2	1:N:936:LEU:HB2	2.50	0.42
1:P:955:LEU:CD1	1:P:983:LEU:N	2.82	0.42
1:K:145:ARG:NH1	1:K:615:ASP:OD2	2.52	0.42
1:F:405:LYS:HE2	1:F:405:LYS:HB3	1.82	0.42
1:H:96:GLU:O	1:H:100:VAL:HG12	2.19	0.42
1:H:991:LEU:HD13	1:H:997:LEU:CD2	2.50	0.42
1:L:854:ASP:OD2	1:L:856:SER:OG	2.34	0.42
1:N:990:VAL:O	1:N:994:LEU:HG	2.20	0.42
1:K:282:GLU:H	1:K:282:GLU:HG3	1.65	0.42
1:K:345:CYS:O	1:K:349:MET:HG3	2.19	0.42
1:K:777:GLU:O	1:K:781:LYS:HG3	2.20	0.42
1:D:677:ILE:HG23	1:D:707:VAL:HG22	2.00	0.42
1:D:764:ASN:HA	1:D:792:LYS:HD3	2.01	0.42
1:L:825:MET:HG2	1:L:827:LEU:HD13	2.02	0.42
1:N:269:HIS:CD2	1:N:269:HIS:H	2.37	0.42
1:N:605:CYS:O	1:N:609:LEU:HG	2.20	0.42
1:N:964:LEU:H	1:N:964:LEU:HG	1.48	0.42
1:P:460:THR:HG21	1:P:498:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:480:ILE:HG13	1:P:514:GLN:O	2.20	0.42
1:P:712:LYS:HD2	1:P:712:LYS:HA	1.93	0.42
1:K:248:ASP:HA	1:K:278:THR:HB	2.01	0.42
1:K:288:ARG:NH2	1:K:522:SER:O	2.47	0.42
1:K:571:LEU:HB3	1:K:575:PHE:HD2	1.85	0.42
1:B:478:VAL:O	1:B:512:VAL:HG13	2.20	0.42
1:B:945:ALA:O	1:B:946:GLY:C	2.58	0.42
1:B:1018:THR:O	1:B:1018:THR:OG1	2.37	0.42
1:D:325:ILE:HD13	1:D:335:MET:HG2	2.01	0.42
1:D:429:LYS:HB2	1:D:439:TYR:CD2	2.55	0.42
1:D:859:TYR:HH	1:D:890:TRP:HD1	1.66	0.42
1:H:582:LYS:O	1:H:610:ASP:N	2.52	0.42
1:H:931:LEU:HD23	1:H:931:LEU:HA	1.81	0.42
1:L:333:ASN:HA	1:L:336:LYS:HZ3	1.85	0.42
1:L:653:PHE:O	1:L:654:ASN:HB2	2.20	0.42
1:L:970:PHE:HZ	1:L:991:LEU:HD11	1.84	0.42
1:K:507:ARG:NH1	1:K:574:GLU:HG3	2.34	0.41
1:K:537:LEU:HD21	1:K:740:ASN:HB3	2.01	0.41
1:K:743:ILE:O	1:K:743:ILE:HG13	2.20	0.41
1:K:813:LYS:HE3	1:K:817:GLU:HG3	2.01	0.41
1:B:282:GLU:H	1:B:282:GLU:HG3	1.63	0.41
1:B:854:ASP:HA	1:B:885:MET:HB2	2.02	0.41
1:B:986:LYS:O	1:B:990:VAL:HG23	2.20	0.41
1:D:925:LYS:O	1:D:929:GLU:HG3	2.19	0.41
1:F:549:ILE:O	1:F:552:ASN:HB2	2.19	0.41
1:L:518:LEU:HA	1:L:521:LEU:HD22	2.02	0.41
1:N:591:ILE:HB	1:N:647:ARG:HG2	2.02	0.41
1:N:740:ASN:ND2	1:N:767:ARG:HB2	2.35	0.41
1:N:770:LEU:HD12	1:N:770:LEU:HA	1.93	0.41
1:P:324:GLN:OE1	1:P:353:GLU:HG2	2.20	0.41
1:P:756:ILE:HG22	1:P:783:LEU:HD13	2.02	0.41
1:P:869:GLN:NE2	1:P:898:LYS:HD3	2.34	0.41
1:D:229:LYS:HB3	1:D:230:PRO:HD3	2.02	0.41
1:F:361:MET:O	1:F:365:THR:OG1	2.29	0.41
1:F:900:LEU:HD22	1:F:930:PHE:CG	2.55	0.41
1:L:817:GLU:HB3	1:L:818:GLU:HG3	2.02	0.41
1:N:339:LEU:O	1:N:343:ILE:HG13	2.20	0.41
1:N:480:ILE:HG23	1:N:514:GLN:O	2.20	0.41
1:N:588:SER:HA	1:N:591:ILE:HD11	2.03	0.41
1:K:173:LYS:HD3	1:K:173:LYS:HA	1.68	0.41
1:B:225:ASP:HB3	1:F:409:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:ARG:HA	1:B:948:CYS:O	2.20	0.41
1:D:891:ASP:OD1	1:D:891:ASP:N	2.44	0.41
1:F:205:LEU:HD12	1:F:205:LEU:HA	1.89	0.41
1:F:345:CYS:O	1:F:349:MET:HG3	2.20	0.41
1:F:824:GLU:HG2	1:F:852:ILE:HB	2.02	0.41
1:H:167:ILE:HB	1:H:278:THR:HG22	2.01	0.41
1:H:230:PRO:HG3	1:L:256:GLN:HG2	2.02	0.41
1:H:492:LEU:HG	1:H:564:GLU:HG3	2.03	0.41
1:H:568:LYS:HD3	1:H:601:TYR:CE1	2.56	0.41
1:L:752:PRO:HA	1:L:757:ASP:OD1	2.20	0.41
1:N:158:LEU:O	1:N:161:LEU:HG	2.20	0.41
1:N:334:LEU:HD13	1:N:334:LEU:HA	1.88	0.41
1:N:479:SER:O	1:N:483:ILE:HG13	2.21	0.41
1:N:619:ARG:HH11	1:N:645:PRO:HB3	1.86	0.41
1:N:906:THR:O	1:N:909:LEU:HB2	2.20	0.41
1:P:776:ASN:H	1:P:779:ASP:HB2	1.85	0.41
1:P:970:PHE:HZ	1:P:991:LEU:HD21	1.84	0.41
1:K:322:TRP:CE3	1:K:325:ILE:HD12	2.55	0.41
1:B:740:ASN:HD22	1:B:767:ARG:HB2	1.86	0.41
1:D:398:LEU:HD23	1:D:398:LEU:HA	1.91	0.41
1:D:418:GLU:H	1:D:418:GLU:HG2	1.59	0.41
1:D:797:HIS:CE1	1:D:826:LYS:HG3	2.56	0.41
1:F:164:PRO:HG2	1:F:290:VAL:HG12	2.02	0.41
1:F:716:THR:HG22	1:F:740:ASN:HD22	1.85	0.41
1:F:1018:THR:O	1:F:1018:THR:OG1	2.39	0.41
1:L:168:GLU:HB3	1:L:284:LEU:HD13	2.01	0.41
1:L:351:ARG:HE	1:L:369:LEU:HG	1.84	0.41
1:N:371:ILE:O	1:N:375:SER:HB3	2.21	0.41
1:N:434:ARG:NH2	1:N:438:THR:HG21	2.34	0.41
1:N:694:ILE:HD12	1:N:719:VAL:HG22	2.03	0.41
1:P:416:MET:O	1:P:420:VAL:HG23	2.20	0.41
1:P:799:THR:HA	1:P:828:VAL:O	2.20	0.41
1:K:228:SER:OG	1:K:231:THR:OG1	2.17	0.41
1:K:361:MET:O	1:K:365:THR:OG1	2.31	0.41
1:B:434:ARG:HB3	1:B:436:LYS:O	2.20	0.41
1:B:595:LEU:HD13	1:B:595:LEU:HA	1.76	0.41
1:D:252:GLU:HA	1:D:406:PHE:CE2	2.55	0.41
1:F:653:PHE:HA	1:F:656:LYS:HD2	2.02	0.41
1:F:888:TRP:HA	1:F:892:VAL:HG11	2.02	0.41
1:H:306:LYS:HD2	1:H:322:TRP:CE2	2.56	0.41
1:H:750:GLN:HG3	1:H:756:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:669:ILE:HB	1:K:697:CYS:SG	2.61	0.41
1:B:832:LEU:HB2	1:B:858:ASN:OD1	2.20	0.41
1:N:968:VAL:O	1:N:998:GLN:N	2.44	0.41
1:P:855:ILE:O	1:P:858:ASN:ND2	2.53	0.41
1:K:890:TRP:CH2	1:F:580:GLN:HG2	2.55	0.41
1:K:920:ARG:HE	1:K:920:ARG:HB2	1.73	0.41
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.96	0.41
1:D:920:ARG:HD2	1:D:920:ARG:HA	1.85	0.41
1:F:347:ILE:O	1:F:351:ARG:N	2.52	0.41
1:F:617:TYR:C	1:F:619:ARG:H	2.23	0.41
1:F:800:HIS:H	1:F:829:ALA:HB3	1.86	0.41
1:F:931:LEU:HD23	1:F:931:LEU:HA	1.83	0.41
1:N:266:LYS:HA	1:N:290:VAL:HG21	2.02	0.41
1:N:274:MET:HE3	1:N:274:MET:HB3	1.73	0.41
1:P:872:ILE:HA	1:P:875:LEU:HG	2.02	0.41
1:P:924:ILE:HD13	1:P:924:ILE:HA	1.70	0.41
1:K:206:ARG:HG2	1:K:207:SER:N	2.35	0.41
1:B:672:LEU:HB2	1:B:699:ALA:HB1	2.02	0.41
1:B:672:LEU:HD12	1:B:676:ASP:HB3	2.02	0.41
1:B:679:TYR:O	1:B:683:ILE:HG13	2.21	0.41
1:B:936:LEU:HD12	1:B:936:LEU:HA	1.78	0.41
1:D:321:LEU:O	1:D:325:ILE:HG13	2.21	0.41
1:D:745:ARG:HA	1:D:772:ASP:HB3	2.03	0.41
1:F:421:LEU:HB2	1:F:427:LEU:HD12	2.02	0.41
1:L:576:GLU:HB2	1:L:604:ASN:HD22	1.85	0.41
1:L:800:HIS:H	1:L:829:ALA:HB3	1.86	0.41
1:N:337:THR:HA	1:N:338:PRO:HD3	1.89	0.41
1:N:719:VAL:HG11	1:N:724:LEU:HD13	2.02	0.41
1:N:744:HIS:NE2	1:N:771:ASP:OD2	2.54	0.41
1:K:531:GLN:NE2	1:K:744:HIS:HE1	2.18	0.41
1:K:918:ARG:NH2	1:K:975:GLU:OE1	2.53	0.41
1:B:376:HIS:HE2	1:H:107:ASP:CG	2.25	0.41
1:B:383:SER:HB3	1:B:384:GLY:H	1.57	0.41
1:B:420:VAL:O	1:B:423:THR:OG1	2.26	0.41
1:B:555:VAL:O	1:B:559:ILE:HG13	2.21	0.41
1:B:645:PRO:HA	1:B:646:PRO:HD3	1.95	0.41
1:B:712:LYS:HD2	1:B:712:LYS:O	2.20	0.41
1:B:746:LEU:HD23	1:B:746:LEU:HA	1.65	0.41
1:B:813:LYS:O	1:B:817:GLU:N	2.53	0.41
1:B:990:VAL:O	1:B:994:LEU:HG	2.20	0.41
1:D:303:ASP:OD2	1:D:303:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LYS:HB3	1:D:601:TYR:CD2	2.56	0.41
1:F:173:LYS:HA	1:F:173:LYS:HD3	1.77	0.41
1:F:832:LEU:HB2	1:F:858:ASN:CG	2.42	0.41
1:L:324:GLN:HE22	1:L:354:PHE:H	1.67	0.41
1:L:477:MET:HE1	1:L:491:LEU:HD21	2.02	0.41
1:N:189:GLY:HA3	1:N:190:GLY:HA2	1.56	0.41
1:N:621:THR:HG21	1:N:679:TYR:HB2	2.03	0.41
1:P:97:ASP:HA	1:P:100:VAL:HG22	2.02	0.41
1:P:338:PRO:O	1:P:342:VAL:HG23	2.21	0.41
1:P:680:LEU:HB3	1:P:684:PHE:CE2	2.55	0.41
1:P:987:LEU:O	1:P:991:LEU:HB2	2.21	0.41
1:K:823:GLN:HA	1:K:850:LEU:HA	2.02	0.41
1:K:914:LEU:HB3	1:K:917:TRP:CD1	2.56	0.41
1:K:925:LYS:HA	1:K:956:TYR:HE2	1.86	0.41
1:B:918:ARG:H	1:B:918:ARG:HG2	1.52	0.41
1:F:859:TYR:CE1	1:F:889:CYS:HA	2.56	0.41
1:H:813:LYS:HD3	1:H:817:GLU:OE2	2.21	0.41
1:B:131:GLU:HA	1:B:181:ARG:HH22	1.86	0.40
1:B:614:LEU:HD23	1:B:616:PHE:CE2	2.56	0.40
1:D:360:THR:OG1	1:D:564:GLU:OE1	2.25	0.40
1:D:665:THR:HG23	1:D:693:HIS:HB3	2.03	0.40
1:F:816:SER:HB2	1:F:843:ASN:CB	2.52	0.40
1:F:822:LEU:HD23	1:F:822:LEU:HA	1.86	0.40
1:N:904:GLU:HG2	1:N:930:PHE:HE1	1.86	0.40
1:P:612:VAL:O	1:P:662:LEU:HD23	2.21	0.40
1:K:266:LYS:HA	1:K:290:VAL:HG21	2.03	0.40
1:K:562:PHE:O	1:K:565:SER:OG	2.32	0.40
1:F:378:TYR:HD2	1:F:386:PHE:CD1	2.34	0.40
1:F:968:VAL:HG12	1:F:998:GLN:HB2	2.02	0.40
1:H:343:ILE:O	1:H:347:ILE:HG13	2.20	0.40
1:H:799:THR:HA	1:H:828:VAL:O	2.20	0.40
1:N:506:MET:HG3	1:N:575:PHE:CE1	2.56	0.40
1:P:751:LEU:HD23	1:P:752:PRO:O	2.22	0.40
1:K:161:LEU:HD21	1:K:276:ILE:HD11	2.03	0.40
1:B:240:HIS:HB3	1:B:241:LYS:H	1.50	0.40
1:D:205:LEU:CD2	1:D:247:LEU:HB3	2.45	0.40
1:D:400:GLY:O	1:D:404:HIS:N	2.55	0.40
1:F:239:LEU:HD22	1:F:239:LEU:HA	1.89	0.40
1:H:134:PHE:CZ	1:H:181:ARG:HG2	2.56	0.40
1:H:816:SER:HB2	1:H:843:ASN:CB	2.51	0.40
1:L:92:GLN:O	1:L:93:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:399:GLU:OE1	1:L:473:TYR:OH	2.29	0.40
1:L:656:LYS:H	1:L:656:LYS:HG2	1.47	0.40
1:N:98:LEU:HD13	1:N:235:LEU:HD21	2.02	0.40
1:N:925:LYS:O	1:N:929:GLU:HG2	2.21	0.40
1:P:882:THR:O	1:P:910:ALA:N	2.51	0.40
1:K:614:LEU:O	1:K:664:VAL:HA	2.21	0.40
1:B:164:PRO:HG2	1:B:290:VAL:CG1	2.52	0.40
1:D:931:LEU:HA	1:D:931:LEU:HD23	1.82	0.40
1:F:876:GLY:N	1:F:902:GLN:HE21	2.19	0.40
1:F:915:LYS:HA	1:F:945:ALA:HB3	2.03	0.40
1:H:216:LEU:HD11	1:H:245:PHE:HE1	1.86	0.40
1:H:495:CYS:HB3	1:H:502:THR:HB	2.02	0.40
1:H:503:ARG:HG3	1:H:571:LEU:CD1	2.51	0.40
1:N:769:ILE:HA	1:N:797:HIS:HB2	2.03	0.40
1:K:416:MET:O	1:K:420:VAL:HG23	2.22	0.40
1:K:781:LYS:O	1:K:785:GLU:HG3	2.21	0.40
1:B:344:THR:HB	1:B:362:LEU:HD11	2.04	0.40
1:B:724:LEU:HG	1:B:728:ASP:HB2	2.04	0.40
1:B:746:LEU:O	1:B:747:HIS:HB2	2.22	0.40
1:D:426:LEU:HD13	1:D:426:LEU:HA	1.82	0.40
1:D:813:LYS:HD2	1:D:839:VAL:HG11	2.04	0.40
1:F:753:GLY:HA3	1:F:754:GLY:HA3	1.73	0.40
1:F:921:ASP:O	1:F:925:LYS:HB2	2.21	0.40
1:H:93:VAL:HG11	1:H:235:LEU:HD22	2.03	0.40
1:N:126:ILE:HG21	1:N:342:VAL:HG13	2.03	0.40
1:N:223:ILE:HA	1:N:224:PRO:HD3	1.91	0.40
1:N:543:GLN:O	1:N:547:LYS:HG3	2.21	0.40
1:N:909:LEU:O	1:N:939:LEU:HA	2.21	0.40
1:P:126:ILE:HG21	1:P:342:VAL:HG13	2.02	0.40
1:P:568:LYS:HB2	1:P:568:LYS:HE2	1.95	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:433:GLN:CD	1:K:433:GLN:NE2[8_555]	1.34	0.86
1:K:433:GLN:OE1	1:K:433:GLN:NE2[8_555]	1.76	0.44

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	896/1024 (88%)	875 (98%)	21 (2%)	0	100	100
1	D	893/1024 (87%)	864 (97%)	28 (3%)	1 (0%)	51	83
1	F	892/1024 (87%)	868 (97%)	23 (3%)	1 (0%)	51	83
1	H	887/1024 (87%)	862 (97%)	25 (3%)	0	100	100
1	K	895/1024 (87%)	878 (98%)	15 (2%)	2 (0%)	47	79
1	L	882/1024 (86%)	859 (97%)	21 (2%)	2 (0%)	47	79
1	N	870/1024 (85%)	847 (97%)	20 (2%)	3 (0%)	41	74
1	P	856/1024 (84%)	824 (96%)	31 (4%)	1 (0%)	51	83
All	All	7071/8192 (86%)	6877 (97%)	184 (3%)	10 (0%)	51	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	93	VAL
1	N	976	GLU
1	N	979	PRO
1	K	568	LYS
1	F	1018	THR
1	K	519	GLN
1	D	519	GLN
1	P	519	GLN
1	L	519	GLN
1	N	947	HIS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	797/912 (87%)	668 (84%)	129 (16%)	2	11
1	D	795/912 (87%)	678 (85%)	117 (15%)	3	14
1	F	795/912 (87%)	679 (85%)	116 (15%)	3	15
1	H	788/912 (86%)	665 (84%)	123 (16%)	2	12
1	K	798/912 (88%)	668 (84%)	130 (16%)	2	11
1	L	785/912 (86%)	663 (84%)	122 (16%)	2	12
1	N	769/912 (84%)	642 (84%)	127 (16%)	2	10
1	P	754/912 (83%)	626 (83%)	128 (17%)	2	10
All	All	6281/7296 (86%)	5289 (84%)	992 (16%)	2	12

All (992) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	95	GLU
1	K	97	ASP
1	K	108	LEU
1	K	111	SER
1	K	115	LEU
1	K	120	LEU
1	K	133	THR
1	K	138	ILE
1	K	139	MET
1	K	143	ASP
1	K	168	GLU
1	K	171	SER
1	K	175	LYS
1	K	177	THR
1	K	178	LEU
1	K	184	MET
1	K	195	LYS
1	K	206	ARG
1	K	209	ARG
1	K	221	LEU
1	K	223	ILE
1	K	231	THR
1	K	233	LYS
1	K	238	LYS

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Mol	Chain	Res	Type
1	K	256	GLN
1	K	266	LYS
1	K	281	THR
1	K	287	ILE
1	K	288	ARG
1	K	301	THR
1	K	314	VAL
1	K	324	GLN
1	K	335	MET
1	K	337	THR
1	K	359	GLN
1	K	369	LEU
1	K	396	LEU
1	K	404	HIS
1	K	409	GLU
1	K	414	SER
1	K	416	MET
1	K	417	ASN
1	K	418	GLU
1	K	423	THR
1	K	433	GLN
1	K	445	SER
1	K	455	LEU
1	K	463	GLU
1	K	481	SER
1	K	498	SER
1	K	507	ARG
1	K	511	MET
1	K	523	VAL
1	K	525	LYS
1	K	531	GLN
1	K	540	THR
1	K	543	GLN
1	K	553	SER
1	K	563	SER
1	K	569	SER
1	K	571	LEU
1	K	573	GLN
1	K	580	GLN
1	K	583	SER
1	K	589	GLU
1	K	591	ILE

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Mol	Chain	Res	Type
1	K	619	ARG
1	K	621	THR
1	K	647	ARG
1	K	650	SER
1	K	651	LEU
1	K	660	LYS
1	K	664	VAL
1	K	675	GLN
1	K	685	SER
1	K	690	LEU
1	K	692	LEU
1	K	703	ARG
1	K	710	THR
1	K	716	THR
1	K	735	VAL
1	K	743	ILE
1	K	745	ARG
1	K	746	LEU
1	K	749	GLN
1	K	751	LEU
1	K	755	LEU
1	K	756	ILE
1	K	762	LEU
1	K	770	LEU
1	K	788	ARG
1	K	789	SER
1	K	790	LEU
1	K	793	MET
1	K	832	LEU
1	K	847	LEU
1	K	848	ILE
1	K	874	ARG
1	K	878	LEU
1	K	886	LEU
1	K	892	VAL
1	K	896	LEU
1	K	900	LEU
1	K	902	GLN
1	K	909	LEU
1	K	911	LYS
1	K	914	LEU
1	K	918	ARG

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Mol	Chain	Res	Type
1	K	924	ILE
1	K	925	LYS
1	K	926	SER
1	K	934	ASN
1	K	936	LEU
1	K	939	LEU
1	K	966	GLN
1	K	976	GLU
1	K	988	SER
1	K	993	LYS
1	K	995	THR
1	K	996	LEU
1	K	997	LEU
1	K	1003	THR
1	K	1008	ASP
1	K	1010	TYR
1	K	1012	ILE
1	K	1013	SER
1	K	1016	LYS
1	K	1018	THR
1	K	1020	LYS
1	K	1023	THR
1	B	97	ASP
1	B	100	VAL
1	B	115	LEU
1	B	120	LEU
1	B	133	THR
1	B	139	MET
1	B	161	LEU
1	B	168	GLU
1	B	171	SER
1	B	184	MET
1	B	188	SER
1	B	195	LYS
1	B	206	ARG
1	B	209	ARG
1	B	221	LEU
1	B	223	ILE
1	B	225	ASP
1	B	231	THR
1	B	237	LEU
1	B	240	HIS

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Mol	Chain	Res	Type
1	B	256	GLN
1	B	274	MET
1	B	281	THR
1	B	287	ILE
1	B	288	ARG
1	B	314	VAL
1	B	319	GLU
1	B	335	MET
1	B	337	THR
1	B	339	LEU
1	B	352	GLN
1	B	353	GLU
1	B	383	SER
1	B	396	LEU
1	B	409	GLU
1	B	411	GLU
1	B	416	MET
1	B	418	GLU
1	B	421	LEU
1	B	434	ARG
1	B	455	LEU
1	B	463	GLU
1	B	497	SER
1	B	498	SER
1	B	499	THR
1	B	502	THR
1	B	503	ARG
1	B	519	GLN
1	B	523	VAL
1	B	526	ARG
1	B	528	LEU
1	B	529	TRP
1	B	530	ARG
1	B	535	GLN
1	B	540	THR
1	B	541	THR
1	B	542	GLU
1	B	543	GLN
1	B	563	SER
1	B	573	GLN
1	B	583	SER
1	B	588	SER

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Mol	Chain	Res	Type
1	B	595	LEU
1	B	621	THR
1	B	647	ARG
1	B	662	LEU
1	B	664	VAL
1	B	670	ASN
1	B	685	SER
1	B	689	ASN
1	B	692	LEU
1	B	706	SER
1	B	712	LYS
1	B	713	ASN
1	B	714	MET
1	B	725	THR
1	B	735	VAL
1	B	744	HIS
1	B	749	GLN
1	B	751	LEU
1	B	755	LEU
1	B	762	LEU
1	B	770	LEU
1	B	774	ARG
1	B	789	SER
1	B	790	LEU
1	B	791	LYS
1	B	793	MET
1	B	802	SER
1	B	806	GLU
1	B	822	LEU
1	B	828	VAL
1	B	832	LEU
1	B	847	LEU
1	B	848	ILE
1	B	850	LEU
1	B	851	SER
1	B	857	GLU
1	B	862	LYS
1	B	878	LEU
1	B	880	GLU
1	B	892	VAL
1	B	896	LEU
1	B	900	LEU

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Mol	Chain	Res	Type
1	B	909	LEU
1	B	911	LYS
1	B	914	LEU
1	B	918	ARG
1	B	920	ARG
1	B	924	ILE
1	B	926	SER
1	B	934	ASN
1	B	936	LEU
1	B	939	LEU
1	B	951	SER
1	B	955	LEU
1	B	962	GLU
1	B	964	LEU
1	B	969	PHE
1	B	975	GLU
1	B	988	SER
1	B	989	GLN
1	B	995	THR
1	B	996	LEU
1	B	1002	LEU
1	B	1007	PHE
1	B	1015	ILE
1	B	1018	THR
1	B	1020	LYS
1	D	115	LEU
1	D	120	LEU
1	D	130	LEU
1	D	133	THR
1	D	138	ILE
1	D	139	MET
1	D	142	LYS
1	D	145	ARG
1	D	168	GLU
1	D	181	ARG
1	D	184	MET
1	D	192	ARG
1	D	200	VAL
1	D	206	ARG
1	D	209	ARG
1	D	221	LEU
1	D	227	ILE

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Mol	Chain	Res	Type
1	D	231	THR
1	D	237	LEU
1	D	278	THR
1	D	287	ILE
1	D	288	ARG
1	D	301	THR
1	D	303	ASP
1	D	314	VAL
1	D	334	LEU
1	D	335	MET
1	D	339	LEU
1	D	351	ARG
1	D	352	GLN
1	D	353	GLU
1	D	359	GLN
1	D	371	ILE
1	D	396	LEU
1	D	409	GLU
1	D	411	GLU
1	D	414	SER
1	D	423	THR
1	D	430	TYR
1	D	436	LYS
1	D	445	SER
1	D	455	LEU
1	D	462	LYS
1	D	463	GLU
1	D	475	ASN
1	D	481	SER
1	D	490	LEU
1	D	498	SER
1	D	507	ARG
1	D	511	MET
1	D	523	VAL
1	D	537	LEU
1	D	541	THR
1	D	543	GLN
1	D	547	LYS
1	D	563	SER
1	D	573	GLN
1	D	580	GLN
1	D	583	SER

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Mol	Chain	Res	Type
1	D	589	GLU
1	D	595	LEU
1	D	614	LEU
1	D	621	THR
1	D	651	LEU
1	D	657	GLN
1	D	664	VAL
1	D	670	ASN
1	D	682	LYS
1	D	685	SER
1	D	689	ASN
1	D	690	LEU
1	D	692	LEU
1	D	696	ARG
1	D	711	CYS
1	D	713	ASN
1	D	725	THR
1	D	730	GLN
1	D	735	VAL
1	D	736	THR
1	D	746	LEU
1	D	755	LEU
1	D	756	ILE
1	D	762	LEU
1	D	770	LEU
1	D	789	SER
1	D	790	LEU
1	D	793	MET
1	D	828	VAL
1	D	832	LEU
1	D	847	LEU
1	D	878	LEU
1	D	886	LEU
1	D	891	ASP
1	D	892	VAL
1	D	900	LEU
1	D	903	LEU
1	D	906	THR
1	D	909	LEU
1	D	914	LEU
1	D	924	ILE
1	D	934	ASN

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Mol	Chain	Res	Type
1	D	936	LEU
1	D	951	SER
1	D	955	LEU
1	D	962	GLU
1	D	964	LEU
1	D	965	LYS
1	D	976	GLU
1	D	978	LEU
1	D	987	LEU
1	D	988	SER
1	D	989	GLN
1	D	993	LYS
1	D	996	LEU
1	D	997	LEU
1	D	1008	ASP
1	D	1018	THR
1	F	97	ASP
1	F	115	LEU
1	F	133	THR
1	F	139	MET
1	F	145	ARG
1	F	161	LEU
1	F	168	GLU
1	F	184	MET
1	F	192	ARG
1	F	205	LEU
1	F	206	ARG
1	F	209	ARG
1	F	219	GLN
1	F	223	ILE
1	F	227	ILE
1	F	231	THR
1	F	239	LEU
1	F	274	MET
1	F	278	THR
1	F	281	THR
1	F	288	ARG
1	F	301	THR
1	F	303	ASP
1	F	308	LEU
1	F	324	GLN
1	F	335	MET

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Mol	Chain	Res	Type
1	F	337	THR
1	F	339	LEU
1	F	344	THR
1	F	351	ARG
1	F	353	GLU
1	F	357	HIS
1	F	369	LEU
1	F	385	ASP
1	F	389	SER
1	F	396	LEU
1	F	404	HIS
1	F	409	GLU
1	F	415	SER
1	F	423	THR
1	F	433	GLN
1	F	434	ARG
1	F	436	LYS
1	F	455	LEU
1	F	481	SER
1	F	497	SER
1	F	498	SER
1	F	499	THR
1	F	507	ARG
1	F	523	VAL
1	F	540	THR
1	F	543	GLN
1	F	553	SER
1	F	560	ASN
1	F	563	SER
1	F	574	GLU
1	F	580	GLN
1	F	583	SER
1	F	591	ILE
1	F	614	LEU
1	F	619	ARG
1	F	656	LYS
1	F	657	GLN
1	F	664	VAL
1	F	672	LEU
1	F	678	LYS
1	F	682	LYS
1	F	685	SER

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Mol	Chain	Res	Type
1	F	692	LEU
1	F	710	THR
1	F	715	HIS
1	F	716	THR
1	F	725	THR
1	F	726	THR
1	F	735	VAL
1	F	736	THR
1	F	743	ILE
1	F	746	LEU
1	F	751	LEU
1	F	755	LEU
1	F	756	ILE
1	F	762	LEU
1	F	770	LEU
1	F	788	ARG
1	F	789	SER
1	F	790	LEU
1	F	793	MET
1	F	811	ILE
1	F	813	LYS
1	F	828	VAL
1	F	832	LEU
1	F	847	LEU
1	F	848	ILE
1	F	878	LEU
1	F	891	ASP
1	F	892	VAL
1	F	918	ARG
1	F	922	GLU
1	F	924	ILE
1	F	933	MET
1	F	936	LEU
1	F	951	SER
1	F	962	GLU
1	F	964	LEU
1	F	978	LEU
1	F	983	LEU
1	F	987	LEU
1	F	988	SER
1	F	993	LYS
1	F	995	THR

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Mol	Chain	Res	Type
1	F	997	LEU
1	F	1003	THR
1	F	1008	ASP
1	F	1015	ILE
1	F	1018	THR
1	F	1023	THR
1	H	103	GLN
1	H	115	LEU
1	H	133	THR
1	H	135	THR
1	H	138	ILE
1	H	139	MET
1	H	143	ASP
1	H	145	ARG
1	H	150	GLU
1	H	154	LEU
1	H	168	GLU
1	H	171	SER
1	H	177	THR
1	H	184	MET
1	H	195	LYS
1	H	205	LEU
1	H	206	ARG
1	H	207	SER
1	H	209	ARG
1	H	220	LEU
1	H	231	THR
1	H	237	LEU
1	H	239	LEU
1	H	254	HIS
1	H	256	GLN
1	H	274	MET
1	H	281	THR
1	H	287	ILE
1	H	289	HIS
1	H	301	THR
1	H	314	VAL
1	H	319	GLU
1	H	324	GLN
1	H	331	LEU
1	H	335	MET
1	H	337	THR

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Mol	Chain	Res	Type
1	H	339	LEU
1	H	353	GLU
1	H	359	GLN
1	H	385	ASP
1	H	396	LEU
1	H	404	HIS
1	H	405	LYS
1	H	409	GLU
1	H	415	SER
1	H	431	THR
1	H	433	GLN
1	H	440	LYS
1	H	445	SER
1	H	462	LYS
1	H	498	SER
1	H	502	THR
1	H	503	ARG
1	H	518	LEU
1	H	537	LEU
1	H	540	THR
1	H	543	GLN
1	H	551	VAL
1	H	563	SER
1	H	573	GLN
1	H	574	GLU
1	H	583	SER
1	H	591	ILE
1	H	595	LEU
1	H	614	LEU
1	H	615	ASP
1	H	621	THR
1	H	647	ARG
1	H	650	SER
1	H	651	LEU
1	H	664	VAL
1	H	665	THR
1	H	685	SER
1	H	692	LEU
1	H	703	ARG
1	H	710	THR
1	H	713	ASN
1	H	735	VAL

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Mol	Chain	Res	Type
1	H	736	THR
1	H	745	ARG
1	H	746	LEU
1	H	755	LEU
1	H	756	ILE
1	H	762	LEU
1	H	770	LEU
1	H	789	SER
1	H	790	LEU
1	H	793	MET
1	H	818	GLU
1	H	827	LEU
1	H	828	VAL
1	H	832	LEU
1	H	847	LEU
1	H	878	LEU
1	H	890	TRP
1	H	892	VAL
1	H	896	LEU
1	H	900	LEU
1	H	901	LYS
1	H	906	THR
1	H	909	LEU
1	H	914	LEU
1	H	922	GLU
1	H	924	ILE
1	H	926	SER
1	H	934	ASN
1	H	936	LEU
1	H	937	ARG
1	H	959	ASN
1	H	962	GLU
1	H	964	LEU
1	H	988	SER
1	H	993	LYS
1	H	995	THR
1	H	997	LEU
1	H	1002	LEU
1	H	1003	THR
1	H	1008	ASP
1	H	1011	ASP
1	H	1012	ILE

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Mol	Chain	Res	Type
1	H	1015	ILE
1	H	1020	LYS
1	H	1023	THR
1	L	105	LEU
1	L	108	LEU
1	L	115	LEU
1	L	120	LEU
1	L	130	LEU
1	L	133	THR
1	L	138	ILE
1	L	139	MET
1	L	145	ARG
1	L	150	GLU
1	L	154	LEU
1	L	168	GLU
1	L	171	SER
1	L	184	MET
1	L	192	ARG
1	L	195	LYS
1	L	205	LEU
1	L	206	ARG
1	L	207	SER
1	L	209	ARG
1	L	231	THR
1	L	239	LEU
1	L	243	VAL
1	L	288	ARG
1	L	293	LEU
1	L	301	THR
1	L	303	ASP
1	L	314	VAL
1	L	319	GLU
1	L	331	LEU
1	L	335	MET
1	L	339	LEU
1	L	351	ARG
1	L	353	GLU
1	L	359	GLN
1	L	373	LYS
1	L	377	ARG
1	L	385	ASP
1	L	396	LEU

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Mol	Chain	Res	Type
1	L	404	HIS
1	L	405	LYS
1	L	409	GLU
1	L	411	GLU
1	L	431	THR
1	L	436	LYS
1	L	445	SER
1	L	455	LEU
1	L	481	SER
1	L	497	SER
1	L	498	SER
1	L	521	LEU
1	L	522	SER
1	L	532	GLU
1	L	536	SER
1	L	538	ARG
1	L	540	THR
1	L	543	GLN
1	L	560	ASN
1	L	561	LEU
1	L	563	SER
1	L	574	GLU
1	L	580	GLN
1	L	583	SER
1	L	591	ILE
1	L	595	LEU
1	L	621	THR
1	L	647	ARG
1	L	651	LEU
1	L	656	LYS
1	L	657	GLN
1	L	664	VAL
1	L	670	ASN
1	L	685	SER
1	L	692	LEU
1	L	710	THR
1	L	713	ASN
1	L	716	THR
1	L	725	THR
1	L	727	ASP
1	L	735	VAL
1	L	736	THR

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Mol	Chain	Res	Type
1	L	751	LEU
1	L	755	LEU
1	L	756	ILE
1	L	762	LEU
1	L	770	LEU
1	L	778	GLU
1	L	788	ARG
1	L	789	SER
1	L	790	LEU
1	L	791	LYS
1	L	793	MET
1	L	813	LYS
1	L	828	VAL
1	L	832	LEU
1	L	847	LEU
1	L	848	ILE
1	L	878	LEU
1	L	886	LEU
1	L	890	TRP
1	L	892	VAL
1	L	896	LEU
1	L	900	LEU
1	L	906	THR
1	L	909	LEU
1	L	914	LEU
1	L	922	GLU
1	L	924	ILE
1	L	926	SER
1	L	936	LEU
1	L	939	LEU
1	L	951	SER
1	L	956	TYR
1	L	964	LEU
1	L	965	LYS
1	L	975	GLU
1	L	986	LYS
1	L	988	SER
1	L	995	THR
1	L	996	LEU
1	L	997	LEU
1	L	1023	THR
1	N	96	GLU

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Mol	Chain	Res	Type
1	N	100	VAL
1	N	103	GLN
1	N	108	LEU
1	N	115	LEU
1	N	120	LEU
1	N	133	THR
1	N	138	ILE
1	N	139	MET
1	N	144	HIS
1	N	145	ARG
1	N	150	GLU
1	N	161	LEU
1	N	168	GLU
1	N	171	SER
1	N	177	THR
1	N	184	MET
1	N	195	LYS
1	N	205	LEU
1	N	207	SER
1	N	223	ILE
1	N	231	THR
1	N	239	LEU
1	N	240	HIS
1	N	274	MET
1	N	288	ARG
1	N	301	THR
1	N	303	ASP
1	N	314	VAL
1	N	319	GLU
1	N	324	GLN
1	N	334	LEU
1	N	335	MET
1	N	339	LEU
1	N	353	GLU
1	N	359	GLN
1	N	370	LEU
1	N	396	LEU
1	N	409	GLU
1	N	415	SER
1	N	416	MET
1	N	436	LYS
1	N	455	LEU

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Mol	Chain	Res	Type
1	N	463	GLU
1	N	475	ASN
1	N	480	ILE
1	N	497	SER
1	N	498	SER
1	N	502	THR
1	N	503	ARG
1	N	511	MET
1	N	518	LEU
1	N	523	VAL
1	N	535	GLN
1	N	536	SER
1	N	540	THR
1	N	541	THR
1	N	543	GLN
1	N	551	VAL
1	N	561	LEU
1	N	563	SER
1	N	580	GLN
1	N	583	SER
1	N	591	ILE
1	N	595	LEU
1	N	614	LEU
1	N	621	THR
1	N	647	ARG
1	N	650	SER
1	N	651	LEU
1	N	657	GLN
1	N	660	LYS
1	N	664	VAL
1	N	685	SER
1	N	692	LEU
1	N	725	THR
1	N	735	VAL
1	N	745	ARG
1	N	746	LEU
1	N	751	LEU
1	N	755	LEU
1	N	761	ASN
1	N	762	LEU
1	N	770	LEU
1	N	789	SER

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Mol	Chain	Res	Type
1	N	790	LEU
1	N	793	MET
1	N	794	ARG
1	N	795	LEU
1	N	802	SER
1	N	809	ASP
1	N	811	ILE
1	N	817	GLU
1	N	818	GLU
1	N	822	LEU
1	N	828	VAL
1	N	832	LEU
1	N	847	LEU
1	N	874	ARG
1	N	878	LEU
1	N	880	GLU
1	N	881	LEU
1	N	886	LEU
1	N	892	VAL
1	N	896	LEU
1	N	900	LEU
1	N	901	LYS
1	N	903	LEU
1	N	914	LEU
1	N	918	ARG
1	N	920	ARG
1	N	924	ILE
1	N	925	LYS
1	N	926	SER
1	N	931	LEU
1	N	936	LEU
1	N	937	ARG
1	N	947	HIS
1	N	955	LEU
1	N	964	LEU
1	N	965	LYS
1	N	975	GLU
1	N	989	GLN
1	N	990	VAL
1	N	993	LYS
1	N	996	LEU
1	N	1003	THR

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Mol	Chain	Res	Type
1	P	103	GLN
1	P	105	LEU
1	P	115	LEU
1	P	120	LEU
1	P	122	GLU
1	P	130	LEU
1	P	133	THR
1	P	138	ILE
1	P	139	MET
1	P	144	HIS
1	P	145	ARG
1	P	147	HIS
1	P	154	LEU
1	P	161	LEU
1	P	168	GLU
1	P	171	SER
1	P	177	THR
1	P	184	MET
1	P	192	ARG
1	P	195	LYS
1	P	205	LEU
1	P	206	ARG
1	P	207	SER
1	P	209	ARG
1	P	227	ILE
1	P	231	THR
1	P	239	LEU
1	P	243	VAL
1	P	274	MET
1	P	275	VAL
1	P	288	ARG
1	P	301	THR
1	P	314	VAL
1	P	319	GLU
1	P	330	CYS
1	P	334	LEU
1	P	335	MET
1	P	339	LEU
1	P	357	HIS
1	P	359	GLN
1	P	369	LEU
1	P	370	LEU

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Mol	Chain	Res	Type
1	P	377	ARG
1	P	396	LEU
1	P	404	HIS
1	P	409	GLU
1	P	410	PRO
1	P	435	LEU
1	P	436	LYS
1	P	455	LEU
1	P	463	GLU
1	P	498	SER
1	P	503	ARG
1	P	517	SER
1	P	521	LEU
1	P	540	THR
1	P	541	THR
1	P	543	GLN
1	P	551	VAL
1	P	561	LEU
1	P	563	SER
1	P	568	LYS
1	P	569	SER
1	P	580	GLN
1	P	583	SER
1	P	589	GLU
1	P	591	ILE
1	P	595	LEU
1	P	614	LEU
1	P	660	LYS
1	P	662	LEU
1	P	664	VAL
1	P	665	THR
1	P	672	LEU
1	P	674	LYS
1	P	677	ILE
1	P	682	LYS
1	P	685	SER
1	P	689	ASN
1	P	692	LEU
1	P	695	LYS
1	P	703	ARG
1	P	710	THR
1	P	725	THR

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Mol	Chain	Res	Type
1	P	735	VAL
1	P	746	LEU
1	P	751	LEU
1	P	755	LEU
1	P	756	ILE
1	P	762	LEU
1	P	770	LEU
1	P	788	ARG
1	P	789	SER
1	P	790	LEU
1	P	793	MET
1	P	802	SER
1	P	813	LYS
1	P	827	LEU
1	P	828	VAL
1	P	832	LEU
1	P	847	LEU
1	P	848	ILE
1	P	859	TYR
1	P	861	GLU
1	P	874	ARG
1	P	878	LEU
1	P	892	VAL
1	P	896	LEU
1	P	901	LYS
1	P	906	THR
1	P	909	LEU
1	P	914	LEU
1	P	922	GLU
1	P	924	ILE
1	P	926	SER
1	P	934	ASN
1	P	936	LEU
1	P	951	SER
1	P	955	LEU
1	P	964	LEU
1	P	975	GLU
1	P	980	ASP
1	P	988	SER
1	P	993	LYS
1	P	995	THR
1	P	996	LEU

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Mol	Chain	Res	Type
1	P	997	LEU
1	P	1003	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	289	HIS
1	K	531	GLN
1	B	268	ASN
1	B	552	ASN
1	B	998	GLN
1	D	364	GLN
1	D	573	GLN
1	D	747	HIS
1	H	433	GLN
1	H	715	HIS
1	H	739	GLN
1	H	740	ASN
1	L	324	GLN
1	L	359	GLN
1	N	269	HIS
1	N	657	GLN
1	N	675	GLN
1	N	693	HIS
1	N	761	ASN
1	P	317	GLN
1	P	324	GLN
1	P	359	GLN
1	P	740	ASN
1	P	941	GLN
1	P	947	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	B	533	1	8,9,10	1.62	1 (12%)	7,12,14	1.57	1 (14%)
1	SEP	L	533	1	8,9,10	1.60	1 (12%)	7,12,14	1.58	1 (14%)
1	SEP	D	533	1	8,9,10	1.59	1 (12%)	7,12,14	1.62	1 (14%)
1	SEP	F	533	1	8,9,10	1.58	1 (12%)	7,12,14	1.34	1 (14%)
1	SEP	N	533	1	4,5,10	0.59	0	1,5,14	0.41	0
1	SEP	H	533	1	8,9,10	1.59	1 (12%)	7,12,14	1.06	0
1	SEP	K	533	1	8,9,10	1.60	1 (12%)	7,12,14	1.45	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	533	1	-	5/6/8/10	-
1	SEP	L	533	1	-	5/6/8/10	-
1	SEP	D	533	1	-	6/6/8/10	-
1	SEP	F	533	1	-	2/6/8/10	-
1	SEP	N	533	1	-	1/2/4/10	-
1	SEP	H	533	1	-	1/6/8/10	-
1	SEP	K	533	1	-	5/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	533	SEP	P-O1P	3.53	1.61	1.50
1	L	533	SEP	P-O1P	3.52	1.61	1.50
1	B	533	SEP	P-O1P	3.50	1.61	1.50
1	D	533	SEP	P-O1P	3.49	1.61	1.50
1	K	533	SEP	P-O1P	3.45	1.61	1.50
1	F	533	SEP	P-O1P	3.45	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	533	SEP	OG-CB-CA	3.79	111.83	108.14
1	B	533	SEP	OG-CB-CA	3.67	111.72	108.14
1	K	533	SEP	OG-CB-CA	3.33	111.39	108.14
1	L	533	SEP	OG-CB-CA	3.23	111.29	108.14
1	F	533	SEP	OG-CB-CA	2.86	110.92	108.14

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	533	SEP	CB-OG-P-O2P
1	B	533	SEP	C-CA-CB-OG
1	B	533	SEP	CB-OG-P-O1P
1	B	533	SEP	CB-OG-P-O3P
1	D	533	SEP	C-CA-CB-OG
1	D	533	SEP	CA-CB-OG-P
1	D	533	SEP	CB-OG-P-O1P
1	D	533	SEP	CB-OG-P-O2P
1	D	533	SEP	CB-OG-P-O3P
1	F	533	SEP	N-CA-CB-OG
1	F	533	SEP	C-CA-CB-OG
1	H	533	SEP	N-CA-CB-OG
1	L	533	SEP	CB-OG-P-O2P
1	L	533	SEP	CB-OG-P-O3P
1	L	533	SEP	CB-OG-P-O1P
1	N	533	SEP	N-CA-CB-OG
1	B	533	SEP	CB-OG-P-O2P
1	K	533	SEP	CA-CB-OG-P
1	L	533	SEP	CA-CB-OG-P
1	K	533	SEP	CB-OG-P-O1P
1	K	533	SEP	N-CA-CB-OG
1	B	533	SEP	N-CA-CB-OG
1	D	533	SEP	N-CA-CB-OG
1	L	533	SEP	N-CA-CB-OG
1	K	533	SEP	CB-OG-P-O3P

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	533	SEP	3	0
1	F	533	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	533	SEP	2	0
1	K	533	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	N	1102	-	4,4,4	0.24	0	6,6,6	0.08	0
2	ADP	N	1101	-	24,29,29	0.96	1 (4%)	29,45,45	1.23	2 (6%)
2	ADP	L	1101	-	24,29,29	0.96	2 (8%)	29,45,45	1.27	4 (13%)
2	ADP	P	1101	-	24,29,29	0.92	0	29,45,45	1.18	2 (6%)
2	ADP	H	1101	-	24,29,29	0.93	1 (4%)	29,45,45	1.17	2 (6%)
2	ADP	B	1101	-	24,29,29	0.90	0	29,45,45	1.19	2 (6%)
2	ADP	D	1101	-	24,29,29	0.92	0	29,45,45	1.25	3 (10%)
2	ADP	K	1101	-	24,29,29	0.93	1 (4%)	29,45,45	1.12	2 (6%)
3	SO4	B	1102	-	4,4,4	0.23	0	6,6,6	0.08	0
2	ADP	F	1101	-	24,29,29	0.91	1 (4%)	29,45,45	1.19	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	N	1101	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	L	1101	-	-	2/12/32/32	0/3/3/3
2	ADP	P	1101	-	-	0/12/32/32	0/3/3/3
2	ADP	H	1101	-	-	3/12/32/32	0/3/3/3
2	ADP	B	1101	-	-	2/12/32/32	0/3/3/3
2	ADP	D	1101	-	-	2/12/32/32	0/3/3/3
2	ADP	K	1101	-	-	0/12/32/32	0/3/3/3
2	ADP	F	1101	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1101	ADP	PA-O3A	2.41	1.62	1.59
2	H	1101	ADP	PA-O3A	2.18	1.61	1.59
2	L	1101	ADP	PA-O3A	2.13	1.61	1.59
2	L	1101	ADP	C2-N3	2.08	1.35	1.32
2	F	1101	ADP	PA-O3A	2.06	1.61	1.59
2	K	1101	ADP	PA-O3A	2.02	1.61	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1101	ADP	N3-C2-N1	-3.58	123.81	128.67
2	F	1101	ADP	N3-C2-N1	-3.56	123.85	128.67
2	N	1101	ADP	N3-C2-N1	-3.53	123.88	128.67
2	D	1101	ADP	N3-C2-N1	-3.51	123.91	128.67
2	H	1101	ADP	N3-C2-N1	-3.50	123.92	128.67
2	B	1101	ADP	N3-C2-N1	-3.48	123.95	128.67
2	P	1101	ADP	N3-C2-N1	-3.23	124.28	128.67
2	L	1101	ADP	O4'-C1'-N9	3.08	112.83	108.75
2	L	1101	ADP	N3-C2-N1	-3.02	124.58	128.67
2	K	1101	ADP	C4-C5-N7	-2.53	106.67	109.34
2	P	1101	ADP	C4-C5-N7	-2.53	106.67	109.34
2	N	1101	ADP	C4-C5-N7	-2.43	106.77	109.34
2	B	1101	ADP	C4-C5-N7	-2.41	106.79	109.34
2	F	1101	ADP	C4-C5-N7	-2.39	106.81	109.34
2	D	1101	ADP	C4-C5-N7	-2.37	106.83	109.34
2	L	1101	ADP	C4'-O4'-C1'	-2.37	107.76	109.92
2	H	1101	ADP	C4-C5-N7	-2.35	106.85	109.34
2	L	1101	ADP	C4-C5-N7	-2.31	106.89	109.34
2	D	1101	ADP	C4'-O4'-C1'	2.23	111.97	109.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	ADP	PA-O3A-PB-O3B
2	L	1101	ADP	C5'-O5'-PA-O3A
2	N	1101	ADP	PA-O3A-PB-O2B
2	N	1101	ADP	C5'-O5'-PA-O1A
2	N	1101	ADP	C5'-O5'-PA-O2A
2	N	1101	ADP	C5'-O5'-PA-O3A
2	H	1101	ADP	O4'-C4'-C5'-O5'
2	D	1101	ADP	PA-O3A-PB-O1B
2	H	1101	ADP	C3'-C4'-C5'-O5'
2	B	1101	ADP	O4'-C4'-C5'-O5'
2	F	1101	ADP	C5'-O5'-PA-O1A
2	H	1101	ADP	C5'-O5'-PA-O1A
2	D	1101	ADP	O4'-C4'-C5'-O5'
2	F	1101	ADP	PB-O3A-PA-O1A
2	L	1101	ADP	PB-O3A-PA-O2A
2	N	1101	ADP	PA-O3A-PB-O1B
2	F	1101	ADP	PB-O3A-PA-O2A

There are no ring outliers.

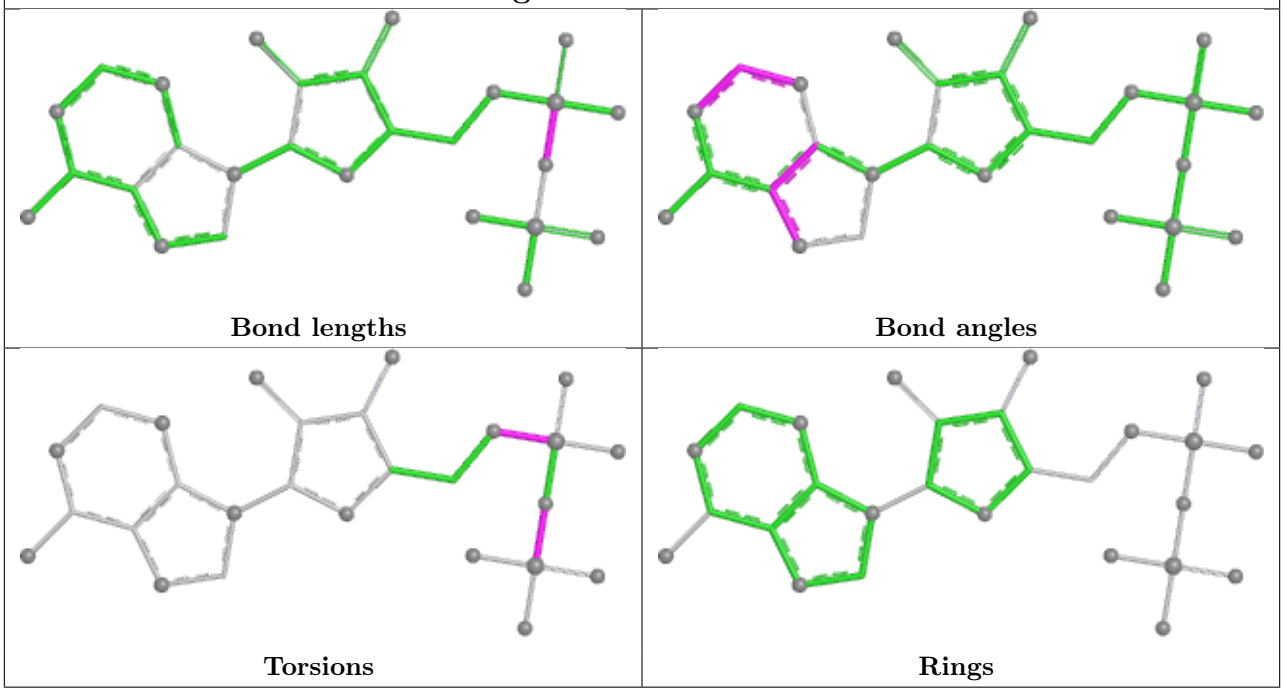
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1101	ADP	1	0
2	P	1101	ADP	2	0
2	B	1101	ADP	1	0
2	D	1101	ADP	1	0
2	K	1101	ADP	2	0
2	F	1101	ADP	1	0

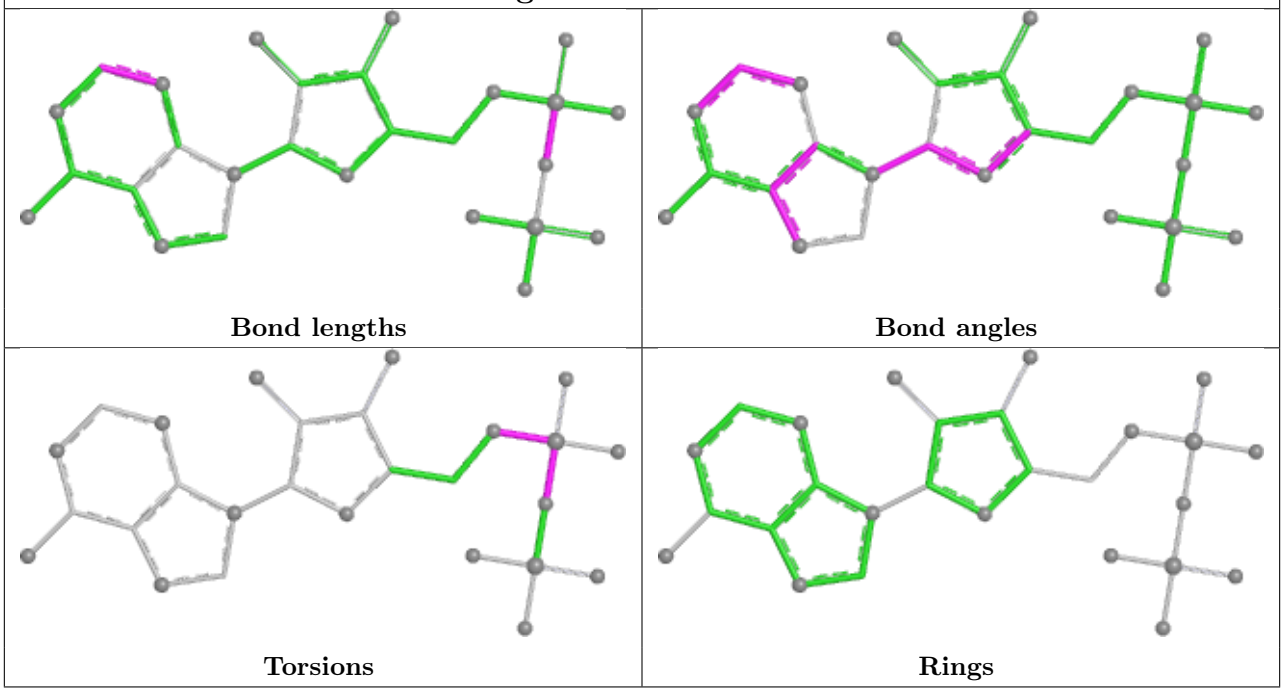
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

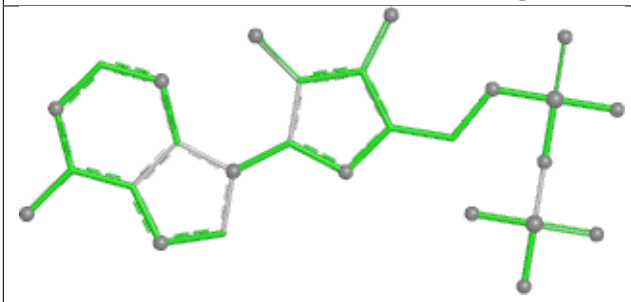
Ligand ADP N 1101



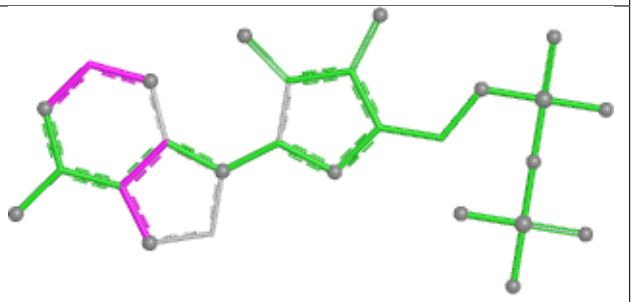
Ligand ADP L 1101



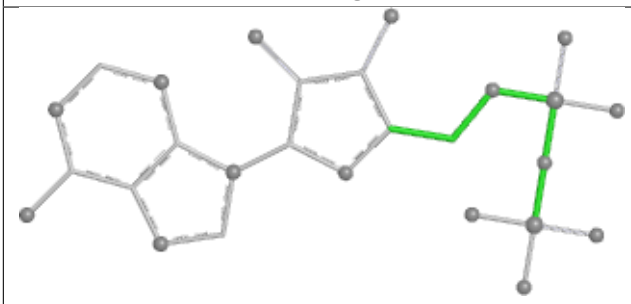
Ligand ADP P 1101



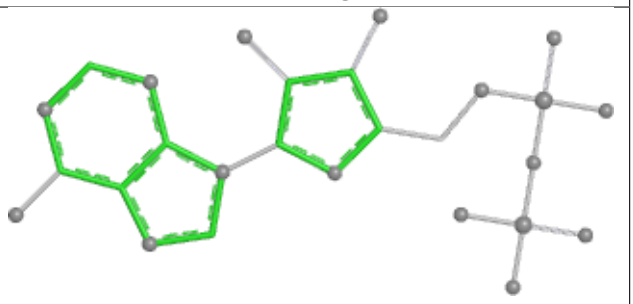
Bond lengths



Bond angles

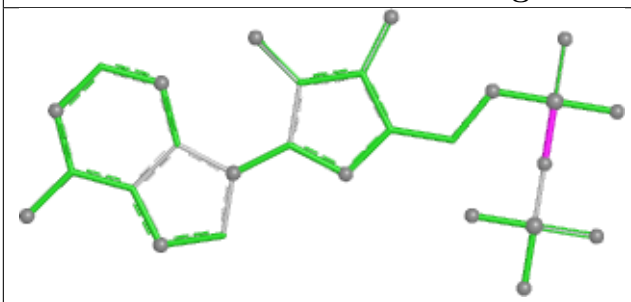


Torsions

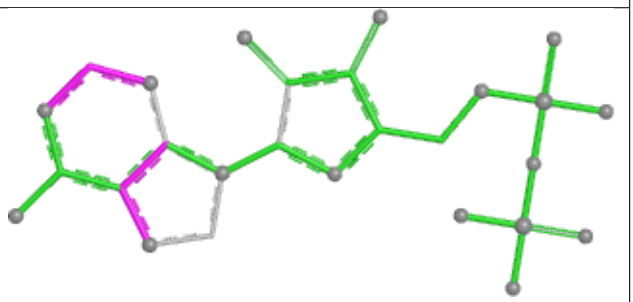


Rings

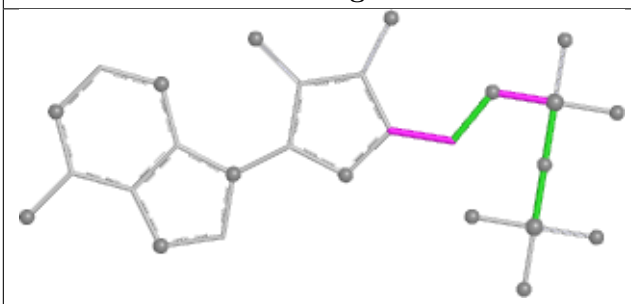
Ligand ADP H 1101



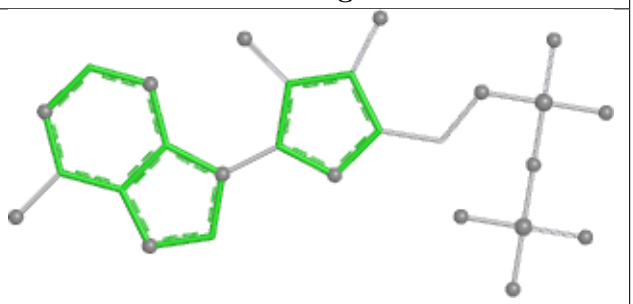
Bond lengths



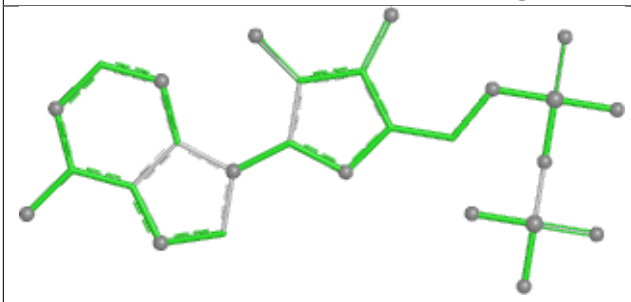
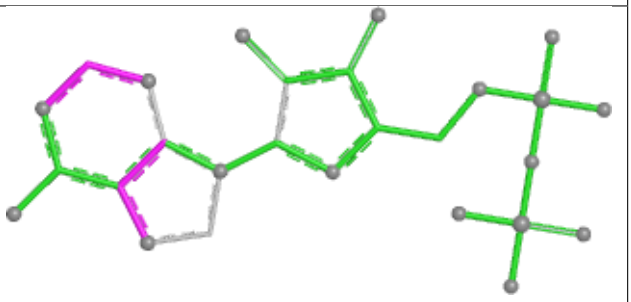
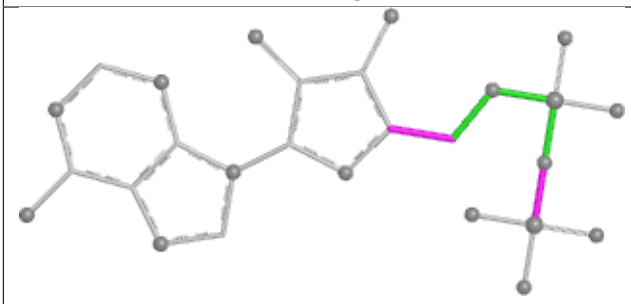
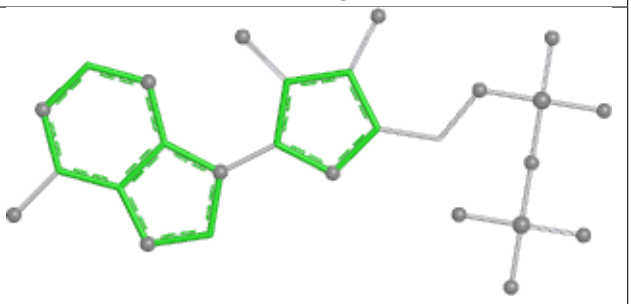
Bond angles

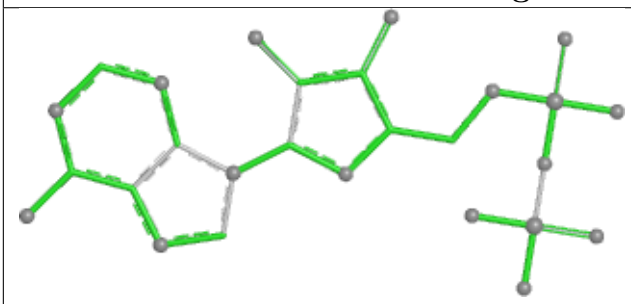
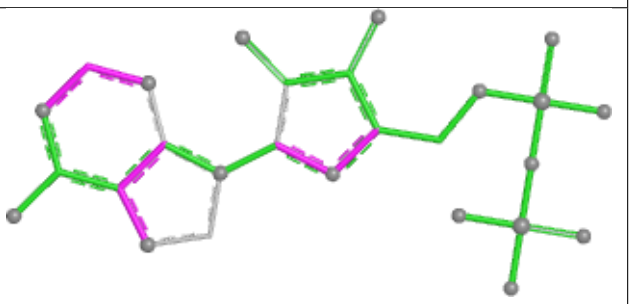
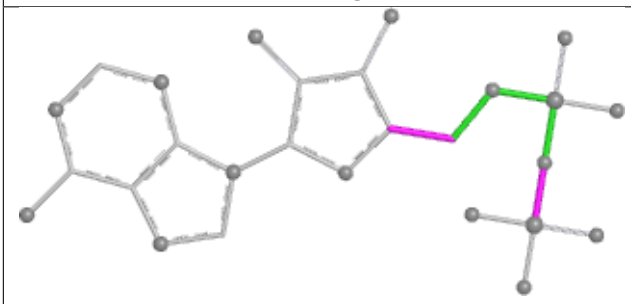
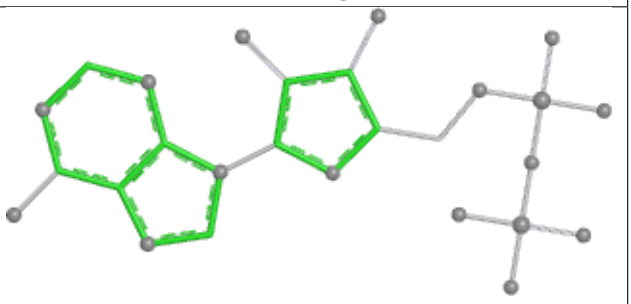


Torsions

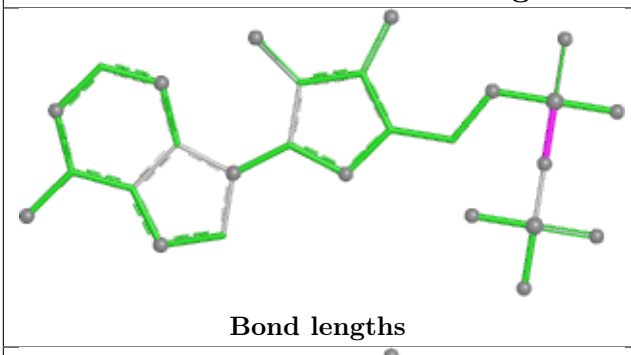


Rings

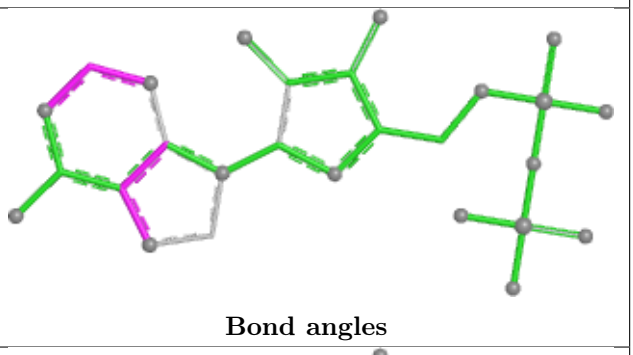
Ligand ADP B 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

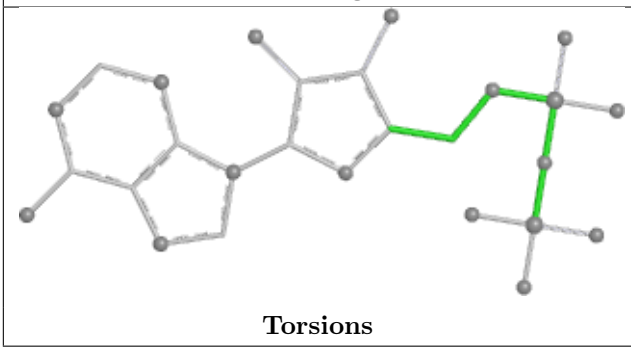
Ligand ADP K 1101



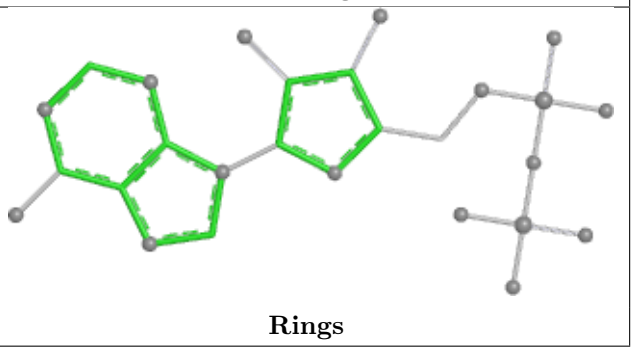
Bond lengths



Bond angles

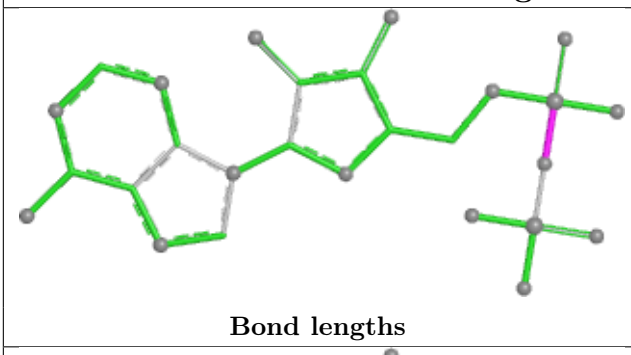


Torsions

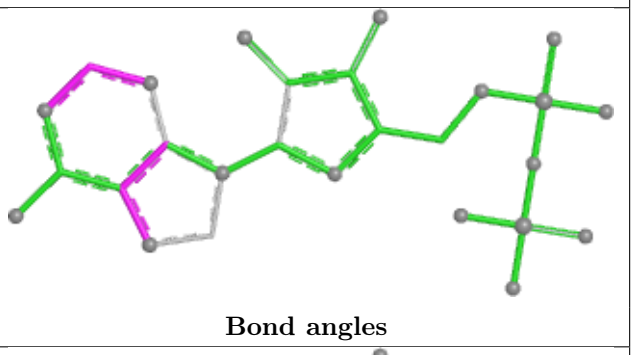


Rings

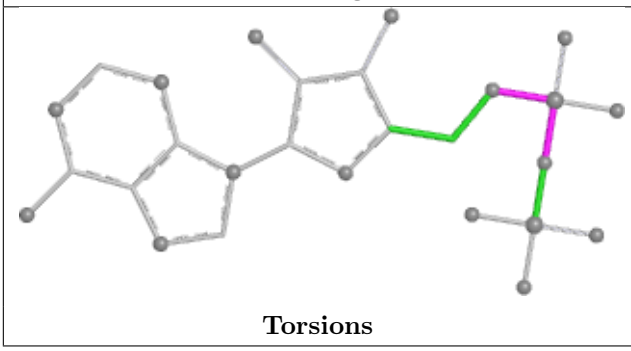
Ligand ADP F 1101



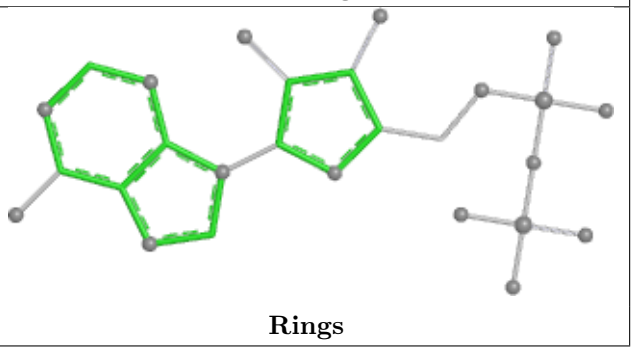
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	902/1024 (88%)	-0.02	18 (1%) 65 51	3, 15, 68, 143	0
1	D	899/1024 (87%)	0.02	29 (3%) 47 31	3, 22, 71, 148	0
1	F	898/1024 (87%)	0.01	24 (2%) 54 39	2, 19, 65, 130	0
1	H	897/1024 (87%)	0.09	33 (3%) 41 26	4, 17, 61, 155	0
1	K	903/1024 (88%)	0.01	24 (2%) 54 39	4, 19, 66, 152	0
1	L	892/1024 (87%)	-0.00	23 (2%) 56 40	2, 15, 66, 146	0
1	N	881/1024 (86%)	0.32	55 (6%) 20 11	4, 41, 106, 178	0
1	P	866/1024 (84%)	0.65	110 (12%) 3 2	5, 53, 156, 254	0
All	All	7138/8192 (87%)	0.13	316 (4%) 34 21	2, 23, 92, 254	0

All (316) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1007	PHE	7.2
1	P	987	LEU	6.8
1	N	980	ASP	6.7
1	N	979	PRO	6.6
1	P	984	VAL	6.2
1	N	1021	LEU	6.2
1	N	978	LEU	6.1
1	P	975	GLU	6.1
1	H	712	LYS	6.0
1	F	1005	TRP	5.8
1	N	961	PHE	5.7
1	P	980	ASP	5.6
1	N	1005	TRP	5.5
1	P	567	SER	5.3
1	B	1007	PHE	5.2
1	P	954	TRP	5.2

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Mol	Chain	Res	Type	RSRZ
1	H	1006	GLU	5.2
1	P	988	SER	5.1
1	P	957	PHE	5.0
1	P	979	PRO	5.0
1	P	974	THR	4.9
1	P	989	GLN	4.9
1	P	958	MET	4.9
1	P	1002	LEU	4.7
1	P	985	ARG	4.7
1	H	1011	ASP	4.6
1	N	712	LYS	4.6
1	P	955	LEU	4.5
1	N	957	PHE	4.5
1	P	1004	GLY	4.5
1	N	1015	ILE	4.5
1	P	932	GLU	4.4
1	K	1005	TRP	4.4
1	H	1015	ILE	4.4
1	D	383	SER	4.4
1	P	670	ASN	4.4
1	P	1005	TRP	4.3
1	P	1021	LEU	4.3
1	F	352	GLN	4.2
1	K	1021	LEU	4.2
1	P	925	LYS	4.2
1	P	357	HIS	4.2
1	P	973	SER	4.2
1	D	1007	PHE	4.1
1	P	863	ASP	4.0
1	K	1006	GLU	4.0
1	P	962	GLU	4.0
1	F	1006	GLU	3.9
1	N	929	GLU	3.9
1	B	384	GLY	3.9
1	P	981	ALA	3.9
1	P	679	TYR	3.9
1	P	672	LEU	3.9
1	D	151	GLN	3.9
1	P	960	VAL	3.9
1	K	1015	ILE	3.9
1	P	992	SER	3.8
1	F	1007	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	P	982	ALA	3.8
1	P	704	LEU	3.8
1	N	987	LEU	3.8
1	H	973	SER	3.8
1	L	987	LEU	3.8
1	N	386	PHE	3.7
1	P	929	GLU	3.7
1	F	983	LEU	3.7
1	N	976	GLU	3.7
1	N	1002	LEU	3.7
1	N	975	GLU	3.7
1	D	352	GLN	3.7
1	F	1015	ILE	3.6
1	N	952	ASP	3.6
1	F	383	SER	3.6
1	P	945	ALA	3.6
1	P	976	GLU	3.6
1	L	378	TYR	3.6
1	L	984	VAL	3.5
1	L	977	PHE	3.5
1	L	1005	TRP	3.5
1	P	331	LEU	3.4
1	K	983	LEU	3.4
1	B	1005	TRP	3.4
1	P	959	ASN	3.4
1	P	931	LEU	3.4
1	N	378	TYR	3.4
1	D	97	ASP	3.3
1	P	927	LEU	3.3
1	F	386	PHE	3.3
1	P	961	PHE	3.3
1	P	141	LYS	3.3
1	B	524	THR	3.3
1	L	956	TYR	3.3
1	H	763	LYS	3.3
1	P	669	ILE	3.2
1	P	1003	THR	3.2
1	N	721	ALA	3.2
1	F	977	PHE	3.2
1	P	991	LEU	3.2
1	N	679	TYR	3.2
1	K	1023	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	P	685	SER	3.2
1	P	802	SER	3.1
1	H	381	GLY	3.1
1	P	983	LEU	3.1
1	P	924	ILE	3.1
1	F	151	GLN	3.1
1	D	323	ALA	3.1
1	P	935	PRO	3.1
1	N	535	GLN	3.1
1	D	1015	ILE	3.0
1	N	977	PHE	3.0
1	P	965	LYS	3.0
1	N	1000	VAL	3.0
1	L	431	THR	3.0
1	P	820	CYS	3.0
1	N	821	ASP	3.0
1	N	958	MET	3.0
1	P	934	ASN	3.0
1	K	386	PHE	3.0
1	P	708	LEU	3.0
1	D	327	GLU	3.0
1	L	412	HIS	3.0
1	B	352	GLN	3.0
1	H	1005	TRP	3.0
1	P	321	LEU	3.0
1	F	1023	THR	3.0
1	H	388	ARG	2.9
1	P	928	GLY	2.9
1	B	353	GLU	2.9
1	P	951	SER	2.9
1	B	1023	THR	2.9
1	P	783	LEU	2.9
1	F	378	TYR	2.9
1	F	353	GLU	2.9
1	B	527	PRO	2.9
1	P	152	LEU	2.9
1	P	926	SER	2.8
1	P	356	ALA	2.8
1	N	371	ILE	2.8
1	D	353	GLU	2.8
1	L	983	LEU	2.8
1	N	388	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	431	THR	2.8
1	H	951	SER	2.8
1	N	513	TYR	2.8
1	D	382	ALA	2.8
1	N	433	GLN	2.8
1	H	378	TYR	2.8
1	H	977	PHE	2.8
1	D	1023	THR	2.8
1	L	386	PHE	2.8
1	P	675	GLN	2.8
1	H	679	TYR	2.8
1	N	802	SER	2.7
1	B	378	TYR	2.7
1	L	1023	THR	2.7
1	N	762	LEU	2.7
1	L	1022	VAL	2.7
1	L	424	ILE	2.7
1	P	464	PRO	2.7
1	K	1016	LYS	2.7
1	B	529	TRP	2.7
1	D	763	LYS	2.7
1	B	411	GLU	2.7
1	P	732	ILE	2.7
1	P	684	PHE	2.7
1	P	1000	VAL	2.7
1	K	981	ALA	2.7
1	P	972	PHE	2.6
1	P	688	THR	2.6
1	K	380	GLY	2.6
1	P	386	PHE	2.6
1	F	389	SER	2.6
1	N	984	VAL	2.6
1	P	615	ASP	2.6
1	D	388	ARG	2.6
1	P	455	LEU	2.6
1	P	389	SER	2.6
1	P	1019	PHE	2.6
1	H	1004	GLY	2.6
1	F	1021	LEU	2.6
1	N	418	GLU	2.6
1	N	713	ASN	2.6
1	P	977	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	1001	LYS	2.5
1	L	979	PRO	2.5
1	P	1001	LYS	2.5
1	P	696	ARG	2.5
1	B	981	ALA	2.5
1	B	995	THR	2.5
1	P	747	HIS	2.5
1	D	976	GLU	2.5
1	L	980	ASP	2.5
1	P	947	HIS	2.5
1	K	1007	PHE	2.5
1	K	979	PRO	2.5
1	F	1004	GLY	2.5
1	P	379	ARG	2.5
1	P	673	ASN	2.5
1	F	994	LEU	2.5
1	H	1008	ASP	2.5
1	K	1022	VAL	2.5
1	D	414	SER	2.5
1	N	988	SER	2.5
1	N	670	ASN	2.5
1	N	761	ASN	2.5
1	H	1022	VAL	2.4
1	N	621	THR	2.4
1	K	322	TRP	2.4
1	H	1024	ALA	2.4
1	P	946	GLY	2.4
1	P	746	LEU	2.4
1	K	607	SER	2.4
1	K	605	CYS	2.4
1	P	668	ASP	2.4
1	N	822	LEU	2.4
1	N	763	LYS	2.4
1	F	380	GLY	2.4
1	N	804	ILE	2.4
1	L	976	GLU	2.3
1	P	762	LEU	2.3
1	D	523	VAL	2.3
1	D	319	GLU	2.3
1	N	617	TYR	2.3
1	D	384	GLY	2.3
1	L	1004	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	700	MET	2.3
1	P	990	VAL	2.3
1	K	606	ALA	2.3
1	P	950	SER	2.3
1	D	302	GLU	2.3
1	H	379	ARG	2.3
1	H	980	ASP	2.3
1	P	495	CYS	2.3
1	P	683	ILE	2.3
1	P	890	TRP	2.3
1	H	1012	ILE	2.3
1	D	1005	TRP	2.3
1	B	431	THR	2.3
1	B	994	LEU	2.3
1	F	993	LYS	2.3
1	H	781	LYS	2.3
1	P	689	ASN	2.2
1	N	430	TYR	2.2
1	D	1006	GLU	2.2
1	L	679	TYR	2.2
1	K	226	PHE	2.2
1	N	810	TYR	2.2
1	H	1009	ASP	2.2
1	P	543	GLN	2.2
1	K	617	TYR	2.2
1	D	620	ALA	2.2
1	F	965	LYS	2.2
1	N	354	PHE	2.2
1	N	981	ALA	2.2
1	P	378	TYR	2.2
1	H	386	PHE	2.2
1	B	531	GLN	2.2
1	N	925	LYS	2.2
1	P	674	LYS	2.2
1	P	325	ILE	2.2
1	D	521	LEU	2.2
1	F	978	LEU	2.2
1	F	1010	TYR	2.2
1	P	355	GLN	2.2
1	N	927	LEU	2.2
1	K	1012	ILE	2.2
1	K	381	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	357	HIS	2.2
1	N	710	THR	2.2
1	L	98	LEU	2.1
1	L	975	GLU	2.1
1	H	762	LEU	2.1
1	P	93	VAL	2.1
1	N	1003	THR	2.1
1	P	936	LEU	2.1
1	D	489	ASN	2.1
1	P	788	ARG	2.1
1	P	996	LEU	2.1
1	P	745	ARG	2.1
1	H	1023	THR	2.1
1	N	764	ASN	2.1
1	P	786	GLY	2.1
1	N	653	PHE	2.1
1	P	682	LYS	2.1
1	B	980	ASP	2.1
1	N	98	LEU	2.1
1	P	933	MET	2.1
1	P	993	LYS	2.1
1	F	617	TYR	2.1
1	N	999	GLU	2.1
1	K	352	GLN	2.1
1	K	987	LEU	2.1
1	H	1002	LEU	2.1
1	P	317	GLN	2.1
1	D	977	PHE	2.1
1	N	806	GLU	2.1
1	L	420	VAL	2.1
1	P	764	ASN	2.1
1	D	966	GLN	2.1
1	H	269	HIS	2.1
1	P	952	ASP	2.1
1	H	713	ASN	2.1
1	H	978	LEU	2.1
1	H	1000	VAL	2.0
1	P	686	SER	2.0
1	L	656	LYS	2.0
1	F	382	ALA	2.0
1	D	965	LYS	2.0
1	H	976	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	948	CYS	2.0
1	K	1011	ASP	2.0
1	B	1016	LYS	2.0
1	N	736	THR	2.0
1	D	379	ARG	2.0
1	P	790	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	N	533	6/11	0.78	0.25	6,7,16,17	0
1	SEP	D	533	10/11	0.83	0.25	59,59,59,59	0
1	SEP	B	533	10/11	0.83	0.21	54,54,54,54	0
1	SEP	F	533	10/11	0.89	0.17	69,69,69,69	0
1	SEP	L	533	10/11	0.90	0.16	69,69,69,69	0
1	SEP	K	533	10/11	0.92	0.15	67,67,67,68	0
1	SEP	H	533	10/11	0.92	0.16	45,46,46,46	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	N	1102	5/5	0.76	0.34	79,86,87,116	0
3	SO4	B	1102	5/5	0.81	0.32	81,93,103,106	0
2	ADP	N	1101	27/27	0.94	0.26	9,20,28,39	0
2	ADP	B	1101	27/27	0.94	0.22	4,5,7,7	0
2	ADP	D	1101	27/27	0.94	0.21	3,4,9,10	0

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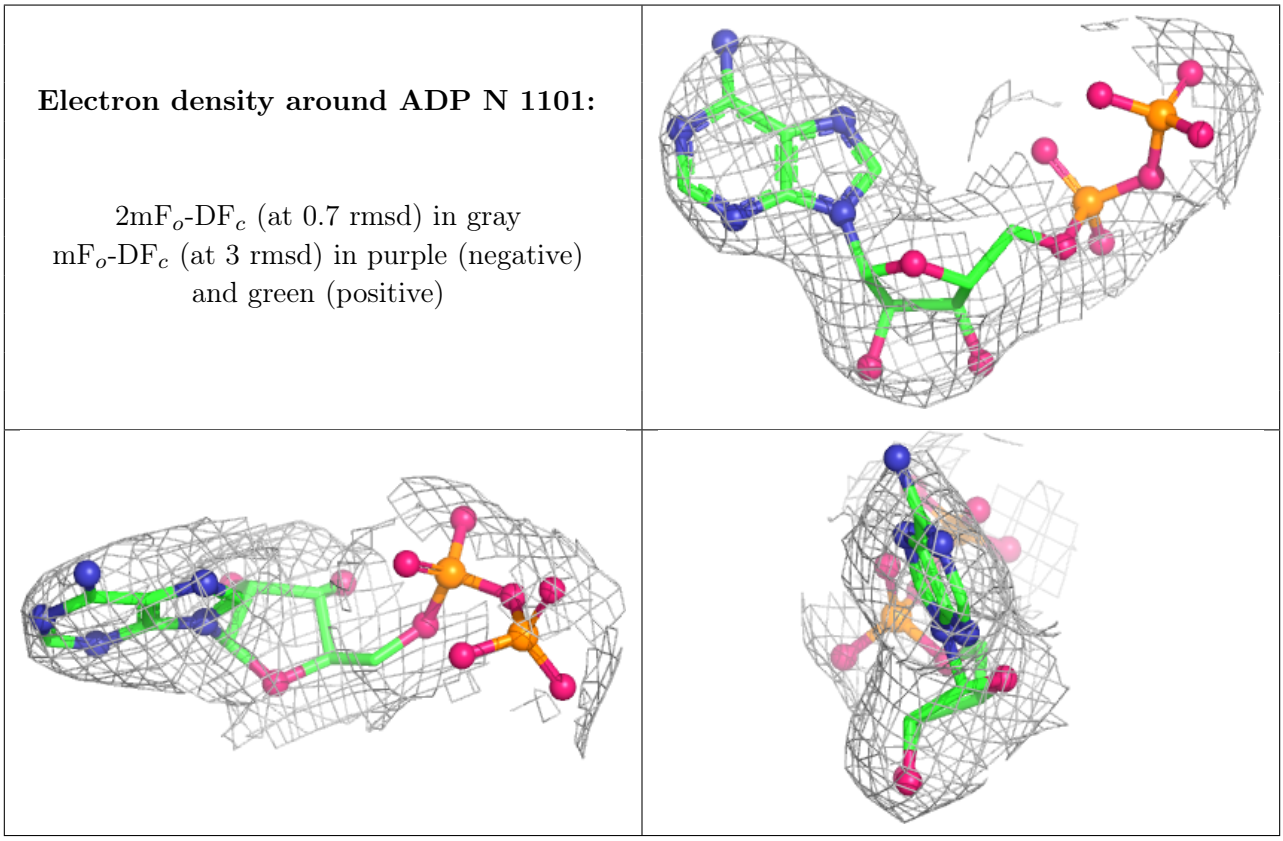
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	P	1101	27/27	0.95	0.23	8,18,28,35	0
2	ADP	L	1101	27/27	0.95	0.24	2,4,6,7	0
2	ADP	F	1101	27/27	0.95	0.21	2,2,3,3	0
2	ADP	H	1101	27/27	0.96	0.26	4,5,6,8	0
2	ADP	K	1101	27/27	0.96	0.20	6,10,15,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

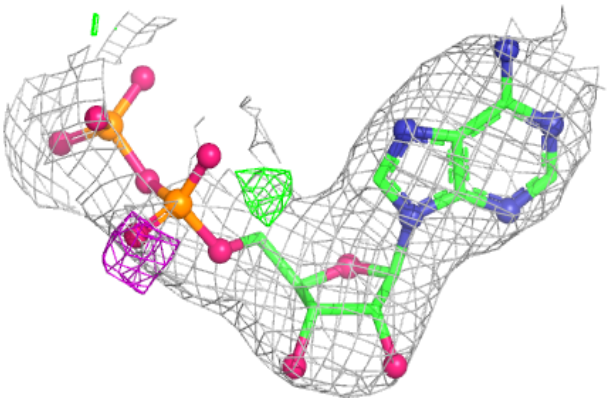
Electron density around ADP N 1101:

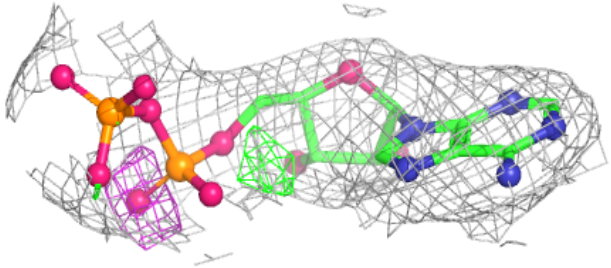
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

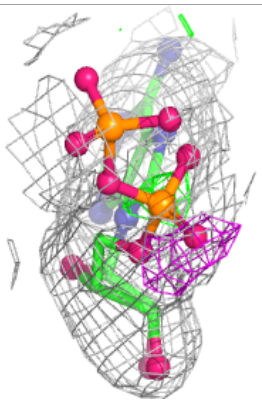


Electron density around ADP B 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

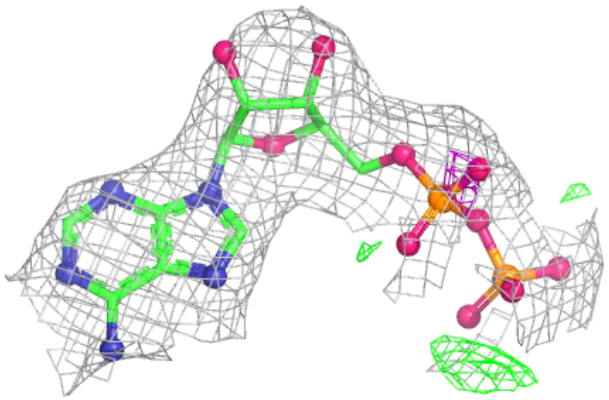


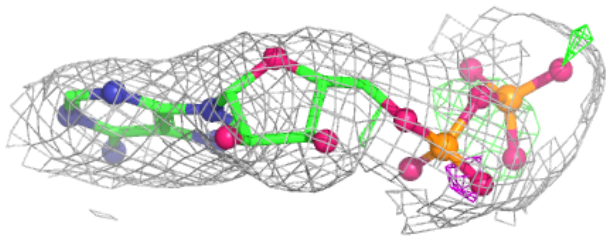


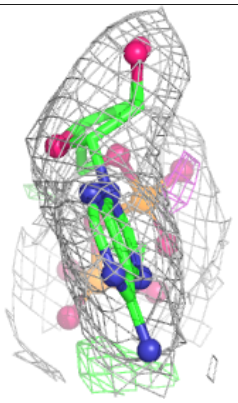


Electron density around ADP D 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

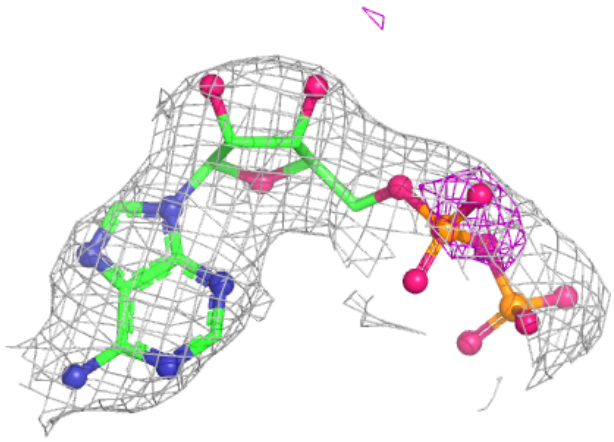


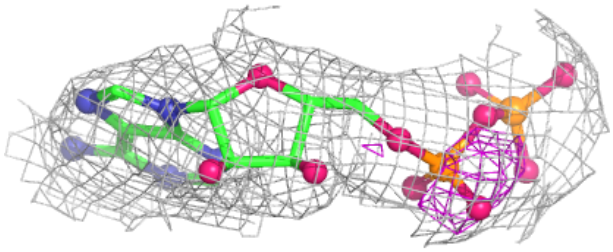


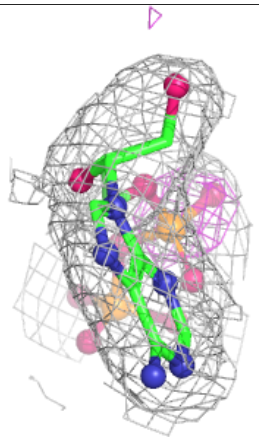


Electron density around ADP P 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

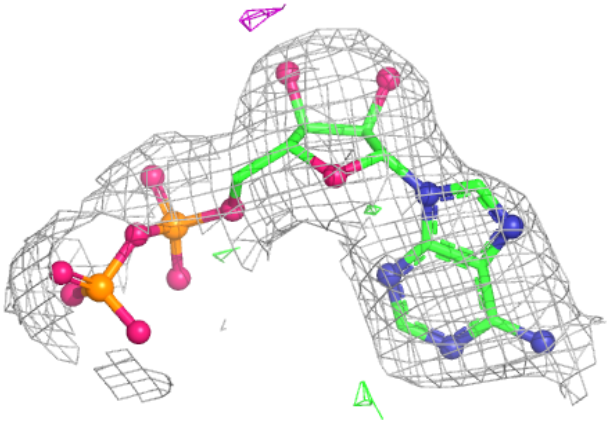


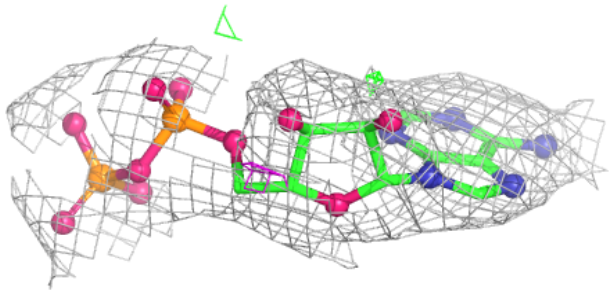


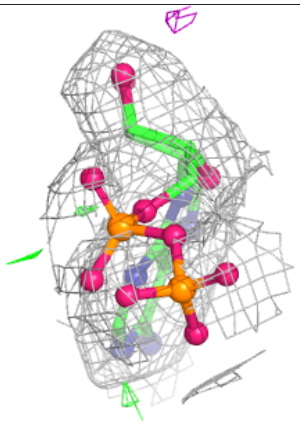


Electron density around ADP L 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

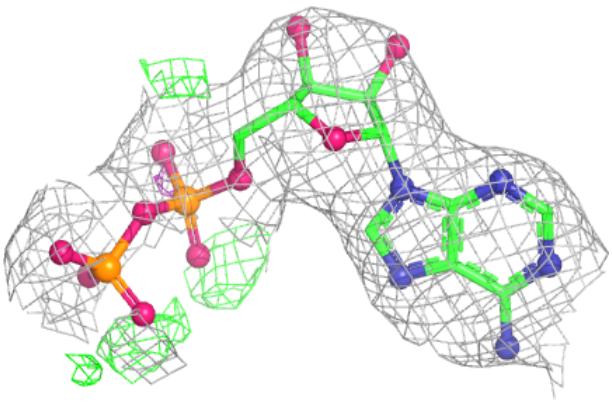


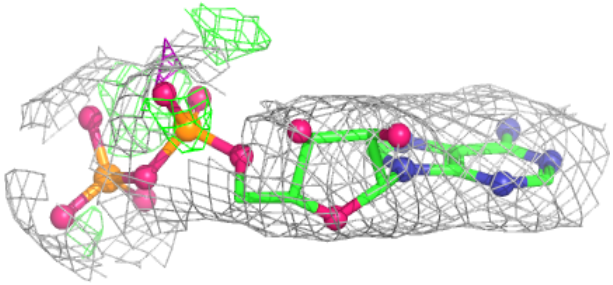


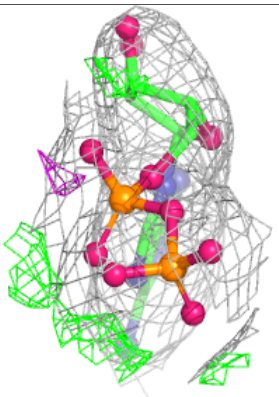


Electron density around ADP F 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

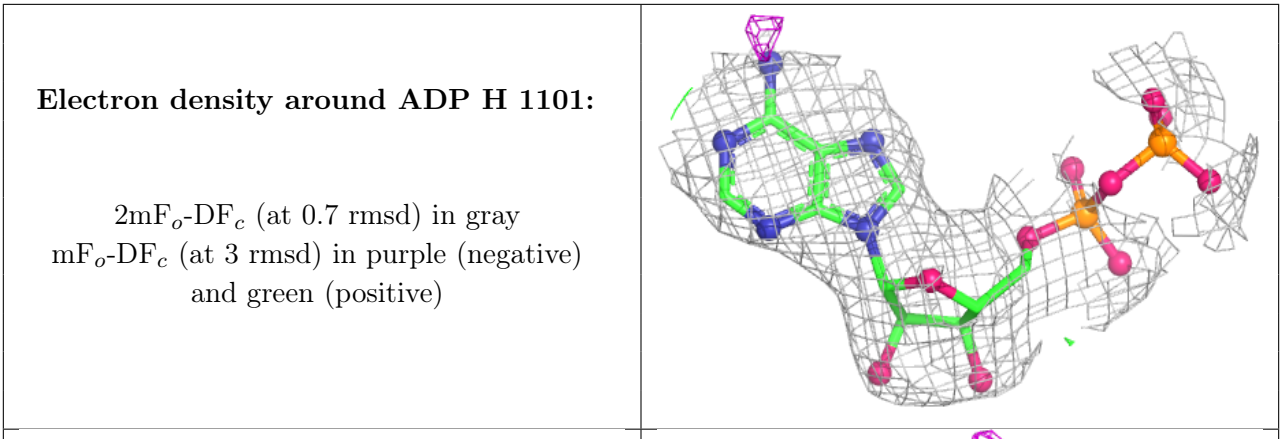






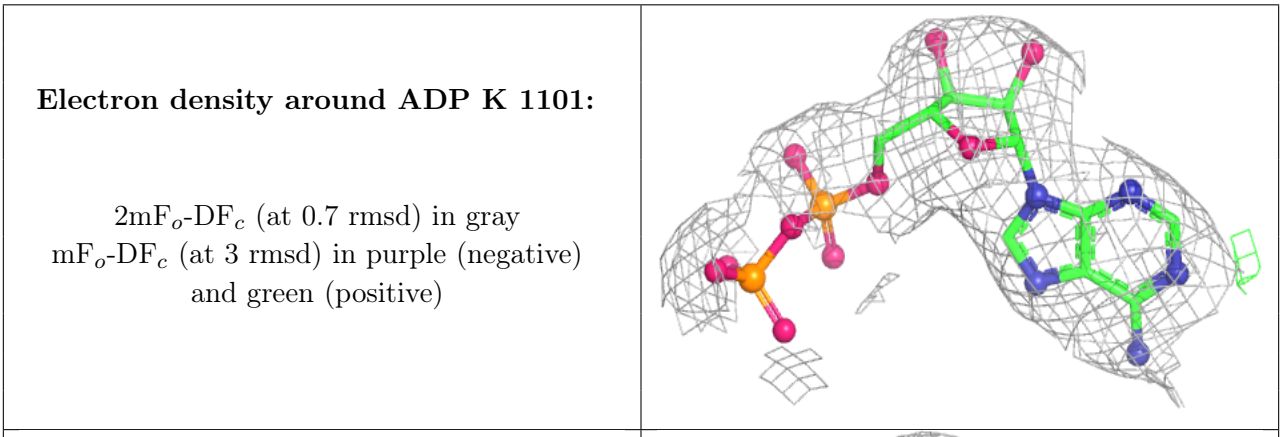
Electron density around ADP H 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP K 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.