Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 02:05 pm BST

PDB ID	:	2IUU
Title	:	P. aeruginosa FtsK motor domain, hexamer
Authors	:	Massey, T.H.; Mercogliano, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on	:	2006-06-07
Resolution	:	2.90 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:

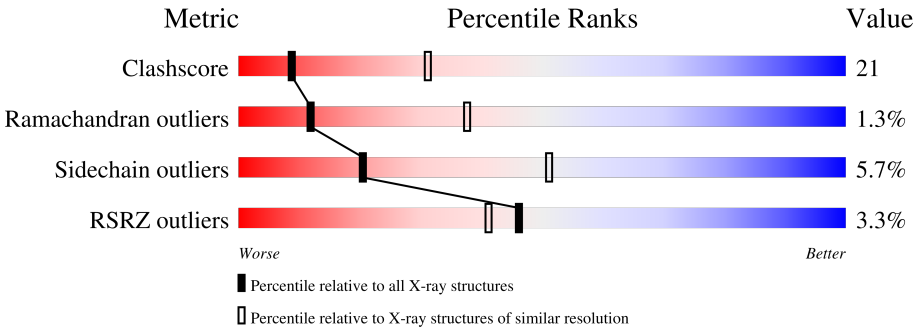
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	A	491	5% 52% 29% • • 17%
1	B	491	2% 51% 29% • 17%
1	C	491	2% 51% 29% • • 17%
1	D	491	% 55% 26% • • 17%
1	E	491	3% 48% 32% • • 17%
1	F	491	4% 52% 28% • 17%

2 Entry composition (i)

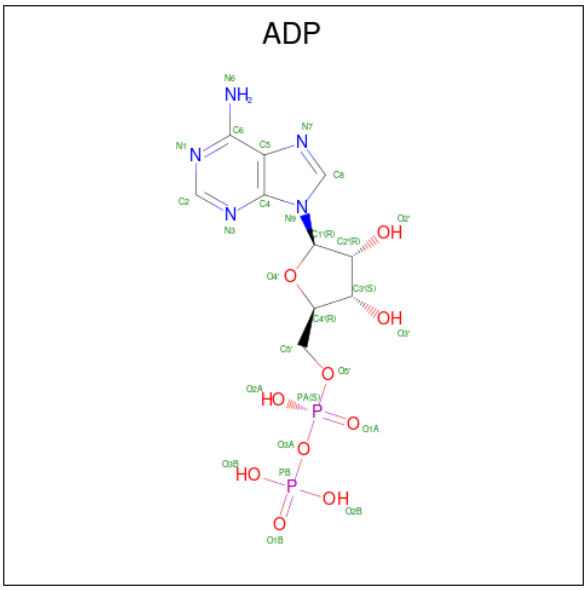
There are 2 unique types of molecules in this entry. The entry contains 18888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	B	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	C	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	D	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	E	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	F	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			

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



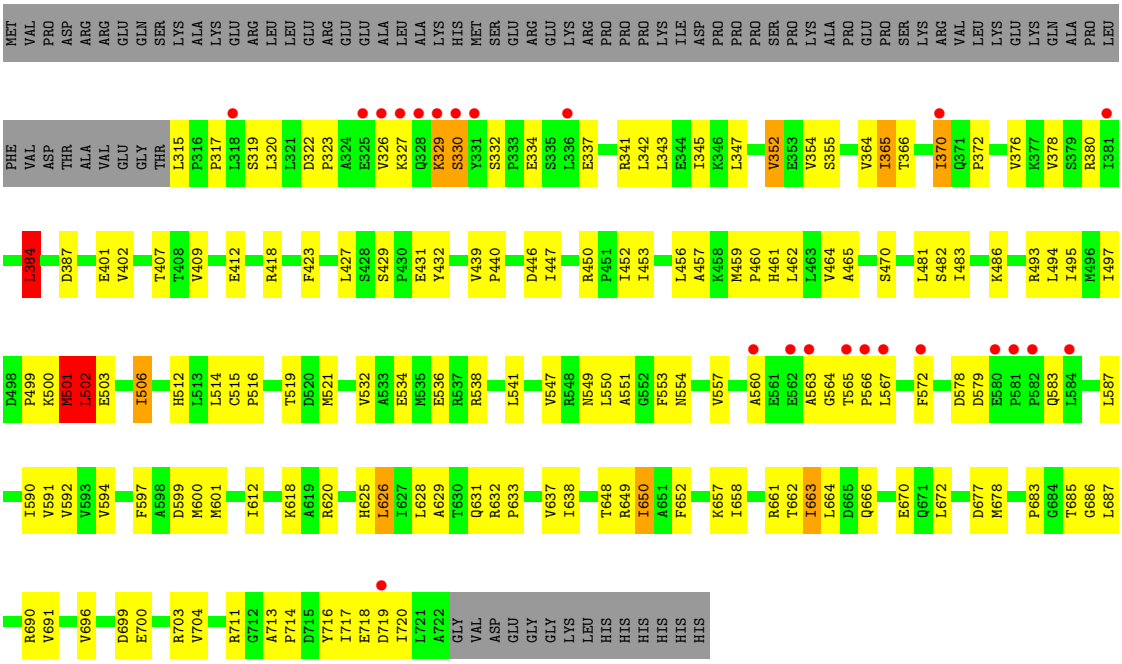
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

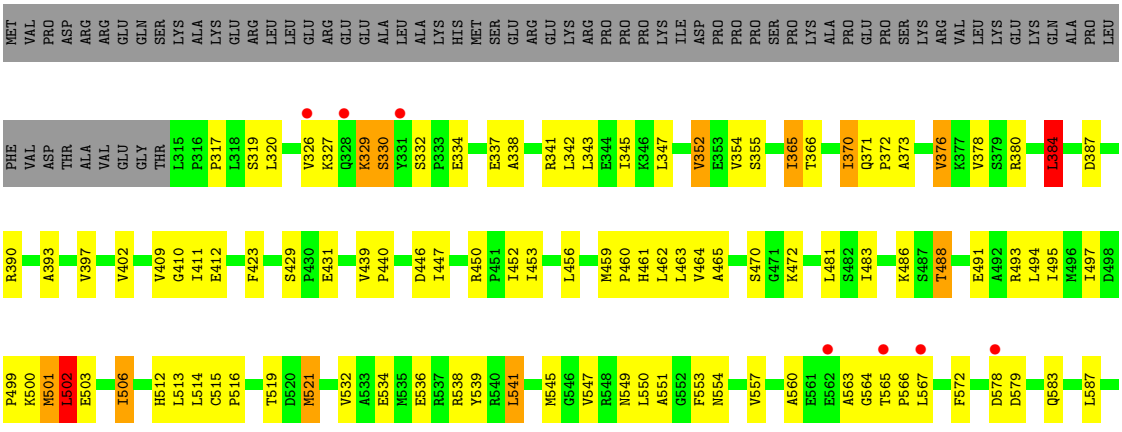
• Molecule 1: DNA TRANSLOCASE FTSK

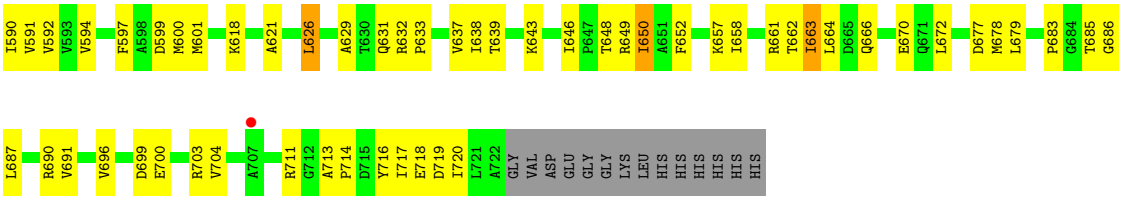
Chain A:



• Molecule 1: DNA TRANSLOCASE FTSK

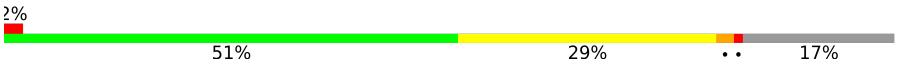
Chain B:

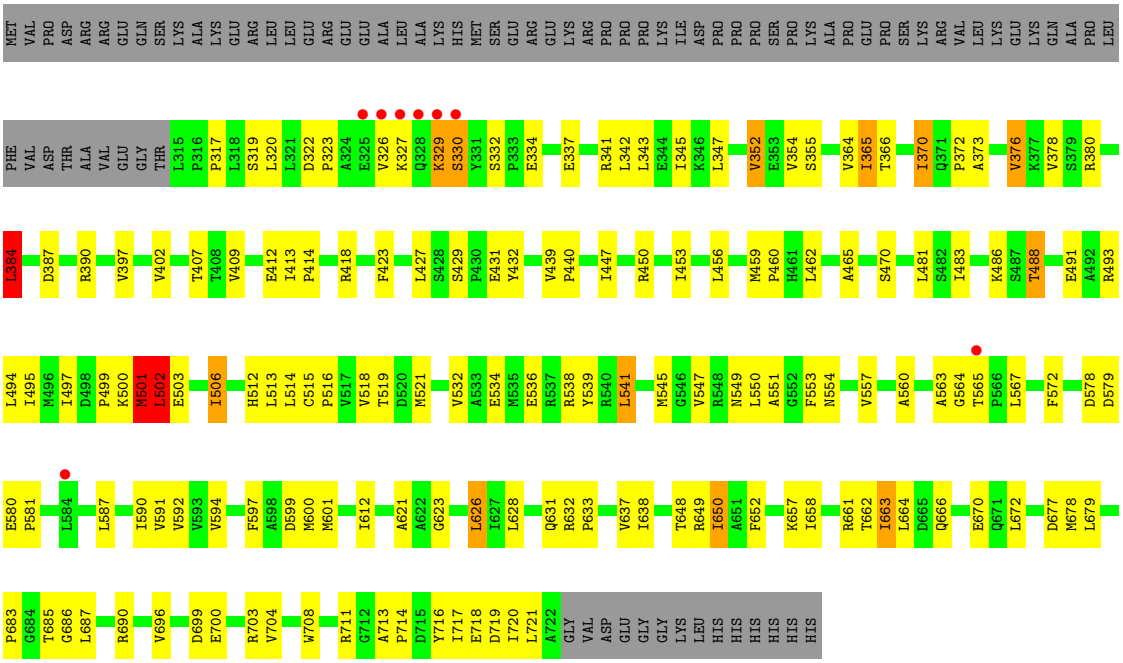




• Molecule 1: DNA TRANSLOCASE FTSK

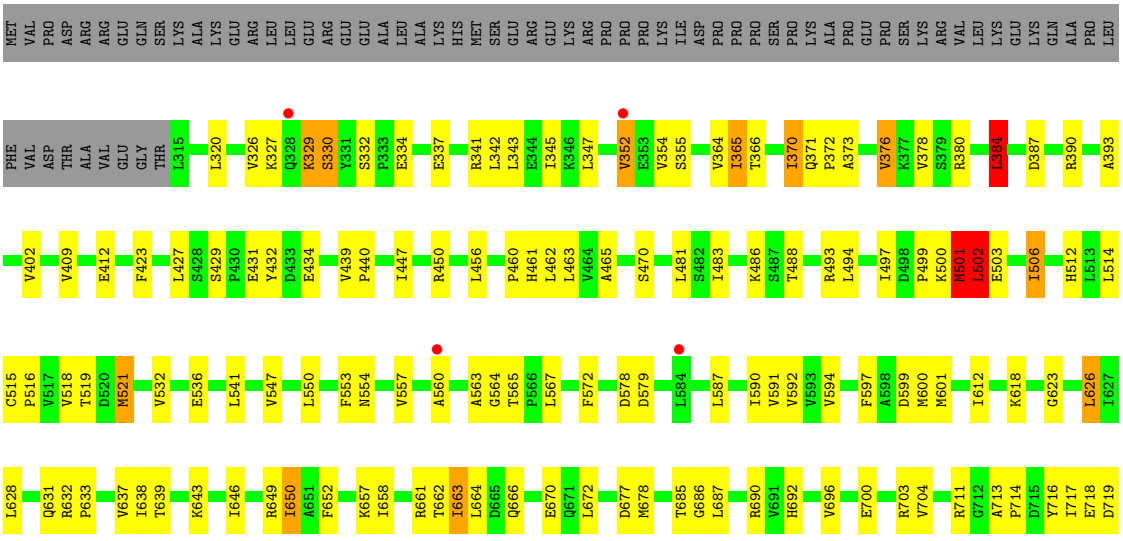
Chain C:

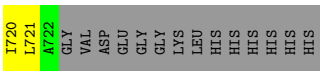




• Molecule 1: DNA TRANSLOCASE FTSK

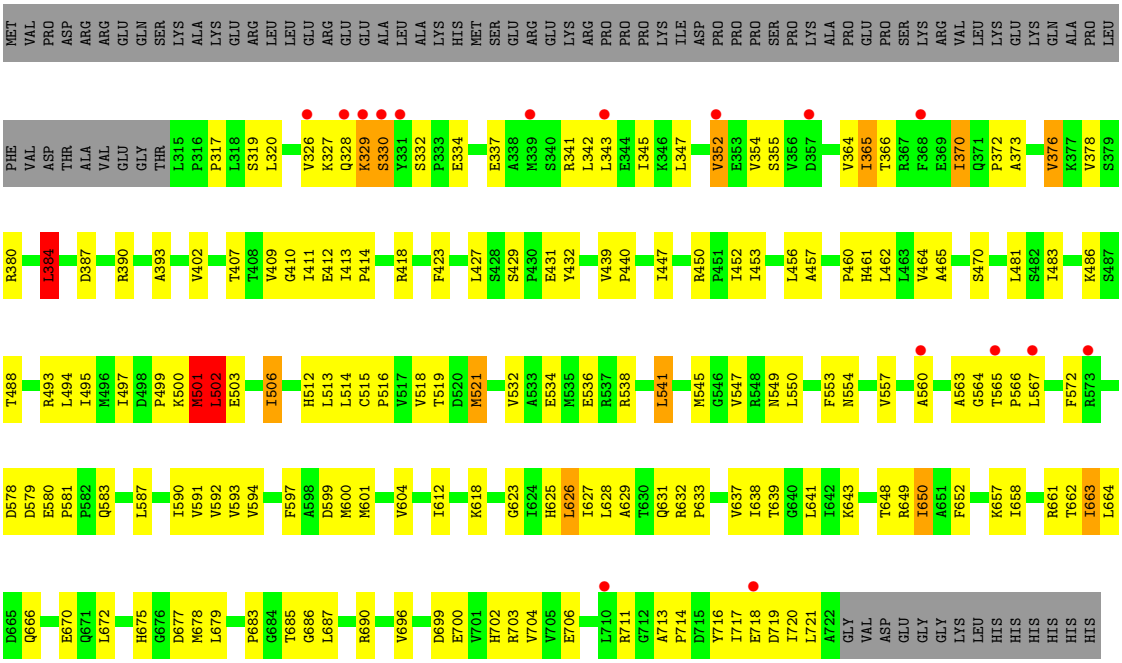
Chain D:





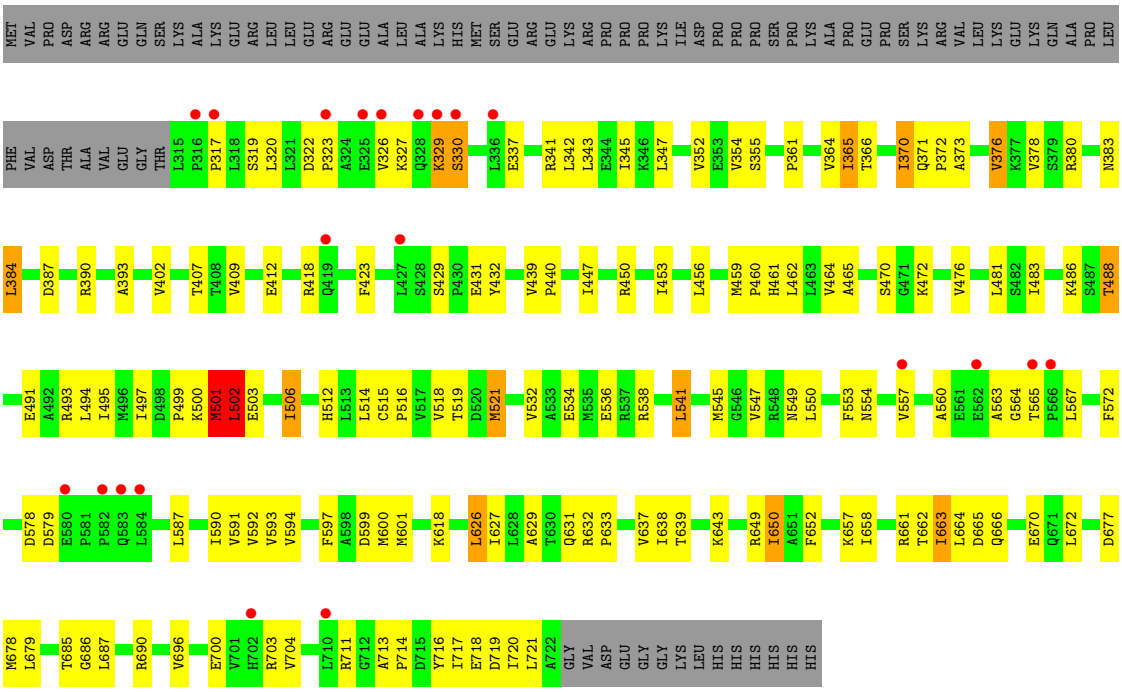
• Molecule 1: DNA TRANSLOCASE FTSK

Chain E:



• Molecule 1: DNA TRANSLOCASE FTSK

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.01Å 221.76Å 134.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90 48.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (100.00-2.90) 99.7 (48.11-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.259 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18888	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: ADP

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	A	0.43	0/3177	0.70	3/4312 (0.1%)
1	B	0.42	0/3177	0.70	3/4312 (0.1%)
1	C	0.43	0/3177	0.70	3/4312 (0.1%)
1	D	0.44	0/3177	0.71	3/4312 (0.1%)
1	E	0.41	0/3177	0.70	3/4312 (0.1%)
1	F	0.44	0/3177	0.70	1/4312 (0.0%)
All	All	0.43	0/19062	0.70	16/25872 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	384	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	502	LEU	CA-CB-CG	5.82	128.69	115.30
1	E	502	LEU	CA-CB-CG	5.81	128.67	115.30
1	C	384	LEU	CA-CB-CG	5.75	128.53	115.30
1	E	384	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	502	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	502	LEU	CA-CB-CG	5.48	127.90	115.30
1	C	502	LEU	CA-CB-CG	5.40	127.72	115.30
1	E	352	VAL	N-CA-C	5.32	125.37	111.00
1	D	384	LEU	CA-CB-CG	5.31	127.52	115.30
1	F	502	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	352	VAL	N-CA-C	5.30	125.31	111.00
1	D	352	VAL	N-CA-C	5.23	125.11	111.00
1	C	352	VAL	N-CA-C	5.16	124.93	111.00
1	A	352	VAL	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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	A	3121	0	3238	132	0
1	B	3121	0	3238	140	1
1	C	3121	0	3238	134	0
1	D	3121	0	3238	124	1
1	E	3121	0	3238	148	0
1	F	3121	0	3238	133	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
All	All	18888	0	19500	788	1

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 21.

All (788) 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:D:502:LEU:HD13	1:D:503:GLU:HG2	1.53	0.91
1:E:502:LEU:HD13	1:E:503:GLU:HG2	1.49	0.91
1:F:502:LEU:HD13	1:F:503:GLU:HG2	1.51	0.90
1:B:502:LEU:HD13	1:B:503:GLU:HG2	1.54	0.88
1:A:502:LEU:HD13	1:A:503:GLU:HG2	1.55	0.87
1:B:521:MET:HE3	1:B:600:MET:HG3	1.55	0.86
1:D:506:ILE:HD13	1:D:506:ILE:O	1.75	0.86
1:C:506:ILE:HD13	1:C:506:ILE:O	1.76	0.85
1:C:502:LEU:HD13	1:C:503:GLU:HG2	1.56	0.85
1:F:506:ILE:HD13	1:F:506:ILE:O	1.77	0.85
1:D:521:MET:HE3	1:D:600:MET:HG3	1.56	0.85
1:C:521:MET:HE3	1:C:600:MET:HG3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:ILE:HD13	1:E:506:ILE:O	1.79	0.83
1:B:506:ILE:O	1:B:506:ILE:HD13	1.78	0.83
1:D:497:ILE:HG21	1:D:600:MET:HE2	1.60	0.82
1:A:497:ILE:HG21	1:A:600:MET:HE2	1.60	0.82
1:B:497:ILE:HG21	1:B:600:MET:HE2	1.59	0.81
1:D:329:LYS:HG2	1:D:330:SER:H	1.46	0.81
1:A:329:LYS:HG2	1:A:330:SER:H	1.46	0.81
1:E:497:ILE:HG21	1:E:600:MET:HE1	1.64	0.80
1:D:500:LYS:O	1:D:502:LEU:N	2.12	0.80
1:A:500:LYS:O	1:A:502:LEU:N	2.15	0.80
1:E:329:LYS:HG2	1:E:330:SER:H	1.46	0.80
1:C:500:LYS:O	1:C:502:LEU:N	2.15	0.79
1:B:500:LYS:O	1:B:502:LEU:N	2.15	0.79
1:D:554:ASN:HD21	1:D:587:LEU:H	1.28	0.79
1:C:329:LYS:HG2	1:C:330:SER:H	1.47	0.79
1:C:497:ILE:HG21	1:C:600:MET:HE2	1.64	0.78
1:C:554:ASN:HD21	1:C:587:LEU:H	1.30	0.78
1:A:663:ILE:HD13	1:A:663:ILE:O	1.84	0.78
1:B:554:ASN:HD21	1:B:587:LEU:H	1.32	0.77
1:E:658:ILE:HD12	1:E:658:ILE:H	1.50	0.77
1:D:638:ILE:HD12	1:D:662:THR:HG22	1.67	0.77
1:B:658:ILE:HD12	1:B:658:ILE:H	1.47	0.77
1:B:329:LYS:HG2	1:B:330:SER:H	1.48	0.76
1:E:521:MET:HE3	1:E:600:MET:HG3	1.67	0.76
1:F:329:LYS:HG2	1:F:330:SER:H	1.49	0.76
1:A:547:VAL:HG11	1:A:553:PHE:N	2.01	0.76
1:F:554:ASN:HD21	1:F:587:LEU:H	1.33	0.76
1:A:554:ASN:HD21	1:A:587:LEU:H	1.34	0.76
1:F:658:ILE:HD12	1:F:658:ILE:H	1.51	0.76
1:F:521:MET:HE3	1:F:600:MET:HG3	1.67	0.75
1:E:380:ARG:O	1:E:384:LEU:HD22	1.87	0.75
1:A:658:ILE:HD12	1:A:658:ILE:H	1.51	0.75
1:E:554:ASN:HD21	1:E:587:LEU:H	1.34	0.75
1:A:506:ILE:HD13	1:A:506:ILE:O	1.86	0.74
1:B:547:VAL:HG11	1:B:553:PHE:N	2.01	0.74
1:E:500:LYS:O	1:E:502:LEU:N	2.19	0.74
1:F:499:PRO:HB3	1:F:521:MET:CE	2.19	0.73
1:C:658:ILE:HD12	1:C:658:ILE:H	1.53	0.73
1:C:440:PRO:HG3	1:C:486:LYS:HD2	1.70	0.73
1:E:499:PRO:HB3	1:E:521:MET:CE	2.18	0.73
1:A:521:MET:HE3	1:A:600:MET:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ARG:O	1:D:384:LEU:HD22	1.88	0.73
1:E:440:PRO:HG3	1:E:486:LYS:HD2	1.71	0.73
1:A:685:THR:HG22	1:A:686:GLY:N	2.04	0.73
1:C:365:ILE:HG13	1:C:412:GLU:HB3	1.71	0.73
1:F:500:LYS:O	1:F:502:LEU:N	2.20	0.73
1:E:547:VAL:HG11	1:E:553:PHE:N	2.03	0.72
1:F:365:ILE:HG13	1:F:412:GLU:HB3	1.70	0.72
1:B:685:THR:HG22	1:B:686:GLY:N	2.05	0.72
1:F:497:ILE:HG21	1:F:600:MET:HE2	1.71	0.72
1:F:638:ILE:HD12	1:F:662:THR:HG22	1.72	0.72
1:A:365:ILE:HG13	1:A:412:GLU:HB3	1.71	0.72
1:E:685:THR:HG22	1:E:686:GLY:N	2.03	0.72
1:B:380:ARG:O	1:B:384:LEU:HD22	1.89	0.71
1:A:638:ILE:HD12	1:A:662:THR:HG22	1.72	0.71
1:B:500:LYS:C	1:B:502:LEU:H	1.94	0.71
1:D:658:ILE:H	1:D:658:ILE:HD12	1.56	0.71
1:F:685:THR:HG22	1:F:686:GLY:N	2.06	0.71
1:F:500:LYS:C	1:F:502:LEU:H	1.94	0.70
1:F:547:VAL:HG11	1:F:553:PHE:N	2.07	0.70
1:C:717:ILE:O	1:C:720:ILE:HG22	1.91	0.70
1:A:380:ARG:O	1:A:384:LEU:HD22	1.90	0.70
1:B:663:ILE:HD13	1:B:663:ILE:O	1.91	0.70
1:F:717:ILE:HG22	1:F:719:ASP:HB3	1.74	0.70
1:D:500:LYS:C	1:D:502:LEU:H	1.94	0.70
1:C:500:LYS:C	1:C:502:LEU:H	1.94	0.70
1:F:711:ARG:HG3	1:F:711:ARG:HH21	1.55	0.69
1:A:500:LYS:C	1:A:502:LEU:H	1.95	0.69
1:E:500:LYS:C	1:E:502:LEU:H	1.95	0.69
1:A:440:PRO:HG3	1:A:486:LYS:HD2	1.73	0.69
1:B:500:LYS:HE3	1:B:599:ASP:OD2	1.93	0.69
1:D:663:ILE:O	1:D:663:ILE:HD13	1.93	0.69
1:E:493:ARG:HD2	1:E:512:HIS:O	1.93	0.69
1:F:717:ILE:O	1:F:720:ILE:HG22	1.92	0.69
1:B:717:ILE:HG22	1:B:719:ASP:HB3	1.75	0.69
1:D:685:THR:HG22	1:D:686:GLY:N	2.07	0.69
1:C:685:THR:HG22	1:C:686:GLY:N	2.06	0.68
1:D:547:VAL:HG11	1:D:553:PHE:N	2.08	0.68
1:F:380:ARG:O	1:F:384:LEU:HD22	1.93	0.68
1:B:711:ARG:HH21	1:B:711:ARG:HG3	1.59	0.68
1:F:601:MET:CE	1:F:637:VAL:HG13	2.23	0.68
1:A:717:ILE:HG22	1:A:719:ASP:HB3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:717:ILE:HG22	1:D:719:ASP:HB3	1.74	0.68
1:F:500:LYS:HE3	1:F:599:ASP:OD2	1.94	0.68
1:C:387:ASP:OD2	1:D:378:VAL:HG23	1.93	0.68
1:C:380:ARG:O	1:C:384:LEU:HD22	1.92	0.68
1:B:497:ILE:HG21	1:B:600:MET:CE	2.24	0.68
1:C:711:ARG:HH21	1:C:711:ARG:HG3	1.58	0.68
1:A:499:PRO:HB3	1:A:521:MET:CE	2.24	0.68
1:B:601:MET:CE	1:B:637:VAL:HG13	2.24	0.68
1:C:717:ILE:HG22	1:C:719:ASP:HB3	1.75	0.67
1:C:663:ILE:HD13	1:C:663:ILE:O	1.95	0.67
1:E:365:ILE:HG13	1:E:412:GLU:HB3	1.75	0.67
1:E:717:ILE:O	1:E:720:ILE:HG22	1.94	0.67
1:E:497:ILE:HD13	1:E:600:MET:HE1	1.77	0.67
1:F:554:ASN:HA	1:F:557:VAL:HG12	1.77	0.67
1:C:547:VAL:HG11	1:C:553:PHE:N	2.11	0.66
1:E:429:SER:HB2	1:E:431:GLU:OE2	1.94	0.66
1:D:601:MET:CE	1:D:637:VAL:HG13	2.26	0.66
1:E:601:MET:CE	1:E:637:VAL:HG13	2.25	0.66
1:E:717:ILE:HG22	1:E:719:ASP:HB3	1.77	0.66
1:F:440:PRO:HG3	1:F:486:LYS:HD2	1.78	0.66
1:A:497:ILE:HG21	1:A:600:MET:CE	2.25	0.66
1:E:341:ARG:O	1:E:345:ILE:HG12	1.96	0.65
1:B:572:PHE:HZ	1:B:579:ASP:HB3	1.61	0.65
1:A:717:ILE:O	1:A:720:ILE:HG22	1.95	0.65
1:F:499:PRO:HB3	1:F:521:MET:HE1	1.78	0.65
1:A:700:GLU:O	1:A:704:VAL:HG23	1.95	0.65
1:B:440:PRO:HG3	1:B:486:LYS:HD2	1.78	0.65
1:D:462:LEU:HD11	1:D:650:ILE:HD13	1.79	0.65
1:F:423:PHE:HE1	1:F:481:LEU:HB3	1.62	0.65
1:A:402:VAL:HG13	1:A:687:LEU:HD11	1.78	0.65
1:E:663:ILE:HD13	1:E:663:ILE:O	1.97	0.65
1:C:497:ILE:HD13	1:C:600:MET:HE2	1.78	0.65
1:E:439:VAL:HG12	1:E:483:ILE:HD12	1.78	0.65
1:D:365:ILE:HG13	1:D:412:GLU:HB3	1.78	0.65
1:D:493:ARG:HD2	1:D:512:HIS:O	1.97	0.65
1:D:554:ASN:HA	1:D:557:VAL:HG12	1.79	0.65
1:C:499:PRO:HB3	1:C:521:MET:CE	2.27	0.64
1:D:717:ILE:O	1:D:720:ILE:HG22	1.97	0.64
1:E:554:ASN:HA	1:E:557:VAL:HG12	1.80	0.64
1:C:638:ILE:HD12	1:C:662:THR:HG22	1.79	0.64
1:F:663:ILE:HD13	1:F:663:ILE:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ILE:O	1:B:720:ILE:HG22	1.97	0.64
1:C:497:ILE:HG21	1:C:600:MET:CE	2.28	0.64
1:E:462:LEU:HD11	1:E:650:ILE:CD1	2.27	0.64
1:A:499:PRO:HB3	1:A:521:MET:HE1	1.78	0.64
1:B:439:VAL:HG12	1:B:483:ILE:HD12	1.79	0.64
1:E:327:LYS:HG3	1:E:327:LYS:O	1.98	0.64
1:B:499:PRO:HB3	1:B:521:MET:CE	2.28	0.64
1:B:499:PRO:HB3	1:B:521:MET:HE1	1.79	0.64
1:E:572:PHE:HZ	1:E:579:ASP:HB3	1.62	0.64
1:E:638:ILE:HD12	1:E:662:THR:HG22	1.79	0.64
1:F:402:VAL:HG13	1:F:687:LEU:HD11	1.79	0.64
1:A:387:ASP:OD2	1:B:378:VAL:HG23	1.98	0.64
1:B:365:ILE:HG13	1:B:412:GLU:HB3	1.78	0.64
1:D:329:LYS:HG2	1:D:330:SER:N	2.13	0.64
1:D:700:GLU:O	1:D:704:VAL:HG23	1.98	0.64
1:A:493:ARG:HD2	1:A:512:HIS:O	1.97	0.63
1:D:327:LYS:O	1:D:327:LYS:HG3	1.98	0.63
1:B:327:LYS:HG3	1:B:327:LYS:O	1.99	0.63
1:C:329:LYS:HG2	1:C:330:SER:N	2.13	0.63
1:E:329:LYS:CG	1:E:330:SER:H	2.11	0.63
1:A:572:PHE:HZ	1:A:579:ASP:HB3	1.63	0.63
1:E:500:LYS:HE3	1:E:599:ASP:OD2	1.98	0.63
1:F:327:LYS:O	1:F:327:LYS:HG3	1.98	0.63
1:F:493:ARG:HD2	1:F:512:HIS:O	1.99	0.63
1:A:711:ARG:HG3	1:A:711:ARG:HH21	1.63	0.63
1:C:327:LYS:O	1:C:327:LYS:HG3	1.97	0.63
1:D:440:PRO:HG3	1:D:486:LYS:HD2	1.80	0.63
1:A:329:LYS:HG2	1:A:330:SER:N	2.13	0.63
1:B:638:ILE:HD12	1:B:662:THR:HG22	1.80	0.63
1:E:499:PRO:HB3	1:E:521:MET:HE1	1.81	0.63
1:F:462:LEU:HD11	1:F:650:ILE:HD13	1.80	0.63
1:B:514:LEU:HD11	1:B:590:ILE:HD12	1.80	0.63
1:F:572:PHE:HZ	1:F:579:ASP:HB3	1.64	0.63
1:A:354:VAL:HG23	1:A:372:PRO:HA	1.81	0.62
1:E:711:ARG:HH21	1:E:711:ARG:HG3	1.64	0.62
1:B:329:LYS:HG2	1:B:330:SER:N	2.14	0.62
1:C:370:ILE:HD13	1:C:409:VAL:O	1.99	0.62
1:C:601:MET:CE	1:C:637:VAL:HG13	2.30	0.62
1:E:387:ASP:OD2	1:F:378:VAL:HG23	2.00	0.62
1:D:370:ILE:HD13	1:D:409:VAL:O	1.99	0.62
1:F:370:ILE:HD13	1:F:409:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:SER:HB2	1:A:431:GLU:OE2	1.99	0.62
1:B:658:ILE:HD12	1:B:658:ILE:N	2.14	0.62
1:B:685:THR:HG22	1:B:686:GLY:H	1.65	0.62
1:C:514:LEU:HD11	1:C:590:ILE:HD12	1.80	0.62
1:A:494:LEU:HD23	1:A:591:VAL:HB	1.81	0.62
1:D:572:PHE:HZ	1:D:579:ASP:HB3	1.65	0.62
1:C:554:ASN:HA	1:C:557:VAL:HG12	1.82	0.62
1:F:370:ILE:HD13	1:F:370:ILE:H	1.65	0.62
1:E:354:VAL:HG23	1:E:372:PRO:HA	1.80	0.62
1:D:439:VAL:HG12	1:D:483:ILE:HD12	1.82	0.61
1:D:711:ARG:HH21	1:D:711:ARG:HG3	1.65	0.61
1:B:341:ARG:O	1:B:345:ILE:HG12	2.01	0.61
1:B:497:ILE:HD12	1:B:594:VAL:HG22	1.82	0.61
1:C:370:ILE:HD13	1:C:370:ILE:H	1.66	0.61
1:D:499:PRO:HB3	1:D:521:MET:HE1	1.83	0.61
1:C:541:LEU:O	1:C:545:MET:HG2	2.01	0.61
1:F:329:LYS:HG2	1:F:330:SER:N	2.15	0.61
1:F:462:LEU:HD11	1:F:650:ILE:CD1	2.30	0.61
1:A:423:PHE:HE1	1:A:481:LEU:HB3	1.63	0.61
1:A:631:GLN:O	1:A:633:PRO:HD3	2.01	0.61
1:E:497:ILE:HG21	1:E:600:MET:CE	2.31	0.61
1:B:429:SER:HB2	1:B:431:GLU:OE2	2.00	0.61
1:C:439:VAL:HG12	1:C:483:ILE:HD12	1.82	0.61
1:E:497:ILE:HD12	1:E:594:VAL:HG22	1.83	0.61
1:F:429:SER:HB2	1:F:431:GLU:OE2	2.00	0.61
1:A:327:LYS:O	1:A:327:LYS:HG3	2.01	0.60
1:D:500:LYS:HE3	1:D:599:ASP:OD2	2.01	0.60
1:A:341:ARG:O	1:A:345:ILE:HG12	2.01	0.60
1:A:370:ILE:HD13	1:A:409:VAL:O	2.02	0.60
1:C:465:ALA:HB3	1:C:663:ILE:HG13	1.83	0.60
1:F:341:ARG:O	1:F:345:ILE:HG12	2.00	0.60
1:A:554:ASN:HA	1:A:557:VAL:HG12	1.82	0.60
1:D:354:VAL:HG23	1:D:372:PRO:HA	1.83	0.60
1:D:497:ILE:HD12	1:D:594:VAL:HG22	1.83	0.60
1:C:429:SER:HB2	1:C:431:GLU:OE2	2.01	0.60
1:C:700:GLU:O	1:C:704:VAL:HG23	2.01	0.60
1:A:658:ILE:HD12	1:A:658:ILE:N	2.17	0.60
1:E:329:LYS:HG2	1:E:330:SER:N	2.14	0.60
1:F:601:MET:HE1	1:F:637:VAL:HG13	1.82	0.60
1:D:429:SER:HB2	1:D:431:GLU:OE2	2.02	0.60
1:E:423:PHE:HE1	1:E:481:LEU:HB3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ILE:HD12	1:C:594:VAL:HG22	1.84	0.59
1:D:499:PRO:HB3	1:D:521:MET:CE	2.32	0.59
1:E:465:ALA:HB3	1:E:663:ILE:HG13	1.84	0.59
1:C:713:ALA:HB1	1:C:714:PRO:HD2	1.84	0.59
1:F:532:VAL:O	1:F:536:GLU:HG2	2.02	0.59
1:A:378:VAL:HG23	1:F:387:ASP:OD2	2.03	0.59
1:E:658:ILE:HD12	1:E:658:ILE:N	2.15	0.59
1:A:685:THR:HG22	1:A:686:GLY:H	1.65	0.59
1:B:423:PHE:HE1	1:B:481:LEU:HB3	1.68	0.59
1:B:554:ASN:HA	1:B:557:VAL:HG12	1.83	0.59
1:D:341:ARG:O	1:D:345:ILE:HG12	2.02	0.59
1:E:370:ILE:HD13	1:E:370:ILE:H	1.66	0.59
1:E:370:ILE:HD13	1:E:409:VAL:O	2.03	0.59
1:E:462:LEU:HD11	1:E:650:ILE:HD13	1.83	0.59
1:A:601:MET:CE	1:A:637:VAL:HG13	2.33	0.59
1:D:497:ILE:HG21	1:D:600:MET:CE	2.32	0.59
1:C:572:PHE:HZ	1:C:579:ASP:HB3	1.66	0.59
1:B:465:ALA:HB1	1:B:633:PRO:HG3	1.83	0.59
1:C:500:LYS:HE3	1:C:599:ASP:OD2	2.02	0.59
1:A:497:ILE:HD12	1:A:594:VAL:HG22	1.85	0.58
1:C:499:PRO:HB3	1:C:521:MET:HE1	1.83	0.58
1:D:465:ALA:HB3	1:D:663:ILE:HG13	1.84	0.58
1:F:700:GLU:O	1:F:704:VAL:HG23	2.03	0.58
1:B:402:VAL:HG13	1:B:687:LEU:HD11	1.85	0.58
1:F:658:ILE:HD12	1:F:658:ILE:N	2.15	0.58
1:C:329:LYS:CG	1:C:330:SER:N	2.66	0.58
1:D:329:LYS:CG	1:D:330:SER:N	2.66	0.58
1:B:497:ILE:HD13	1:B:600:MET:HE2	1.85	0.58
1:D:329:LYS:H	1:D:329:LYS:HD3	1.69	0.58
1:E:601:MET:HE1	1:E:637:VAL:HG13	1.84	0.58
1:C:341:ARG:O	1:C:345:ILE:HG12	2.04	0.58
1:F:354:VAL:HG23	1:F:372:PRO:HA	1.85	0.58
1:F:439:VAL:HG12	1:F:483:ILE:HD12	1.85	0.58
1:C:465:ALA:HB1	1:C:633:PRO:HG3	1.86	0.58
1:A:500:LYS:HE3	1:A:599:ASP:OD2	2.03	0.58
1:C:597:PHE:CE1	1:C:601:MET:HE1	2.39	0.58
1:D:599:ASP:OD1	1:D:632:ARG:NH1	2.37	0.58
1:D:462:LEU:HD11	1:D:650:ILE:CD1	2.32	0.57
1:F:514:LEU:HD11	1:F:590:ILE:HD12	1.84	0.57
1:C:402:VAL:HG13	1:C:687:LEU:HD11	1.86	0.57
1:C:550:LEU:HD11	1:C:587:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:THR:HG22	1:C:686:GLY:H	1.67	0.57
1:F:494:LEU:HD23	1:F:591:VAL:HB	1.86	0.57
1:A:661:ARG:HA	1:A:666:GLN:H	1.68	0.57
1:E:329:LYS:CG	1:E:330:SER:N	2.67	0.57
1:E:685:THR:CG2	1:E:686:GLY:N	2.67	0.57
1:B:329:LYS:CG	1:B:330:SER:N	2.68	0.57
1:B:370:ILE:HD13	1:B:370:ILE:H	1.70	0.57
1:B:550:LEU:HD11	1:B:587:LEU:HB2	1.85	0.57
1:B:493:ARG:HD2	1:B:512:HIS:O	2.05	0.57
1:A:329:LYS:CG	1:A:330:SER:N	2.67	0.57
1:B:601:MET:HE1	1:B:637:VAL:HG13	1.87	0.57
1:D:423:PHE:HE1	1:D:481:LEU:HB3	1.68	0.57
1:A:462:LEU:HD11	1:A:650:ILE:HD13	1.87	0.57
1:D:514:LEU:HD11	1:D:590:ILE:HD12	1.87	0.57
1:F:365:ILE:HG12	1:F:366:THR:N	2.19	0.57
1:A:465:ALA:HB3	1:A:663:ILE:HG13	1.87	0.57
1:A:685:THR:CG2	1:A:686:GLY:N	2.68	0.57
1:B:365:ILE:HD11	1:B:447:ILE:HB	1.86	0.57
1:F:497:ILE:HG21	1:F:600:MET:CE	2.35	0.56
1:C:354:VAL:HG23	1:C:372:PRO:HA	1.87	0.56
1:C:658:ILE:HD12	1:C:658:ILE:N	2.18	0.56
1:A:439:VAL:HG12	1:A:483:ILE:HD12	1.87	0.56
1:B:465:ALA:HB3	1:B:663:ILE:HG13	1.87	0.56
1:B:521:MET:HE3	1:B:600:MET:CG	2.30	0.56
1:B:685:THR:CG2	1:B:686:GLY:N	2.69	0.56
1:B:700:GLU:O	1:B:704:VAL:HG23	2.04	0.56
1:E:365:ILE:HD11	1:E:447:ILE:HB	1.86	0.56
1:E:470:SER:HB2	1:E:652:PHE:HB3	1.87	0.56
1:A:560:ALA:CB	1:A:567:LEU:HG	2.34	0.56
1:D:658:ILE:HD12	1:D:658:ILE:N	2.20	0.56
1:E:685:THR:HG22	1:E:686:GLY:H	1.69	0.56
1:D:370:ILE:HD13	1:D:370:ILE:H	1.71	0.56
1:E:550:LEU:HD11	1:E:587:LEU:HB2	1.86	0.56
1:E:658:ILE:H	1:E:658:ILE:CD1	2.18	0.56
1:F:329:LYS:H	1:F:329:LYS:HD3	1.70	0.56
1:F:560:ALA:CB	1:F:567:LEU:HG	2.35	0.56
1:D:365:ILE:HD11	1:D:447:ILE:HB	1.87	0.56
1:D:387:ASP:OD2	1:E:378:VAL:HG23	2.05	0.56
1:E:329:LYS:HD3	1:E:329:LYS:H	1.71	0.56
1:E:532:VAL:O	1:E:536:GLU:HG2	2.05	0.56
1:A:514:LEU:HD11	1:A:590:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:ASP:OD1	1:C:632:ARG:NH1	2.39	0.56
1:F:470:SER:HB2	1:F:652:PHE:HB3	1.88	0.56
1:E:402:VAL:HG13	1:E:687:LEU:HD11	1.88	0.56
1:F:550:LEU:HD11	1:F:587:LEU:HB2	1.87	0.56
1:B:462:LEU:HD11	1:B:650:ILE:CD1	2.36	0.56
1:A:470:SER:HB2	1:A:652:PHE:HB3	1.88	0.56
1:F:685:THR:CG2	1:F:686:GLY:N	2.69	0.56
1:C:493:ARG:HD2	1:C:512:HIS:O	2.06	0.55
1:C:423:PHE:HE1	1:C:481:LEU:HB3	1.69	0.55
1:A:370:ILE:HD13	1:A:370:ILE:H	1.71	0.55
1:C:685:THR:CG2	1:C:686:GLY:N	2.69	0.55
1:E:499:PRO:HB3	1:E:521:MET:HE2	1.86	0.55
1:B:354:VAL:HG23	1:B:372:PRO:HA	1.88	0.55
1:B:488:THR:HG23	1:B:491:GLU:OE2	2.06	0.55
1:C:560:ALA:CB	1:C:567:LEU:HG	2.35	0.55
1:E:465:ALA:HB1	1:E:633:PRO:HG3	1.88	0.55
1:A:347:LEU:HB3	1:A:352:VAL:HG23	1.89	0.55
1:A:462:LEU:HD11	1:A:650:ILE:CD1	2.35	0.55
1:D:532:VAL:O	1:D:536:GLU:HG2	2.06	0.55
1:E:494:LEU:HD23	1:E:591:VAL:HB	1.87	0.55
1:E:560:ALA:CB	1:E:567:LEU:HG	2.36	0.55
1:F:658:ILE:H	1:F:658:ILE:CD1	2.19	0.55
1:F:661:ARG:HA	1:F:666:GLN:H	1.71	0.55
1:C:494:LEU:HD23	1:C:591:VAL:HB	1.89	0.55
1:F:713:ALA:HB1	1:F:714:PRO:HD2	1.89	0.55
1:A:713:ALA:HB1	1:A:714:PRO:HD2	1.89	0.55
1:E:661:ARG:HA	1:E:666:GLN:H	1.71	0.54
1:E:700:GLU:O	1:E:704:VAL:HG23	2.07	0.54
1:A:677:ASP:OD1	1:A:690:ARG:NH1	2.36	0.54
1:A:658:ILE:H	1:A:658:ILE:CD1	2.19	0.54
1:D:465:ALA:HB1	1:D:633:PRO:HG3	1.89	0.54
1:F:347:LEU:HB3	1:F:352:VAL:HG23	1.89	0.54
1:D:550:LEU:HD11	1:D:587:LEU:HB2	1.90	0.54
1:C:329:LYS:H	1:C:329:LYS:HD3	1.71	0.54
1:D:685:THR:CG2	1:D:686:GLY:N	2.70	0.54
1:F:329:LYS:CG	1:F:330:SER:N	2.68	0.54
1:A:329:LYS:H	1:A:329:LYS:HD3	1.72	0.54
1:F:649:ARG:HB3	1:F:663:ILE:CD1	2.37	0.54
1:A:365:ILE:HD11	1:A:447:ILE:HB	1.88	0.54
1:C:462:LEU:HD11	1:C:650:ILE:CD1	2.38	0.54
1:D:554:ASN:HA	1:D:557:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:VAL:HB	1:B:626:LEU:HD12	1.89	0.54
1:E:599:ASP:OD1	1:E:632:ARG:NH1	2.40	0.54
1:A:550:LEU:HD11	1:A:587:LEU:HB2	1.89	0.54
1:B:370:ILE:HD13	1:B:409:VAL:O	2.08	0.53
1:E:713:ALA:HB1	1:E:714:PRO:HD2	1.90	0.53
1:A:465:ALA:HB1	1:A:633:PRO:HG3	1.88	0.53
1:B:685:THR:CG2	1:B:686:GLY:H	2.21	0.53
1:C:521:MET:HE3	1:C:600:MET:CG	2.33	0.53
1:C:717:ILE:N	1:C:717:ILE:HD12	2.23	0.53
1:D:560:ALA:CB	1:D:567:LEU:HG	2.38	0.53
1:E:516:PRO:HG3	1:E:716:TYR:CE1	2.44	0.53
1:D:677:ASP:OD1	1:D:690:ARG:NH1	2.39	0.53
1:F:717:ILE:N	1:F:717:ILE:HD12	2.23	0.53
1:F:554:ASN:HA	1:F:557:VAL:CG1	2.39	0.53
1:C:661:ARG:HA	1:C:666:GLN:H	1.73	0.53
1:A:365:ILE:HG12	1:A:366:THR:N	2.24	0.53
1:D:494:LEU:HD23	1:D:591:VAL:HB	1.90	0.53
1:B:329:LYS:H	1:B:329:LYS:HD3	1.74	0.53
1:B:663:ILE:HD13	1:B:663:ILE:C	2.29	0.53
1:B:717:ILE:HD12	1:B:717:ILE:N	2.24	0.53
1:E:514:LEU:HD11	1:E:590:ILE:HD12	1.90	0.53
1:F:685:THR:HG22	1:F:686:GLY:H	1.73	0.53
1:A:663:ILE:HD13	1:A:663:ILE:C	2.29	0.53
1:B:534:GLU:O	1:B:538:ARG:HG3	2.09	0.53
1:B:658:ILE:H	1:B:658:ILE:CD1	2.17	0.53
1:C:532:VAL:O	1:C:536:GLU:HG2	2.09	0.53
1:A:717:ILE:N	1:A:717:ILE:HD12	2.24	0.53
1:C:534:GLU:O	1:C:538:ARG:HG3	2.09	0.53
1:F:497:ILE:HD12	1:F:594:VAL:HG22	1.91	0.53
1:F:541:LEU:O	1:F:545:MET:HG2	2.08	0.52
1:F:497:ILE:HD13	1:F:600:MET:HE2	1.92	0.52
1:D:657:LYS:HG2	1:D:670:GLU:OE1	2.09	0.52
1:B:560:ALA:CB	1:B:567:LEU:HG	2.38	0.52
1:D:601:MET:HE1	1:D:637:VAL:HG13	1.91	0.52
1:A:685:THR:CG2	1:A:686:GLY:H	2.21	0.52
1:D:470:SER:HB2	1:D:652:PHE:HB3	1.92	0.52
1:D:661:ARG:HA	1:D:666:GLN:H	1.74	0.52
1:D:672:LEU:HD13	1:D:678:MET:HA	1.91	0.52
1:F:465:ALA:HB1	1:F:633:PRO:HG3	1.92	0.52
1:D:685:THR:HG22	1:D:686:GLY:H	1.74	0.52
1:F:464:VAL:O	1:F:629:ALA:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:CG	1:C:330:SER:H	2.12	0.52
1:D:402:VAL:HG13	1:D:687:LEU:HD11	1.92	0.52
1:B:657:LYS:HG2	1:B:670:GLU:OE1	2.10	0.52
1:B:500:LYS:C	1:B:502:LEU:N	2.62	0.51
1:C:354:VAL:HG22	1:C:355:SER:N	2.25	0.51
1:C:462:LEU:HD11	1:C:650:ILE:HD13	1.92	0.51
1:D:460:PRO:HG2	1:D:461:HIS:CD2	2.45	0.51
1:E:685:THR:CG2	1:E:686:GLY:H	2.24	0.51
1:A:329:LYS:CG	1:A:330:SER:H	2.11	0.51
1:A:699:ASP:HB3	1:A:703:ARG:HH11	1.75	0.51
1:F:465:ALA:HB3	1:F:663:ILE:HG13	1.92	0.51
1:B:387:ASP:OD2	1:C:378:VAL:HG23	2.10	0.51
1:E:677:ASP:OD1	1:E:690:ARG:NH1	2.36	0.51
1:D:347:LEU:HB3	1:D:352:VAL:HG23	1.92	0.51
1:D:390:ARG:HE	1:E:378:VAL:CG2	2.22	0.51
1:C:516:PRO:HG3	1:C:716:TYR:CE1	2.44	0.51
1:C:354:VAL:HG22	1:C:355:SER:H	1.76	0.51
1:F:677:ASP:OD1	1:F:690:ARG:NH1	2.39	0.51
1:C:685:THR:CG2	1:C:686:GLY:H	2.23	0.51
1:A:547:VAL:HG12	1:A:549:ASN:H	1.76	0.51
1:F:488:THR:HG23	1:F:491:GLU:OE2	2.12	0.51
1:A:354:VAL:HG21	1:A:370:ILE:CG1	2.41	0.50
1:C:495:ILE:HG13	1:C:514:LEU:HD12	1.93	0.50
1:B:462:LEU:HD11	1:B:650:ILE:HD13	1.92	0.50
1:B:470:SER:HB2	1:B:652:PHE:HB3	1.93	0.50
1:B:494:LEU:HD23	1:B:591:VAL:HB	1.93	0.50
1:F:499:PRO:HB3	1:F:521:MET:HE2	1.93	0.50
1:B:713:ALA:HB1	1:B:714:PRO:HD2	1.92	0.50
1:A:554:ASN:HA	1:A:557:VAL:CG1	2.41	0.50
1:B:599:ASP:OD1	1:B:632:ARG:NH1	2.44	0.50
1:D:354:VAL:HG21	1:D:370:ILE:CG1	2.41	0.50
1:E:592:VAL:HB	1:E:626:LEU:HD12	1.94	0.50
1:E:717:ILE:O	1:E:719:ASP:N	2.45	0.50
1:D:501:MET:HE1	1:E:618:LYS:HE2	1.93	0.50
1:E:373:ALA:O	1:E:376:VAL:HG13	2.11	0.50
1:F:592:VAL:HB	1:F:626:LEU:HD12	1.94	0.50
1:B:672:LEU:HD13	1:B:678:MET:HA	1.94	0.50
1:E:663:ILE:HG23	1:E:664:LEU:HG	1.93	0.50
1:D:717:ILE:HD12	1:D:717:ILE:N	2.26	0.50
1:F:599:ASP:OD1	1:F:632:ARG:NH1	2.45	0.49
1:C:501:MET:CE	1:D:618:LYS:HE2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:VAL:HB	1:C:626:LEU:HD12	1.94	0.49
1:E:380:ARG:O	1:E:384:LEU:CD2	2.59	0.49
1:E:699:ASP:HB3	1:E:703:ARG:HH11	1.76	0.49
1:A:717:ILE:O	1:A:719:ASP:N	2.46	0.49
1:D:373:ALA:O	1:D:376:VAL:HG13	2.12	0.49
1:D:497:ILE:HD13	1:D:600:MET:HE2	1.94	0.49
1:E:462:LEU:HD11	1:E:650:ILE:HD12	1.94	0.49
1:E:717:ILE:N	1:E:717:ILE:HD12	2.27	0.49
1:A:592:VAL:HB	1:A:626:LEU:HD12	1.94	0.49
1:B:563:ALA:O	1:B:565:THR:N	2.46	0.49
1:B:717:ILE:O	1:B:719:ASP:N	2.46	0.49
1:C:365:ILE:HG12	1:C:366:THR:N	2.28	0.49
1:E:460:PRO:HG2	1:E:461:HIS:CD2	2.48	0.49
1:B:373:ALA:O	1:B:376:VAL:HG13	2.12	0.49
1:D:717:ILE:O	1:D:719:ASP:N	2.46	0.49
1:F:364:VAL:HG22	1:F:418:ARG:HG3	1.95	0.49
1:D:597:PHE:CD1	1:D:601:MET:HE2	2.48	0.49
1:E:390:ARG:HE	1:F:378:VAL:CG2	2.26	0.49
1:A:549:ASN:OD1	1:A:551:ALA:HB3	2.13	0.49
1:B:393:ALA:HB2	1:C:407:THR:CG2	2.43	0.49
1:C:672:LEU:HD13	1:C:678:MET:HA	1.93	0.49
1:D:713:ALA:HB1	1:D:714:PRO:HD2	1.94	0.49
1:B:452:ILE:C	1:B:453:ILE:HD12	2.33	0.49
1:C:364:VAL:HG22	1:C:418:ARG:HG3	1.95	0.49
1:B:639:THR:O	1:B:643:LYS:HG3	2.13	0.48
1:D:500:LYS:C	1:D:502:LEU:N	2.62	0.48
1:F:672:LEU:HD13	1:F:678:MET:HA	1.95	0.48
1:F:711:ARG:HG3	1:F:711:ARG:NH2	2.24	0.48
1:A:500:LYS:C	1:A:502:LEU:N	2.63	0.48
1:B:332:SER:OG	1:B:334:GLU:HG3	2.13	0.48
1:F:663:ILE:HD13	1:F:663:ILE:C	2.33	0.48
1:B:516:PRO:HG3	1:B:716:TYR:CE1	2.49	0.48
1:D:663:ILE:HD13	1:D:663:ILE:C	2.32	0.48
1:E:493:ARG:NH2	1:E:513:LEU:O	2.46	0.48
1:E:534:GLU:O	1:E:538:ARG:HG3	2.13	0.48
1:C:493:ARG:NH2	1:C:513:LEU:O	2.46	0.48
1:B:549:ASN:OD1	1:B:551:ALA:HB3	2.14	0.48
1:C:500:LYS:C	1:C:502:LEU:N	2.62	0.48
1:D:631:GLN:O	1:D:633:PRO:HD3	2.13	0.48
1:F:515:CYS:HB3	1:F:720:ILE:HG21	1.95	0.48
1:B:365:ILE:HG12	1:B:366:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:O	1:B:384:LEU:CD2	2.61	0.48
1:B:554:ASN:HA	1:B:557:VAL:CG1	2.43	0.48
1:E:521:MET:HE3	1:E:600:MET:CG	2.38	0.48
1:F:380:ARG:O	1:F:384:LEU:CD2	2.61	0.48
1:C:677:ASP:OD1	1:C:690:ARG:NH1	2.40	0.48
1:F:597:PHE:CE1	1:F:601:MET:HE1	2.49	0.48
1:F:717:ILE:O	1:F:719:ASP:N	2.47	0.48
1:B:631:GLN:C	1:B:633:PRO:HD3	2.33	0.48
1:C:470:SER:HB2	1:C:652:PHE:HB3	1.95	0.48
1:D:463:LEU:HG	1:D:646:ILE:HG21	1.96	0.48
1:E:457:ALA:HA	1:E:625:HIS:CD2	2.48	0.48
1:A:532:VAL:O	1:A:536:GLU:HG2	2.14	0.48
1:C:717:ILE:O	1:C:719:ASP:N	2.46	0.48
1:E:347:LEU:HB3	1:E:352:VAL:HG23	1.96	0.48
1:B:354:VAL:HG21	1:B:370:ILE:CG1	2.44	0.48
1:B:532:VAL:O	1:B:536:GLU:HG2	2.13	0.48
1:B:661:ARG:HA	1:B:666:GLN:H	1.79	0.48
1:C:601:MET:HE3	1:C:637:VAL:HG13	1.96	0.48
1:E:554:ASN:HA	1:E:557:VAL:CG1	2.43	0.48
1:F:521:MET:HE3	1:F:600:MET:CG	2.43	0.47
1:A:648:THR:OG1	1:A:683:PRO:HD3	2.13	0.47
1:B:711:ARG:HG3	1:B:711:ARG:NH2	2.27	0.47
1:C:354:VAL:HG21	1:C:370:ILE:CG1	2.43	0.47
1:C:649:ARG:HB3	1:C:663:ILE:CD1	2.44	0.47
1:E:663:ILE:HD13	1:E:663:ILE:C	2.34	0.47
1:C:649:ARG:HB3	1:C:663:ILE:HD13	1.96	0.47
1:E:500:LYS:C	1:E:502:LEU:N	2.63	0.47
1:E:639:THR:O	1:E:643:LYS:HG3	2.14	0.47
1:F:354:VAL:HG21	1:F:370:ILE:CG1	2.45	0.47
1:A:317:PRO:C	1:A:319:SER:H	2.18	0.47
1:C:365:ILE:HD11	1:C:447:ILE:HB	1.96	0.47
1:D:521:MET:CE	1:D:600:MET:HG3	2.37	0.47
1:D:658:ILE:H	1:D:658:ILE:CD1	2.23	0.47
1:E:354:VAL:HG23	1:E:372:PRO:CA	2.45	0.47
1:F:460:PRO:HG2	1:F:461:HIS:CD2	2.49	0.47
1:F:631:GLN:O	1:F:633:PRO:HD3	2.13	0.47
1:A:631:GLN:C	1:A:633:PRO:HD3	2.33	0.47
1:B:460:PRO:HG2	1:B:461:HIS:CD2	2.49	0.47
1:C:658:ILE:H	1:C:658:ILE:CD1	2.23	0.47
1:B:354:VAL:HG22	1:B:355:SER:N	2.30	0.47
1:C:631:GLN:C	1:C:633:PRO:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:VAL:HG22	1:D:355:SER:N	2.30	0.47
1:A:515:CYS:HB3	1:A:720:ILE:HG21	1.96	0.47
1:A:601:MET:HE1	1:A:637:VAL:HG13	1.97	0.47
1:C:663:ILE:HD13	1:C:663:ILE:C	2.35	0.47
1:D:516:PRO:HG3	1:D:716:TYR:CE1	2.50	0.47
1:F:365:ILE:HD11	1:F:447:ILE:HB	1.96	0.47
1:A:663:ILE:HG23	1:A:664:LEU:HG	1.97	0.47
1:D:354:VAL:HG22	1:D:355:SER:H	1.80	0.47
1:F:685:THR:CG2	1:F:686:GLY:H	2.26	0.47
1:F:373:ALA:O	1:F:376:VAL:HG13	2.14	0.47
1:A:460:PRO:HG2	1:A:461:HIS:CD2	2.50	0.46
1:A:534:GLU:O	1:A:538:ARG:HG3	2.14	0.46
1:F:597:PHE:CD1	1:F:601:MET:HE2	2.50	0.46
1:B:699:ASP:HB3	1:B:703:ARG:HH11	1.80	0.46
1:D:550:LEU:HD22	1:D:623:GLY:HA3	1.96	0.46
1:D:601:MET:HE3	1:D:637:VAL:HG13	1.96	0.46
1:C:320:LEU:O	1:C:703:ARG:NH2	2.45	0.46
1:D:501:MET:CE	1:E:618:LYS:HE2	2.45	0.46
1:F:354:VAL:HG22	1:F:355:SER:H	1.80	0.46
1:A:516:PRO:HG3	1:A:716:TYR:CE1	2.51	0.46
1:B:663:ILE:HG23	1:B:664:LEU:HG	1.97	0.46
1:C:317:PRO:C	1:C:319:SER:H	2.17	0.46
1:D:663:ILE:HG23	1:D:664:LEU:HG	1.96	0.46
1:E:464:VAL:O	1:E:629:ALA:HA	2.15	0.46
1:F:495:ILE:HG13	1:F:514:LEU:HD12	1.97	0.46
1:F:516:PRO:HG3	1:F:716:TYR:CE1	2.51	0.46
1:C:465:ALA:CB	1:C:663:ILE:HG13	2.45	0.46
1:B:601:MET:HE3	1:B:637:VAL:HG13	1.97	0.46
1:D:685:THR:CG2	1:D:686:GLY:H	2.27	0.46
1:C:554:ASN:HA	1:C:557:VAL:CG1	2.45	0.46
1:C:601:MET:HE1	1:C:637:VAL:HG13	1.97	0.46
1:E:541:LEU:O	1:E:545:MET:HG2	2.15	0.46
1:B:648:THR:OG1	1:B:683:PRO:HD3	2.16	0.46
1:D:329:LYS:H	1:D:329:LYS:CD	2.28	0.46
1:D:521:MET:HE3	1:D:600:MET:CG	2.35	0.46
1:D:592:VAL:HB	1:D:626:LEU:HD12	1.98	0.46
1:F:547:VAL:HG12	1:F:549:ASN:H	1.79	0.46
1:A:597:PHE:CD1	1:A:601:MET:HE2	2.52	0.46
1:B:329:LYS:CG	1:B:330:SER:H	2.13	0.46
1:B:354:VAL:HG23	1:B:371:GLN:C	2.36	0.46
1:F:500:LYS:C	1:F:502:LEU:N	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:657:LYS:HG2	1:F:670:GLU:OE1	2.15	0.45
1:F:663:ILE:HG23	1:F:664:LEU:HG	1.97	0.45
1:B:390:ARG:HE	1:C:378:VAL:CG2	2.29	0.45
1:B:631:GLN:O	1:B:633:PRO:HD3	2.16	0.45
1:A:494:LEU:CD2	1:A:591:VAL:HB	2.44	0.45
1:A:672:LEU:HD13	1:A:678:MET:HA	1.98	0.45
1:C:699:ASP:HB3	1:C:703:ARG:HH11	1.81	0.45
1:D:597:PHE:CE1	1:D:601:MET:HE1	2.51	0.45
1:F:329:LYS:HD3	1:F:329:LYS:N	2.31	0.45
1:B:541:LEU:O	1:B:545:MET:HG2	2.16	0.45
1:C:560:ALA:HB2	1:C:567:LEU:HG	1.98	0.45
1:E:317:PRO:C	1:E:319:SER:H	2.20	0.45
1:F:649:ARG:HB3	1:F:663:ILE:HD13	1.98	0.45
1:A:364:VAL:HG22	1:A:418:ARG:HG3	1.98	0.45
1:C:711:ARG:HG3	1:C:711:ARG:NH2	2.28	0.45
1:F:560:ALA:HB2	1:F:567:LEU:HG	1.98	0.45
1:B:317:PRO:C	1:B:319:SER:H	2.19	0.45
1:B:320:LEU:O	1:B:703:ARG:NH2	2.42	0.45
1:C:515:CYS:SG	1:C:720:ILE:HD13	2.57	0.45
1:E:329:LYS:H	1:E:329:LYS:CD	2.30	0.45
1:F:354:VAL:HG22	1:F:355:SER:N	2.32	0.45
1:C:329:LYS:H	1:C:329:LYS:CD	2.30	0.45
1:C:432:TYR:HB2	1:C:453:ILE:HG12	1.99	0.45
1:D:649:ARG:HB3	1:D:663:ILE:CD1	2.46	0.45
1:E:332:SER:OG	1:E:334:GLU:HG3	2.16	0.45
1:F:354:VAL:HG23	1:F:372:PRO:CA	2.46	0.45
1:F:672:LEU:HD21	1:F:679:LEU:HG	1.98	0.45
1:B:347:LEU:HB3	1:B:352:VAL:HG23	1.98	0.45
1:B:545:MET:HE1	1:B:553:PHE:CE1	2.52	0.45
1:C:663:ILE:HG23	1:C:664:LEU:HG	1.98	0.45
1:D:521:MET:HE2	1:D:600:MET:HA	1.99	0.45
1:D:639:THR:O	1:D:643:LYS:HG3	2.17	0.45
1:A:378:VAL:CG1	1:A:401:GLU:HG2	2.46	0.45
1:A:657:LYS:HG2	1:A:670:GLU:OE1	2.17	0.45
1:B:409:VAL:HG12	1:B:410:GLY:N	2.32	0.45
1:C:332:SER:OG	1:C:334:GLU:HG3	2.16	0.45
1:D:465:ALA:CB	1:D:663:ILE:HG13	2.47	0.45
1:E:354:VAL:HG21	1:E:370:ILE:CG1	2.46	0.45
1:E:450:ARG:HG2	1:E:450:ARG:HH21	1.82	0.45
1:E:672:LEU:HD21	1:E:679:LEU:HG	1.99	0.45
1:F:459:MET:N	1:F:460:PRO:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:LYS:O	1:F:476:VAL:HG23	2.17	0.45
1:A:464:VAL:O	1:A:629:ALA:HA	2.16	0.45
1:B:563:ALA:C	1:B:565:THR:H	2.19	0.45
1:E:672:LEU:HD13	1:E:678:MET:HA	1.99	0.45
1:A:354:VAL:HG23	1:A:372:PRO:CA	2.46	0.44
1:B:465:ALA:CB	1:B:663:ILE:HG13	2.47	0.44
1:D:329:LYS:HD3	1:D:329:LYS:N	2.29	0.44
1:E:649:ARG:HB3	1:E:663:ILE:CD1	2.47	0.44
1:B:495:ILE:HG13	1:B:514:LEU:HD12	1.98	0.44
1:B:649:ARG:HB3	1:B:663:ILE:CD1	2.48	0.44
1:E:393:ALA:HB2	1:F:407:THR:CG2	2.48	0.44
1:F:329:LYS:H	1:F:329:LYS:CD	2.29	0.44
1:A:599:ASP:OD1	1:A:632:ARG:NH1	2.51	0.44
1:C:373:ALA:O	1:C:376:VAL:HG13	2.17	0.44
1:C:459:MET:N	1:C:460:PRO:HA	2.33	0.44
1:E:365:ILE:HG12	1:E:366:THR:N	2.32	0.44
1:A:329:LYS:H	1:A:329:LYS:CD	2.31	0.44
1:A:378:VAL:CG2	1:F:390:ARG:HE	2.31	0.44
1:D:354:VAL:HG23	1:D:372:PRO:CA	2.46	0.44
1:D:393:ALA:HB2	1:E:407:THR:CG2	2.48	0.44
1:B:450:ARG:HG2	1:B:450:ARG:HH21	1.82	0.44
1:C:427:LEU:HD22	1:C:432:TYR:CZ	2.52	0.44
1:D:332:SER:OG	1:D:334:GLU:HG3	2.18	0.44
1:E:593:VAL:HG12	1:E:627:ILE:HB	1.99	0.44
1:F:450:ARG:HG2	1:F:450:ARG:HH21	1.83	0.44
1:C:380:ARG:O	1:C:384:LEU:CD2	2.62	0.44
1:C:550:LEU:HD22	1:C:623:GLY:HA3	1.99	0.44
1:C:563:ALA:C	1:C:565:THR:H	2.21	0.44
1:C:631:GLN:O	1:C:633:PRO:HD3	2.18	0.44
1:D:320:LEU:O	1:D:703:ARG:NH2	2.43	0.44
1:F:534:GLU:O	1:F:538:ARG:HG3	2.18	0.44
1:A:322:ASP:HA	1:A:323:PRO:HD3	1.83	0.44
1:A:612:ILE:HD12	1:A:628:LEU:HD11	1.99	0.44
1:C:612:ILE:HD12	1:C:628:LEU:HD11	1.99	0.44
1:F:317:PRO:C	1:F:319:SER:H	2.21	0.44
1:F:432:TYR:HB2	1:F:453:ILE:HG12	1.99	0.44
1:A:563:ALA:O	1:A:565:THR:N	2.51	0.44
1:B:354:VAL:HG23	1:B:372:PRO:CA	2.48	0.44
1:B:597:PHE:CD1	1:B:601:MET:HE2	2.53	0.44
1:C:518:VAL:HG22	1:C:721:LEU:HD21	2.00	0.44
1:A:329:LYS:HD3	1:A:329:LYS:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:TYR:C	1:C:717:ILE:HD12	2.39	0.43
1:F:494:LEU:CD2	1:F:591:VAL:HB	2.48	0.43
1:E:521:MET:HB3	1:E:604:VAL:HG23	2.00	0.43
1:E:578:ASP:O	1:E:579:ASP:C	2.56	0.43
1:E:631:GLN:O	1:E:633:PRO:HD3	2.18	0.43
1:A:332:SER:OG	1:A:334:GLU:HG3	2.18	0.43
1:C:563:ALA:O	1:C:565:THR:N	2.51	0.43
1:E:329:LYS:HD3	1:E:329:LYS:N	2.32	0.43
1:E:409:VAL:HG12	1:E:410:GLY:N	2.33	0.43
1:C:547:VAL:HG12	1:C:549:ASN:H	1.82	0.43
1:B:446:ASP:OD2	1:B:450:ARG:HB2	2.19	0.43
1:D:364:VAL:HB	1:D:692:HIS:CE1	2.54	0.43
1:E:432:TYR:HB2	1:E:453:ILE:HG12	2.01	0.43
1:C:450:ARG:HG2	1:C:450:ARG:HH21	1.82	0.43
1:E:494:LEU:CD2	1:E:591:VAL:HB	2.49	0.43
1:E:547:VAL:HG12	1:E:549:ASN:H	1.81	0.43
1:E:597:PHE:CE1	1:E:601:MET:HE1	2.53	0.43
1:A:427:LEU:HD22	1:A:432:TYR:CE2	2.54	0.43
1:B:678:MET:HG2	1:B:691:VAL:O	2.19	0.43
1:C:347:LEU:HB3	1:C:352:VAL:HG23	2.01	0.43
1:D:341:ARG:N	1:D:341:ARG:HD2	2.34	0.43
1:D:515:CYS:HB3	1:D:720:ILE:HG21	2.01	0.43
1:F:320:LEU:O	1:F:703:ARG:NH2	2.44	0.43
1:E:515:CYS:HB3	1:E:720:ILE:HG21	2.00	0.43
1:A:452:ILE:C	1:A:453:ILE:HD12	2.38	0.43
1:A:597:PHE:CE1	1:A:601:MET:HE1	2.54	0.43
1:B:497:ILE:HD13	1:B:600:MET:CE	2.49	0.43
1:B:515:CYS:HB3	1:B:720:ILE:HG21	2.00	0.43
1:E:560:ALA:HB2	1:E:567:LEU:HG	2.00	0.43
1:E:648:THR:OG1	1:E:683:PRO:HD3	2.19	0.43
1:A:563:ALA:C	1:A:565:THR:H	2.22	0.43
1:A:566:PRO:HB2	1:A:583:GLN:OE1	2.19	0.43
1:A:678:MET:HG2	1:A:691:VAL:O	2.19	0.43
1:B:541:LEU:HD22	1:B:553:PHE:CE1	2.54	0.43
1:C:322:ASP:HA	1:C:323:PRO:HD3	1.84	0.43
1:D:563:ALA:O	1:D:565:THR:N	2.52	0.43
1:D:578:ASP:O	1:D:579:ASP:C	2.57	0.43
1:D:711:ARG:HG3	1:D:711:ARG:NH2	2.31	0.43
1:F:518:VAL:HG22	1:F:721:LEU:HD21	2.01	0.43
1:B:329:LYS:H	1:B:329:LYS:CD	2.32	0.42
1:F:373:ALA:O	1:F:376:VAL:CG1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:563:ALA:O	1:F:565:THR:N	2.52	0.42
1:A:446:ASP:OD2	1:A:450:ARG:HB2	2.20	0.42
1:A:711:ARG:HG3	1:A:711:ARG:NH2	2.31	0.42
1:B:521:MET:HE2	1:B:600:MET:HA	2.01	0.42
1:B:547:VAL:HG12	1:B:549:ASN:H	1.84	0.42
1:C:329:LYS:HD3	1:C:329:LYS:N	2.32	0.42
1:F:361:PRO:HA	1:F:366:THR:HG23	2.00	0.42
1:B:566:PRO:CB	1:B:583:GLN:OE1	2.67	0.42
1:A:618:LYS:HE2	1:F:501:MET:CE	2.49	0.42
1:B:493:ARG:NH2	1:B:513:LEU:O	2.53	0.42
1:C:539:TYR:OH	1:C:621:ALA:HB3	2.19	0.42
1:C:657:LYS:HG2	1:C:670:GLU:OE1	2.20	0.42
1:D:380:ARG:O	1:D:384:LEU:CD2	2.61	0.42
1:D:518:VAL:HG22	1:D:721:LEU:HD21	2.01	0.42
1:E:364:VAL:HG22	1:E:418:ARG:HG3	2.00	0.42
1:E:465:ALA:CB	1:E:663:ILE:HG13	2.49	0.42
1:A:450:ARG:HG2	1:A:450:ARG:HH21	1.84	0.42
1:A:465:ALA:CB	1:A:663:ILE:HG13	2.49	0.42
1:C:597:PHE:CD1	1:C:601:MET:HE2	2.54	0.42
1:E:702:HIS:O	1:E:706:GLU:HG2	2.20	0.42
1:A:495:ILE:HG13	1:A:514:LEU:HD12	2.02	0.42
1:A:649:ARG:HB3	1:A:663:ILE:CD1	2.49	0.42
1:B:464:VAL:O	1:B:629:ALA:HA	2.20	0.42
1:B:566:PRO:HB2	1:B:583:GLN:OE1	2.18	0.42
1:C:317:PRO:C	1:C:319:SER:N	2.73	0.42
1:C:578:ASP:O	1:C:579:ASP:C	2.57	0.42
1:D:720:ILE:HG23	1:D:721:LEU:N	2.35	0.42
1:E:495:ILE:HG13	1:E:514:LEU:HD12	2.02	0.42
1:E:711:ARG:HG3	1:E:711:ARG:NH2	2.30	0.42
1:F:563:ALA:C	1:F:565:THR:H	2.23	0.42
1:A:427:LEU:HD22	1:A:432:TYR:CZ	2.54	0.42
1:A:501:MET:CE	1:B:618:LYS:HE2	2.50	0.42
1:D:365:ILE:HG12	1:D:366:THR:N	2.34	0.42
1:D:427:LEU:HD22	1:D:432:TYR:CE2	2.55	0.42
1:E:390:ARG:HH11	1:F:378:VAL:CG2	2.33	0.42
1:E:563:ALA:C	1:E:565:THR:H	2.23	0.42
1:E:550:LEU:HD22	1:E:623:GLY:HA3	2.02	0.42
1:F:578:ASP:O	1:F:579:ASP:C	2.58	0.42
1:D:354:VAL:HG23	1:D:371:GLN:C	2.40	0.42
1:E:370:ILE:HD12	1:E:411:ILE:HG13	2.01	0.42
1:E:413:ILE:HA	1:E:414:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:HD3	1:B:329:LYS:N	2.34	0.41
1:B:370:ILE:HD12	1:B:411:ILE:HG13	2.02	0.41
1:E:328:GLN:HE21	1:E:328:GLN:HB2	1.66	0.41
1:E:612:ILE:HD12	1:E:628:LEU:HD11	2.01	0.41
1:E:638:ILE:HG22	1:E:643:LYS:CG	2.50	0.41
1:A:560:ALA:HB2	1:A:567:LEU:HG	2.00	0.41
1:B:638:ILE:HG22	1:B:643:LYS:CG	2.51	0.41
1:C:390:ARG:HH11	1:D:378:VAL:CG2	2.33	0.41
1:A:459:MET:N	1:A:460:PRO:HA	2.36	0.41
1:B:462:LEU:HD11	1:B:650:ILE:HD12	2.02	0.41
1:A:515:CYS:SG	1:A:720:ILE:HD13	2.60	0.41
1:A:566:PRO:CB	1:A:583:GLN:OE1	2.69	0.41
1:B:672:LEU:HD21	1:B:679:LEU:HG	2.02	0.41
1:D:390:ARG:NE	1:E:378:VAL:HG22	2.36	0.41
1:D:560:ALA:HB2	1:D:567:LEU:HG	2.01	0.41
1:A:317:PRO:C	1:A:319:SER:N	2.74	0.41
1:A:407:THR:CG2	1:F:393:ALA:HB2	2.51	0.41
1:C:373:ALA:O	1:C:376:VAL:CG1	2.68	0.41
1:E:580:GLU:HA	1:E:581:PRO:HD3	1.93	0.41
1:C:497:ILE:HD13	1:C:600:MET:CE	2.47	0.41
1:E:354:VAL:HG22	1:E:355:SER:N	2.35	0.41
1:A:315:LEU:N	1:A:711:ARG:HE	2.19	0.41
1:A:578:ASP:O	1:A:579:ASP:C	2.58	0.41
1:B:317:PRO:C	1:B:319:SER:N	2.74	0.41
1:B:354:VAL:HG21	1:B:370:ILE:HG13	2.03	0.41
1:B:459:MET:N	1:B:460:PRO:HA	2.35	0.41
1:B:716:TYR:C	1:B:717:ILE:HD12	2.41	0.41
1:E:563:ALA:O	1:E:565:THR:N	2.53	0.41
1:E:631:GLN:C	1:E:633:PRO:HD3	2.40	0.41
1:A:354:VAL:HG21	1:A:370:ILE:HG13	2.03	0.41
1:B:463:LEU:HG	1:B:646:ILE:HG21	2.02	0.41
1:C:580:GLU:HA	1:C:581:PRO:HD3	1.95	0.41
1:E:320:LEU:O	1:E:703:ARG:NH2	2.47	0.41
1:F:341:ARG:N	1:F:341:ARG:HD2	2.35	0.41
1:B:373:ALA:O	1:B:376:VAL:CG1	2.68	0.41
1:B:578:ASP:O	1:B:579:ASP:C	2.58	0.41
1:C:512:HIS:HE1	1:C:708:TRP:CD2	2.39	0.41
1:C:549:ASN:OD1	1:C:551:ALA:HB3	2.21	0.41
1:E:341:ARG:N	1:E:341:ARG:HD2	2.35	0.41
1:E:347:LEU:HD23	1:E:347:LEU:HA	1.92	0.41
1:F:665:ASP:O	1:F:666:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG22	1:A:355:SER:H	1.86	0.41
1:A:457:ALA:HA	1:A:625:HIS:CD2	2.56	0.41
1:B:677:ASP:OD1	1:B:690:ARG:NH1	2.43	0.41
1:C:672:LEU:HD21	1:C:679:LEU:HG	2.02	0.41
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.95	0.41
1:E:501:MET:CE	1:F:618:LYS:HE2	2.51	0.41
1:E:641:LEU:HD23	1:E:641:LEU:HA	1.86	0.41
1:A:521:MET:HE3	1:A:600:MET:CG	2.46	0.40
1:A:716:TYR:C	1:A:717:ILE:HD12	2.41	0.40
1:C:413:ILE:HA	1:C:414:PRO:HD3	1.91	0.40
1:D:354:VAL:HG21	1:D:370:ILE:HG13	2.02	0.40
1:E:427:LEU:HD22	1:E:432:TYR:CE2	2.56	0.40
1:F:593:VAL:HG12	1:F:627:ILE:HB	2.03	0.40
1:A:453:ILE:HD12	1:A:453:ILE:N	2.36	0.40
1:B:472:LYS:HE2	1:B:472:LYS:HB3	1.99	0.40
1:B:539:TYR:OH	1:B:621:ALA:HB3	2.21	0.40
1:C:648:THR:OG1	1:C:683:PRO:HD3	2.21	0.40
1:D:450:ARG:HH21	1:D:450:ARG:HG2	1.86	0.40
1:D:563:ALA:C	1:D:565:THR:H	2.25	0.40
1:E:518:VAL:HG22	1:E:721:LEU:HD21	2.03	0.40
1:F:322:ASP:HA	1:F:323:PRO:HD3	1.79	0.40
1:A:440:PRO:O	1:A:482:SER:HB3	2.22	0.40
1:B:560:ALA:HB2	1:B:567:LEU:HG	2.03	0.40
1:C:488:THR:HG23	1:C:491:GLU:OE2	2.20	0.40
1:D:612:ILE:HD12	1:D:628:LEU:HD11	2.04	0.40
1:E:452:ILE:C	1:E:453:ILE:HD12	2.41	0.40
1:E:457:ALA:HA	1:E:625:HIS:NE2	2.36	0.40
1:E:566:PRO:HB2	1:E:583:GLN:OE1	2.22	0.40
1:E:566:PRO:CB	1:E:583:GLN:OE1	2.70	0.40
1:E:657:LYS:HG2	1:E:670:GLU:OE1	2.21	0.40
1:F:639:THR:O	1:F:643:LYS:HG3	2.22	0.40
1:D:427:LEU:HD22	1:D:432:TYR:CZ	2.57	0.40
1:F:383:ASN:HD22	1:F:383:ASN:HA	1.63	0.40
1:A:320:LEU:O	1:A:703:ARG:NH2	2.44	0.40
1:E:418:ARG:NH2	1:E:675:HIS:HB2	2.36	0.40
1:F:354:VAL:HG23	1:F:371:GLN:C	2.41	0.40
1:F:593:VAL:O	1:F:593:VAL:HG23	2.20	0.40
1:F:711:ARG:HH21	1:F:711:ARG:CG	2.29	0.40

All (1) 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:B:338:ALA:O	1:D:434:GLU:OE2[4_554]	2.00	0.20

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	A	406/491 (83%)	373 (92%)	27 (7%)	6 (2%)	10	34
1	B	406/491 (83%)	376 (93%)	25 (6%)	5 (1%)	13	40
1	C	406/491 (83%)	377 (93%)	24 (6%)	5 (1%)	13	40
1	D	406/491 (83%)	380 (94%)	21 (5%)	5 (1%)	13	40
1	E	406/491 (83%)	375 (92%)	26 (6%)	5 (1%)	13	40
1	F	406/491 (83%)	375 (92%)	26 (6%)	5 (1%)	13	40
All	All	2436/2946 (83%)	2256 (93%)	149 (6%)	31 (1%)	12	37

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	MET
1	B	501	MET
1	C	501	MET
1	D	501	MET
1	E	501	MET
1	F	501	MET
1	A	330	SER
1	A	564	GLY
1	A	718	GLU
1	B	330	SER
1	B	564	GLY
1	B	718	GLU
1	C	330	SER
1	C	564	GLY
1	C	718	GLU

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Mol	Chain	Res	Type
1	D	330	SER
1	D	564	GLY
1	D	718	GLU
1	E	330	SER
1	E	718	GLU
1	F	330	SER
1	F	564	GLY
1	F	718	GLU
1	E	564	GLY
1	A	620	ARG
1	E	326	VAL
1	F	326	VAL
1	C	326	VAL
1	A	326	VAL
1	B	326	VAL
1	D	326	VAL

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	A	346/419 (83%)	328 (95%)	18 (5%)	23	55
1	B	346/419 (83%)	325 (94%)	21 (6%)	18	48
1	C	346/419 (83%)	326 (94%)	20 (6%)	20	50
1	D	346/419 (83%)	326 (94%)	20 (6%)	20	50
1	E	346/419 (83%)	326 (94%)	20 (6%)	20	50
1	F	346/419 (83%)	326 (94%)	20 (6%)	20	50
All	All	2076/2514 (83%)	1957 (94%)	119 (6%)	20	51

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	LYS
1	A	337	GLU

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	343	LEU
1	A	365	ILE
1	A	370	ILE
1	A	376	VAL
1	A	384	LEU
1	A	456	LEU
1	A	501	MET
1	A	502	LEU
1	A	506	ILE
1	A	519	THR
1	A	541	LEU
1	A	626	LEU
1	A	650	ILE
1	A	663	ILE
1	A	696	VAL
1	B	329	LYS
1	B	337	GLU
1	B	342	LEU
1	B	343	LEU
1	B	365	ILE
1	B	370	ILE
1	B	376	VAL
1	B	384	LEU
1	B	397	VAL
1	B	456	LEU
1	B	488	THR
1	B	501	MET
1	B	502	LEU
1	B	506	ILE
1	B	519	THR
1	B	521	MET
1	B	541	LEU
1	B	626	LEU
1	B	650	ILE
1	B	663	ILE
1	B	696	VAL
1	C	329	LYS
1	C	337	GLU
1	C	342	LEU
1	C	343	LEU
1	C	365	ILE

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Mol	Chain	Res	Type
1	C	370	ILE
1	C	376	VAL
1	C	384	LEU
1	C	397	VAL
1	C	456	LEU
1	C	488	THR
1	C	501	MET
1	C	502	LEU
1	C	506	ILE
1	C	519	THR
1	C	541	LEU
1	C	626	LEU
1	C	650	ILE
1	C	663	ILE
1	C	696	VAL
1	D	329	LYS
1	D	337	GLU
1	D	342	LEU
1	D	343	LEU
1	D	365	ILE
1	D	370	ILE
1	D	376	VAL
1	D	384	LEU
1	D	456	LEU
1	D	488	THR
1	D	501	MET
1	D	502	LEU
1	D	506	ILE
1	D	519	THR
1	D	521	MET
1	D	541	LEU
1	D	626	LEU
1	D	650	ILE
1	D	663	ILE
1	D	696	VAL
1	E	329	LYS
1	E	337	GLU
1	E	342	LEU
1	E	343	LEU
1	E	365	ILE
1	E	370	ILE
1	E	376	VAL

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Mol	Chain	Res	Type
1	E	384	LEU
1	E	456	LEU
1	E	488	THR
1	E	501	MET
1	E	502	LEU
1	E	506	ILE
1	E	519	THR
1	E	521	MET
1	E	541	LEU
1	E	626	LEU
1	E	650	ILE
1	E	663	ILE
1	E	696	VAL
1	F	329	LYS
1	F	337	GLU
1	F	342	LEU
1	F	343	LEU
1	F	365	ILE
1	F	370	ILE
1	F	376	VAL
1	F	384	LEU
1	F	456	LEU
1	F	488	THR
1	F	501	MET
1	F	502	LEU
1	F	506	ILE
1	F	519	THR
1	F	521	MET
1	F	541	LEU
1	F	626	LEU
1	F	650	ILE
1	F	663	ILE
1	F	696	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	383	ASN
1	A	415	ASN
1	A	554	ASN
1	A	631	GLN

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Mol	Chain	Res	Type
1	A	666	GLN
1	B	328	GLN
1	B	383	ASN
1	B	415	ASN
1	B	554	ASN
1	B	631	GLN
1	C	328	GLN
1	C	383	ASN
1	C	415	ASN
1	C	554	ASN
1	C	625	HIS
1	C	631	GLN
1	D	328	GLN
1	D	383	ASN
1	D	415	ASN
1	D	554	ASN
1	D	631	GLN
1	D	666	GLN
1	E	328	GLN
1	E	383	ASN
1	E	415	ASN
1	E	554	ASN
1	E	631	GLN
1	E	666	GLN
1	F	328	GLN
1	F	383	ASN
1	F	415	ASN
1	F	554	ASN
1	F	631	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
2	ADP	E	1723	-	24,29,29	1.03	1 (4%)	29,45,45	1.58	5 (17%)
2	ADP	D	1723	-	24,29,29	0.98	1 (4%)	29,45,45	1.58	5 (17%)
2	ADP	F	1723	-	24,29,29	1.07	1 (4%)	29,45,45	1.59	5 (17%)
2	ADP	C	1723	-	24,29,29	1.00	1 (4%)	29,45,45	1.51	5 (17%)
2	ADP	B	1723	-	24,29,29	0.98	1 (4%)	29,45,45	1.58	5 (17%)
2	ADP	A	1723	-	24,29,29	1.02	1 (4%)	29,45,45	1.57	5 (17%)

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	E	1723	-	-	2/12/32/32	0/3/3/3
2	ADP	D	1723	-	-	3/12/32/32	0/3/3/3
2	ADP	F	1723	-	-	2/12/32/32	0/3/3/3
2	ADP	C	1723	-	-	2/12/32/32	0/3/3/3
2	ADP	B	1723	-	-	3/12/32/32	0/3/3/3
2	ADP	A	1723	-	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1723	ADP	C2-N1	3.58	1.40	1.33
2	A	1723	ADP	C2-N1	3.48	1.40	1.33
2	E	1723	ADP	C2-N1	3.47	1.40	1.33
2	C	1723	ADP	C2-N1	3.37	1.40	1.33
2	D	1723	ADP	C2-N1	3.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1723	ADP	C2-N1	3.25	1.39	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1723	ADP	C5-C6-N6	3.81	126.14	120.35
2	E	1723	ADP	C5-C6-N6	3.71	126.00	120.35
2	A	1723	ADP	C5-C6-N6	3.63	125.87	120.35
2	D	1723	ADP	C5-C6-N6	3.59	125.81	120.35
2	F	1723	ADP	C5-C6-N6	3.58	125.79	120.35
2	C	1723	ADP	C5-C6-N6	3.56	125.77	120.35
2	D	1723	ADP	N3-C2-N1	-3.51	123.19	128.68
2	A	1723	ADP	N3-C2-N1	-3.46	123.26	128.68
2	E	1723	ADP	N3-C2-N1	-3.43	123.31	128.68
2	C	1723	ADP	N3-C2-N1	-3.37	123.41	128.68
2	B	1723	ADP	N3-C2-N1	-3.30	123.51	128.68
2	F	1723	ADP	N3-C2-N1	-3.27	123.56	128.68
2	A	1723	ADP	C3'-C2'-C1'	3.23	105.84	100.98
2	B	1723	ADP	C3'-C2'-C1'	3.16	105.73	100.98
2	F	1723	ADP	C3'-C2'-C1'	3.14	105.71	100.98
2	D	1723	ADP	C3'-C2'-C1'	3.04	105.56	100.98
2	E	1723	ADP	C3'-C2'-C1'	3.01	105.50	100.98
2	F	1723	ADP	C5-C6-N1	-2.94	113.70	120.35
2	D	1723	ADP	C5-C6-N1	-2.91	113.76	120.35
2	D	1723	ADP	C2-N1-C6	2.88	123.68	118.75
2	E	1723	ADP	C5-C6-N1	-2.86	113.86	120.35
2	C	1723	ADP	C3'-C2'-C1'	2.81	105.21	100.98
2	A	1723	ADP	C5-C6-N1	-2.80	114.00	120.35
2	F	1723	ADP	C2-N1-C6	2.80	123.54	118.75
2	B	1723	ADP	C2-N1-C6	2.78	123.51	118.75
2	B	1723	ADP	C5-C6-N1	-2.76	114.11	120.35
2	E	1723	ADP	C2-N1-C6	2.75	123.47	118.75
2	C	1723	ADP	C2-N1-C6	2.74	123.45	118.75
2	C	1723	ADP	C5-C6-N1	-2.71	114.20	120.35
2	A	1723	ADP	C2-N1-C6	2.66	123.30	118.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1723	ADP	PA-O3A-PB-O3B
2	B	1723	ADP	PA-O3A-PB-O3B

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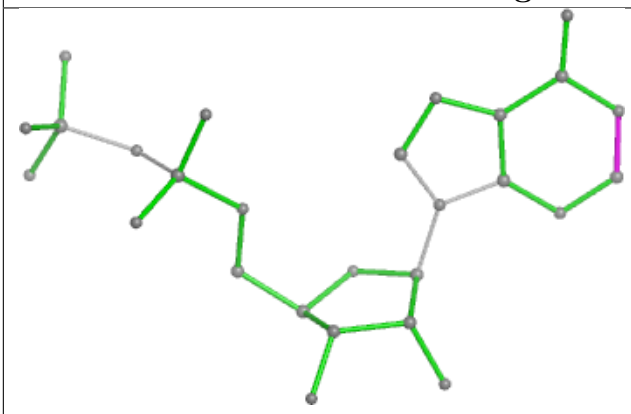
Mol	Chain	Res	Type	Atoms
2	C	1723	ADP	PA-O3A-PB-O3B
2	D	1723	ADP	PA-O3A-PB-O3B
2	E	1723	ADP	PA-O3A-PB-O3B
2	F	1723	ADP	PA-O3A-PB-O3B
2	A	1723	ADP	PA-O3A-PB-O2B
2	B	1723	ADP	PA-O3A-PB-O2B
2	C	1723	ADP	PA-O3A-PB-O2B
2	D	1723	ADP	PA-O3A-PB-O2B
2	E	1723	ADP	PA-O3A-PB-O2B
2	F	1723	ADP	PA-O3A-PB-O2B
2	B	1723	ADP	PA-O3A-PB-O1B
2	D	1723	ADP	PA-O3A-PB-O1B

There are no ring outliers.

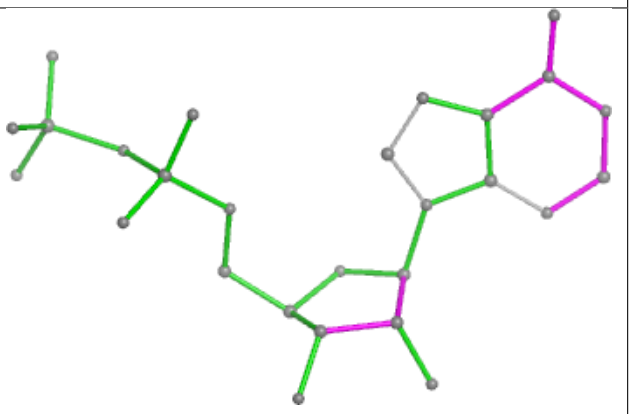
No monomer is involved in short contacts.

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.

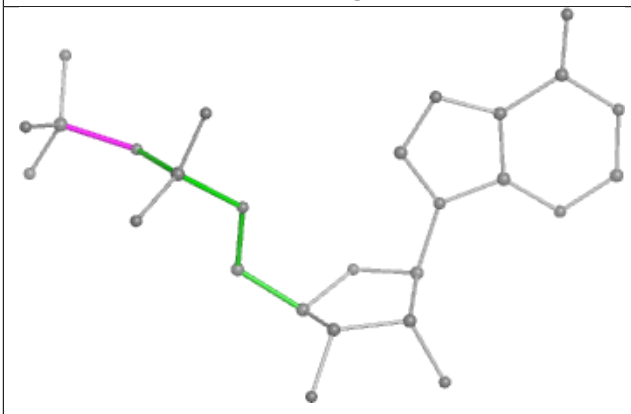
Ligand ADP E 1723



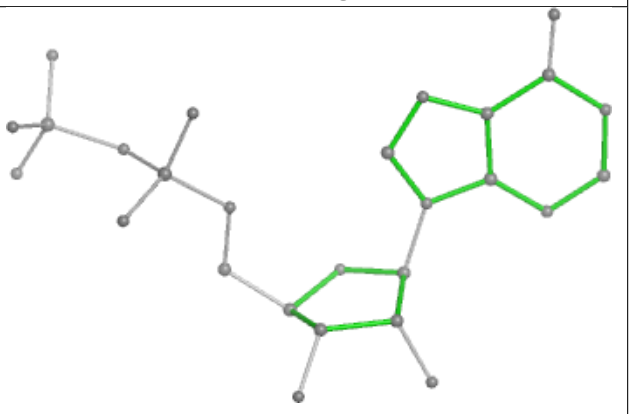
Bond lengths



Bond angles

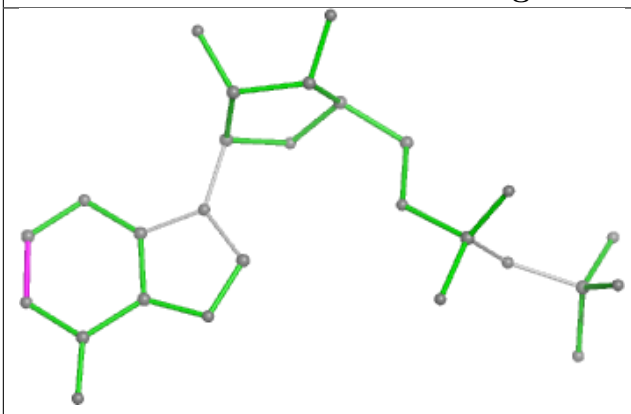


Torsions

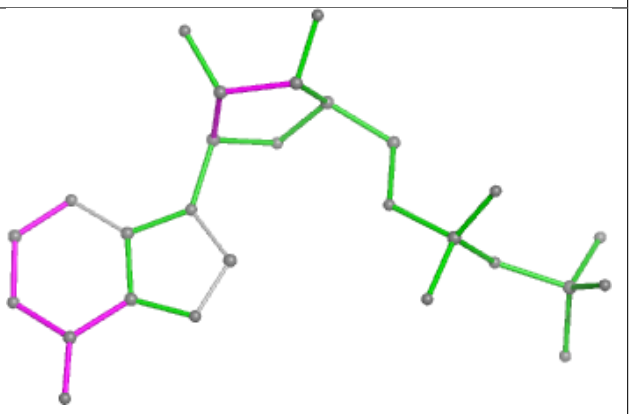


Rings

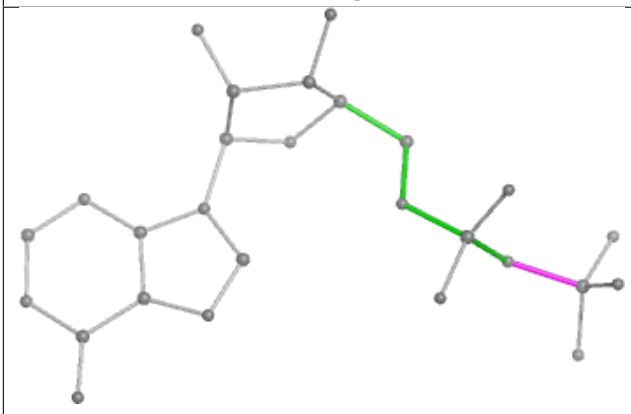
Ligand ADP D 1723



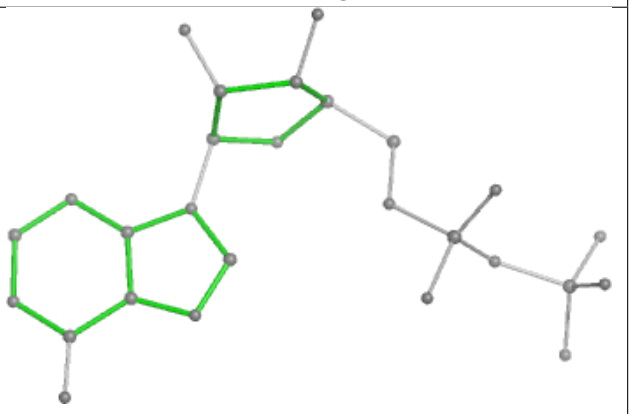
Bond lengths



Bond angles

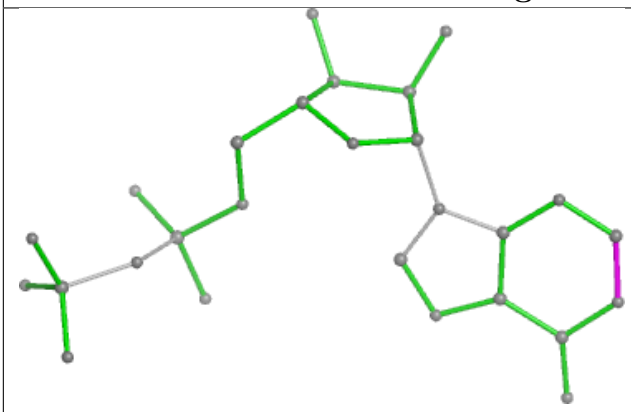


Torsions

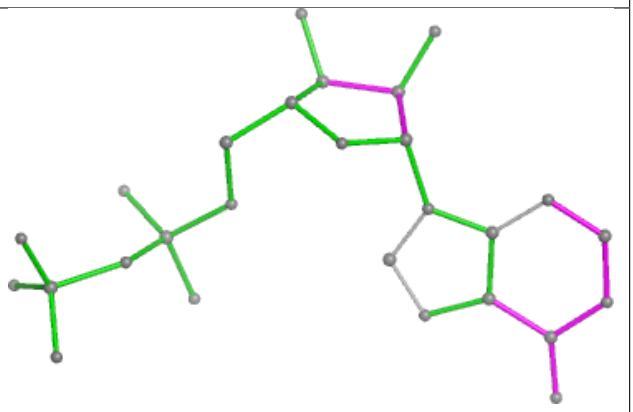


Rings

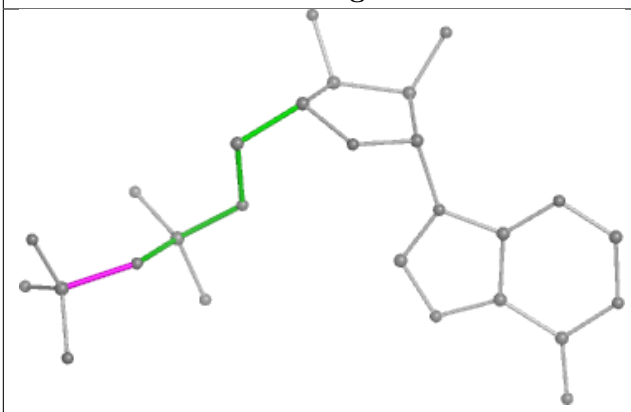
Ligand ADP F 1723



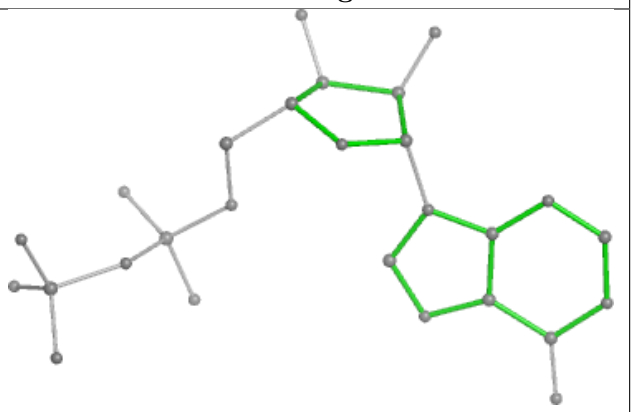
Bond lengths



Bond angles

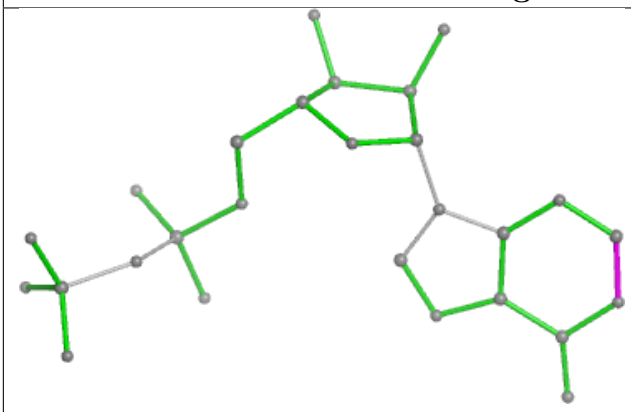


Torsions

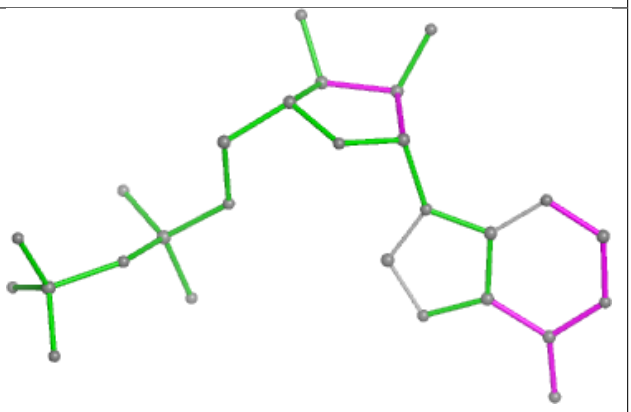


Rings

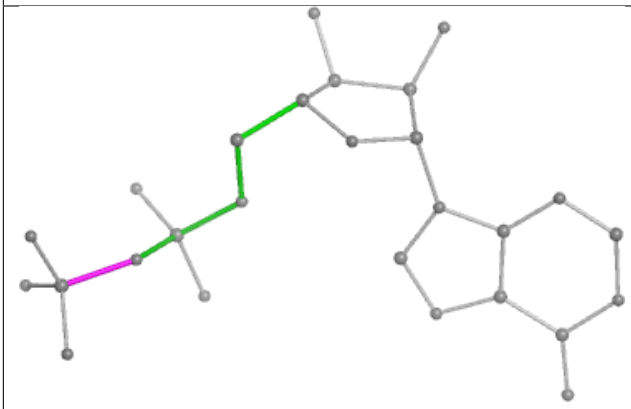
Ligand ADP C 1723



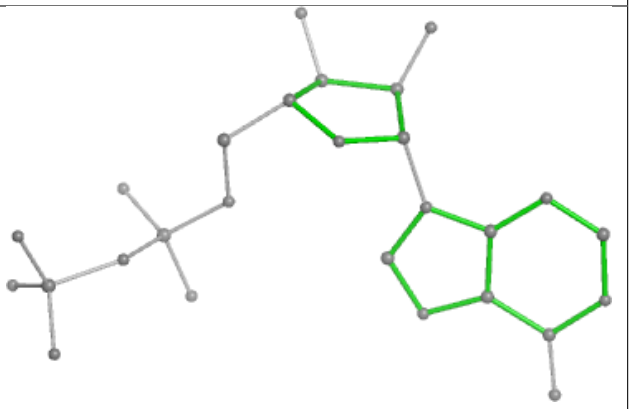
Bond lengths



Bond angles

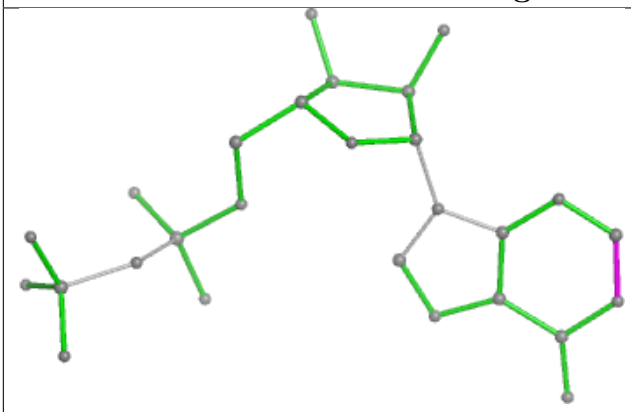


Torsions

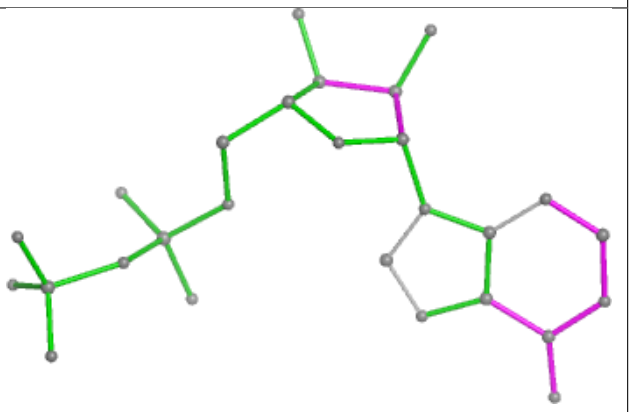


Rings

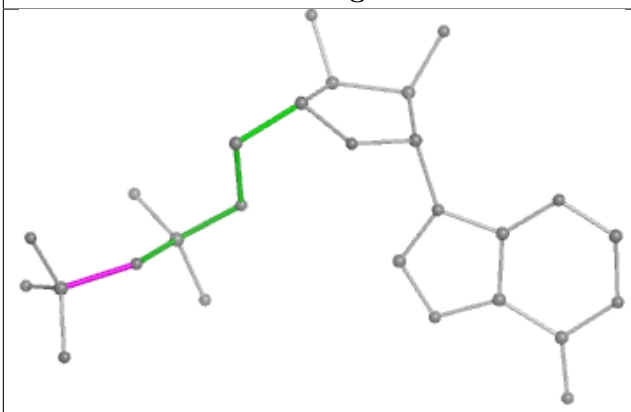
Ligand ADP B 1723



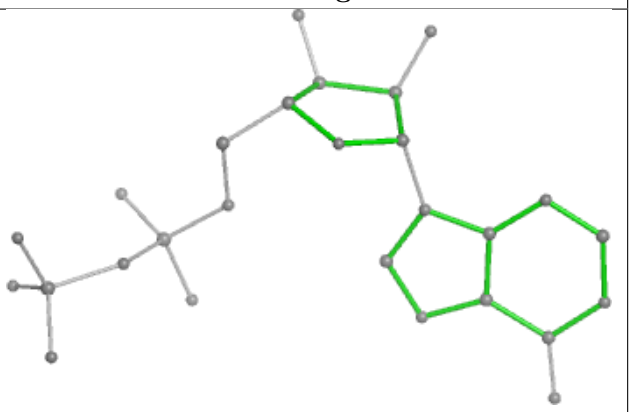
Bond lengths



Bond angles

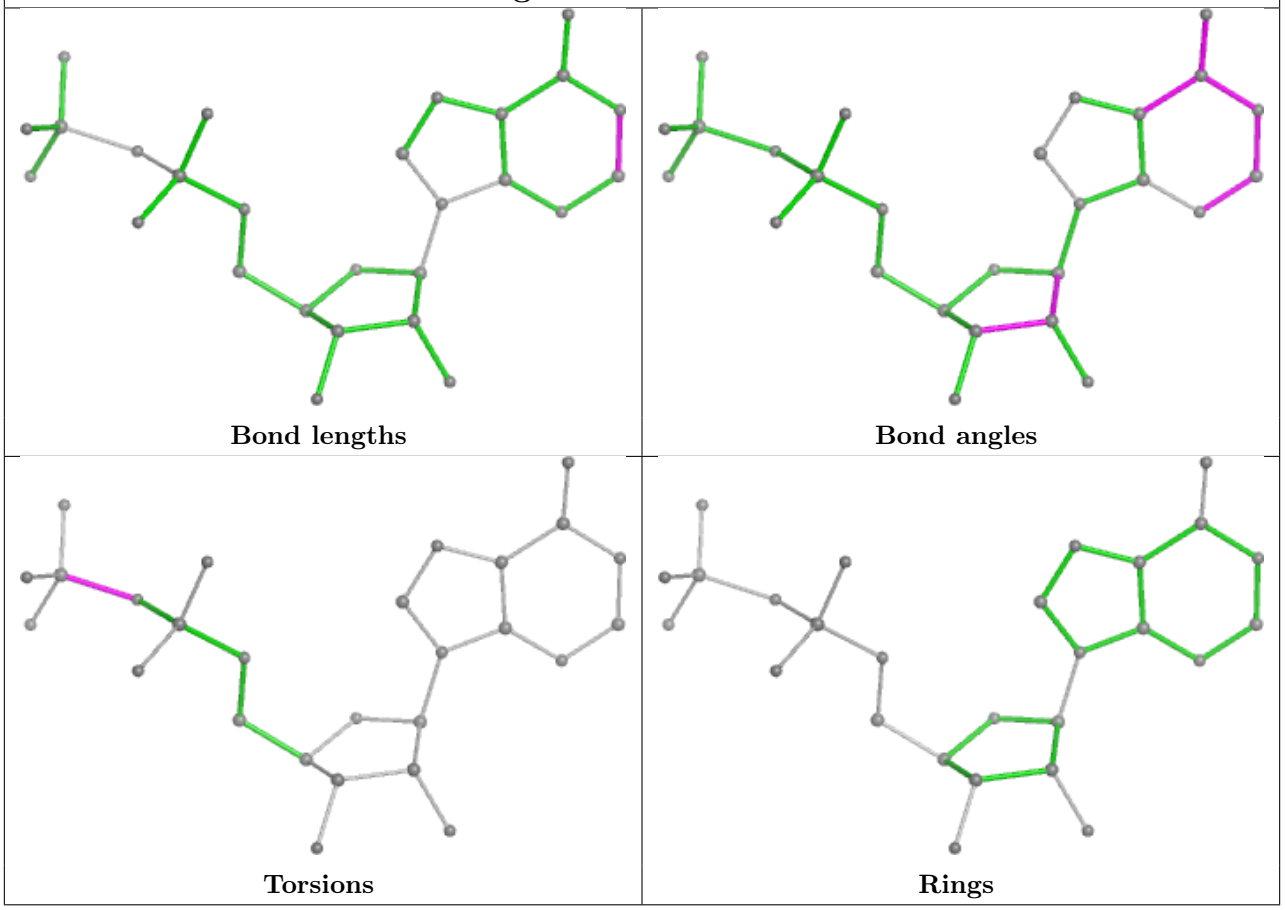


Torsions



Rings

Ligand ADP A 1723



5.7 Other polymers (i)

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	A	408/491 (83%)	0.40	23 (5%)	24	20	48, 72, 110, 136	0
1	B	408/491 (83%)	0.16	8 (1%)	65	63	37, 57, 97, 127	0
1	C	408/491 (83%)	0.11	8 (1%)	65	63	31, 51, 93, 140	0
1	D	408/491 (83%)	0.09	4 (0%)	82	82	32, 49, 85, 131	0
1	E	408/491 (83%)	0.27	16 (3%)	39	35	42, 65, 102, 142	0
1	F	408/491 (83%)	0.33	21 (5%)	28	24	47, 73, 108, 140	0
All	All	2448/2946 (83%)	0.23	80 (3%)	46	41	31, 62, 103, 142	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	328	GLN	8.4
1	E	329	LYS	6.1
1	C	328	GLN	4.3
1	F	326	VAL	4.2
1	C	329	LYS	4.0
1	A	326	VAL	3.9
1	C	326	VAL	3.8
1	A	336	LEU	3.6
1	A	328	GLN	3.6
1	E	567	LEU	3.5
1	F	328	GLN	3.5
1	B	328	GLN	3.5
1	B	326	VAL	3.3
1	F	565	THR	3.3
1	E	326	VAL	3.3
1	B	331	TYR	3.3
1	F	316	PRO	3.3
1	A	581	PRO	3.3
1	F	584	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	329	LYS	3.2
1	E	331	TYR	3.2
1	C	327	LYS	3.2
1	A	318	LEU	3.2
1	A	584	LEU	3.1
1	F	427	LEU	3.1
1	A	562	GLU	3.0
1	A	325	GLU	3.0
1	F	419	GLN	2.9
1	C	330	SER	2.9
1	A	567	LEU	2.8
1	B	565	THR	2.8
1	E	352	VAL	2.7
1	A	580	GLU	2.7
1	A	565	THR	2.7
1	A	572	PHE	2.7
1	F	330	SER	2.7
1	A	566	PRO	2.7
1	A	327	LYS	2.7
1	D	328	GLN	2.7
1	E	560	ALA	2.7
1	A	381	ILE	2.6
1	A	719	ASP	2.6
1	C	584	LEU	2.6
1	F	566	PRO	2.6
1	B	562	GLU	2.6
1	D	584	LEU	2.6
1	E	357	ASP	2.6
1	E	710	LEU	2.5
1	F	580	GLU	2.4
1	A	563	ALA	2.4
1	E	343	LEU	2.4
1	B	707	ALA	2.4
1	C	325	GLU	2.4
1	D	352	VAL	2.4
1	C	565	THR	2.4
1	F	583	GLN	2.3
1	F	702	HIS	2.3
1	F	557	VAL	2.3
1	E	368	PHE	2.3
1	A	560	ALA	2.3
1	E	573	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	LYS	2.3
1	B	567	LEU	2.2
1	F	710	LEU	2.2
1	E	330	SER	2.2
1	F	317	PRO	2.2
1	F	323	PRO	2.2
1	A	331	TYR	2.2
1	A	330	SER	2.1
1	F	325	GLU	2.1
1	F	336	LEU	2.1
1	A	370	ILE	2.1
1	E	718	GLU	2.1
1	D	560	ALA	2.1
1	E	339	MET	2.1
1	B	578	ASP	2.0
1	F	562	GLU	2.0
1	E	565	THR	2.0
1	F	582	PRO	2.0
1	A	582	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
2	ADP	A	1723	27/27	0.85	0.23	93,96,103,104	0
2	ADP	F	1723	27/27	0.86	0.22	87,100,105,105	0
2	ADP	E	1723	27/27	0.90	0.22	87,90,91,91	0
2	ADP	D	1723	27/27	0.92	0.22	62,72,76,81	0

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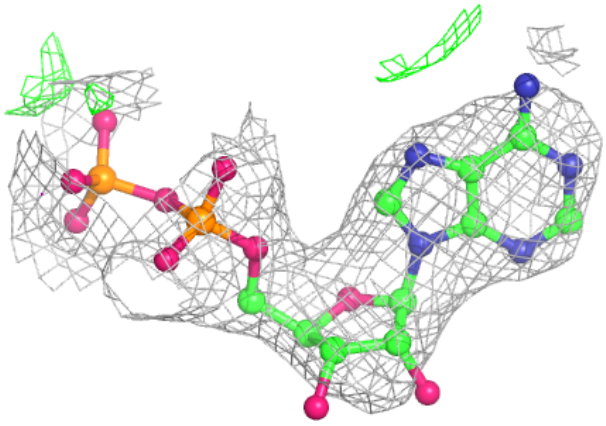
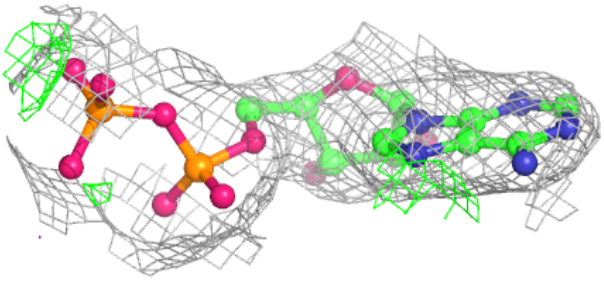
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	1723	27/27	0.92	0.21	75,82,85,88	0
2	ADP	C	1723	27/27	0.92	0.22	67,82,87,88	0

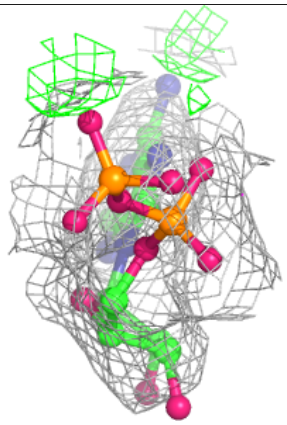
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1723:

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

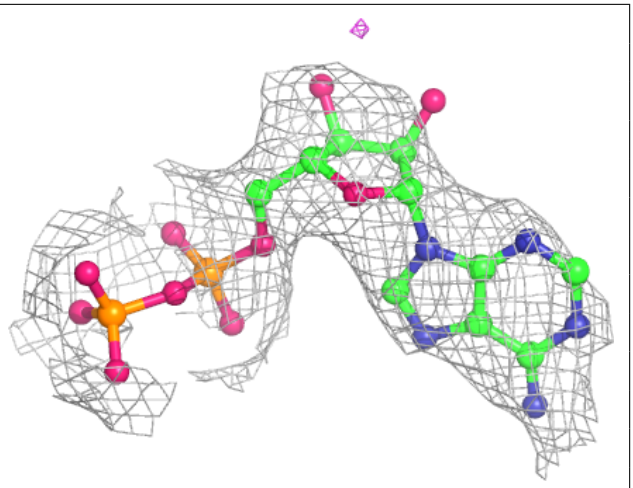


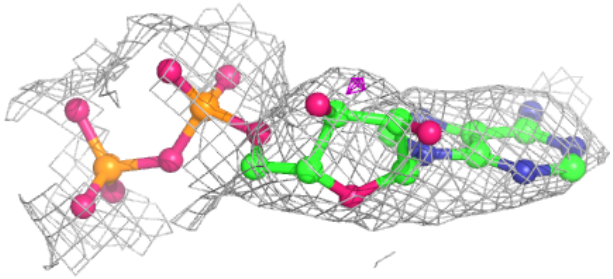


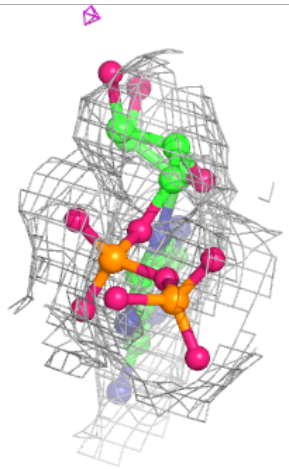


Electron density around ADP F 1723:

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

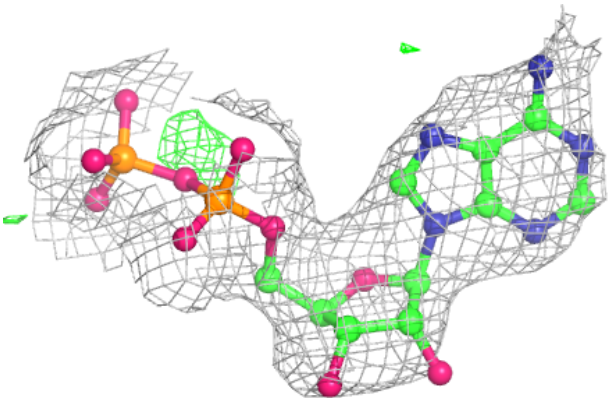


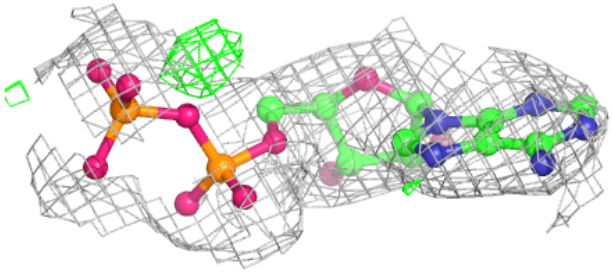


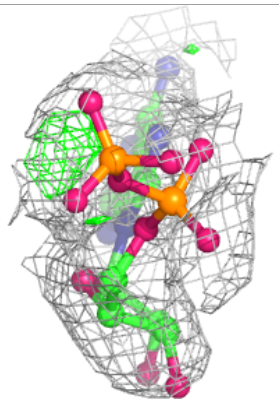


Electron density around ADP E 1723:

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

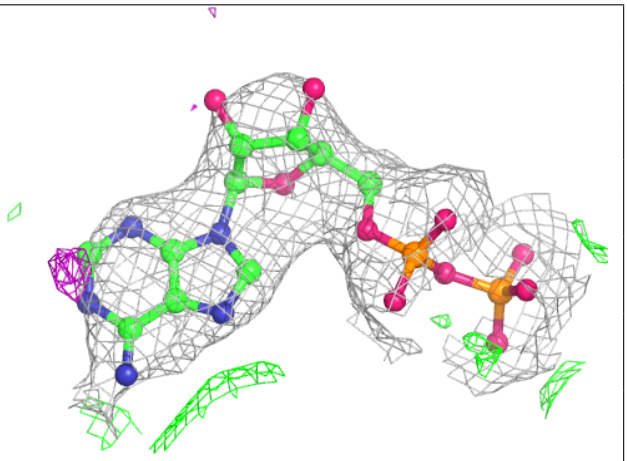


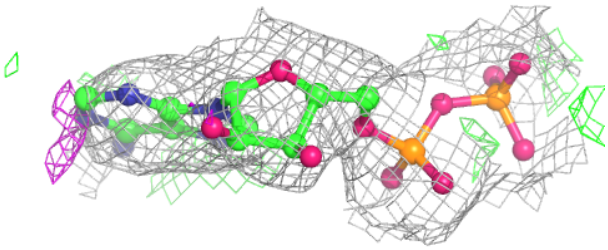


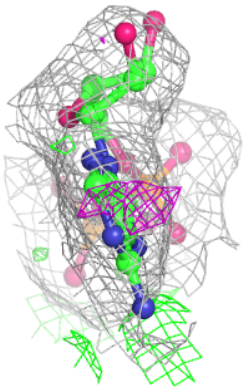


Electron density around ADP D 1723:

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

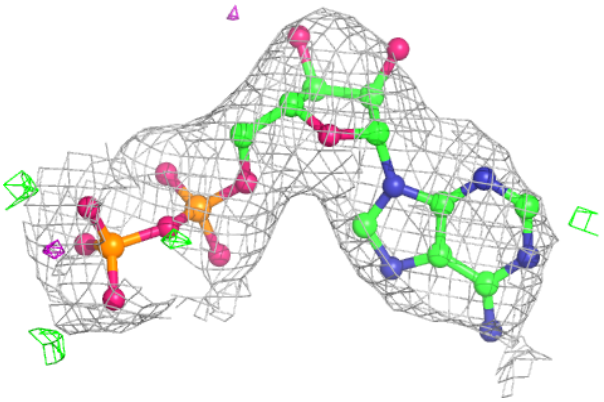


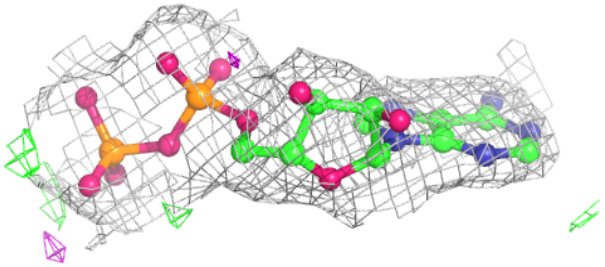


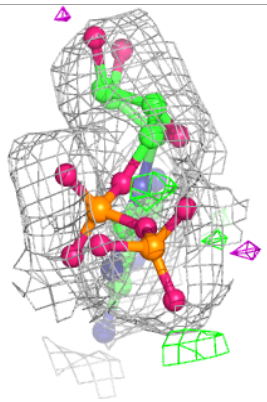


Electron density around ADP B 1723:

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

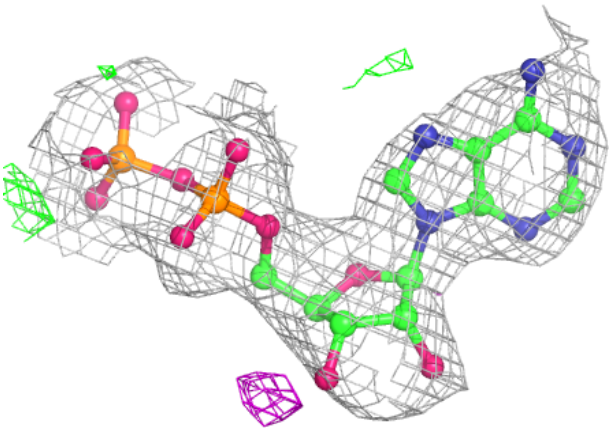


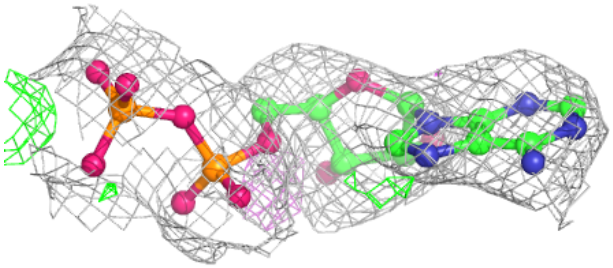


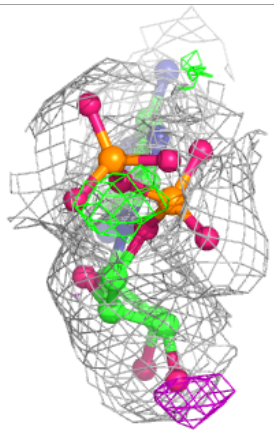


Electron density around ADP C 1723:

$2mF_o$-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.