Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 12:49 PM EDT

PDB ID	:	3JV2
Title	:	Crystal Structure of B. subtilis SecA with bound peptide
Authors	:	Zimmer, J.
Deposited on	:	2009-09-15
Resolution	:	2.50 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:

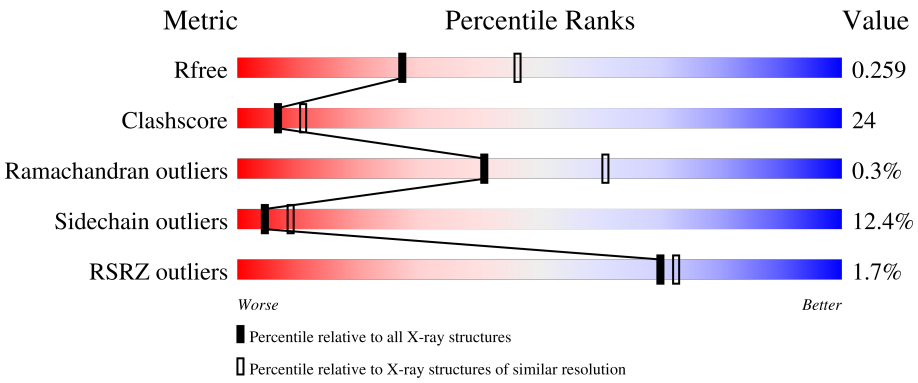
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	783	2% 66% 25% 5% • •
1	B	783	% 69% 21% 6% • •
2	C	3	67% 33%
2	D	3	67% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12364 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 Protein translocase subunit SecA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	758	6043	3782	1053	1175	33	0	0	0
1	B	762	6083	3804	1063	1183	33	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A085C4M4
A	-1	PRO	-	expression tag	UNP A0A085C4M4
A	0	HIS	-	expression tag	UNP A0A085C4M4
B	-2	GLY	-	expression tag	UNP A0A085C4M4
B	-1	PRO	-	expression tag	UNP A0A085C4M4
B	0	HIS	-	expression tag	UNP A0A085C4M4

- Molecule 2 is a protein called peptide.

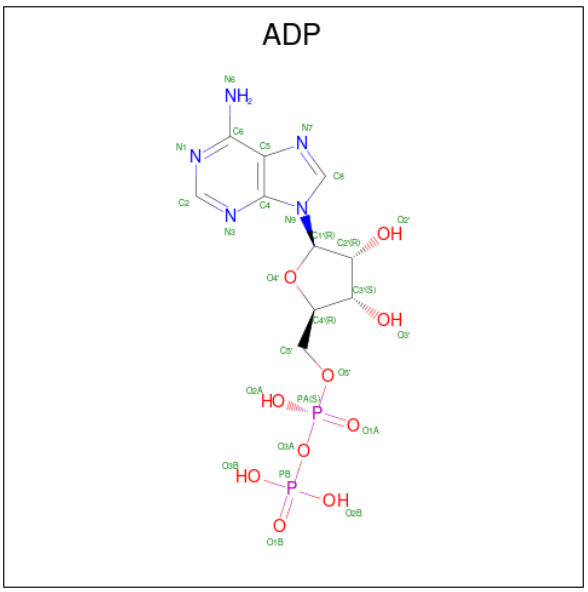
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	15	9	3	3	0	0	0
2	D	3	15	9	3	3	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

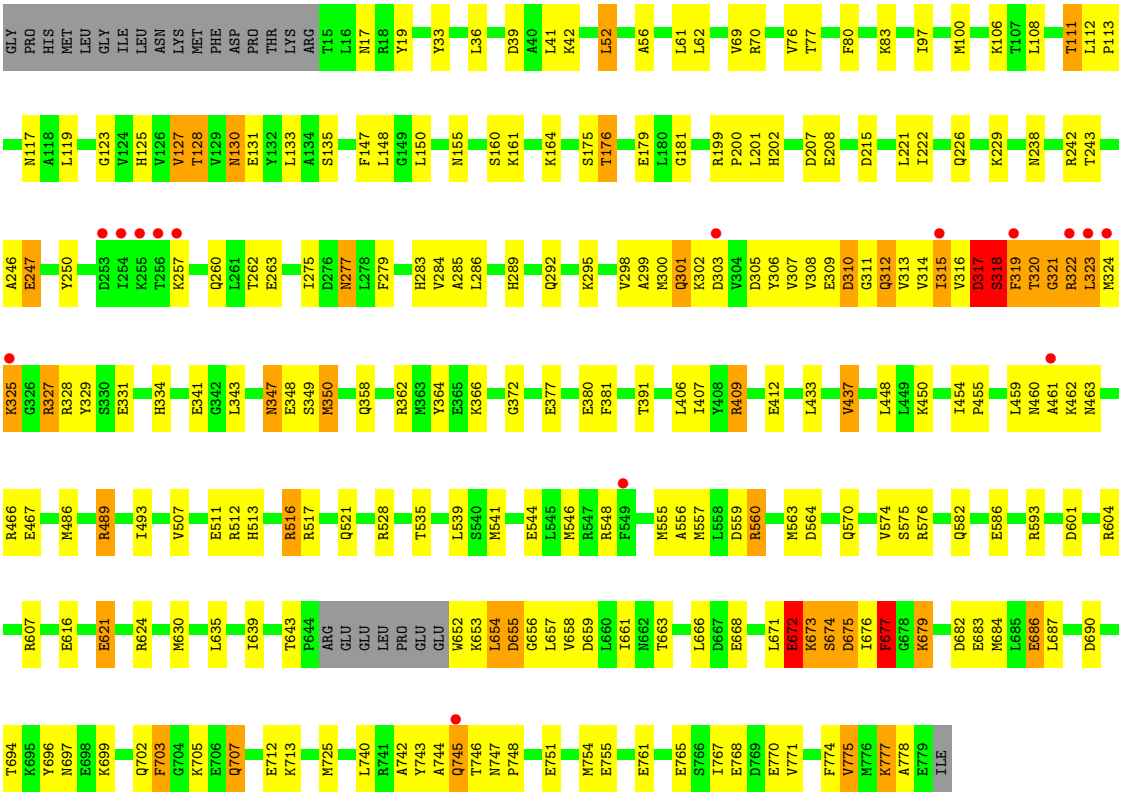
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	71	Total	O	0	0
			71	71		

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.

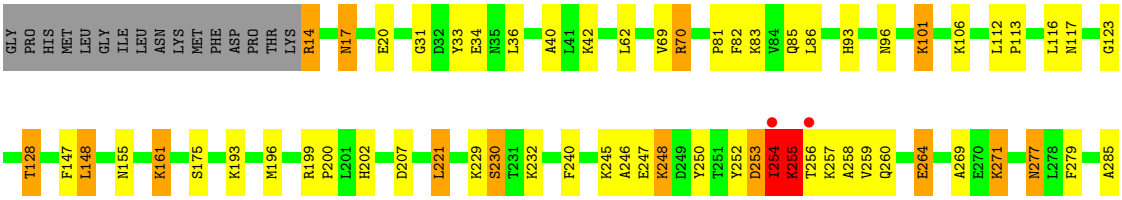
• Molecule 1: Protein translocase subunit SecA

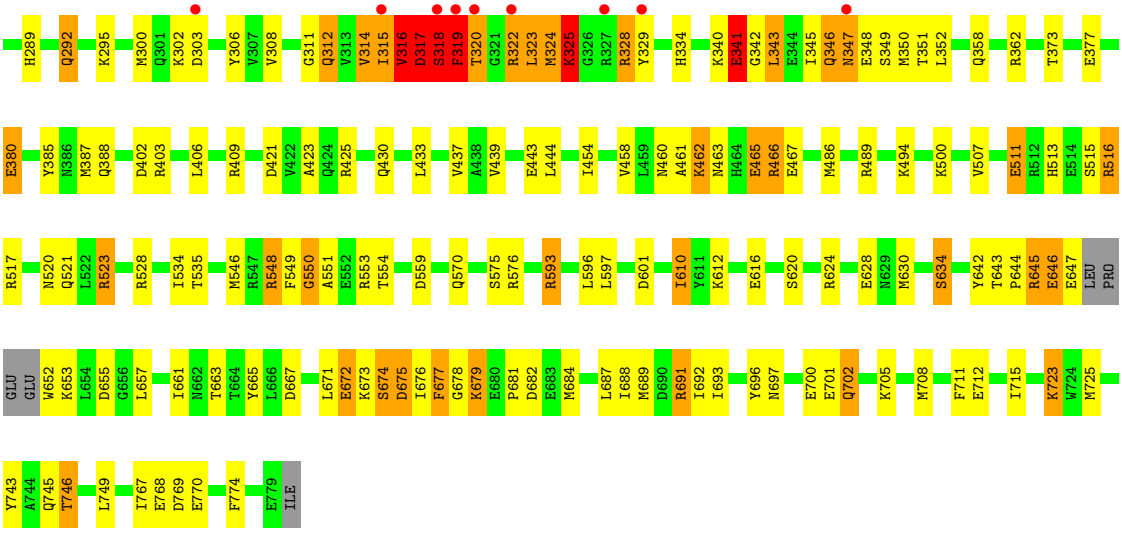
Chain A:



• Molecule 1: Protein translocase subunit SecA

Chain B:





- Molecule 2: peptide

Chain C: 67% 33%

- Molecule 2: peptide

Chain D: 67% 33%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	106.72Å 106.72Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 32.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.50) 99.7 (32.31-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.208 , 0.258 0.210 , 0.259	Depositor DCC
R_{free} test set	3443 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 12.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12364	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.48	0/6127	0.60	5/8239 (0.1%)
1	B	0.50	0/6167	1.10	21/8291 (0.3%)
All	All	0.49	0/12294	0.89	26/16530 (0.2%)

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	A	0	1
1	B	0	5
All	All	0	6

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	341	GLU	CA-C-N	29.99	176.18	116.20
1	B	325	LYS	CA-C-N	27.76	171.72	116.20
1	B	318	SER	CA-C-N	26.39	175.26	117.20
1	B	255	LYS	CA-C-N	24.04	170.09	117.20
1	B	319	PHE	O-C-N	-23.70	84.78	122.70
1	B	255	LYS	O-C-N	-22.22	87.14	122.70
1	B	325	LYS	O-C-N	-21.54	86.58	123.20
1	B	319	PHE	CA-C-O	20.89	163.97	120.10
1	B	318	SER	O-C-N	-19.74	91.11	122.70
1	B	341	GLU	O-C-N	-19.10	90.73	123.20
1	B	255	LYS	CA-C-O	-17.67	82.99	120.10
1	B	319	PHE	CA-C-N	-17.27	79.20	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	318	SER	CA-C-O	-16.82	84.78	120.10
1	B	325	LYS	CA-C-O	-16.63	85.18	120.10
1	B	341	GLU	CA-C-O	-15.05	88.50	120.10
1	A	319	PHE	N-CA-C	8.58	134.16	111.00
1	A	321	GLY	N-CA-C	-7.18	95.15	113.10
1	B	319	PHE	C-N-CA	6.60	138.19	121.70
1	B	254	ILE	N-CA-C	-6.38	93.77	111.00
1	B	671	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	316	VAL	CB-CA-C	-5.84	100.30	111.40
1	A	317	ASP	N-CA-C	5.58	126.07	111.00
1	A	672	GLU	N-CA-C	5.46	125.74	111.00
1	B	259	VAL	N-CA-C	-5.43	96.34	111.00
1	B	318	SER	N-CA-C	-5.30	96.68	111.00
1	A	318	SER	C-N-CA	5.05	134.32	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	742	ALA	Peptide
1	B	255	LYS	Mainchain
1	B	318	SER	Mainchain
1	B	325	LYS	Mainchain
1	B	341	GLU	Peptide,Mainchain

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	6043	0	6031	292	0
1	B	6083	0	6069	281	0
2	C	15	0	5	1	0
2	D	15	0	6	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	81	0	0	8	0
5	B	71	0	0	6	0
All	All	12364	0	12135	573	0

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 24.

All (573) 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:A:316:VAL:HG12	1:A:320:THR:CG2	1.37	1.50
1:A:316:VAL:CG1	1:A:320:THR:HG21	1.41	1.49
1:A:673:LYS:HA	1:A:676:ILE:CD1	1.41	1.45
1:A:677:PHE:CE1	1:A:679:LYS:HD3	1.60	1.36
1:A:317:ASP:HB3	1:A:322:ARG:CG	1.55	1.35
1:B:323:LEU:HD12	1:B:323:LEU:C	1.53	1.27
1:B:221:LEU:HD12	2:D:1:UNK:CB	1.66	1.24
1:A:541:MET:HG2	1:A:555:MET:CE	1.66	1.24
1:B:315:ILE:C	1:B:315:ILE:HD13	1.58	1.23
1:A:672:GLU:OE1	1:A:675:ASP:HB2	1.40	1.19
1:B:252:TYR:OH	1:B:257:LYS:HG3	1.37	1.17
1:B:673:LYS:HA	1:B:676:ILE:CG2	1.75	1.17
1:B:548:ARG:HD3	1:B:548:ARG:O	1.46	1.15
1:B:221:LEU:CD1	2:D:1:UNK:CB	2.25	1.14
1:B:548:ARG:HH11	1:B:548:ARG:HG3	1.11	1.13
1:A:317:ASP:CG	1:A:322:ARG:HD2	1.69	1.13
1:A:541:MET:HG2	1:A:555:MET:HE2	1.17	1.12
1:A:322:ARG:HH21	1:A:325:LYS:HE3	1.12	1.12
1:B:343:LEU:N	1:B:343:LEU:HD23	1.53	1.12
1:B:645:ARG:NH1	1:B:645:ARG:HG3	1.47	1.11
1:A:320:THR:N	1:A:321:GLY:HA3	1.58	1.11
1:A:320:THR:HA	1:A:322:ARG:N	1.66	1.11
1:A:673:LYS:HA	1:A:676:ILE:HD11	1.15	1.09
1:B:647:GLU:HG3	1:B:652:TRP:CD1	1.86	1.09
1:A:316:VAL:O	1:A:320:THR:HG22	1.52	1.09
1:A:673:LYS:CA	1:A:676:ILE:CD1	2.30	1.09
1:B:673:LYS:HA	1:B:676:ILE:HG21	1.24	1.08
1:A:317:ASP:CB	1:A:322:ARG:CG	2.30	1.08
1:B:323:LEU:HD12	1:B:323:LEU:O	1.52	1.08
1:B:645:ARG:HH11	1:B:645:ARG:CG	1.66	1.07
1:A:676:ILE:HA	1:A:677:PHE:HB2	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASP:CB	1:A:322:ARG:HG3	1.85	1.05
1:A:677:PHE:CE1	1:A:679:LYS:CD	2.39	1.05
1:B:691:ARG:HG3	1:B:691:ARG:HH11	1.18	1.05
1:B:676:ILE:HG23	1:B:677:PHE:N	1.70	1.03
1:A:322:ARG:NH2	1:A:325:LYS:HE3	1.72	1.03
1:B:292:GLN:HE21	1:B:292:GLN:HA	1.21	1.03
1:A:322:ARG:HH21	1:A:325:LYS:CE	1.72	1.03
1:A:673:LYS:HA	1:A:676:ILE:HD12	1.40	1.03
1:B:315:ILE:HD13	1:B:316:VAL:N	1.75	1.01
1:A:560:ARG:HH11	1:A:560:ARG:HG3	0.84	1.00
1:A:624:ARG:NH2	1:A:697:ASN:OD1	1.94	1.00
1:A:322:ARG:NE	1:A:325:LYS:HZ2	1.59	1.00
1:A:560:ARG:HH11	1:A:560:ARG:CG	1.74	1.00
1:B:691:ARG:HH11	1:B:691:ARG:CG	1.73	0.99
1:A:675:ASP:O	1:A:677:PHE:HA	1.60	0.99
1:B:255:LYS:O	1:B:255:LYS:HD3	1.63	0.98
1:A:560:ARG:HG3	1:A:560:ARG:NH1	1.66	0.98
1:A:516:ARG:CD	1:A:582:GLN:NE2	2.27	0.97
1:B:248:LYS:HE3	1:B:264:GLU:HG3	1.46	0.97
1:A:677:PHE:HE1	1:A:679:LYS:CD	1.75	0.97
1:B:341:GLU:HB2	1:B:343:LEU:HG	1.45	0.96
1:A:317:ASP:CG	1:A:322:ARG:CD	2.33	0.96
1:A:317:ASP:HB3	1:A:322:ARG:HG3	0.96	0.96
1:A:317:ASP:OD1	1:A:322:ARG:HD2	1.65	0.96
1:B:548:ARG:HD3	1:B:548:ARG:C	1.87	0.95
1:B:549:PHE:O	1:B:551:ALA:N	1.98	0.95
1:B:255:LYS:N	1:B:255:LYS:CD	2.30	0.95
1:B:323:LEU:C	1:B:323:LEU:CD1	2.30	0.95
1:B:255:LYS:CD	1:B:255:LYS:H	1.77	0.95
1:B:315:ILE:C	1:B:315:ILE:CD1	2.29	0.95
1:A:677:PHE:HE1	1:A:679:LYS:HD3	0.80	0.94
1:B:676:ILE:CG2	1:B:677:PHE:N	2.30	0.93
1:A:322:ARG:CZ	1:A:325:LYS:NZ	2.30	0.93
1:A:320:THR:N	1:A:321:GLY:CA	2.30	0.92
1:B:343:LEU:HD23	1:B:343:LEU:H	1.30	0.92
1:B:255:LYS:H	1:B:255:LYS:HD2	1.33	0.92
1:B:548:ARG:HG3	1:B:548:ARG:NH1	1.76	0.92
1:A:516:ARG:CD	1:A:582:GLN:HE22	1.83	0.92
1:A:654:LEU:O	1:A:654:LEU:HD23	1.68	0.92
1:B:82:PHE:H	1:B:85:GLN:HE21	1.18	0.92
1:A:322:ARG:NH2	1:A:325:LYS:CE	2.30	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:HD3	1:B:462:LYS:N	1.85	0.90
1:B:463:ASN:HD22	1:B:466:ARG:HB2	1.36	0.90
1:A:516:ARG:HH11	1:A:516:ARG:CG	1.84	0.90
1:A:320:THR:H	1:A:321:GLY:HA3	1.34	0.90
1:B:647:GLU:CG	1:B:652:TRP:HD1	1.85	0.90
1:B:462:LYS:HD3	1:B:462:LYS:H	1.35	0.90
1:B:500:LYS:HG3	5:B:817:HOH:O	1.70	0.90
1:B:676:ILE:CG2	1:B:677:PHE:H	1.84	0.90
1:A:673:LYS:CA	1:A:676:ILE:HD12	1.98	0.89
1:A:317:ASP:OD1	1:A:322:ARG:HG2	1.73	0.89
1:B:343:LEU:N	1:B:343:LEU:CD2	2.31	0.89
1:A:461:ALA:HA	1:A:467:GLU:OE1	1.73	0.89
1:A:516:ARG:HH11	1:A:516:ARG:HG2	1.37	0.88
1:A:516:ARG:HD3	1:A:582:GLN:NE2	1.86	0.88
1:B:691:ARG:HG3	1:B:691:ARG:NH1	1.87	0.88
1:A:316:VAL:C	1:A:320:THR:HG22	1.94	0.87
1:A:673:LYS:HA	1:A:676:ILE:CG1	2.04	0.87
1:B:647:GLU:CG	1:B:652:TRP:CD1	2.55	0.87
1:A:673:LYS:O	1:A:676:ILE:HB	1.75	0.87
1:B:463:ASN:ND2	1:B:466:ARG:HB2	1.88	0.86
1:B:255:LYS:HD3	1:B:255:LYS:N	1.88	0.86
1:B:323:LEU:HD11	1:B:325:LYS:HG2	1.55	0.86
1:B:461:ALA:HA	1:B:467:GLU:OE1	1.74	0.86
1:B:696:TYR:OH	1:B:712:GLU:OE2	1.94	0.86
1:B:317:ASP:OD2	1:B:319:PHE:CD1	2.30	0.85
1:A:541:MET:CG	1:A:555:MET:HE2	2.05	0.85
1:A:675:ASP:O	1:A:677:PHE:CG	2.29	0.85
1:A:323:LEU:N	1:A:323:LEU:HD23	1.89	0.85
1:A:541:MET:CG	1:A:555:MET:CE	2.54	0.85
1:A:673:LYS:C	1:A:676:ILE:HG13	1.96	0.85
1:B:548:ARG:C	1:B:548:ARG:CD	2.45	0.85
1:B:317:ASP:OD2	1:B:319:PHE:CE1	2.30	0.84
1:B:673:LYS:CA	1:B:676:ILE:CG2	2.55	0.84
1:A:460:ASN:HB2	1:A:462:LYS:HE2	1.60	0.84
1:A:322:ARG:CZ	1:A:325:LYS:HZ1	1.90	0.83
1:B:322:ARG:O	1:B:322:ARG:HG2	1.77	0.83
1:B:647:GLU:HG3	1:B:652:TRP:HD1	1.38	0.82
1:A:229:LYS:HE3	1:A:350:MET:CE	2.10	0.81
1:B:316:VAL:HG22	1:B:316:VAL:O	1.78	0.81
1:B:315:ILE:HD13	1:B:315:ILE:O	1.80	0.81
1:A:317:ASP:OD1	1:A:322:ARG:CD	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASP:CB	1:A:322:ARG:CD	2.58	0.80
1:A:699:LYS:NZ	1:A:778:ALA:O	2.15	0.80
1:B:316:VAL:HA	1:B:323:LEU:HA	1.61	0.80
1:B:549:PHE:C	1:B:551:ALA:H	1.84	0.80
1:B:645:ARG:HG3	1:B:645:ARG:HH11	0.74	0.80
1:A:675:ASP:O	1:A:677:PHE:CA	2.30	0.80
1:B:255:LYS:O	1:B:255:LYS:CD	2.30	0.80
1:B:673:LYS:CA	1:B:676:ILE:HG22	2.13	0.79
1:B:643:THR:HB	1:B:653:LYS:HE3	1.64	0.79
1:A:316:VAL:O	1:A:320:THR:CG2	2.30	0.79
1:A:673:LYS:O	1:A:676:ILE:CG1	2.30	0.79
1:A:673:LYS:HG2	1:A:674:SER:N	1.96	0.79
1:A:677:PHE:CD1	1:A:679:LYS:CD	2.66	0.79
1:B:229:LYS:HG2	1:B:350:MET:HG2	1.63	0.79
1:A:654:LEU:O	1:A:654:LEU:CD2	2.30	0.79
1:A:322:ARG:NE	1:A:325:LYS:NZ	2.30	0.79
1:A:322:ARG:NH2	1:A:325:LYS:NZ	2.30	0.79
1:A:320:THR:CA	1:A:322:ARG:N	2.46	0.78
1:A:673:LYS:O	1:A:676:ILE:CB	2.30	0.78
1:B:323:LEU:O	1:B:323:LEU:CD1	2.30	0.78
1:B:676:ILE:O	1:B:679:LYS:HG3	1.83	0.78
1:A:673:LYS:O	1:A:676:ILE:HG13	1.81	0.78
1:A:677:PHE:CD1	1:A:679:LYS:HD2	2.20	0.77
1:B:323:LEU:HD12	1:B:324:MET:N	1.99	0.77
1:A:317:ASP:OD1	1:A:322:ARG:CG	2.32	0.77
1:A:654:LEU:O	1:A:654:LEU:CG	2.30	0.77
1:A:679:LYS:O	1:A:684:MET:CE	2.33	0.77
1:B:14:ARG:N	1:B:14:ARG:HD3	2.00	0.76
1:B:328:ARG:HH12	1:B:346:GLN:CG	1.99	0.76
1:A:409:ARG:NH1	1:A:559:ASP:OD1	2.18	0.76
1:A:437:VAL:HG23	1:A:513:HIS:NE2	2.00	0.75
1:B:255:LYS:O	1:B:255:LYS:CG	2.33	0.75
1:A:275:ILE:HG23	1:A:283:HIS:CE1	2.21	0.75
1:B:673:LYS:HA	1:B:676:ILE:HG22	1.63	0.75
1:B:677:PHE:C	1:B:677:PHE:CD2	2.60	0.75
1:A:260:GLN:HE21	1:A:740:LEU:HD22	1.52	0.74
1:B:93:HIS:HD2	1:B:117:ASN:HD21	1.34	0.74
1:B:246:ALA:HA	1:B:250:TYR:CZ	2.22	0.74
1:A:317:ASP:HB3	1:A:322:ARG:HG2	1.66	0.74
1:B:193:LYS:HG3	1:B:196:MET:HE3	1.69	0.74
1:A:309:GLU:O	1:A:310:ASP:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:TYR:O	1:A:746:THR:HG22	1.88	0.74
1:A:486:MET:HA	1:A:486:MET:HE2	1.70	0.73
1:B:257:LYS:O	1:B:257:LYS:HG2	1.89	0.73
1:A:176:THR:HG22	1:A:179:GLU:H	1.54	0.72
1:B:315:ILE:HD13	1:B:316:VAL:CA	2.18	0.72
1:A:380:GLU:OE2	1:A:593:ARG:HD2	1.88	0.72
1:B:358:GLN:HE21	1:B:362:ARG:HD3	1.54	0.72
1:A:229:LYS:HE3	1:A:350:MET:HE3	1.70	0.72
1:A:307:VAL:HG23	1:A:308:VAL:N	2.04	0.72
1:A:556:ALA:O	1:A:560:ARG:NH1	2.22	0.72
1:A:635:LEU:O	1:A:639:ILE:HG12	1.89	0.72
1:A:676:ILE:CA	1:A:677:PHE:HB2	2.14	0.72
1:B:612:LYS:O	1:B:616:GLU:HG2	1.90	0.72
1:B:85:GLN:HE22	4:B:873:ADP:HN61	1.37	0.71
1:A:673:LYS:CA	1:A:676:ILE:HG13	2.18	0.71
1:A:516:ARG:HD2	1:A:582:GLN:HE22	1.55	0.71
1:A:516:ARG:HD2	1:A:582:GLN:NE2	2.04	0.71
1:B:252:TYR:OH	1:B:257:LYS:CG	2.29	0.71
1:B:317:ASP:O	1:B:318:SER:C	2.29	0.71
1:B:674:SER:C	1:B:675:ASP:OD1	2.30	0.71
1:A:317:ASP:CG	1:A:322:ARG:CG	2.58	0.70
1:A:676:ILE:HA	1:A:677:PHE:CB	2.13	0.70
1:A:311:GLY:C	1:A:312:GLN:OE1	2.29	0.70
1:B:308:VAL:HG13	1:B:343:LEU:HD11	1.74	0.70
1:B:646:GLU:O	1:B:647:GLU:C	2.30	0.70
1:A:301:GLN:N	1:A:305:ASP:OD1	2.24	0.70
1:A:486:MET:HA	1:A:486:MET:CE	2.22	0.70
1:B:253:ASP:OD1	1:B:253:ASP:C	2.30	0.70
1:B:252:TYR:CZ	1:B:257:LYS:HG3	2.25	0.69
1:A:309:GLU:OE1	1:A:324:MET:SD	2.51	0.69
1:A:246:ALA:HA	1:A:250:TYR:CZ	2.28	0.69
1:A:673:LYS:CA	1:A:676:ILE:CG1	2.67	0.69
1:A:246:ALA:HA	1:A:250:TYR:CE1	2.28	0.69
1:B:292:GLN:HA	1:B:292:GLN:NE2	2.02	0.69
1:A:130:ASN:ND2	1:A:133:LEU:H	1.89	0.69
1:B:643:THR:N	1:B:644:PRO:HD3	2.07	0.69
1:A:320:THR:CA	1:A:321:GLY:C	2.60	0.68
1:A:679:LYS:O	1:A:684:MET:HE3	1.94	0.67
1:B:128:THR:HG21	5:B:784:HOH:O	1.95	0.67
1:A:275:ILE:HD11	1:A:286:LEU:HD21	1.75	0.67
1:A:69:VAL:HG11	1:A:111:THR:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:THR:HG22	1:A:263:GLU:H	1.59	0.66
1:A:320:THR:HA	1:A:321:GLY:C	2.15	0.66
1:B:271:LYS:HD2	1:B:271:LYS:O	1.95	0.66
1:B:319:PHE:CD2	1:B:319:PHE:N	2.63	0.66
1:B:672:GLU:OE2	1:B:673:LYS:N	2.29	0.66
1:B:675:ASP:HA	1:B:679:LYS:HE3	1.77	0.66
1:B:316:VAL:O	1:B:317:ASP:HB2	1.95	0.66
1:B:647:GLU:HG3	1:B:652:TRP:NE1	2.10	0.66
1:A:320:THR:HA	1:A:322:ARG:H	1.58	0.66
1:A:658:VAL:HG22	1:A:671:LEU:HD23	1.76	0.66
1:B:253:ASP:OD1	1:B:254:ILE:N	2.30	0.65
1:B:675:ASP:C	1:B:679:LYS:HE3	2.17	0.65
1:A:322:ARG:NH2	1:A:325:LYS:HZ1	1.92	0.65
1:B:642:TYR:C	1:B:644:PRO:HD3	2.17	0.65
1:B:316:VAL:O	1:B:317:ASP:CB	2.37	0.65
1:A:128:THR:HG21	5:A:782:HOH:O	1.95	0.65
1:B:106:LYS:HE2	5:B:800:HOH:O	1.96	0.65
1:B:341:GLU:N	1:B:341:GLU:OE1	2.29	0.65
1:A:229:LYS:HE3	1:A:350:MET:HE1	1.77	0.64
1:A:275:ILE:HD11	1:A:286:LEU:CD2	2.27	0.64
1:B:324:MET:N	1:B:324:MET:HE2	2.12	0.64
1:B:409:ARG:NH2	1:B:559:ASP:OD1	2.30	0.64
1:A:322:ARG:HE	1:A:325:LYS:HZ2	1.43	0.64
1:B:319:PHE:H	1:B:319:PHE:HD2	1.42	0.64
1:B:385:TYR:HB3	1:B:387:MET:HE2	1.78	0.64
1:B:548:ARG:NH1	1:B:548:ARG:CG	2.54	0.64
1:A:777:LYS:HB2	1:A:777:LYS:NZ	2.13	0.63
1:B:306:TYR:OH	1:B:340:LYS:HE2	1.97	0.63
1:B:256:THR:HG23	1:B:256:THR:O	1.97	0.63
1:B:548:ARG:HH11	1:B:548:ARG:CG	1.95	0.63
1:B:323:LEU:HD11	1:B:325:LYS:CG	2.25	0.63
1:B:675:ASP:OD1	1:B:675:ASP:N	2.30	0.63
1:B:676:ILE:HG22	1:B:677:PHE:H	1.63	0.62
1:B:675:ASP:CA	1:B:679:LYS:HE3	2.29	0.62
1:A:654:LEU:O	1:A:654:LEU:HG	1.97	0.62
1:B:316:VAL:HA	1:B:323:LEU:CA	2.29	0.62
1:A:655:ASP:N	1:A:655:ASP:OD1	2.30	0.61
1:B:123:GLY:O	1:B:202:HIS:HD2	1.83	0.61
1:B:341:GLU:CB	1:B:343:LEU:HG	2.24	0.61
1:B:681:PRO:HA	1:B:684:MET:CE	2.30	0.61
1:A:316:VAL:C	1:A:320:THR:CG2	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LEU:O	1:A:777:LYS:HE2	2.00	0.61
1:B:630:MET:HE1	1:B:767:ILE:HG22	1.83	0.61
1:A:315:ILE:HD12	1:A:329:TYR:OH	2.01	0.61
1:B:315:ILE:CD1	1:B:315:ILE:O	2.43	0.61
1:B:341:GLU:OE1	1:B:341:GLU:CA	2.49	0.61
1:A:128:THR:HG23	1:A:207:ASP:HB3	1.81	0.61
1:A:770:GLU:HG3	1:A:774:PHE:CE1	2.36	0.61
1:B:770:GLU:HG3	1:B:774:PHE:CE2	2.35	0.61
1:A:541:MET:HG2	1:A:555:MET:HE3	1.74	0.60
1:B:343:LEU:H	1:B:343:LEU:CD2	1.95	0.60
1:B:745:GLN:HA	1:B:745:GLN:OE1	1.99	0.60
1:A:643:THR:HG22	1:A:643:THR:O	2.00	0.60
1:B:672:GLU:O	1:B:674:SER:N	2.29	0.60
1:A:516:ARG:CG	1:A:516:ARG:NH1	2.57	0.60
1:B:523:ARG:NH2	5:B:842:HOH:O	2.34	0.60
1:A:319:PHE:C	1:A:320:THR:HG23	2.22	0.60
1:A:513:HIS:HB3	5:A:798:HOH:O	2.01	0.60
1:A:673:LYS:C	1:A:676:ILE:CG1	2.70	0.60
1:A:262:THR:HG22	1:A:263:GLU:N	2.16	0.59
1:A:377:GLU:OE2	1:A:517:ARG:NH1	2.35	0.59
1:B:328:ARG:HB3	1:B:334:HIS:CE1	2.37	0.59
1:A:450:LYS:HD3	5:A:783:HOH:O	2.01	0.59
1:A:652:TRP:CD1	1:A:652:TRP:O	2.56	0.59
1:B:248:LYS:HE3	1:B:264:GLU:CG	2.29	0.59
1:B:460:ASN:C	1:B:462:LYS:HD2	2.23	0.59
1:B:711:PHE:O	1:B:715:ILE:HG12	2.03	0.59
1:A:130:ASN:HD22	1:A:130:ASN:C	2.06	0.58
1:A:322:ARG:HB3	1:A:325:LYS:HD3	1.85	0.58
1:B:311:GLY:C	1:B:312:GLN:HG2	2.23	0.58
1:B:516:ARG:NH2	5:B:785:HOH:O	2.36	0.58
1:A:309:GLU:O	1:A:310:ASP:CB	2.50	0.58
1:B:340:LYS:C	1:B:341:GLU:O	2.41	0.58
1:B:423:ALA:HA	1:B:454:ILE:CD1	2.33	0.58
1:A:690:ASP:O	1:A:694:THR:HG23	2.04	0.58
1:A:703:PHE:O	1:A:707:GLN:HG3	2.03	0.58
1:B:347:ASN:HD22	1:B:347:ASN:N	2.01	0.58
1:A:672:GLU:CD	1:A:672:GLU:H	2.05	0.58
1:A:295:LYS:O	1:A:299:ALA:HB3	2.04	0.58
1:A:655:ASP:OD2	1:A:676:ILE:HG23	2.04	0.58
1:A:657:LEU:O	1:A:661:ILE:HG13	2.03	0.58
1:A:696:TYR:OH	1:A:712:GLU:OE1	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ASP:O	1:A:677:PHE:CB	2.52	0.57
1:B:247:GLU:OE1	1:B:247:GLU:HA	2.04	0.57
1:B:306:TYR:OH	1:B:340:LYS:CE	2.53	0.57
1:B:689:MET:O	1:B:693:ILE:HG12	2.05	0.57
1:A:285:ALA:O	1:A:289:HIS:HD2	1.88	0.57
1:A:461:ALA:CA	1:A:467:GLU:OE1	2.50	0.57
1:A:673:LYS:CB	1:A:676:ILE:HD12	2.34	0.57
1:B:128:THR:HG23	1:B:207:ASP:HB3	1.86	0.56
1:B:549:PHE:C	1:B:551:ALA:N	2.51	0.56
1:B:672:GLU:C	1:B:674:SER:H	2.07	0.56
1:B:676:ILE:HG23	1:B:677:PHE:H	1.46	0.56
1:A:316:VAL:CG1	1:A:320:THR:CG2	2.30	0.56
1:B:229:LYS:HD3	1:B:348:GLU:HG3	1.87	0.56
1:A:238:ASN:O	1:A:242:ARG:HG3	2.06	0.56
1:A:671:LEU:HG	1:A:672:GLU:N	2.20	0.56
1:B:358:GLN:NE2	1:B:362:ARG:HD3	2.21	0.56
1:A:97:ILE:CD1	1:A:381:PHE:CD2	2.88	0.56
1:B:645:ARG:NH1	1:B:645:ARG:CG	2.34	0.56
1:A:41:LEU:HD12	1:A:147:PHE:HE2	1.70	0.56
1:B:350:MET:HB2	1:B:725:MET:CE	2.35	0.55
1:B:437:VAL:HG12	1:B:513:HIS:CE1	2.41	0.55
1:A:677:PHE:HD1	1:A:679:LYS:HD2	1.69	0.55
1:A:770:GLU:HG3	1:A:774:PHE:HE1	1.70	0.55
1:B:155:ASN:HB3	1:B:175:SER:HB2	1.89	0.55
1:B:193:LYS:HA	1:B:196:MET:HE2	1.87	0.55
1:B:340:LYS:O	1:B:341:GLU:O	2.25	0.55
1:B:256:THR:HG23	1:B:258:ALA:CB	2.36	0.55
1:B:462:LYS:N	1:B:462:LYS:CD	2.58	0.55
1:A:322:ARG:HE	1:A:325:LYS:HD3	1.70	0.55
1:A:125:HIS:HD2	1:A:364:TYR:OH	1.90	0.54
1:A:493:ILE:O	1:A:528:ARG:HD3	2.06	0.54
1:B:252:TYR:CD2	1:B:252:TYR:O	2.60	0.54
1:B:672:GLU:C	1:B:674:SER:N	2.61	0.54
1:A:686:GLU:CA	1:A:686:GLU:OE2	2.53	0.54
1:A:52:LEU:HD12	1:A:56:ALA:O	2.08	0.54
1:A:771:VAL:O	1:A:775:VAL:HG13	2.07	0.54
1:B:681:PRO:HA	1:B:684:MET:HE2	1.88	0.54
1:B:385:TYR:HB3	1:B:387:MET:CE	2.38	0.54
1:A:516:ARG:NE	1:A:582:GLN:HE22	2.06	0.54
1:A:686:GLU:OE2	1:A:686:GLU:HA	2.08	0.54
1:B:315:ILE:CD1	1:B:316:VAL:N	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:THR:N	1:B:644:PRO:CD	2.71	0.53
1:B:82:PHE:H	1:B:85:GLN:NE2	1.96	0.53
1:B:489:ARG:HH21	1:B:521:GLN:HE22	1.57	0.53
1:B:229:LYS:CG	1:B:350:MET:HG2	2.37	0.53
1:B:256:THR:HG23	1:B:258:ALA:HB3	1.91	0.53
1:A:516:ARG:HG2	1:A:516:ARG:NH1	2.15	0.53
1:B:147:PHE:HD2	1:B:148:LEU:HD13	1.74	0.53
1:B:548:ARG:O	1:B:548:ARG:CD	2.36	0.53
1:A:176:THR:CG2	1:A:179:GLU:H	2.20	0.52
1:B:328:ARG:HH12	1:B:346:GLN:HG2	1.72	0.52
1:B:676:ILE:O	1:B:679:LYS:CG	2.54	0.52
1:B:350:MET:HB2	1:B:725:MET:HE2	1.92	0.52
1:B:708:MET:O	1:B:712:GLU:HG3	2.09	0.52
1:A:70:ARG:HG2	1:A:80:PHE:CE1	2.45	0.52
1:B:112:LEU:HB2	1:B:113:PRO:CD	2.40	0.52
1:B:316:VAL:HA	1:B:323:LEU:HB2	1.92	0.52
1:A:160:SER:OG	1:A:161:LYS:N	2.42	0.52
1:A:673:LYS:HB2	1:A:676:ILE:HD12	1.92	0.52
1:B:229:LYS:HG2	1:B:350:MET:CG	2.37	0.52
1:B:320:THR:O	1:B:320:THR:CG2	2.58	0.52
1:B:673:LYS:C	1:B:676:ILE:HG22	2.30	0.52
1:A:672:GLU:CD	1:A:672:GLU:N	2.63	0.52
1:B:460:ASN:O	1:B:462:LYS:HD2	2.10	0.52
1:A:315:ILE:HD13	1:A:329:TYR:CE1	2.44	0.52
1:A:672:GLU:CD	1:A:675:ASP:HB2	2.25	0.52
1:B:101:LYS:N	1:B:101:LYS:HD2	2.24	0.52
1:B:322:ARG:O	1:B:324:MET:CE	2.57	0.51
1:B:323:LEU:CD1	1:B:325:LYS:N	2.73	0.51
1:B:328:ARG:NH1	1:B:346:GLN:CG	2.72	0.51
1:B:302:LYS:O	1:B:303:ASP:HB2	2.10	0.51
1:B:421:ASP:OD2	1:B:425:ARG:NH1	2.43	0.51
1:B:688:ILE:O	1:B:692:ILE:HG12	2.11	0.51
1:A:350:MET:HG2	1:A:725:MET:CG	2.40	0.51
1:B:439:VAL:O	1:B:443:GLU:HG2	2.10	0.51
1:B:520:ASN:OD1	1:B:523:ARG:NH2	2.43	0.51
1:B:256:THR:O	1:B:256:THR:CG2	2.59	0.51
1:A:630:MET:HE1	1:A:767:ILE:HG22	1.93	0.51
1:B:42:LYS:HG2	1:B:147:PHE:O	2.10	0.51
1:A:123:GLY:O	1:A:202:HIS:HD2	1.94	0.51
1:A:560:ARG:CG	1:A:560:ARG:NH1	2.45	0.51
1:B:81:PRO:HA	1:B:85:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASP:O	1:A:317:ASP:OD2	2.29	0.51
1:B:253:ASP:O	1:B:256:THR:O	2.29	0.51
1:A:127:VAL:HA	1:A:175:SER:O	2.11	0.50
1:A:327:ARG:HG3	1:A:328:ARG:N	2.26	0.50
1:A:437:VAL:HG23	1:A:513:HIS:CD2	2.46	0.50
1:B:271:LYS:HD2	1:B:271:LYS:C	2.31	0.50
1:A:679:LYS:O	1:A:684:MET:HE2	2.11	0.50
1:A:128:THR:CG2	1:A:207:ASP:HB3	2.42	0.50
1:B:324:MET:N	1:B:324:MET:CE	2.73	0.50
1:A:320:THR:C	1:A:323:LEU:CD2	2.80	0.50
1:A:621:GLU:OE1	1:A:621:GLU:HA	2.11	0.50
1:B:743:TYR:O	1:B:746:THR:OG1	2.30	0.50
1:A:320:THR:O	1:A:320:THR:OG1	2.29	0.50
1:A:328:ARG:HB2	1:A:334:HIS:ND1	2.27	0.50
1:A:489:ARG:HH12	1:A:521:GLN:NE2	2.10	0.50
1:B:33:TYR:HA	1:B:36:LEU:CD1	2.42	0.50
1:B:230:SER:OG	1:B:232:LYS:HG3	2.12	0.50
1:B:665:TYR:HB3	1:B:692:ILE:HD12	1.93	0.50
1:B:292:GLN:HE21	1:B:292:GLN:CA	2.05	0.50
1:B:82:PHE:N	1:B:85:GLN:HE21	1.99	0.49
1:B:677:PHE:C	1:B:677:PHE:HD2	2.11	0.49
1:A:229:LYS:CE	1:A:350:MET:HE3	2.38	0.49
1:A:668:GLU:CD	1:A:668:GLU:H	2.14	0.49
1:A:155:ASN:HB3	1:A:175:SER:HB2	1.94	0.49
1:A:672:GLU:OE1	1:A:672:GLU:CA	2.59	0.49
1:A:672:GLU:OE1	1:A:672:GLU:O	2.30	0.49
5:A:811:HOH:O	1:B:702:GLN:HG2	2.13	0.49
1:A:659:ASP:O	1:A:659:ASP:OD2	2.30	0.49
1:B:17:ASN:OD1	1:B:20:GLU:HG3	2.13	0.49
1:A:682:ASP:O	1:A:682:ASP:OD2	2.30	0.49
1:B:246:ALA:HA	1:B:250:TYR:OH	2.13	0.49
1:B:647:GLU:HG2	1:B:652:TRP:HD1	1.73	0.49
1:B:465:GLU:OE1	1:B:465:GLU:O	2.30	0.49
1:B:646:GLU:O	1:B:647:GLU:O	2.30	0.49
1:A:247:GLU:O	1:A:247:GLU:OE2	2.29	0.49
1:A:604:ARG:NH1	1:A:604:ARG:HG2	2.28	0.49
1:A:672:GLU:OE2	1:A:675:ASP:OD2	2.30	0.49
1:A:412:GLU:CD	1:A:412:GLU:H	2.16	0.49
1:B:630:MET:HE2	1:B:768:GLU:HA	1.94	0.49
1:A:76:VAL:HG23	1:A:77:THR:HG23	1.93	0.49
5:A:811:HOH:O	1:B:702:GLN:CG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLU:OE2	1:B:593:ARG:NH1	2.45	0.49
1:B:385:TYR:CB	1:B:387:MET:CE	2.90	0.49
1:A:42:LYS:HG2	1:A:147:PHE:O	2.13	0.48
1:B:328:ARG:HB3	1:B:334:HIS:ND1	2.28	0.48
1:A:663:THR:O	1:A:663:THR:OG1	2.30	0.48
1:B:681:PRO:HA	1:B:684:MET:HE3	1.95	0.48
1:A:671:LEU:HG	1:A:672:GLU:H	1.79	0.48
1:B:221:LEU:HD13	2:D:1:UNK:CB	2.38	0.48
1:B:316:VAL:O	1:B:317:ASP:OD1	2.30	0.48
1:B:673:LYS:CA	1:B:676:ILE:HG21	2.16	0.48
1:A:277:ASN:ND2	1:A:279:PHE:H	2.11	0.48
1:A:316:VAL:CG1	1:A:320:THR:CB	2.88	0.48
1:A:673:LYS:HG2	1:A:674:SER:H	1.78	0.48
1:B:675:ASP:CB	1:B:687:LEU:HD11	2.43	0.48
1:A:604:ARG:HG2	1:A:604:ARG:HH11	1.79	0.48
1:A:155:ASN:HD21	1:A:164:LYS:HG2	1.79	0.48
1:A:260:GLN:NE2	1:A:740:LEU:HD22	2.26	0.48
1:B:83:LYS:HA	1:B:86:LEU:HD12	1.96	0.48
1:B:285:ALA:O	1:B:289:HIS:HD2	1.96	0.48
1:A:17:ASN:HD22	1:A:19:TYR:H	1.60	0.48
1:B:316:VAL:HA	1:B:323:LEU:CB	2.44	0.48
1:B:624:ARG:NH1	1:B:628:GLU:OE1	2.45	0.48
1:A:199:ARG:HB3	1:A:200:PRO:CD	2.44	0.47
1:B:634:SER:HB2	1:B:769:ASP:OD2	2.14	0.47
1:A:284:VAL:HG12	5:A:814:HOH:O	2.13	0.47
1:A:407:ILE:CD1	1:A:574:VAL:HG11	2.44	0.47
1:A:316:VAL:O	1:A:320:THR:CB	2.62	0.47
1:A:643:THR:HG23	1:A:653:LYS:NZ	2.30	0.47
1:B:315:ILE:O	1:B:315:ILE:HG23	2.14	0.47
1:A:323:LEU:HD23	1:A:323:LEU:H	1.72	0.47
1:A:512:ARG:HG3	1:A:539:LEU:HD21	1.96	0.47
1:B:33:TYR:HA	1:B:36:LEU:HD12	1.95	0.47
1:B:647:GLU:HG2	1:B:652:TRP:CD1	2.43	0.47
1:A:117:ASN:HD21	1:A:366:LYS:NZ	2.12	0.47
1:A:348:GLU:OE2	1:A:348:GLU:N	2.48	0.47
1:B:406:LEU:HD23	1:B:570:GLN:HB2	1.96	0.47
1:A:302:LYS:O	1:A:303:ASP:HB2	2.15	0.47
1:A:317:ASP:CG	1:A:317:ASP:O	2.52	0.47
1:A:318:SER:O	1:A:318:SER:OG	2.30	0.47
1:A:407:ILE:CD1	1:A:574:VAL:CG1	2.93	0.47
1:A:672:GLU:OE1	1:A:672:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:MET:HG3	1:B:521:GLN:HE21	1.80	0.47
1:A:556:ALA:C	1:A:560:ARG:HH12	2.15	0.47
1:A:747:ASN:HA	1:A:748:PRO:HD3	1.73	0.47
1:B:314:VAL:HG11	1:B:323:LEU:HD22	1.97	0.47
1:A:312:GLN:OE1	1:A:312:GLN:N	2.48	0.47
1:A:320:THR:O	1:A:323:LEU:HD22	2.14	0.47
1:A:321:GLY:O	1:A:323:LEU:HD23	2.15	0.47
1:A:155:ASN:ND2	1:A:164:LYS:HG2	2.30	0.46
1:B:358:GLN:O	1:B:362:ARG:HG3	2.15	0.46
1:A:347:ASN:C	1:A:347:ASN:HD22	2.18	0.46
1:A:17:ASN:ND2	1:A:19:TYR:H	2.13	0.46
1:B:323:LEU:O	1:B:323:LEU:CG	2.62	0.46
1:B:770:GLU:HG3	1:B:774:PHE:HE2	1.80	0.46
1:B:691:ARG:CG	1:B:691:ARG:NH1	2.45	0.46
1:A:744:ALA:HA	1:A:745:GLN:HA	1.59	0.46
1:B:256:THR:O	1:B:258:ALA:N	2.49	0.46
1:B:643:THR:CB	1:B:653:LYS:HE3	2.40	0.46
1:B:657:LEU:O	1:B:661:ILE:HG12	2.16	0.46
1:A:328:ARG:NH2	1:A:334:HIS:CD2	2.84	0.45
1:B:328:ARG:HH12	1:B:346:GLN:CB	2.29	0.45
1:B:385:TYR:CB	1:B:387:MET:HE3	2.46	0.45
1:A:652:TRP:CD1	1:A:652:TRP:C	2.87	0.45
1:B:322:ARG:O	1:B:324:MET:HE2	2.17	0.45
1:B:676:ILE:C	1:B:679:LYS:HG3	2.35	0.45
1:A:310:ASP:HB3	1:A:311:GLY:H	1.32	0.45
1:B:62:LEU:HD23	1:B:62:LEU:C	2.37	0.45
1:B:403:ARG:CZ	1:B:534:ILE:HD11	2.46	0.45
1:B:663:THR:HG22	1:B:663:THR:O	2.16	0.45
1:A:247:GLU:OE2	1:A:247:GLU:CA	2.60	0.45
1:B:322:ARG:O	1:B:324:MET:HE1	2.17	0.45
1:A:658:VAL:HG22	1:A:671:LEU:CD2	2.44	0.45
1:B:610:ILE:HD13	1:B:610:ILE:HA	1.78	0.45
1:B:342:GLY:O	1:B:343:LEU:C	2.54	0.44
1:B:630:MET:CE	1:B:767:ILE:HG22	2.45	0.44
1:B:697:ASN:O	1:B:701:GLU:HG2	2.18	0.44
1:A:767:ILE:O	1:A:771:VAL:HG23	2.17	0.44
1:A:350:MET:HG2	1:A:725:MET:SD	2.57	0.44
1:B:93:HIS:CD2	1:B:116:LEU:HD23	2.52	0.44
1:B:437:VAL:HG13	1:B:511:GLU:HG3	1.99	0.44
1:B:546:MET:HA	1:B:546:MET:CE	2.48	0.44
1:A:507:VAL:HB	1:A:535:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:ASP:OD1	1:B:673:LYS:HD3	2.17	0.44
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.48	0.44
1:B:106:LYS:CE	5:B:800:HOH:O	2.62	0.44
1:B:123:GLY:O	1:B:202:HIS:CD2	2.68	0.44
1:B:341:GLU:OE1	1:B:341:GLU:HA	2.18	0.44
1:B:657:LEU:HD23	1:B:657:LEU:C	2.37	0.44
1:A:130:ASN:ND2	1:A:130:ASN:C	2.72	0.44
1:B:423:ALA:HA	1:B:454:ILE:HD11	1.99	0.44
1:A:707:GLN:H	1:A:707:GLN:HG2	1.35	0.43
1:B:350:MET:HB2	1:B:725:MET:HE1	2.00	0.43
1:A:316:VAL:O	1:A:317:ASP:HB3	2.18	0.43
1:A:406:LEU:HD23	1:A:570:GLN:HB2	2.00	0.43
1:A:546:MET:HA	1:A:546:MET:CE	2.48	0.43
1:A:676:ILE:O	1:A:676:ILE:HG22	2.18	0.43
1:A:311:GLY:O	1:A:312:GLN:OE1	2.36	0.43
1:A:321:GLY:O	1:A:323:LEU:CD2	2.65	0.43
1:A:486:MET:HG3	1:A:521:GLN:NE2	2.33	0.43
1:A:306:TYR:HA	1:A:316:VAL:HG23	2.00	0.43
1:A:285:ALA:O	1:A:289:HIS:CD2	2.69	0.43
1:A:659:ASP:OD2	1:A:659:ASP:C	2.55	0.43
1:B:70:ARG:HG3	1:B:81:PRO:HD2	2.00	0.43
1:A:52:LEU:HD13	1:A:61:LEU:HD22	2.01	0.43
1:A:676:ILE:CA	1:A:677:PHE:CB	2.86	0.43
1:A:751:GLU:O	1:A:755:GLU:HG3	2.19	0.43
1:B:31:GLY:HA2	1:B:34:GLU:HG2	2.00	0.43
1:B:317:ASP:O	1:B:320:THR:HA	2.19	0.43
1:B:402:ASP:OD2	1:B:535:THR:HB	2.19	0.43
1:A:215:ASP:OD2	1:A:517:ARG:NH2	2.52	0.43
1:A:222:ILE:HG13	2:C:2:UNK:HA	1.99	0.43
1:A:229:LYS:HB2	1:A:348:GLU:O	2.19	0.43
1:A:624:ARG:HG3	1:A:696:TYR:CE2	2.54	0.43
1:A:314:VAL:HG13	1:A:315:ILE:N	2.34	0.42
1:A:630:MET:HE2	1:A:768:GLU:HA	2.00	0.42
1:A:761:GLU:O	1:A:765:GLU:HG3	2.18	0.42
1:B:36:LEU:HB3	1:B:40:ALA:HB3	2.01	0.42
1:B:693:ILE:HG12	1:B:693:ILE:H	1.72	0.42
1:A:106:LYS:HE2	5:A:810:HOH:O	2.19	0.42
1:A:407:ILE:HD12	1:A:574:VAL:HG11	2.00	0.42
1:A:463:ASN:OD1	1:A:466:ARG:HB2	2.19	0.42
1:B:323:LEU:HD12	1:B:324:MET:CA	2.48	0.42
1:A:677:PHE:CE1	1:A:679:LYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:O	1:A:372:GLY:HA2	2.19	0.42
1:A:705:LYS:HE3	1:A:705:LYS:HB3	1.77	0.42
1:A:643:THR:HA	1:A:653:LYS:HD2	2.01	0.42
1:A:682:ASP:OD2	1:A:682:ASP:C	2.57	0.42
1:B:624:ARG:NH2	1:B:700:GLU:OE1	2.53	0.42
1:A:454:ILE:HA	1:A:455:PRO:HD3	1.89	0.42
1:B:254:ILE:O	1:B:254:ILE:HG12	2.06	0.42
1:B:328:ARG:NH1	1:B:346:GLN:HG3	2.35	0.42
1:B:723:LYS:N	1:B:723:LYS:HD2	2.33	0.42
1:A:292:GLN:OE1	1:A:292:GLN:HA	2.19	0.42
1:B:341:GLU:HB2	1:B:343:LEU:CG	2.31	0.42
1:B:677:PHE:CD2	1:B:678:GLY:N	2.87	0.42
1:A:112:LEU:HB2	1:A:113:PRO:HD3	2.02	0.41
1:B:199:ARG:HB3	1:B:200:PRO:CD	2.50	0.41
1:B:240:PHE:CZ	1:B:269:ALA:HA	2.55	0.41
1:A:130:ASN:HD21	1:A:133:LEU:H	1.62	0.41
1:B:112:LEU:CB	1:B:113:PRO:CD	2.98	0.41
1:B:277:ASN:ND2	1:B:279:PHE:H	2.18	0.41
1:A:655:ASP:HA	1:A:656:GLY:HA3	1.76	0.41
1:B:425:ARG:HD3	1:B:430:GLN:OE1	2.21	0.41
1:B:295:LYS:O	1:B:300:MET:HG2	2.21	0.41
1:A:33:TYR:HA	1:A:36:LEU:HD22	2.02	0.41
1:B:549:PHE:CG	1:B:550:GLY:N	2.88	0.41
1:A:319:PHE:O	1:A:320:THR:HG23	2.21	0.41
1:B:285:ALA:O	1:B:289:HIS:CD2	2.73	0.41
1:A:199:ARG:HB3	1:A:200:PRO:HD2	2.02	0.41
1:A:306:TYR:CD2	1:A:306:TYR:N	2.88	0.41
1:A:322:ARG:HG2	1:A:322:ARG:H	1.52	0.41
1:A:486:MET:HG3	1:A:521:GLN:HE21	1.86	0.41
1:A:675:ASP:O	1:A:677:PHE:CD1	2.73	0.41
1:A:675:ASP:C	1:A:677:PHE:HA	2.34	0.41
1:A:677:PHE:CZ	1:A:684:MET:HG2	2.56	0.41
1:B:161:LYS:N	1:B:161:LYS:HD2	2.36	0.41
1:B:314:VAL:HG13	1:B:315:ILE:N	2.34	0.41
1:B:437:VAL:HG13	1:B:511:GLU:CG	2.51	0.41
1:A:607:ARG:HD3	5:A:809:HOH:O	2.20	0.41
1:B:700:GLU:OE2	1:B:705:LYS:HG2	2.20	0.41
1:A:130:ASN:HD22	1:A:133:LEU:H	1.67	0.40
1:A:292:GLN:NE2	1:A:331:GLU:O	2.46	0.40
1:B:317:ASP:OD2	1:B:319:PHE:CZ	2.73	0.40
1:B:319:PHE:HA	1:B:320:THR:HA	0.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:MET:HE2	1:A:563:MET:HB3	1.99	0.40
1:B:96:ASN:HB3	1:B:388:GLN:O	2.20	0.40
1:A:131:GLU:O	1:A:135:SER:HB3	2.22	0.40
1:A:672:GLU:HB2	1:A:674:SER:HB3	2.03	0.40
1:B:373:THR:HB	1:B:517:ARG:HG3	2.03	0.40
1:B:675:ASP:HB3	1:B:687:LEU:HD11	2.02	0.40
1:A:317:ASP:CB	1:A:322:ARG:HD3	2.50	0.40
1:A:181:GLY:HA3	1:A:221:LEU:CD1	2.52	0.40
1:B:546:MET:HA	1:B:546:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

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	754/783 (96%)	724 (96%)	28 (4%)	2 (0%)	41 61
1	B	758/783 (97%)	732 (97%)	24 (3%)	2 (0%)	41 61
All	All	1512/1566 (97%)	1456 (96%)	52 (3%)	4 (0%)	41 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	550	GLY
1	A	677	PHE
1	B	317	ASP
1	A	318	SER

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	649/672 (97%)	570 (88%)	79 (12%)	5 9
1	B	653/672 (97%)	571 (87%)	82 (13%)	4 8
All	All	1302/1344 (97%)	1141 (88%)	161 (12%)	4 9

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	52	LEU
1	A	62	LEU
1	A	83	LYS
1	A	108	LEU
1	A	111	THR
1	A	119	LEU
1	A	127	VAL
1	A	128	THR
1	A	130	ASN
1	A	148	LEU
1	A	150	LEU
1	A	176	THR
1	A	201	LEU
1	A	208	GLU
1	A	226	GLN
1	A	243	THR
1	A	247	GLU
1	A	257	LYS
1	A	277	ASN
1	A	298	VAL
1	A	300	MET
1	A	301	GLN
1	A	310	ASP
1	A	312	GLN
1	A	313	VAL
1	A	315	ILE

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Mol	Chain	Res	Type
1	A	317	ASP
1	A	320	THR
1	A	322	ARG
1	A	323	LEU
1	A	325	LYS
1	A	327	ARG
1	A	341	GLU
1	A	343	LEU
1	A	347	ASN
1	A	349	SER
1	A	350	MET
1	A	358	GLN
1	A	362	ARG
1	A	391	THR
1	A	409	ARG
1	A	433	LEU
1	A	437	VAL
1	A	448	LEU
1	A	459	LEU
1	A	489	ARG
1	A	511	GLU
1	A	516	ARG
1	A	544	GLU
1	A	548	ARG
1	A	557	MET
1	A	560	ARG
1	A	564	ASP
1	A	575	SER
1	A	576	ARG
1	A	586	GLU
1	A	601	ASP
1	A	616	GLU
1	A	621	GLU
1	A	654	LEU
1	A	655	ASP
1	A	672	GLU
1	A	673	LYS
1	A	674	SER
1	A	675	ASP
1	A	677	PHE
1	A	679	LYS
1	A	683	GLU

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Mol	Chain	Res	Type
1	A	686	GLU
1	A	687	LEU
1	A	702	GLN
1	A	703	PHE
1	A	707	GLN
1	A	713	LYS
1	A	745	GLN
1	A	754	MET
1	A	775	VAL
1	A	777	LYS
1	B	14	ARG
1	B	17	ASN
1	B	69	VAL
1	B	70	ARG
1	B	101	LYS
1	B	128	THR
1	B	148	LEU
1	B	161	LYS
1	B	221	LEU
1	B	230	SER
1	B	245	LYS
1	B	248	LYS
1	B	253	ASP
1	B	254	ILE
1	B	255	LYS
1	B	260	GLN
1	B	264	GLU
1	B	271	LYS
1	B	277	ASN
1	B	292	GLN
1	B	312	GLN
1	B	314	VAL
1	B	315	ILE
1	B	316	VAL
1	B	317	ASP
1	B	319	PHE
1	B	320	THR
1	B	322	ARG
1	B	323	LEU
1	B	324	MET
1	B	325	LYS
1	B	328	ARG

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Mol	Chain	Res	Type
1	B	329	TYR
1	B	341	GLU
1	B	343	LEU
1	B	345	ILE
1	B	346	GLN
1	B	347	ASN
1	B	349	SER
1	B	351	THR
1	B	352	LEU
1	B	377	GLU
1	B	380	GLU
1	B	433	LEU
1	B	444	LEU
1	B	458	VAL
1	B	462	LYS
1	B	465	GLU
1	B	466	ARG
1	B	494	LYS
1	B	507	VAL
1	B	511	GLU
1	B	515	SER
1	B	516	ARG
1	B	523	ARG
1	B	528	ARG
1	B	548	ARG
1	B	553	ARG
1	B	554	THR
1	B	575	SER
1	B	576	ARG
1	B	593	ARG
1	B	596	LEU
1	B	597	LEU
1	B	601	ASP
1	B	610	ILE
1	B	620	SER
1	B	634	SER
1	B	645	ARG
1	B	646	GLU
1	B	667	ASP
1	B	672	GLU
1	B	674	SER
1	B	675	ASP

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Mol	Chain	Res	Type
1	B	677	PHE
1	B	679	LYS
1	B	682	ASP
1	B	691	ARG
1	B	702	GLN
1	B	723	LYS
1	B	746	THR
1	B	749	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	24	ASN
1	A	96	ASN
1	A	117	ASN
1	A	125	HIS
1	A	130	ASN
1	A	155	ASN
1	A	202	HIS
1	A	260	GLN
1	A	277	ASN
1	A	283	HIS
1	A	289	HIS
1	A	291	ASN
1	A	301	GLN
1	A	347	ASN
1	A	386	ASN
1	A	463	ASN
1	A	485	ASN
1	A	520	ASN
1	A	521	GLN
1	A	582	GLN
1	A	588	ASN
1	A	629	ASN
1	B	24	ASN
1	B	85	GLN
1	B	93	HIS
1	B	202	HIS
1	B	226	GLN
1	B	260	GLN
1	B	277	ASN

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Mol	Chain	Res	Type
1	B	283	HIS
1	B	289	HIS
1	B	292	GLN
1	B	301	GLN
1	B	312	GLN
1	B	347	ASN
1	B	358	GLN
1	B	460	ASN
1	B	463	ASN
1	B	521	GLN
1	B	529	GLN
1	B	570	GLN
1	B	606	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ADP	A	873	3	24,29,29	0.97	1 (4%)	29,45,45	1.31	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	B	873	3	24,29,29	0.99	1 (4%)	29,45,45	1.41	4 (13%)

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
4	ADP	A	873	3	-	6/12/32/32	0/3/3/3
4	ADP	B	873	3	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	873	ADP	C5-C4	2.58	1.47	1.40
4	A	873	ADP	C5-C4	2.50	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	873	ADP	N3-C2-N1	-3.36	123.43	128.68
4	B	873	ADP	N3-C2-N1	-3.22	123.64	128.68
4	B	873	ADP	C4-C5-N7	-3.08	106.19	109.40
4	B	873	ADP	PA-O3A-PB	-2.83	123.13	132.83
4	A	873	ADP	PA-O3A-PB	-2.72	123.48	132.83
4	A	873	ADP	C4-C5-N7	-2.70	106.59	109.40
4	B	873	ADP	C2-N1-C6	2.07	122.30	118.75
4	A	873	ADP	C2-N1-C6	2.02	122.20	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	873	ADP	C5'-O5'-PA-O1A
4	A	873	ADP	C5'-O5'-PA-O2A
4	A	873	ADP	C5'-O5'-PA-O3A
4	A	873	ADP	C3'-C4'-C5'-O5'
4	A	873	ADP	O4'-C4'-C5'-O5'
4	B	873	ADP	PA-O3A-PB-O1B
4	A	873	ADP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
4	B	873	ADP	C3'-C4'-C5'-O5'
4	B	873	ADP	PA-O3A-PB-O2B
4	B	873	ADP	PA-O3A-PB-O3B
4	B	873	ADP	O4'-C4'-C5'-O5'

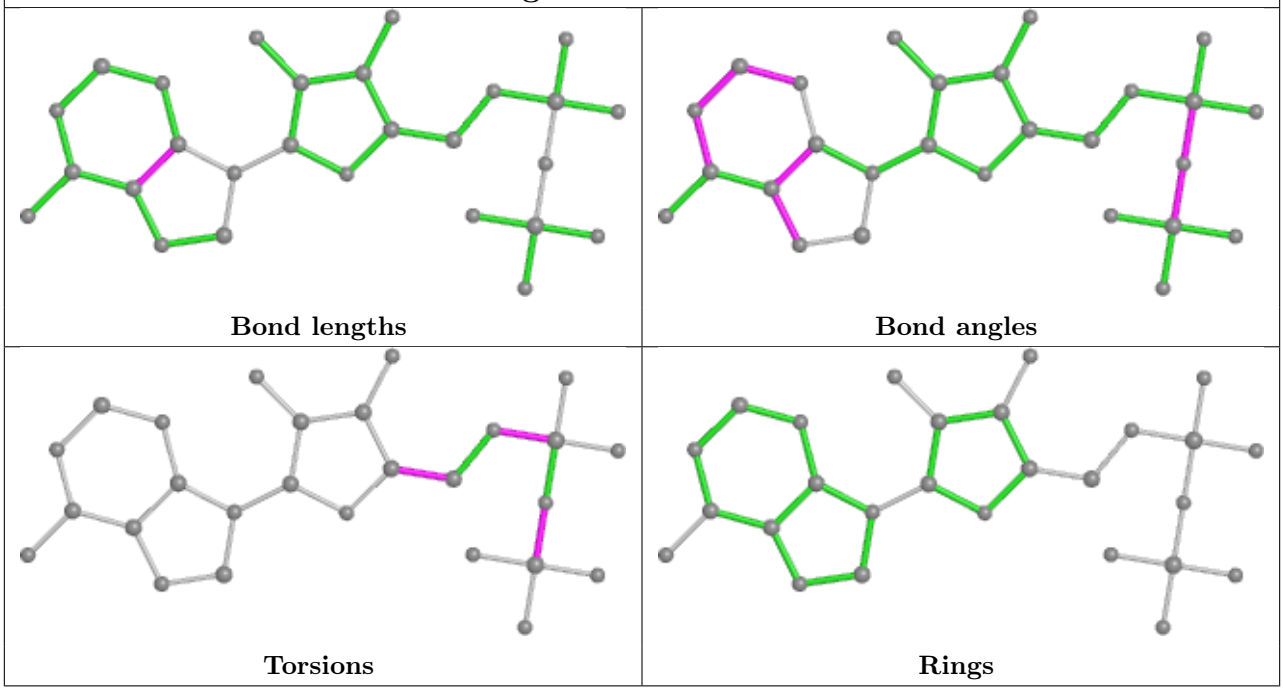
There are no ring outliers.

1 monomer is involved in 1 short contact:

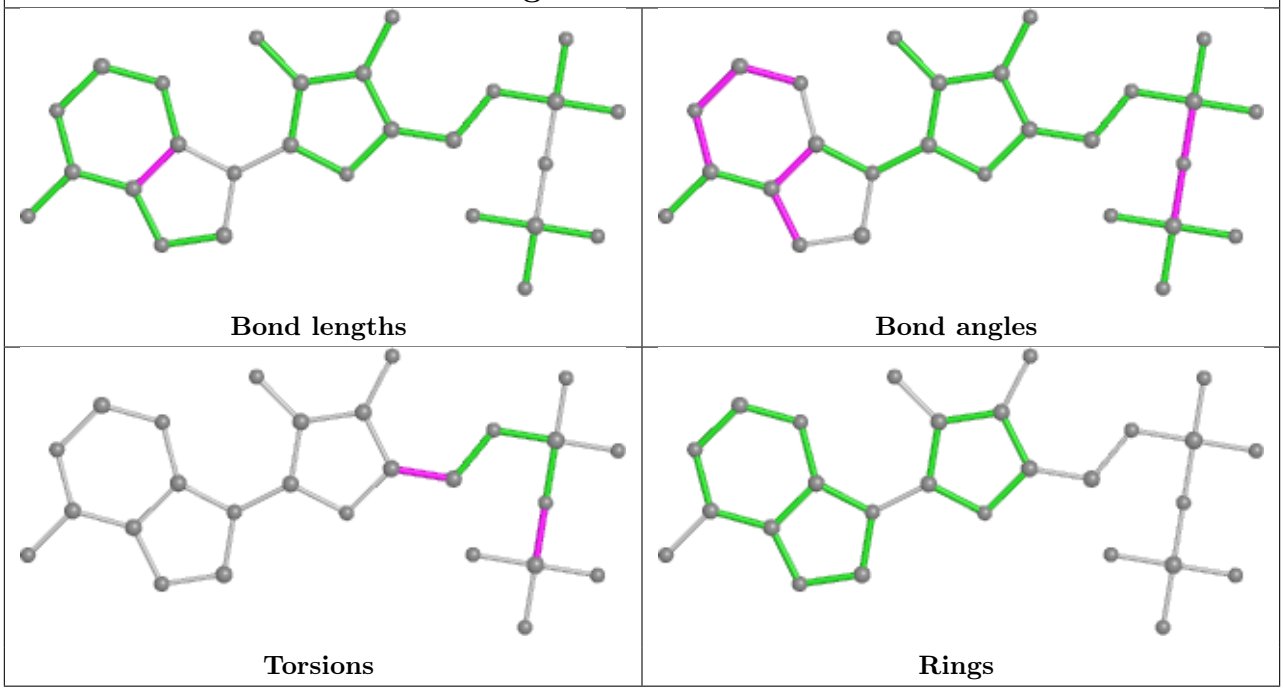
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	873	ADP	1	0

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 A 873



Ligand ADP B 873



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	758/783 (96%)	-0.30	15 (1%)	65	68	21, 48, 106, 178	0
1	B	762/783 (97%)	-0.34	11 (1%)	75	77	21, 49, 104, 171	0
2	C	0/3	-	-			-	-
2	D	0/3	-	-			-	-
All	All	1520/1572 (96%)	-0.32	26 (1%)	70	72	21, 49, 106, 178	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	PHE	5.7
1	A	256	THR	5.6
1	A	254	ILE	4.3
1	A	257	LYS	4.2
1	A	253	ASP	3.6
1	A	461	ALA	3.6
1	A	315	ILE	3.5
1	B	319	PHE	3.4
1	A	255	LYS	3.3
1	B	322	ARG	3.1
1	A	325	LYS	2.8
1	B	315	ILE	2.8
1	A	303	ASP	2.8
1	B	320	THR	2.7
1	B	303	ASP	2.6
1	B	329	TYR	2.5
1	A	324	MET	2.5
1	B	254	ILE	2.4
1	A	549	PHE	2.2
1	A	322	ARG	2.2
1	B	327	ARG	2.1
1	A	745	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	318	SER	2.1
1	B	256	THR	2.1
1	B	347	ASN	2.0
1	A	323	LEU	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)

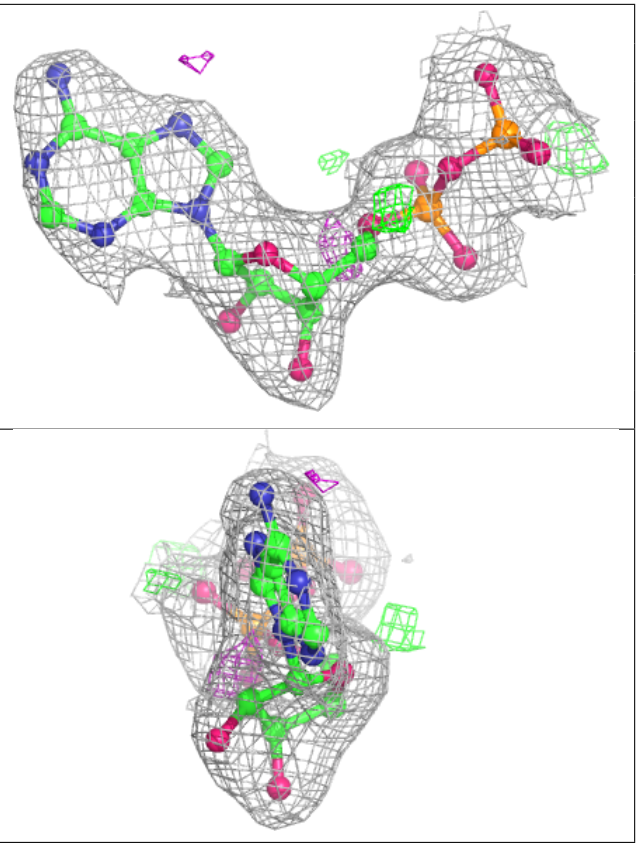
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	872	1/1	0.84	0.24	69,69,69,69	0
3	MG	A	872	1/1	0.95	0.18	60,60,60,60	0
4	ADP	B	873	27/27	0.96	0.14	49,66,76,78	0
4	ADP	A	873	27/27	0.97	0.15	50,73,78,80	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.

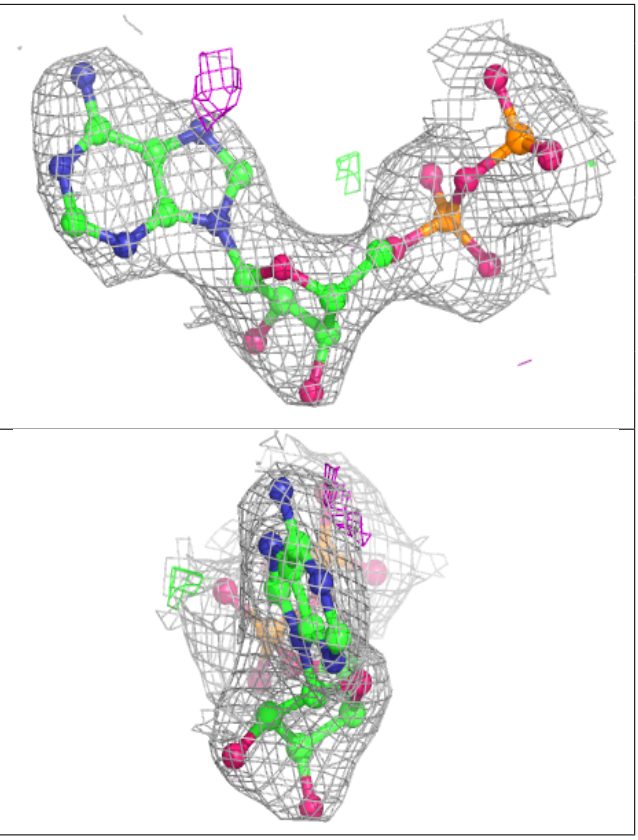
Electron density around ADP B 873:

$2mF_o$-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 A 873:

$2mF_o$-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.