Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 05:13 am GMT

PDB ID	:	2VF8
Title	:	Crystal structure of UvrA2 from Deinococcus radiodurans
Authors	:	Timmins, J.; Gordon, E.; Caria, S.; Leonard, G.; Kuo, M.S.; Monchois, V.; McSweeney, S.
Deposited on	:	2007-10-31
Resolution	:	3.00 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 ⓘ 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 ⓘ) were used in the production of this report:

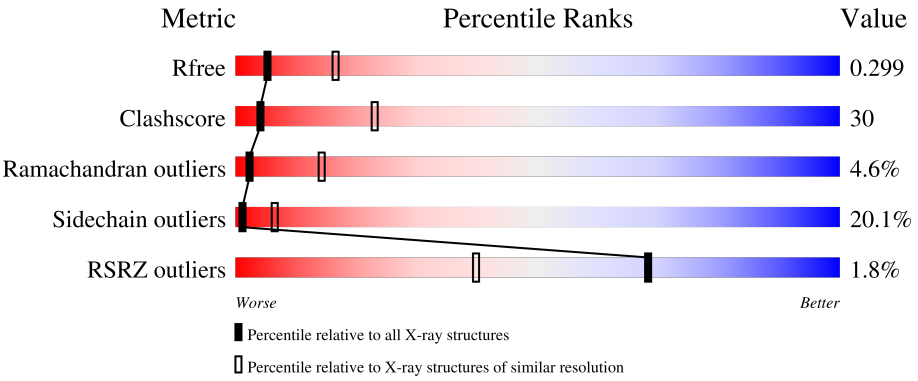
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	842	45% 38% 11%
1	B	842	3% 43% 41% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12843 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.

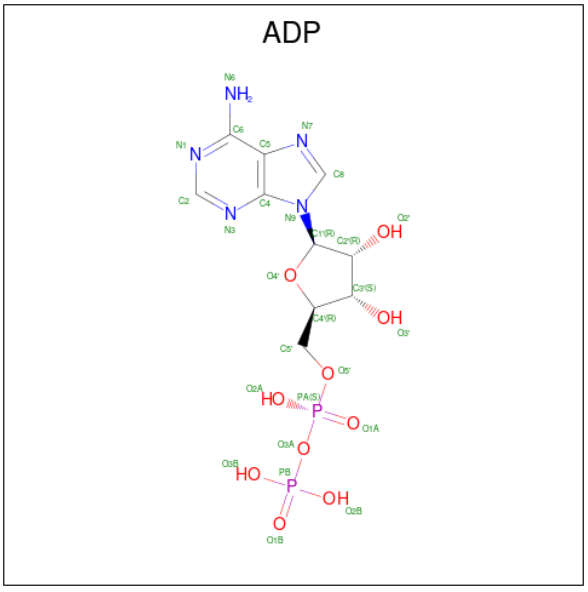
- Molecule 1 is a protein called EXCINUCLEASE ABC SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	806	Total	C	N	O	S	0	26	0
			6182	3879	1119	1165	19			
1	B	835	Total	C	N	O	S	0	26	0
			6402	4014	1154	1215	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	746	ARG	GLN	engineered mutation	UNP Q9RYW8
B	746	ARG	GLN	engineered mutation	UNP Q9RYW8

- 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		

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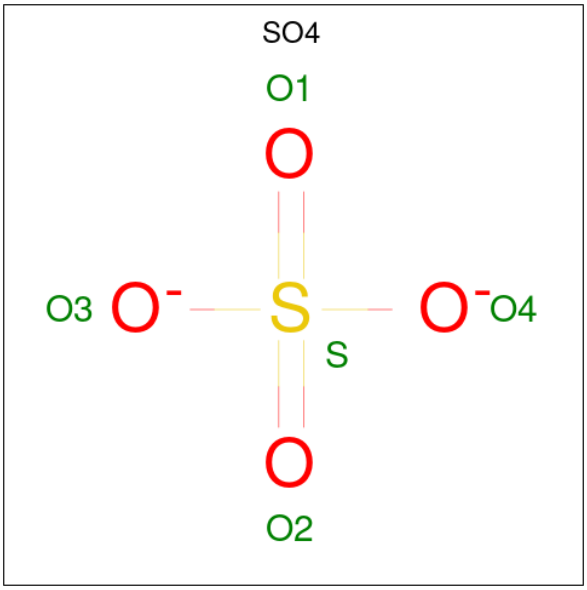
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 27 10 5 10 2	0	0
2	B	1	Total C N O P 27 10 5 10 2	0	0
2	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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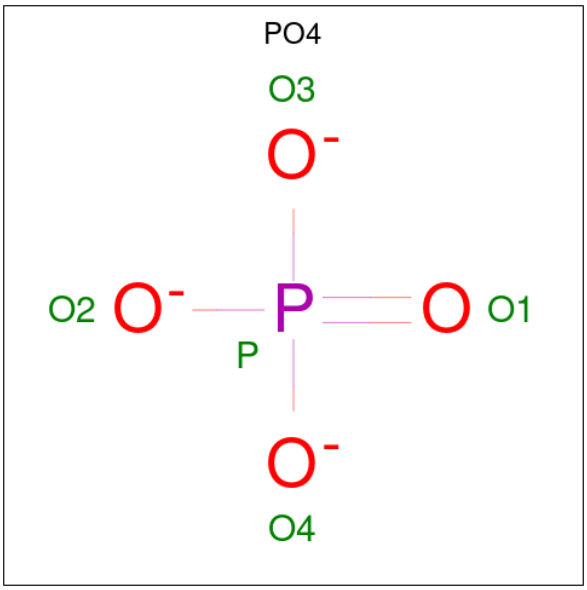
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	1
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	1
4	B	1	Total O S 5 4 1	0	1

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	1

- Molecule 6 is water.

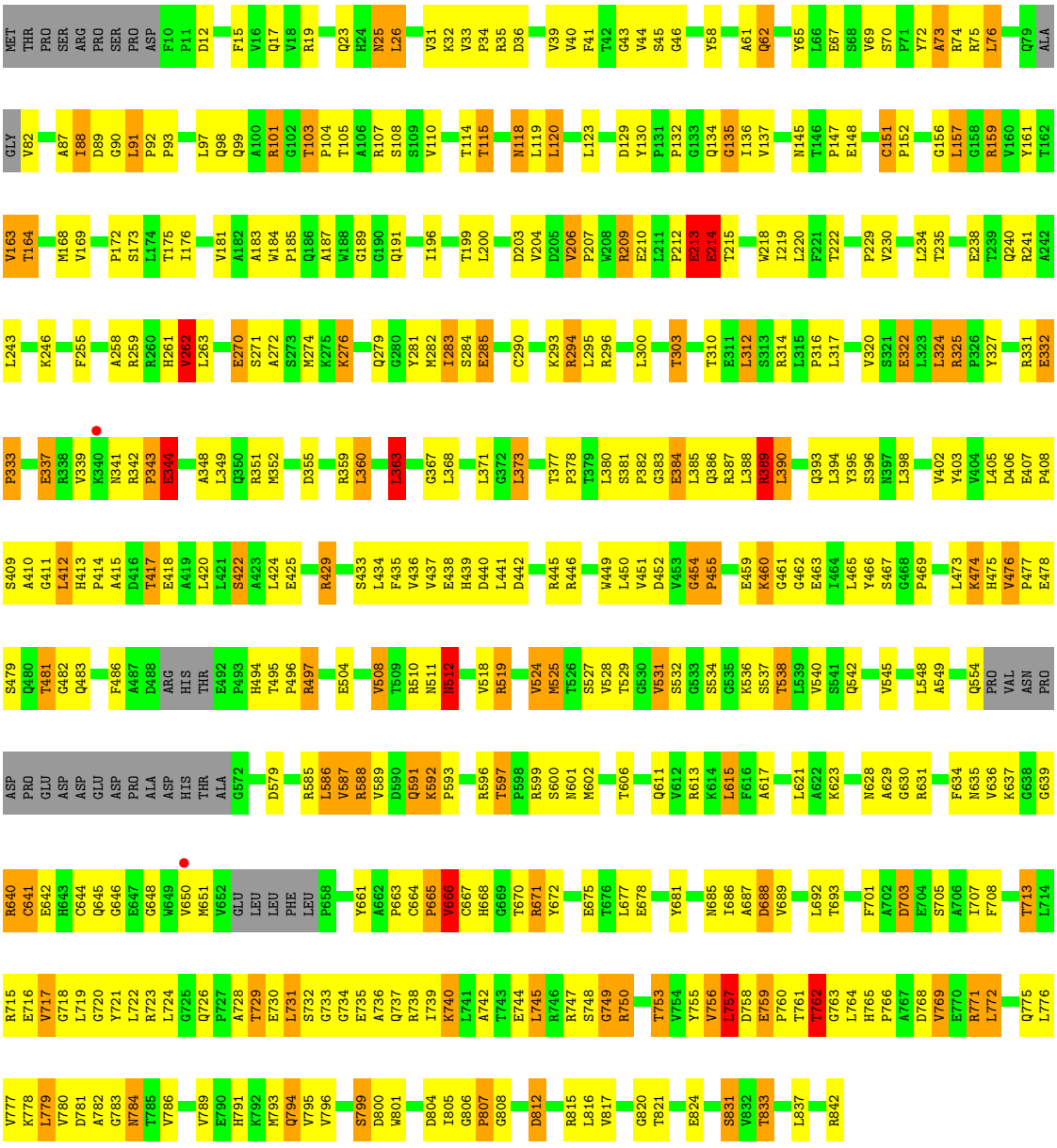
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	37	Total O 37 37	0	0
6	B	65	Total O 65 65	0	0

3 Residue-property plots (i)

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

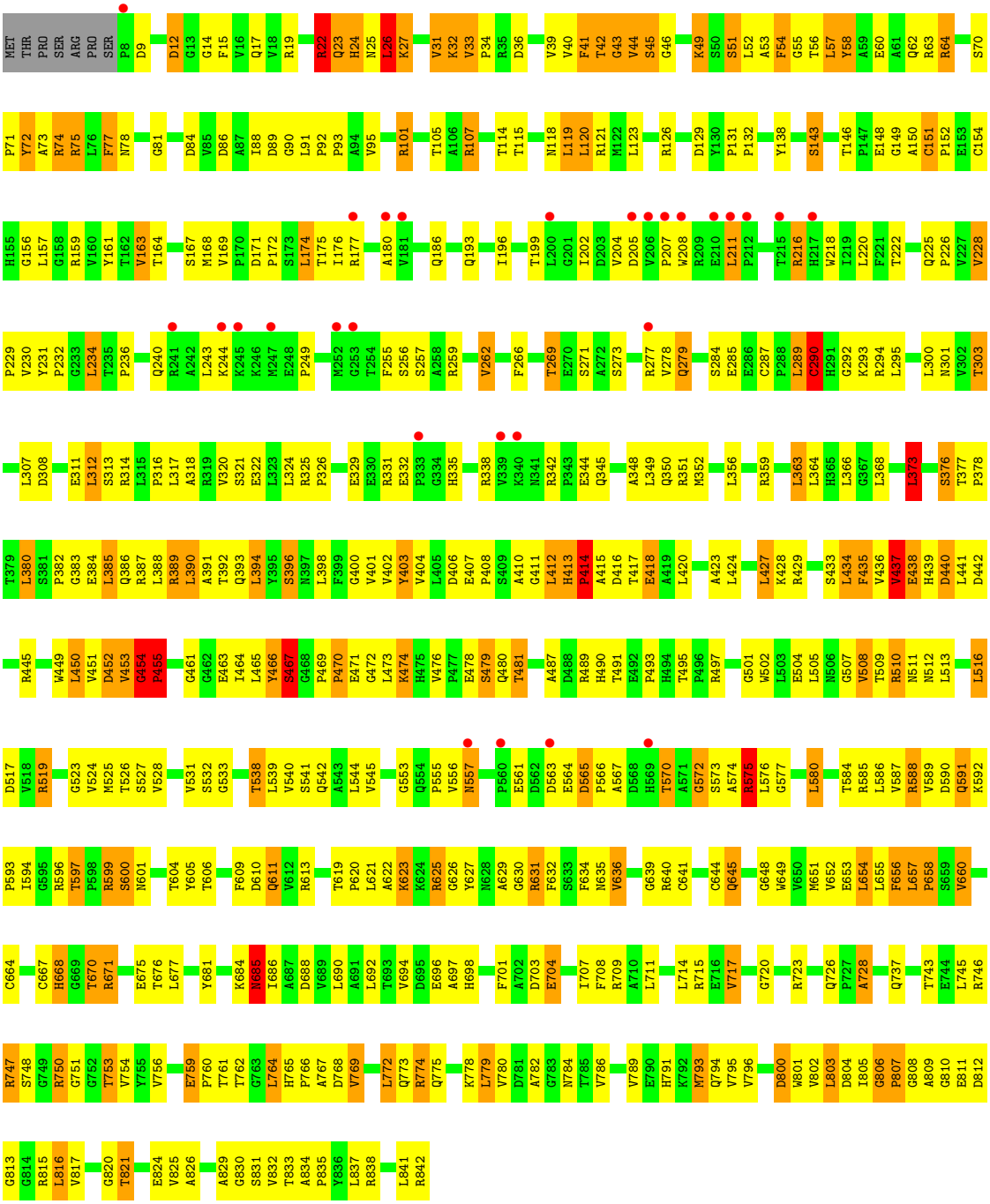
• Molecule 1: EXCINUCLEASE ABC SUBUNIT A

Chain A:



• Molecule 1: EXCINUCLEASE ABC SUBUNIT A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	149.63Å 171.04Å 204.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.06 – 3.00 49.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (102.06-3.00) 96.0 (49.31-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.294 0.235 , 0.299	Depositor DCC
R_{free} test set	2543 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12843	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: ZN, ADP, SO4, PO4

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	0.87	3/6312 (0.0%)	0.88	8/8572 (0.1%)
1	B	0.95	23/6543 (0.4%)	1.02	22/8899 (0.2%)
All	All	0.91	26/12855 (0.2%)	0.95	30/17471 (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	3
1	B	0	4
All	All	0	7

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CD-OE2	29.64	1.58	1.25
1	A	270	GLU	CD-OE1	17.04	1.44	1.25
1	B	290	CYS	CB-SG	-12.89	1.60	1.82
1	B	438	GLU	N-CA	11.50	1.69	1.46
1	B	466	TYR	C-O	10.13	1.42	1.23
1	B	455	PRO	C-O	8.81	1.40	1.23
1	B	467	SER	CB-OG	8.62	1.53	1.42
1	B	43	GLY	CA-C	8.29	1.65	1.51
1	A	276	LYS	CE-NZ	8.19	1.69	1.49
1	B	45	SER	CB-OG	7.63	1.52	1.42
1	B	467	SER	CA-CB	7.44	1.64	1.52
1	B	57	LEU	N-CA	6.92	1.60	1.46
1	B	44	VAL	CA-CB	-6.89	1.40	1.54
1	B	438	GLU	CB-CG	6.89	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	453	VAL	CB-CG1	6.64	1.66	1.52
1	B	455	PRO	N-CD	-6.55	1.38	1.47
1	B	452	ASP	C-O	6.45	1.35	1.23
1	B	454	GLY	N-CA	6.35	1.55	1.46
1	B	452	ASP	CB-CG	-6.18	1.38	1.51
1	B	42	THR	C-N	6.11	1.44	1.33
1	B	41	PHE	CB-CG	-6.02	1.41	1.51
1	B	403	TYR	CE2-CZ	5.99	1.46	1.38
1	B	437	VAL	CA-C	-5.98	1.37	1.52
1	B	438	GLU	CA-C	5.87	1.68	1.52
1	B	435	PHE	CD1-CE1	5.25	1.49	1.39
1	B	45	SER	CA-CB	5.16	1.60	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	452	ASP	CB-CG-OD1	-18.46	101.69	118.30
1	B	452	ASP	CB-CG-OD2	10.81	128.03	118.30
1	B	436	VAL	CG1-CB-CG2	8.45	124.42	110.90
1	B	44	VAL	O-C-N	-7.97	109.95	122.70
1	A	157	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	B	465	LEU	CA-CB-CG	-6.18	101.08	115.30
1	A	389	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	436	VAL	CA-CB-CG1	-6.13	101.70	110.90
1	B	467	SER	N-CA-CB	6.04	119.57	110.50
1	B	36	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	324	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	270	GLU	OE1-CD-OE2	5.93	130.41	123.30
1	A	241[A]	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	44	VAL	CG1-CB-CG2	5.80	120.18	110.90
1	A	135	GLY	N-CA-C	5.60	127.09	113.10
1	B	772	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	757	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	575	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	435	PHE	N-CA-CB	-5.38	100.92	110.60
1	B	441	LEU	CA-CB-CG	-5.35	103.00	115.30
1	B	44	VAL	CA-CB-CG1	5.27	118.80	110.90
1	B	373	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	324	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	454	GLY	CA-C-O	-5.14	111.35	120.60
1	B	33	VAL	CB-CA-C	-5.09	101.72	111.40
1	B	22	ARG	NE-CZ-NH1	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	363	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	31	VAL	CB-CA-C	-5.01	101.87	111.40
1	B	84	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	GLY	Peptide
1	A	666	VAL	Peptide
1	A	806	GLY	Peptide
1	B	45	SER	Mainchain
1	B	455	PRO	Mainchain
1	B	565	ASP	Peptide
1	B	806	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6182	0	6036	368	0
1	B	6402	0	6222	382	0
2	A	54	0	24	5	0
2	B	54	0	24	10	0
3	A	2	0	0	0	0
3	B	2	0	0	1	0
4	A	15	0	0	0	0
4	B	25	0	0	0	0
5	B	5	0	0	0	0
6	A	37	0	0	5	0
6	B	65	0	0	9	0
All	All	12843	0	12306	750	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 30.

All (750) 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:276:LYS:CE	1:A:276:LYS:NZ	1.69	1.52
1:B:438:GLU:N	1:B:438:GLU:CA	1.69	1.51
1:A:759:GLU:OE2	1:A:791[A]:HIS:CD2	1.83	1.30
1:B:413:HIS:CE1	1:B:833:THR:HG22	1.77	1.19
1:B:413:HIS:HE1	1:B:833:THR:HG22	1.06	1.17
1:B:487:ALA:HB1	1:B:490:HIS:NE2	1.65	1.11
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.15	1.09
1:A:764:LEU:HD12	1:A:768:ASP:HB3	1.32	1.06
1:A:120:LEU:H	1:A:120:LEU:HD12	1.23	1.00
1:B:685:ASN:HD22	1:B:686:ILE:H	1.02	0.99
1:A:343:PRO:HD2	1:A:344:GLU:OE1	1.63	0.97
1:B:412:LEU:HD21	1:B:416:ASP:HB2	1.45	0.97
1:A:413:HIS:HE1	1:A:833:THR:HG22	1.27	0.96
1:B:196:ILE:HG23	1:B:228:VAL:HG21	1.48	0.96
1:A:452:ASP:OD1	1:A:481:THR:HG21	1.66	0.96
1:A:670:THR:HG21	1:A:677:LEU:HD11	1.47	0.96
1:A:418:GLU:OE1	1:A:446:ARG:NH2	1.98	0.95
1:A:592:LYS:HG3	1:A:593:PRO:HD2	1.47	0.94
1:A:804:ASP:HB3	1:A:817:VAL:HG23	1.48	0.93
1:A:386:GLN:NE2	1:A:406:ASP:H	1.65	0.93
1:A:753:THR:N	1:A:784:ASN:HD21	1.66	0.93
1:A:585:ARG:HB2	1:A:753:THR:HB	1.49	0.91
1:A:538:THR:HG23	2:A:1844:ADP:O2A	1.70	0.91
1:B:599:ARG:HH11	1:B:599:ARG:CG	1.82	0.91
1:A:753:THR:H	1:A:784:ASN:HD21	1.13	0.91
1:A:755:TYR:HB2	1:A:786:VAL:HG12	1.51	0.90
1:A:599:ARG:HD2	1:A:635:ASN:ND2	1.86	0.89
1:A:386:GLN:HE22	1:A:406:ASP:H	0.90	0.88
1:A:108:SER:O	1:A:377:THR:HG23	1.73	0.87
1:A:644:CYS:SG	1:A:648:GLY:N	2.47	0.87
1:B:287:CYS:SG	1:B:290:CYS:HB2	2.15	0.86
1:A:412:LEU:O	1:A:791[B]:HIS:HD2	1.57	0.86
1:A:46:GLY:O	2:A:1843:ADP:H5'2	1.76	0.86
1:A:670:THR:O	1:A:671:ARG:HB2	1.76	0.86
1:B:504:GLU:HB2	1:B:577:GLY:O	1.77	0.85
1:B:159:ARG:HD3	1:B:284:SER:OG	1.76	0.85
1:A:413:HIS:CE1	1:A:833:THR:HG22	2.10	0.84
1:B:599:ARG:HE	1:B:635:ASN:ND2	1.75	0.84
1:B:580:LEU:HD12	1:B:580:LEU:H	1.44	0.83
1:A:527:SER:HB3	1:A:796:VAL:HG22	1.60	0.83
1:B:759:GLU:CG	1:B:791:HIS:HD2	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:VAL:HG13	1:B:586:LEU:HD21	1.62	0.82
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.43	0.82
1:B:807:PRO:HG3	1:B:815[A]:ARG:NH1	1.93	0.82
1:A:120:LEU:HD12	1:A:120:LEU:N	1.93	0.82
1:A:199:THR:HG21	1:A:229:PRO:O	1.80	0.82
1:B:413:HIS:HD2	1:B:415:ALA:H	1.28	0.82
1:A:411:GLY:HA2	1:A:791[A]:HIS:CD2	2.14	0.81
1:B:759:GLU:CG	1:B:791:HIS:CD2	2.64	0.81
1:A:478:GLU:N	1:A:478:GLU:OE1	2.14	0.81
1:B:338:ARG:HH11	1:B:345:GLN:HE22	1.30	0.80
1:B:685:ASN:HD22	1:B:686:ILE:N	1.80	0.80
1:A:181:VAL:HG11	1:A:184:TRP:CE3	2.17	0.80
1:B:487:ALA:CB	1:B:490:HIS:NE2	2.43	0.80
1:B:599:ARG:HG2	1:B:599:ARG:NH1	1.97	0.79
1:A:615:LEU:HD11	1:A:681:TYR:CE1	2.16	0.79
1:A:804:ASP:OD2	1:A:831:SER:HB2	1.82	0.79
1:B:176:ILE:HD12	1:B:204:VAL:HA	1.65	0.79
1:A:670:THR:HG22	1:A:672:TYR:H	1.45	0.79
1:A:497:ARG:HH11	1:A:497:ARG:CG	1.96	0.78
1:A:750:ARG:HA	1:A:750:ARG:NH1	1.99	0.78
1:B:413:HIS:HE1	1:B:833:THR:CG2	1.94	0.78
1:A:589:VAL:HB	1:A:757:LEU:HB3	1.65	0.78
1:B:175:THR:HG23	1:B:205:ASP:HA	1.65	0.78
1:A:173:SER:HA	1:A:209:ARG:HD3	1.65	0.78
1:B:759:GLU:HG2	1:B:791:HIS:CD2	2.18	0.77
1:A:762:THR:HG23	1:A:763:GLY:N	2.00	0.77
1:A:327:TYR:HA	1:A:332:GLU:HG2	1.66	0.77
1:A:386:GLN:HE22	1:A:406:ASP:N	1.75	0.76
1:A:438:GLU:HG3	1:A:440:ASP:H	1.50	0.76
1:B:163:VAL:HA	6:B:2011:HOH:O	1.84	0.76
1:A:373:LEU:HD23	1:A:373:LEU:H	1.50	0.76
1:A:762:THR:CG2	1:A:763:GLY:H	1.98	0.76
1:B:698:HIS:CD2	1:B:715:ARG:HD2	2.19	0.76
1:B:413:HIS:CD2	1:B:415:ALA:H	2.04	0.76
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.49	0.76
1:A:413:HIS:HE1	1:A:833:THR:CG2	1.97	0.76
1:B:287:CYS:HG	3:B:1845:ZN:ZN	0.99	0.76
1:B:538:THR:HG21	2:B:1844:ADP:H5'1	1.65	0.75
1:A:40:VAL:HG12	1:A:450:LEU:HD12	1.67	0.75
1:B:226:PRO:HD2	1:B:255:PHE:HB3	1.67	0.75
1:A:412:LEU:O	1:A:791[B]:HIS:CD2	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:GLN:HE22	1:B:760:PRO:HA	1.52	0.74
1:B:796:VAL:HG12	1:B:837:LEU:HD21	1.68	0.74
1:A:450:LEU:HG	1:A:451:VAL:N	2.02	0.74
1:A:599:ARG:CD	1:A:635:ASN:HD21	1.99	0.74
1:B:829:ALA:HA	6:B:2058:HOH:O	1.86	0.74
1:B:77:PHE:CZ	1:B:654:LEU:CB	2.71	0.73
1:B:380:LEU:HD23	1:B:385:LEU:HB3	1.69	0.73
1:B:508:VAL:HA	1:B:574:ALA:HB2	1.69	0.73
1:B:22:ARG:NH2	1:B:86:ASP:OD1	2.15	0.73
1:A:529:THR:HG22	1:A:796:VAL:HG21	1.70	0.72
1:A:599:ARG:CD	1:A:635:ASN:ND2	2.51	0.72
1:A:586:LEU:O	1:A:586:LEU:HG	1.88	0.72
1:A:642:GLU:OE1	1:A:642:GLU:HA	1.89	0.72
1:B:348:ALA:O	1:B:352:MET:HB2	1.89	0.72
1:B:320:VAL:HG21	1:B:373:LEU:HD21	1.70	0.72
1:B:454:GLY:HA2	1:B:463:GLU:HB2	1.72	0.72
1:B:77:PHE:CZ	1:B:654:LEU:HB3	2.25	0.71
1:A:279:GLN:HA	1:A:282:MET:HE2	1.71	0.71
1:A:511:ASN:HD22	1:A:538:THR:HG21	1.54	0.71
1:A:531:VAL:HG12	1:A:534:SER:HB3	1.72	0.71
1:A:641:CYS:SG	1:A:667:CYS:HB3	2.30	0.71
1:B:290:CYS:SG	1:B:293:LYS:O	2.48	0.71
1:A:602:MET:HG3	1:A:739:ILE:HD11	1.72	0.71
1:B:807:PRO:HD2	1:B:813:GLY:HA2	1.72	0.71
1:B:311:GLU:HG2	6:B:2018:HOH:O	1.90	0.71
1:A:25:ASN:H	1:A:25:ASN:HD22	1.39	0.70
1:A:719:LEU:HD22	1:A:722:LEU:HD11	1.72	0.70
1:B:450:LEU:O	1:B:467:SER:HA	1.91	0.70
1:B:49:LYS:HE3	1:B:439:HIS:NE2	2.06	0.70
1:A:425:GLU:HA	1:A:425:GLU:OE1	1.90	0.70
1:B:44:VAL:HG13	1:B:768:ASP:OD1	1.90	0.70
1:B:77:PHE:CE1	1:B:654:LEU:HB2	2.27	0.69
1:B:196:ILE:HG23	1:B:228:VAL:CG2	2.22	0.69
1:A:597:THR:HB	1:A:599:ARG:H	1.58	0.69
1:B:307:LEU:HB3	1:B:311:GLU:HB3	1.74	0.69
1:B:580:LEU:HD12	1:B:580:LEU:N	2.07	0.69
1:B:538:THR:CG2	2:B:1844:ADP:H5'1	2.23	0.69
1:B:580:LEU:H	1:B:580:LEU:CD1	2.05	0.69
1:A:759:GLU:OE2	1:A:791[A]:HIS:NE2	2.25	0.69
1:A:762:THR:HG23	1:A:763:GLY:H	1.54	0.69
1:A:613:ARG:HH11	1:A:630:GLY:HA3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ARG:HH11	1:B:575:ARG:CG	2.06	0.69
1:A:367:GLY:HA2	6:A:2020:HOH:O	1.93	0.68
1:A:411:GLY:HA2	1:A:791[A]:HIS:NE2	2.07	0.68
1:B:773[A]:GLN:NE2	1:B:795:VAL:HG23	2.08	0.68
1:A:769:VAL:HG21	1:A:794:GLN:OE1	1.93	0.68
1:B:42:THR:OG1	1:B:452:ASP:OD1	2.10	0.68
1:A:344:GLU:HA	6:A:2016:HOH:O	1.94	0.68
1:A:466:TYR:OH	1:A:469:PRO:O	2.10	0.68
1:B:508:VAL:HA	1:B:574:ALA:CB	2.23	0.67
1:B:619:THR:HB	1:B:620:PRO:HD2	1.75	0.67
1:A:776:LEU:HA	1:A:779:LEU:HD22	1.76	0.67
1:B:146:THR:HB	1:B:148:GLU:OE2	1.94	0.67
1:B:386:GLN:HE22	1:B:406:ASP:H	1.43	0.67
1:B:453:VAL:O	1:B:454:GLY:O	2.13	0.67
1:A:764:LEU:CD1	1:A:768:ASP:HB3	2.19	0.67
1:A:295:LEU:HB2	1:A:300:LEU:CD1	2.25	0.67
1:B:412:LEU:CD2	1:B:416:ASP:HB2	2.23	0.66
1:B:759:GLU:HG3	1:B:791:HIS:CD2	2.30	0.66
1:A:675:GLU:O	1:A:678:GLU:N	2.27	0.66
1:A:747:ARG:O	1:A:749:GLY:N	2.27	0.66
1:A:762:THR:CG2	1:A:763:GLY:N	2.56	0.66
1:A:497:ARG:HG2	1:A:497:ARG:NH1	1.95	0.66
1:B:159:ARG:HB2	1:B:285:GLU:O	1.96	0.66
1:B:53:ALA:HA	1:B:57:LEU:HD12	1.77	0.66
1:B:290:CYS:HB3	1:B:292:GLY:H	1.60	0.66
1:B:424:LEU:HD22	1:B:434:LEU:HD22	1.77	0.66
1:B:77:PHE:CZ	1:B:654:LEU:HB2	2.30	0.65
1:A:529:THR:CG2	1:A:796:VAL:HG21	2.25	0.65
1:A:670:THR:O	1:A:671:ARG:CB	2.44	0.65
1:A:613:ARG:HD2	1:A:630:GLY:HA2	1.79	0.65
1:A:646:GLY:O	1:A:671:ARG:HG2	1.97	0.65
1:B:599:ARG:HH11	1:B:599:ARG:HG3	1.62	0.65
1:A:393:GLN:HA	1:A:396:SER:HB3	1.79	0.65
1:A:413:HIS:HD2	1:A:415:ALA:H	1.42	0.65
1:A:405:LEU:HB2	1:A:436:VAL:HG22	1.79	0.65
1:A:753:THR:N	1:A:784:ASN:ND2	2.44	0.64
1:B:807:PRO:HG3	1:B:815[A]:ARG:HH11	1.59	0.64
1:B:622:ALA:HA	1:B:627:TYR:HB2	1.79	0.64
1:B:428:LYS:HB2	1:B:434:LEU:HD11	1.79	0.64
1:B:466:TYR:OH	1:B:472:GLY:HA3	1.97	0.64
1:B:211:LEU:O	1:B:216:ARG:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:TRP:CH2	1:B:820:GLY:HA2	2.33	0.64
1:B:385:LEU:HD12	1:B:385:LEU:H	1.63	0.64
1:A:322:GLU:HG3	1:A:325:ARG:HH21	1.63	0.63
1:A:168:MET:HE2	1:A:258:ALA:HB1	1.81	0.63
1:B:90:GLY:O	1:B:92:PRO:HD3	1.99	0.63
1:B:600:SER:O	1:B:728:ALA:HB2	1.99	0.63
1:B:509:THR:HA	1:B:513:LEU:O	1.97	0.63
1:A:349:LEU:O	1:A:349:LEU:HD23	1.99	0.63
1:B:403:TYR:CE1	1:B:427:LEU:HD22	2.33	0.63
1:B:750:ARG:HB3	1:B:750:ARG:CZ	2.28	0.63
1:A:723:ARG:HB2	1:A:726:GLN:HB2	1.81	0.62
1:A:295:LEU:HB2	1:A:300:LEU:HD13	1.81	0.62
1:A:615:LEU:HD11	1:A:681:TYR:CD1	2.34	0.62
1:A:235:THR:O	1:A:238:GLU:HG2	1.99	0.62
1:B:631:ARG:NH2	1:B:676:THR:OG1	2.28	0.62
1:B:644:CYS:O	1:B:645:GLN:HB2	1.99	0.62
1:B:176:ILE:HB	1:B:204:VAL:HG13	1.82	0.62
1:A:359:ARG:HH11	1:A:395:TYR:HD1	1.48	0.62
1:A:17:GLN:HE22	1:A:32:LYS:HB3	1.65	0.61
1:A:591[A]:GLN:OE1	1:A:762:THR:OG1	2.18	0.61
1:B:805:ILE:HG22	1:B:806:GLY:N	2.15	0.61
1:B:807:PRO:CD	1:B:813:GLY:HA2	2.30	0.61
1:A:25:ASN:ND2	2:A:1843:ADP:H4'	2.15	0.61
1:A:110:VAL:O	1:A:114:THR:HG23	2.00	0.61
1:A:776:LEU:HA	1:A:779:LEU:CD2	2.30	0.61
1:A:73:ALA:HA	1:A:76:LEU:HB2	1.82	0.61
1:B:403:TYR:CE1	1:B:427:LEU:CD2	2.84	0.61
1:A:672:TYR:HB2	1:A:677:LEU:HD21	1.82	0.61
1:A:807:PRO:HD2	1:A:812:ASP:O	1.99	0.61
1:B:12:ASP:C	1:B:14:GLY:H	2.04	0.61
1:A:271:SER:HB3	1:A:274:MET:HB3	1.83	0.61
1:A:599:ARG:HD2	1:A:635:ASN:HD22	1.64	0.61
1:B:49:LYS:CE	1:B:439:HIS:NE2	2.64	0.60
1:A:183:ALA:HA	1:A:281:TYR:CE2	2.36	0.60
1:B:597:THR:OG1	1:B:599:ARG:HB2	2.01	0.60
1:A:729:THR:O	1:A:730:GLU:HG3	2.01	0.60
1:B:222:THR:O	1:B:257:SER:OG	2.17	0.60
1:A:235:THR:HG22	1:A:238:GLU:CD	2.22	0.60
1:B:143:SER:O	1:B:149:GLY:HA3	2.02	0.60
1:B:388:LEU:O	1:B:391:ALA:HB3	2.02	0.60
1:A:103:THR:HG22	1:A:104:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:CYS:HB2	1:A:293:LYS:O	2.01	0.60
1:A:147:PRO:HG2	1:A:148:GLU:OE2	2.01	0.60
1:A:592:LYS:HG3	1:A:593:PRO:CD	2.27	0.60
1:B:538:THR:HG23	2:B:1844:ADP:O2A	2.02	0.60
1:A:734:GLY:HA2	1:A:762:THR:HG21	1.82	0.60
1:A:161:TYR:OH	1:A:279:GLN:HG2	2.01	0.60
1:B:599:ARG:NE	1:B:635:ASN:ND2	2.48	0.60
1:A:164:THR:O	1:A:168:MET:HG3	2.01	0.59
1:B:231:TYR:HB2	1:B:234:LEU:HD11	1.84	0.59
1:B:657:LEU:HB2	1:B:658:PRO:HD2	1.84	0.59
1:A:524:VAL:HG13	1:A:800:ASP:HB2	1.84	0.59
1:B:613:ARG:HB3	1:B:629:ALA:HB1	1.84	0.59
1:A:455:PRO:HD2	1:A:461:GLY:HA2	1.82	0.59
1:A:176:ILE:HB	1:A:204:VAL:HG13	1.83	0.59
1:A:508:VAL:HG22	1:A:508:VAL:O	2.01	0.59
1:A:769:VAL:HG21	1:A:794:GLN:CD	2.23	0.59
1:B:49:LYS:HG3	2:B:1843:ADP:O1B	2.03	0.59
1:B:491:THR:HG22	1:B:842:ARG:OXT	2.03	0.59
1:B:694:VAL:HG12	1:B:720:GLY:HA2	1.85	0.59
1:B:714:LEU:O	1:B:717:VAL:HG12	2.02	0.59
1:A:343:PRO:HG2	1:A:344:GLU:HG3	1.85	0.59
1:B:193:GLN:HE22	1:B:255:PHE:HA	1.67	0.59
1:B:313:SER:HA	1:B:373:LEU:HD23	1.83	0.59
1:B:807:PRO:HD2	1:B:812:ASP:O	2.02	0.59
1:A:527:SER:CB	1:A:796:VAL:HG22	2.31	0.59
1:A:168:MET:HE2	1:A:258:ALA:CB	2.33	0.58
1:A:398:LEU:HD23	1:B:64:ARG:HB3	1.85	0.58
1:A:613:ARG:HH11	1:A:630:GLY:CA	2.15	0.58
1:A:821:THR:OG1	1:A:824:GLU:HG3	2.03	0.58
1:B:294:ARG:NH2	6:B:2017:HOH:O	2.36	0.58
1:A:666:VAL:HG23	1:A:666:VAL:O	2.04	0.58
1:B:779:LEU:N	1:B:779:LEU:HD23	2.19	0.58
1:A:327:TYR:HA	1:A:332:GLU:CG	2.33	0.58
1:B:516:LEU:HD11	1:B:816:LEU:HB2	1.84	0.58
1:B:711:LEU:O	1:B:715:ARG:HG3	2.04	0.58
1:A:479:SER:O	1:A:482:GLY:N	2.36	0.58
1:B:553:GLY:O	1:B:555:PRO:HD3	2.03	0.58
1:A:93:PRO:HG2	1:B:93:PRO:HG2	1.86	0.57
1:A:807:PRO:HD2	1:A:808:GLY:H	1.68	0.57
1:A:312:LEU:HD11	1:A:320:VAL:HG13	1.86	0.57
1:A:454:GLY:O	1:A:465:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:HD3	1:A:635:ASN:HD21	1.69	0.57
1:B:373:LEU:HD22	1:B:373:LEU:H	1.69	0.57
1:A:615:LEU:CD1	1:A:681:TYR:CD1	2.86	0.57
1:A:759:GLU:OE1	1:A:759:GLU:HA	2.03	0.57
1:B:694:VAL:CG1	1:B:720:GLY:HA2	2.35	0.57
1:B:834:ALA:HB3	1:B:835:PRO:HD3	1.86	0.57
1:B:563:ASP:HB3	1:B:564:GLU:HG2	1.86	0.57
1:A:588:ARG:HB2	1:A:588:ARG:CZ	2.34	0.57
1:A:644:CYS:HG	1:A:648:GLY:H	1.49	0.57
1:B:363:LEU:O	1:B:368:LEU:HB2	2.05	0.57
1:A:343:PRO:HG2	1:A:344:GLU:H	1.69	0.57
1:B:393:GLN:HA	1:B:393:GLN:NE2	2.20	0.56
1:B:631:ARG:O	1:B:639:GLY:HA3	2.06	0.56
1:A:61:ALA:HB2	1:A:91:LEU:HD13	1.87	0.56
1:A:148:GLU:OE2	1:A:148:GLU:N	2.30	0.56
1:A:717:VAL:HG13	1:A:738:ARG:HB3	1.86	0.56
1:B:163:VAL:HG21	1:B:262:VAL:HG11	1.87	0.56
1:A:450:LEU:HG	1:A:451:VAL:H	1.69	0.56
1:A:351:ARG:HD3	6:A:2017:HOH:O	2.04	0.56
1:B:307:LEU:HB3	1:B:311:GLU:CB	2.35	0.56
1:A:587:VAL:HG22	1:A:755:TYR:CD2	2.41	0.56
6:A:2003:HOH:O	1:B:396:SER:HB2	2.04	0.56
1:B:12:ASP:O	1:B:14:GLY:N	2.39	0.56
1:B:33:VAL:CG1	1:B:39:VAL:HG11	2.35	0.56
1:A:383:GLY:O	1:A:384:GLU:C	2.43	0.56
1:B:126[A]:ARG:HH21	1:B:138:TYR:HD1	1.53	0.56
1:B:826:ALA:HB2	1:B:837:LEU:HB3	1.88	0.56
1:A:728:ALA:HA	1:A:731:LEU:HD12	1.86	0.56
2:B:1843:ADP:PA	2:B:1843:ADP:H8	2.29	0.56
1:A:745:LEU:HD11	1:A:775:GLN:HB3	1.88	0.56
1:B:74:ARG:O	1:B:74:ARG:HD3	2.06	0.56
1:B:526:THR:HG23	1:B:801:TRP:HB3	1.88	0.56
1:A:602:MET:HG3	1:A:739:ILE:CD1	2.37	0.55
1:B:318:ALA:O	1:B:322:GLU:HG3	2.06	0.55
1:B:400:GLY:C	1:B:401:VAL:HG13	2.26	0.55
1:A:747:ARG:C	1:A:749:GLY:H	2.08	0.55
1:A:779:LEU:O	1:A:784:ASN:HB2	2.06	0.55
1:B:46:GLY:N	2:B:1843:ADP:O2B	2.40	0.55
1:B:366:LEU:O	1:B:368:LEU:N	2.39	0.55
1:B:533:GLY:N	2:B:1844:ADP:O1B	2.33	0.55
1:A:759:GLU:OE2	1:A:791[A]:HIS:HD2	1.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:MET:HE1	1:B:833:THR:HB	1.87	0.55
1:B:174:LEU:HB2	1:B:180:ALA:HB2	1.88	0.55
1:A:753:THR:O	1:A:784:ASN:ND2	2.39	0.55
1:A:40:VAL:HA	1:A:436:VAL:O	2.07	0.55
1:B:23:GLN:HG3	1:B:24:HIS:N	2.23	0.54
1:B:759:GLU:HG3	1:B:791:HIS:HD2	1.65	0.54
1:A:120:LEU:N	1:A:120:LEU:CD1	2.67	0.54
1:A:176:ILE:HD12	1:A:204:VAL:HA	1.89	0.54
1:A:617:ALA:HB2	1:A:629:ALA:HA	1.90	0.54
1:B:42:THR:OG1	1:B:452:ASP:HA	2.07	0.54
1:A:152:PRO:HG3	1:A:296:ARG:HE	1.72	0.54
1:B:54:PHE:CZ	1:B:404:VAL:HG12	2.42	0.54
1:A:481:THR:HB	1:A:765:HIS:HE2	1.73	0.54
1:B:619:THR:O	1:B:623:LYS:HD3	2.08	0.54
1:A:452:ASP:OD1	1:A:481:THR:CG2	2.49	0.54
1:A:587:VAL:CG2	1:A:755:TYR:CD2	2.91	0.54
1:B:119:LEU:HB3	1:B:356:LEU:HD21	1.89	0.54
1:B:464:ILE:HG22	1:B:464:ILE:O	2.07	0.54
1:B:805:ILE:CG2	1:B:806:GLY:N	2.71	0.54
1:A:689:VAL:O	1:A:692:LEU:HB2	2.07	0.53
1:B:377:THR:N	1:B:378:PRO:HD2	2.23	0.53
1:A:368:LEU:HB3	1:A:371:LEU:HD12	1.90	0.53
1:A:438:GLU:HG3	1:A:439:HIS:N	2.22	0.53
1:A:451:VAL:HG22	1:A:467:SER:HB2	1.90	0.53
1:A:757:LEU:HD23	1:A:760:PRO:HG3	1.91	0.53
1:B:129:ASP:N	1:B:303:THR:O	2.40	0.53
1:B:473:LEU:HD12	1:B:476:VAL:CG2	2.39	0.53
1:B:74:ARG:HH12	1:B:78:ASN:HA	1.72	0.53
1:B:539:LEU:HG	1:B:539:LEU:O	2.09	0.53
1:A:322:GLU:HG3	1:A:325:ARG:NH2	2.24	0.53
1:B:159:ARG:HD3	1:B:284:SER:HG	1.71	0.53
1:A:234:LEU:HB3	1:A:238:GLU:HG3	1.91	0.52
1:A:719:LEU:HB3	1:A:722:LEU:HD12	1.89	0.52
1:A:644:CYS:C	1:A:646:GLY:N	2.60	0.52
1:A:218:TRP:O	1:A:222:THR:HG22	2.10	0.52
1:B:782:ALA:HB3	1:B:784:ASN:ND2	2.25	0.52
1:A:781:ASP:C	1:A:783:GLY:H	2.13	0.52
1:B:599:ARG:CG	1:B:599:ARG:NH1	2.48	0.52
1:B:538:THR:HA	1:B:542:GLN:HB2	1.92	0.52
1:B:577:GLY:HA2	1:B:580:LEU:HD11	1.91	0.52
1:A:650:VAL:HG21	1:A:665:PRO:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HA	1:B:388:LEU:HB2	1.93	0.51
1:B:452:ASP:OD2	1:B:479:SER:HB2	2.09	0.51
1:B:466:TYR:CD2	1:B:467:SER:N	2.79	0.51
1:A:483:GLN:O	1:A:486:PHE:N	2.42	0.51
1:A:666:VAL:O	1:A:666:VAL:CG2	2.58	0.51
1:B:386:GLN:HE22	1:B:406:ASP:N	2.06	0.51
1:A:722:LEU:HD21	1:A:735:GLU:OE1	2.11	0.51
1:B:199:THR:HG21	1:B:229:PRO:O	2.08	0.51
1:A:473:LEU:HB3	1:A:486:PHE:HE2	1.75	0.51
1:B:32:LYS:HD3	6:B:2030:HOH:O	2.11	0.51
1:B:523:GLY:HA2	1:B:784:ASN:O	2.10	0.51
1:A:390:LEU:HD22	1:A:390:LEU:O	2.11	0.51
1:A:613:ARG:NH1	1:A:630:GLY:HA3	2.23	0.51
1:A:758[A]:ASP:OD2	1:A:759:GLU:N	2.32	0.51
1:A:316:PRO:O	1:A:320:VAL:HG23	2.11	0.51
1:A:736:ALA:O	1:A:740:LYS:HD2	2.11	0.51
1:B:175:THR:HG22	1:B:177:ARG:H	1.75	0.51
1:A:181:VAL:HG13	1:A:184:TRP:HB2	1.93	0.51
1:B:383:GLY:HA3	1:B:387:ARG:NH2	2.26	0.51
1:B:440:ASP:OD1	1:B:442:ASP:N	2.44	0.51
1:B:150:ALA:HB1	1:B:156:GLY:HA3	1.92	0.51
1:B:556:VAL:O	1:B:557:ASN:CB	2.59	0.51
1:B:775:GLN:HE22	1:B:778:LYS:NZ	2.09	0.51
1:A:776:LEU:O	1:A:780:VAL:HG23	2.11	0.50
1:B:33:VAL:HG13	1:B:39:VAL:HG11	1.91	0.50
1:B:806:GLY:HA2	1:B:815[A]:ARG:H	1.75	0.50
1:A:349:LEU:HD23	1:A:349:LEU:C	2.31	0.50
1:B:400:GLY:C	1:B:401:VAL:CG1	2.79	0.50
1:A:39:VAL:HA	1:A:449:TRP:O	2.11	0.50
1:B:428:LYS:HB2	1:B:434:LEU:CD1	2.40	0.50
1:B:575:ARG:CG	1:B:575:ARG:NH1	2.72	0.50
1:B:667:CYS:HB2	1:B:670:THR:HG22	1.94	0.50
1:B:677:LEU:HA	1:B:685:ASN:HD21	1.76	0.50
1:B:524:VAL:HG13	1:B:800:ASP:HB2	1.92	0.50
1:B:805:ILE:CG2	1:B:806:GLY:H	2.25	0.50
1:A:23:GLN:O	1:A:26:LEU:HB2	2.12	0.50
1:A:414:PRO:HA	1:A:417:THR:CG2	2.41	0.50
1:A:631:ARG:O	1:A:639:GLY:HA3	2.11	0.50
1:B:652:VAL:C	1:B:654:LEU:H	2.14	0.50
1:A:441:LEU:O	1:A:445:ARG:HB2	2.12	0.50
1:A:271:SER:CB	1:A:274:MET:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG13	1:A:805:ILE:HD13	1.93	0.50
1:B:440:ASP:OD1	1:B:440:ASP:C	2.50	0.50
1:A:341:ASN:O	1:A:342:ARG:HG3	2.11	0.50
1:B:75:ARG:HH11	1:B:75:ARG:HB3	1.77	0.50
1:A:713:THR:HG21	1:A:742:ALA:O	2.12	0.49
1:B:588:ARG:NH1	1:B:588:ARG:HB2	2.27	0.49
1:B:575:ARG:HH11	1:B:575:ARG:HG2	1.77	0.49
1:B:772:LEU:O	1:B:775:GLN:HB2	2.13	0.49
1:A:163:VAL:HG22	1:A:168:MET:CG	2.42	0.49
1:B:24:HIS:CE1	2:B:1843:ADP:C5	3.00	0.49
1:B:382:PRO:HA	1:B:385:LEU:CD1	2.43	0.49
1:B:491:THR:C	1:B:493:PRO:HD3	2.32	0.49
1:A:525:MET:HG2	1:A:786:VAL:CG2	2.43	0.49
1:B:131:PRO:HG3	1:B:301:ASN:HB3	1.94	0.49
1:B:528:VAL:HG21	1:B:540:VAL:HG21	1.95	0.49
1:A:380:LEU:HD23	1:A:385:LEU:HD13	1.95	0.49
1:A:640:ARG:HG2	1:A:640:ARG:HH11	1.77	0.49
1:A:750:ARG:HA	1:A:750:ARG:CZ	2.41	0.49
1:B:636:VAL:O	1:B:640:ARG:HD3	2.13	0.49
1:B:838:ARG:HH11	1:B:838:ARG:HB3	1.76	0.49
1:B:504:GLU:CG	1:B:519:ARG:HG2	2.43	0.49
1:B:754:VAL:HG13	1:B:754:VAL:O	2.13	0.49
1:A:17:GLN:O	1:A:88:ILE:HA	2.12	0.49
1:A:793:MET:O	1:A:794:GLN:C	2.52	0.49
1:B:387:ARG:NH2	1:B:410:ALA:O	2.46	0.49
1:B:806:GLY:HA2	1:B:815[B]:ARG:H	1.76	0.49
1:A:159:ARG:NH1	1:A:284:SER:HB3	2.28	0.48
1:A:677:LEU:HD22	1:A:685:ASN:HD22	1.78	0.48
1:B:507:GLY:N	1:B:517:ASP:OD2	2.46	0.48
1:A:440:ASP:OD1	1:A:442:ASP:HB2	2.13	0.48
1:A:775:GLN:HE22	1:A:778:LYS:NZ	2.11	0.48
1:A:156:GLY:O	1:A:294:ARG:HD2	2.14	0.48
1:A:765:HIS:ND1	1:A:766:PRO:HD2	2.28	0.48
1:B:156:GLY:O	1:B:294:ARG:HB3	2.13	0.48
1:B:575:ARG:HH11	1:B:575:ARG:HG3	1.76	0.48
1:B:656:PHE:CD1	1:B:657:LEU:HD23	2.49	0.48
1:B:657:LEU:CB	1:B:658:PRO:HD2	2.43	0.48
1:A:67:GLU:HB3	1:A:75:ARG:HD3	1.95	0.48
1:A:118:ASN:O	1:A:118:ASN:ND2	2.46	0.48
1:A:753:THR:H	1:A:784:ASN:ND2	1.94	0.48
1:B:398:LEU:HD22	1:B:401:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:GLU:HA	1:B:596:ARG:HH22	1.78	0.48
1:A:538:THR:CG2	2:A:1844:ADP:O2A	2.54	0.48
1:A:545:VAL:HG23	1:A:756:VAL:HG21	1.95	0.48
1:A:602:MET:O	1:A:606:THR:HG23	2.13	0.48
1:A:804:ASP:OD1	1:A:833:THR:CG2	2.62	0.48
1:B:407:GLU:HG2	1:B:410:ALA:HB2	1.94	0.48
1:B:588:ARG:HB2	1:B:588:ARG:HH11	1.77	0.48
1:B:648:GLY:C	1:B:649:TRP:CD1	2.86	0.48
1:A:130:TYR:HE2	1:A:137:VAL:HG23	1.79	0.48
1:A:717:VAL:CG1	1:A:738:ARG:HB3	2.43	0.48
1:B:455:PRO:HB3	1:B:478:GLU:HG3	1.95	0.48
1:B:533:GLY:HA3	1:B:809:ALA:HB1	1.96	0.48
1:B:540:VAL:O	1:B:545:VAL:HG23	2.14	0.48
1:A:281:TYR:O	1:A:282:MET:HG2	2.13	0.48
1:A:390:LEU:HD11	1:A:424:LEU:HD23	1.95	0.48
1:B:609:PHE:O	1:B:610:ASP:C	2.50	0.48
1:B:385:LEU:HD12	1:B:385:LEU:N	2.27	0.48
1:B:408:PRO:HB2	1:B:420:LEU:HD11	1.96	0.48
1:A:90:GLY:O	1:A:92:PRO:HD3	2.13	0.48
1:A:412:LEU:HD12	1:A:417:THR:HA	1.96	0.48
1:B:218:TRP:O	1:B:222:THR:HG22	2.14	0.48
1:B:811:GLU:HB2	6:B:2019:HOH:O	2.12	0.48
1:B:510:ARG:HD2	1:B:572:GLY:O	2.14	0.47
1:B:765:HIS:HD1	1:B:767:ALA:H	1.62	0.47
1:B:765:HIS:ND1	1:B:766:PRO:HD2	2.29	0.47
1:A:343:PRO:CG	1:A:344:GLU:H	2.27	0.47
1:A:713:THR:CG2	1:A:742:ALA:O	2.62	0.47
1:A:801:TRP:CZ3	1:A:820:GLY:HA2	2.49	0.47
1:B:150:ALA:HB1	1:B:156:GLY:CA	2.45	0.47
1:B:262:VAL:HG22	1:B:278:VAL:HG13	1.96	0.47
1:A:156:GLY:O	1:A:294:ARG:HB3	2.14	0.47
1:B:510:ARG:HB2	1:B:570:THR:HG21	1.95	0.47
1:B:692:LEU:HD23	1:B:697:ALA:HA	1.96	0.47
1:A:159:ARG:HH11	1:A:284:SER:HB3	1.78	0.47
1:A:455:PRO:HD2	1:A:460:LYS:O	2.14	0.47
1:A:549:ALA:HB1	1:A:554:GLN:HG2	1.96	0.47
1:B:49:LYS:CG	2:B:1843:ADP:O1B	2.63	0.47
1:B:95:VAL:O	1:B:403:TYR:HA	2.14	0.47
1:B:317:LEU:CD2	1:B:373:LEU:HD13	2.43	0.47
1:B:470:PRO:O	1:B:472:GLY:N	2.48	0.47
1:A:601:ASN:OD1	1:A:724:LEU:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ASP:OD2	1:A:703:ASP:N	2.47	0.47
1:B:77:PHE:HZ	1:B:654:LEU:HB3	1.78	0.47
1:A:118:ASN:ND2	1:A:118:ASN:C	2.68	0.47
1:A:213[A]:GLU:HG3	1:A:214[A]:GLU:HG3	1.96	0.47
1:A:348:ALA:O	1:A:352:MET:HG3	2.15	0.47
1:B:167:SER:OG	1:B:168:MET:N	2.48	0.47
1:B:402:VAL:HG13	1:B:433:SER:HB2	1.96	0.47
1:B:745:LEU:HD21	1:B:775:GLN:HE21	1.79	0.47
1:B:793:MET:CE	1:B:833:THR:HB	2.45	0.47
1:B:403:TYR:CE1	1:B:427:LEU:HD21	2.50	0.47
1:A:585:ARG:HB2	1:A:753:THR:CB	2.32	0.47
1:B:204:VAL:HG12	1:B:204:VAL:O	2.14	0.47
1:B:802:VAL:HB	1:B:825:VAL:HG21	1.96	0.47
1:A:360:LEU:O	1:A:363:LEU:HB2	2.16	0.46
1:B:753:THR:HG23	1:B:784:ASN:OD1	2.15	0.46
1:A:418:GLU:CD	1:A:446:ARG:HH22	2.09	0.46
1:B:545:VAL:CG1	1:B:586:LEU:HD21	2.40	0.46
1:B:651:MET:HG2	1:B:652:VAL:H	1.80	0.46
1:B:652:VAL:HG22	1:B:660:VAL:O	2.15	0.46
1:A:58:TYR:CZ	1:A:62:GLN:HG2	2.50	0.46
1:A:393:GLN:OE1	1:A:403:TYR:HE2	1.98	0.46
1:B:17:GLN:O	1:B:88:ILE:HA	2.15	0.46
1:B:512:ASN:HD21	1:B:810:GLY:HA2	1.80	0.46
1:B:773[A]:GLN:CD	1:B:795:VAL:HG23	2.35	0.46
1:B:157:LEU:O	1:B:294:ARG:HD2	2.16	0.46
1:A:35:ARG:O	1:A:36:ASP:HB2	2.15	0.46
1:A:759:GLU:OE1	1:A:759:GLU:CA	2.63	0.46
1:A:123:LEU:C	1:A:123:LEU:HD23	2.36	0.46
1:A:640:ARG:HA	1:A:672:TYR:HA	1.98	0.46
1:A:196:ILE:HG21	1:A:255:PHE:HB2	1.97	0.46
1:A:807:PRO:CD	1:A:808:GLY:H	2.29	0.46
1:B:685:ASN:ND2	1:B:686:ILE:H	1.87	0.46
1:B:764:LEU:HB3	1:B:769:VAL:HG12	1.97	0.46
1:A:97:LEU:HD12	1:A:405:LEU:HD21	1.98	0.46
1:A:716:GLU:C	1:A:718:GLY:H	2.19	0.46
1:A:271:SER:HB3	1:A:274:MET:CB	2.46	0.46
1:A:373:LEU:H	1:A:373:LEU:CD2	2.25	0.46
1:B:41:PHE:N	1:B:41:PHE:CD2	2.81	0.46
1:B:685:ASN:HB3	1:B:688:ASP:H	1.80	0.46
1:A:62:GLN:OE1	1:A:62:GLN:HA	2.16	0.45
1:A:393:GLN:OE1	1:A:403:TYR:CE2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PRO:HD3	1:B:449:TRP:CG	2.51	0.45
1:B:411:GLY:HA2	1:B:791:HIS:CD2	2.51	0.45
1:B:664:CYS:O	1:B:668:HIS:HA	2.17	0.45
1:B:698:HIS:CD2	1:B:715:ARG:CD	2.97	0.45
1:B:62:GLN:O	1:B:63:ARG:C	2.55	0.45
1:B:804:ASP:OD1	1:B:833:THR:CG2	2.65	0.45
1:A:420:LEU:C	1:A:422:SER:N	2.70	0.45
1:A:585:ARG:CB	1:A:753:THR:HB	2.34	0.45
1:A:640:ARG:HG2	1:A:640:ARG:NH1	2.31	0.45
1:B:151:CYS:HA	1:B:152:PRO:HD3	1.77	0.45
1:B:175:THR:HG22	1:B:177:ARG:N	2.32	0.45
1:B:747:ARG:NH1	6:B:2049:HOH:O	2.49	0.45
1:A:403:TYR:HB2	1:A:434:LEU:CD2	2.46	0.45
1:A:733:GLY:HA2	1:A:736:ALA:HB3	1.98	0.45
1:B:794:GLN:HA	6:B:2054:HOH:O	2.16	0.45
1:A:39:VAL:HG22	1:A:449:TRP:HB3	1.99	0.45
1:B:413:HIS:CD2	1:B:413:HIS:C	2.89	0.45
1:B:423:ALA:O	1:B:427:LEU:HB2	2.17	0.45
1:B:625:ARG:O	1:B:627:TYR:N	2.50	0.45
1:B:703:ASP:OD2	1:B:703:ASP:N	2.48	0.45
1:A:185:PRO:HB2	1:A:189:GLY:HA3	1.99	0.45
1:B:15:PHE:CD2	1:B:32:LYS:HG3	2.51	0.45
1:B:222:THR:O	1:B:257:SER:CB	2.64	0.45
1:A:203:ASP:OD2	1:A:206:VAL:HG22	2.17	0.45
1:B:577:GLY:CA	1:B:580:LEU:HD11	2.45	0.45
1:B:750:ARG:HB2	1:B:751:GLY:H	1.46	0.45
1:A:15:PHE:HA	1:A:34:PRO:HA	1.99	0.45
1:A:44:VAL:HG12	1:A:45:SER:O	2.17	0.45
1:A:413:HIS:CG	1:A:414:PRO:HD2	2.52	0.45
1:B:585:ARG:HB2	1:B:753:THR:HB	1.99	0.45
1:A:164:THR:HG23	1:A:283:ILE:HD11	1.99	0.44
1:A:801:TRP:CH2	1:A:820:GLY:HA2	2.51	0.44
1:B:60:GLU:HG2	1:B:88:ILE:HD12	1.98	0.44
1:B:231:TYR:CE1	1:B:249:PRO:HA	2.52	0.44
1:B:454:GLY:O	1:B:455:PRO:C	2.55	0.44
1:B:575:ARG:NH1	1:B:575:ARG:HG2	2.32	0.44
1:A:101:ARG:HD3	1:A:730:GLU:O	2.17	0.44
1:A:461:GLY:O	1:A:463:GLU:N	2.50	0.44
1:A:473:LEU:O	1:A:476:VAL:HG22	2.17	0.44
1:B:107:ARG:NH2	1:B:565:ASP:HB3	2.32	0.44
1:B:202:ILE:O	1:B:204:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:PHE:HD2	1:B:704:GLU:HG3	1.82	0.44
1:A:402:VAL:HG13	1:A:433:SER:HB3	1.99	0.44
1:A:719:LEU:HD22	1:A:722:LEU:CD1	2.46	0.44
1:B:312:LEU:HD22	1:B:320:VAL:HG22	2.00	0.44
1:B:808:GLY:N	1:B:812:ASP:O	2.50	0.44
1:A:310:THR:O	1:A:314:ARG:HG2	2.18	0.44
1:A:511:ASN:HB3	1:A:512:ASN:H	1.63	0.44
1:A:587:VAL:HG21	1:A:744:GLU:HG3	1.99	0.44
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.75	0.44
1:B:590:ASP:OD1	1:B:592:LYS:HB2	2.17	0.44
1:B:630:GLY:H	1:B:632:PHE:H	1.64	0.44
1:B:782:ALA:HB3	1:B:784:ASN:HD22	1.82	0.44
1:A:537:SER:OG	2:A:1844:ADP:O2B	2.22	0.44
1:B:177:ARG:NH2	1:B:205:ASP:OD2	2.49	0.44
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.27	0.44
1:B:435:PHE:CD1	1:B:435:PHE:N	2.84	0.44
1:B:452:ASP:OD1	1:B:481:THR:HG21	2.18	0.44
1:B:703:ASP:HB3	6:B:2046:HOH:O	2.17	0.44
1:B:820:GLY:HA3	1:B:824:GLU:OE1	2.18	0.44
1:A:43:GLY:C	1:A:765:HIS:HD2	2.20	0.44
1:A:634:PHE:O	1:A:640:ARG:NH1	2.51	0.44
1:A:732:SER:HB3	1:A:735:GLU:OE2	2.18	0.44
1:B:332:GLU:HG3	1:B:335:HIS:HB2	1.99	0.44
1:B:387:ARG:O	1:B:391:ALA:HB2	2.18	0.44
1:B:761:THR:HA	1:B:764:LEU:HD22	2.00	0.44
1:A:159:ARG:NH2	1:A:285:GLU:HA	2.33	0.44
1:A:331:ARG:O	1:A:333:PRO:HD3	2.18	0.44
1:A:504:GLU:HG2	1:A:519:ARG:HG3	1.99	0.44
1:A:644:CYS:C	1:A:646:GLY:H	2.19	0.44
1:B:19:ARG:NH2	1:B:89:ASP:OD2	2.45	0.44
1:B:266:PHE:HE1	1:B:279:GLN:HE22	1.63	0.44
1:B:383:GLY:CA	1:B:387:ARG:NH2	2.81	0.44
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.57	0.44
1:B:428:LYS:CB	1:B:434:LEU:HD11	2.46	0.44
1:A:337:GLU:O	1:A:341:ASN:ND2	2.44	0.43
1:A:473:LEU:HD12	1:A:476:VAL:HG21	1.99	0.43
1:A:510:ARG:O	1:A:511:ASN:HB2	2.17	0.43
1:B:41:PHE:CD1	1:B:53:ALA:HB2	2.53	0.43
1:B:25:ASN:O	1:B:26:LEU:C	2.56	0.43
1:B:413:HIS:HA	1:B:414:PRO:HD2	1.57	0.43
1:B:504:GLU:HG3	1:B:519:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:SER:HB3	1:B:834:ALA:HB2	2.00	0.43
1:A:675:GLU:O	1:A:678:GLU:HB2	2.19	0.43
1:A:25:ASN:HD22	1:A:25:ASN:N	2.13	0.43
1:A:412:LEU:HD22	1:A:412:LEU:HA	1.91	0.43
1:B:12:ASP:C	1:B:14:GLY:N	2.70	0.43
1:B:511:ASN:HD22	1:B:538:THR:HB	1.83	0.43
1:B:611:GLN:HB3	1:B:707:ILE:HD11	2.00	0.43
1:B:817:VAL:HG21	1:B:830:GLY:O	2.17	0.43
1:B:821:THR:HG23	1:B:824:GLU:CD	2.39	0.43
1:A:373:LEU:HD23	1:A:373:LEU:N	2.26	0.43
1:A:41:PHE:HB2	1:A:437:VAL:HA	2.00	0.43
1:A:99[A]:GLN:HE22	1:A:105:THR:HG23	1.82	0.43
1:B:594:ILE:HB	1:B:605:TYR:CD1	2.53	0.43
1:A:207:PRO:O	1:A:210:GLU:HB2	2.18	0.43
1:A:651:MET:HB2	1:A:661:TYR:HE2	1.84	0.43
1:A:716:GLU:C	1:A:718:GLY:N	2.71	0.43
1:B:70:SER:O	1:B:72:TYR:N	2.46	0.43
1:B:473:LEU:HD12	1:B:473:LEU:HA	1.67	0.43
1:B:804:ASP:OD1	1:B:833:THR:HG23	2.19	0.43
1:A:719:LEU:O	1:A:721:TYR:N	2.51	0.43
1:A:719:LEU:C	1:A:721:TYR:H	2.22	0.43
1:B:487:ALA:CB	1:B:490:HIS:CE1	3.01	0.43
1:B:801:TRP:CZ3	1:B:820:GLY:HA2	2.53	0.43
1:A:19:ARG:NH2	1:A:89:ASP:OD2	2.52	0.43
1:B:118:ASN:HA	1:B:121:ARG:NH1	2.33	0.43
1:B:402:VAL:HG11	1:B:435:PHE:CE2	2.54	0.43
1:A:407:GLU:C	1:A:409:SER:H	2.22	0.43
1:A:701:PHE:O	1:A:708:PHE:HB2	2.18	0.43
1:A:701:PHE:CD2	1:A:707:ILE:HG21	2.54	0.43
1:B:803:LEU:HD12	1:B:803:LEU:HA	1.69	0.43
1:A:181:VAL:HG11	1:A:184:TRP:HE3	1.75	0.42
1:A:677:LEU:HD22	1:A:685:ASN:ND2	2.34	0.42
1:A:685:ASN:OD1	1:A:688:ASP:HB2	2.18	0.42
1:B:58:TYR:HB2	1:B:404:VAL:HG21	2.01	0.42
1:B:417:THR:O	1:B:418:GLU:C	2.55	0.42
1:B:417:THR:O	1:B:420:LEU:N	2.52	0.42
1:A:796:VAL:O	1:A:799:SER:HB2	2.20	0.42
1:B:70:SER:O	1:B:73:ALA:N	2.49	0.42
1:B:599:ARG:NH2	1:B:645:GLN:O	2.52	0.42
1:B:723:ARG:HB2	1:B:726:GLN:HB2	2.00	0.42
1:A:17:GLN:HB3	1:A:89:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG22	1:A:168:MET:HG2	2.01	0.42
1:A:262:VAL:HG12	1:A:263:LEU:N	2.33	0.42
1:A:454:GLY:HA2	1:A:461:GLY:C	2.40	0.42
1:A:579:ASP:OD1	1:A:579:ASP:N	2.51	0.42
1:A:717:VAL:HG12	1:A:719:LEU:HG	2.01	0.42
1:A:775:GLN:NE2	1:A:778:LYS:NZ	2.67	0.42
1:B:27:LYS:HD3	1:B:461:GLY:O	2.19	0.42
1:A:169:VAL:HG23	1:A:169:VAL:O	2.19	0.42
1:A:474:LYS:HG3	1:A:486:PHE:CE1	2.55	0.42
1:A:536:LYS:HD2	1:A:789:VAL:HG13	2.01	0.42
1:A:651:MET:HB2	1:A:661:TYR:CE2	2.54	0.42
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.72	0.42
1:B:114:THR:HA	1:B:392:THR:OG1	2.19	0.42
1:B:449:TRP:CZ3	1:B:469:PRO:HD3	2.55	0.42
1:B:589:VAL:HG12	1:B:737:GLN:HG2	2.01	0.42
1:A:41:PHE:HE2	1:A:435:PHE:HB3	1.84	0.42
1:A:481:THR:HB	1:A:765:HIS:NE2	2.35	0.42
1:A:70:SER:C	1:A:72:TYR:H	2.23	0.42
1:A:528:VAL:HG21	1:A:540:VAL:HG21	2.01	0.42
1:B:26:LEU:HD21	1:B:52:LEU:HB2	2.01	0.42
1:B:681:TYR:N	1:B:684:LYS:O	2.46	0.42
1:A:413:HIS:CD2	1:A:415:ALA:H	2.30	0.42
1:A:70:SER:C	1:A:72:TYR:N	2.73	0.42
1:A:390:LEU:O	1:A:390:LEU:CD2	2.67	0.42
1:A:418:GLU:O	1:A:418:GLU:HG3	2.20	0.42
1:A:476:VAL:HA	1:A:477:PRO:HD2	1.80	0.42
1:B:49:LYS:NZ	2:B:1843:ADP:O1B	2.50	0.42
1:B:350:GLN:OE1	1:B:351:ARG:N	2.53	0.42
1:B:690:LEU:HD23	1:B:690:LEU:HA	1.85	0.42
1:A:114:THR:C	1:A:115:THR:HG23	2.41	0.41
1:A:387:ARG:NH2	1:A:410:ALA:O	2.53	0.41
1:A:538:THR:HA	1:A:542:GLN:HB2	2.01	0.41
1:A:717:VAL:HG13	1:A:738:ARG:HD2	2.02	0.41
1:A:87:ALA:C	1:A:88:ILE:HG12	2.40	0.41
1:A:114:THR:CG2	1:A:388:LEU:HD22	2.51	0.41
1:A:151:CYS:HA	1:A:152:PRO:HD3	1.88	0.41
1:A:359:ARG:O	1:A:360:LEU:C	2.58	0.41
1:B:161:TYR:CE2	1:B:284:SER:HB2	2.55	0.41
1:B:402:VAL:HG11	1:B:435:PHE:CZ	2.55	0.41
1:A:159:ARG:CZ	1:A:285:GLU:HA	2.50	0.41
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:VAL:HG21	1:A:755:TYR:CD2	2.56	0.41
1:B:293:LYS:HE3	1:B:308:ASP:OD2	2.20	0.41
1:B:390:LEU:HD22	1:B:394:LEU:HD11	2.02	0.41
1:B:565:ASP:O	1:B:567:ALA:N	2.53	0.41
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.89	0.41
1:B:670:THR:C	1:B:671:ARG:HG3	2.41	0.41
1:A:276:LYS:NZ	1:A:276:LYS:CD	2.68	0.41
1:A:382:PRO:HG3	1:A:591[A]:GLN:NE2	2.35	0.41
1:A:548:LEU:HA	1:A:548:LEU:HD23	1.76	0.41
1:B:43:GLY:C	1:B:765:HIS:HD2	2.23	0.41
1:B:437:VAL:C	1:B:438:GLU:CA	2.71	0.41
1:B:451:VAL:HA	1:B:466:TYR:O	2.20	0.41
1:B:599:ARG:NE	1:B:635:ASN:HD21	2.17	0.41
1:B:619:THR:HB	1:B:620:PRO:CD	2.47	0.41
1:A:494:HIS:O	1:A:496:PRO:HD3	2.20	0.41
1:B:107:ARG:CZ	1:B:376:SER:OG	2.69	0.41
1:A:129:ASP:HB2	1:A:303:THR:HG22	2.03	0.41
1:A:631:ARG:HG3	1:A:631:ARG:HH11	1.86	0.41
1:A:737:GLN:HE22	1:A:762:THR:HB	1.86	0.41
1:B:24:HIS:ND1	1:B:51:SER:OG	2.54	0.41
1:B:580:LEU:N	1:B:580:LEU:CD1	2.74	0.41
1:A:152:PRO:HG3	1:A:296:ARG:HH21	1.86	0.41
1:B:269:THR:HB	1:B:271:SER:HB3	2.01	0.41
1:B:366:LEU:HD23	1:B:387:ARG:HG2	2.03	0.41
1:B:438:GLU:HA	1:B:438:GLU:OE2	2.21	0.41
1:B:466:TYR:CG	1:B:467:SER:N	2.89	0.41
1:A:91:LEU:HA	1:A:92:PRO:HD3	1.92	0.41
1:A:215:THR:O	1:A:219:ILE:HG13	2.20	0.41
1:A:262:VAL:CG1	1:A:263:LEU:N	2.84	0.41
1:A:408:PRO:HB2	1:A:420:LEU:HD11	2.02	0.41
1:A:420:LEU:O	1:A:422:SER:N	2.54	0.41
1:A:686:ILE:HG23	1:A:687:ALA:N	2.36	0.41
1:B:123:LEU:HD23	1:B:123:LEU:C	2.40	0.41
1:B:325:ARG:N	1:B:326:PRO:HD2	2.36	0.41
1:B:329:GLU:OE1	1:B:331:ARG:NH1	2.54	0.41
1:B:385:LEU:CD1	1:B:385:LEU:N	2.83	0.41
1:B:601:ASN:ND2	1:B:634:PHE:CZ	2.88	0.41
1:B:22:ARG:O	1:B:23:GLN:O	2.39	0.41
1:B:491:THR:O	1:B:493:PRO:HD3	2.20	0.41
1:B:621:LEU:HD13	1:B:621:LEU:HA	1.97	0.41
1:A:327:TYR:CA	1:A:332:GLU:HG2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:CYS:HB3	1:B:287:CYS:SG	2.61	0.40
1:B:208:TRP:HZ2	1:B:220:LEU:HD22	1.86	0.40
1:B:592:LYS:HA	1:B:593:PRO:HD2	1.84	0.40
1:B:232:PRO:O	1:B:234:LEU:HD23	2.20	0.40
1:B:413:HIS:CD2	1:B:414:PRO:N	2.89	0.40
1:B:497:ARG:HB2	1:B:524:VAL:HG22	2.04	0.40
1:B:501:GLY:O	1:B:502:TRP:CD1	2.75	0.40
1:B:841:LEU:HD23	1:B:841:LEU:HA	1.71	0.40
1:A:377:THR:N	1:A:378:PRO:CD	2.84	0.40
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.93	0.40
1:A:784:ASN:HD22	1:A:784:ASN:HA	1.56	0.40
1:B:70:SER:C	1:B:72:TYR:H	2.24	0.40
1:B:120:LEU:HD12	1:B:120:LEU:C	2.42	0.40
1:B:171:ASP:HA	1:B:172:PRO:HD3	1.85	0.40
1:A:473:LEU:O	1:A:476:VAL:CG2	2.69	0.40
1:B:196:ILE:HG21	1:B:255:PHE:HB2	2.03	0.40
1:B:501:GLY:O	1:B:502:TRP:CG	2.75	0.40
1:B:544:LEU:O	1:B:544:LEU:HG	2.21	0.40
1:B:692:LEU:HG	1:B:696:GLU:HB3	2.03	0.40
1:B:775:GLN:HE22	1:B:778:LYS:HZ3	1.70	0.40
1:A:65:TYR:CE2	1:A:69:VAL:HG21	2.56	0.40
1:A:103:THR:CG2	1:A:104:PRO:HD2	2.51	0.40
1:A:148:GLU:H	1:A:148:GLU:CD	2.21	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	797/842 (95%)	652 (82%)	110 (14%)	35 (4%)	2 15
1	B	834/842 (99%)	675 (81%)	119 (14%)	40 (5%)	2 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1631/1684 (97%)	1327 (81%)	229 (14%)	75 (5%)	2 14

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213[A]	GLU
1	A	214[A]	GLU
1	A	262	VAL
1	A	455	PRO
1	A	663	PRO
1	A	665	PRO
1	A	748	SER
1	A	762	THR
1	A	807	PRO
1	B	23	GLN
1	B	55	GLY
1	B	454	GLY
1	B	557	ASN
1	B	566	PRO
1	B	645	GLN
1	B	685	ASN
1	B	807	PRO
1	A	135	GLY
1	A	272	ALA
1	A	343	PRO
1	A	462	GLY
1	A	512	ASN
1	A	705	SER
1	A	749	GLY
1	B	259	ARG
1	B	418	GLU
1	B	471[A]	GLU
1	B	489	ARG
1	B	653	GLU
1	B	671	ARG
1	B	675	GLU
1	B	774[A]	ARG
1	A	187	ALA
1	A	344	GLU
1	A	459[A]	GLU
1	A	782	ALA
1	B	81	GLY

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Mol	Chain	Res	Type
1	B	236	PRO
1	B	384	GLU
1	B	470	PRO
1	B	572	GLY
1	B	658	PRO
1	B	668	HIS
1	A	261	HIS
1	A	317	LEU
1	A	384	GLU
1	A	645	GLN
1	A	759	GLU
1	A	794	GLN
1	B	26	LEU
1	B	58	TYR
1	B	273	SER
1	B	704	GLU
1	B	728	ALA
1	B	759	GLU
1	A	132	PRO
1	A	333	PRO
1	A	474	LYS
1	A	637	LYS
1	A	668	HIS
1	A	671	ARG
1	A	720	GLY
1	B	24	HIS
1	B	71	PRO
1	B	101	ARG
1	B	207	PRO
1	B	708	PHE
1	A	73	ALA
1	B	12	ASP
1	B	54	PHE
1	B	77	PHE
1	B	414	PRO
1	B	626	GLY
1	B	132	PRO
1	A	172	PRO

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	652/683 (96%)	523 (80%)	129 (20%)	1 7
1	B	676/683 (99%)	538 (80%)	138 (20%)	1 6
All	All	1328/1366 (97%)	1061 (80%)	267 (20%)	1 6

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	25	ASN
1	A	26	LEU
1	A	31	VAL
1	A	33	VAL
1	A	62	GLN
1	A	74	ARG
1	A	76	LEU
1	A	82	VAL
1	A	88	ILE
1	A	91	LEU
1	A	98	GLN
1	A	101	ARG
1	A	103	THR
1	A	107	ARG
1	A	115	THR
1	A	118	ASN
1	A	119	LEU
1	A	120	LEU
1	A	134	GLN
1	A	136	ILE
1	A	145	ASN
1	A	151	CYS
1	A	157	LEU
1	A	159	ARG
1	A	163	VAL
1	A	164	THR

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Mol	Chain	Res	Type
1	A	175	THR
1	A	191	GLN
1	A	200	LEU
1	A	206	VAL
1	A	209	ARG
1	A	212	PRO
1	A	213[A]	GLU
1	A	214[A]	GLU
1	A	220	LEU
1	A	230	VAL
1	A	243	LEU
1	A	246	LYS
1	A	259	ARG
1	A	262	VAL
1	A	270	GLU
1	A	283	ILE
1	A	285	GLU
1	A	294	ARG
1	A	303	THR
1	A	312	LEU
1	A	322	GLU
1	A	324	LEU
1	A	325	ARG
1	A	332	GLU
1	A	337	GLU
1	A	339	VAL
1	A	344	GLU
1	A	355	ASP
1	A	360	LEU
1	A	363	LEU
1	A	373	LEU
1	A	381	SER
1	A	389	ARG
1	A	390	LEU
1	A	412	LEU
1	A	417	THR
1	A	422	SER
1	A	429[A]	ARG
1	A	460	LYS
1	A	475	HIS
1	A	476	VAL
1	A	481	THR

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Mol	Chain	Res	Type
1	A	495	THR
1	A	497	ARG
1	A	508	VAL
1	A	512	ASN
1	A	518	VAL
1	A	519	ARG
1	A	524	VAL
1	A	525	MET
1	A	531	VAL
1	A	532	SER
1	A	538	THR
1	A	586	LEU
1	A	587	VAL
1	A	588	ARG
1	A	591[A]	GLN
1	A	592	LYS
1	A	596	ARG
1	A	597	THR
1	A	600	SER
1	A	611	GLN
1	A	615	LEU
1	A	621	LEU
1	A	623	LYS
1	A	628	ASN
1	A	636	VAL
1	A	640	ARG
1	A	641	CYS
1	A	664	CYS
1	A	666	VAL
1	A	688	ASP
1	A	693	THR
1	A	703	ASP
1	A	713	THR
1	A	715	ARG
1	A	717	VAL
1	A	729	THR
1	A	731	LEU
1	A	740	LYS
1	A	745	LEU
1	A	750	ARG
1	A	753	THR
1	A	756	VAL

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Mol	Chain	Res	Type
1	A	757	LEU
1	A	761	THR
1	A	762	THR
1	A	769	VAL
1	A	771[A]	ARG
1	A	772	LEU
1	A	777	VAL
1	A	779	LEU
1	A	784	ASN
1	A	795	VAL
1	A	799	SER
1	A	812	ASP
1	A	815[A]	ARG
1	A	816	LEU
1	A	831	SER
1	A	833	THR
1	A	837	LEU
1	A	842	ARG
1	B	9	ASP
1	B	22	ARG
1	B	26	LEU
1	B	27	LYS
1	B	31	VAL
1	B	32	LYS
1	B	40	VAL
1	B	49	LYS
1	B	51	SER
1	B	56	THR
1	B	64	ARG
1	B	72	TYR
1	B	74	ARG
1	B	75	ARG
1	B	91	LEU
1	B	101	ARG
1	B	105	THR
1	B	107	ARG
1	B	115	THR
1	B	119	LEU
1	B	120	LEU
1	B	143	SER
1	B	151	CYS
1	B	163	VAL

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Mol	Chain	Res	Type
1	B	164	THR
1	B	169	VAL
1	B	174	LEU
1	B	186	GLN
1	B	211	LEU
1	B	216	ARG
1	B	225	GLN
1	B	228	VAL
1	B	230	VAL
1	B	234	LEU
1	B	243	LEU
1	B	244[A]	LYS
1	B	256	SER
1	B	262	VAL
1	B	269	THR
1	B	277	ARG
1	B	279	GLN
1	B	289	LEU
1	B	290	CYS
1	B	300	LEU
1	B	303	THR
1	B	312	LEU
1	B	314	ARG
1	B	321	SER
1	B	342	ARG
1	B	344	GLU
1	B	349	LEU
1	B	359	ARG
1	B	363	LEU
1	B	364	LEU
1	B	373	LEU
1	B	376	SER
1	B	380	LEU
1	B	385	LEU
1	B	389[A]	ARG
1	B	390	LEU
1	B	394	LEU
1	B	396	SER
1	B	412	LEU
1	B	413	HIS
1	B	414	PRO
1	B	427	LEU

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Mol	Chain	Res	Type
1	B	429[A]	ARG
1	B	434	LEU
1	B	437	VAL
1	B	440	ASP
1	B	445	ARG
1	B	450	LEU
1	B	467	SER
1	B	474	LYS
1	B	479	SER
1	B	480	GLN
1	B	481	THR
1	B	495	THR
1	B	505	LEU
1	B	508	VAL
1	B	510	ARG
1	B	516	LEU
1	B	519	ARG
1	B	525	MET
1	B	527	SER
1	B	531	VAL
1	B	532	SER
1	B	538	THR
1	B	541	SER
1	B	570	THR
1	B	573	SER
1	B	575	ARG
1	B	576	LEU
1	B	580	LEU
1	B	584	THR
1	B	587	VAL
1	B	588	ARG
1	B	591[A]	GLN
1	B	597	THR
1	B	599	ARG
1	B	600	SER
1	B	604	THR
1	B	606	THR
1	B	611	GLN
1	B	623	LYS
1	B	625	ARG
1	B	631	ARG
1	B	636	VAL

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Mol	Chain	Res	Type
1	B	641	CYS
1	B	654	LEU
1	B	655	LEU
1	B	656	PHE
1	B	657	LEU
1	B	660	VAL
1	B	670	THR
1	B	685	ASN
1	B	709	ARG
1	B	717	VAL
1	B	743	THR
1	B	746	ARG
1	B	747	ARG
1	B	748	SER
1	B	750	ARG
1	B	753	THR
1	B	756	VAL
1	B	762	THR
1	B	764	LEU
1	B	769	VAL
1	B	779	LEU
1	B	780	VAL
1	B	786	VAL
1	B	789	VAL
1	B	793	MET
1	B	800	ASP
1	B	803	LEU
1	B	816	LEU
1	B	821	THR
1	B	832	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	25	ASN
1	A	78	ASN
1	A	98	GLN
1	A	118	ASN
1	A	134	GLN
1	A	192	ASN
1	A	240[A]	GLN

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Mol	Chain	Res	Type
1	A	335	HIS
1	A	386	GLN
1	A	413	HIS
1	A	483	GLN
1	A	511	ASN
1	A	512	ASN
1	A	551	HIS
1	A	582	GLN
1	A	628	ASN
1	A	635	ASN
1	A	737	GLN
1	A	775	GLN
1	A	784	ASN
1	B	186	GLN
1	B	192	ASN
1	B	217	HIS
1	B	345	GLN
1	B	386	GLN
1	B	413	HIS
1	B	511	ASN
1	B	512	ASN
1	B	557	ASN
1	B	582	GLN
1	B	591[A]	GLN
1	B	635	ASN
1	B	668	HIS
1	B	685	ASN
1	B	737	GLN
1	B	773[A]	GLN
1	B	775	GLN
1	B	791	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	SO4	A	1849[A]	-	4,4,4	0.17	0	6,6,6	0.18	0
2	ADP	B	1844	-	24,29,29	1.12	3 (12%)	29,45,45	1.44	5 (17%)
4	SO4	B	1849	-	4,4,4	0.21	0	6,6,6	0.37	0
5	PO4	B	1852[A]	-	4,4,4	0.69	0	6,6,6	0.71	0
4	SO4	B	1851[A]	-	4,4,4	0.20	0	6,6,6	0.36	0
4	SO4	A	1847[A]	-	4,4,4	0.11	0	6,6,6	0.43	0
2	ADP	B	1843	-	24,29,29	1.29	3 (12%)	29,45,45	1.62	5 (17%)
4	SO4	B	1847	-	4,4,4	0.23	0	6,6,6	0.39	0
4	SO4	B	1848[A]	-	4,4,4	0.28	0	6,6,6	0.10	0
2	ADP	A	1844	-	24,29,29	1.10	1 (4%)	29,45,45	1.79	11 (37%)
2	ADP	A	1843	-	24,29,29	1.12	2 (8%)	29,45,45	1.54	4 (13%)
4	SO4	B	1850[A]	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	A	1848[A]	-	4,4,4	0.13	0	6,6,6	0.23	0

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	A	1844	-	-	0/12/32/32	0/3/3/3
2	ADP	A	1843	-	-	2/12/32/32	0/3/3/3
2	ADP	B	1843	-	-	3/12/32/32	0/3/3/3
2	ADP	B	1844	-	-	4/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1843	ADP	C5-C4	3.09	1.49	1.40
2	A	1843	ADP	C5-C4	2.64	1.47	1.40
2	A	1844	ADP	C2'-C1'	-2.43	1.50	1.53
2	B	1843	ADP	C2'-C1'	-2.37	1.50	1.53
2	B	1844	ADP	O4'-C4'	-2.22	1.40	1.45
2	B	1843	ADP	C2-N3	2.18	1.35	1.32
2	A	1843	ADP	O4'-C1'	2.11	1.44	1.41
2	B	1844	ADP	C5-N7	-2.09	1.32	1.39
2	B	1844	ADP	C5-C4	2.02	1.46	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1843	ADP	PA-O3A-PB	-4.21	118.37	132.83
2	B	1843	ADP	N6-C6-N1	4.18	127.26	118.57
2	A	1844	ADP	N3-C2-N1	-4.16	122.17	128.68
2	B	1843	ADP	N3-C2-N1	-3.67	122.94	128.68
2	B	1844	ADP	N3-C2-N1	-3.51	123.19	128.68
2	A	1843	ADP	N3-C2-N1	-3.46	123.26	128.68
2	B	1843	ADP	O3B-PB-O2B	3.06	119.34	107.64
2	B	1843	ADP	C5-C6-N6	-3.06	115.70	120.35
2	A	1844	ADP	C1'-N9-C4	-3.06	121.27	126.64
2	A	1844	ADP	O3'-C3'-C4'	-2.93	102.57	111.05
2	B	1844	ADP	C4-C5-N7	-2.86	106.42	109.40
2	A	1843	ADP	C2-N1-C6	2.75	123.47	118.75
2	A	1844	ADP	O3B-PB-O1B	2.63	120.98	110.68
2	A	1844	ADP	O2A-PA-O5'	2.60	119.83	107.75
2	B	1844	ADP	PA-O3A-PB	-2.44	124.45	132.83
2	A	1843	ADP	N6-C6-N1	2.44	123.63	118.57
2	B	1843	ADP	C2-N1-C6	2.40	122.87	118.75
2	A	1844	ADP	O3B-PB-O3A	-2.40	96.58	104.64
2	A	1844	ADP	C2'-C3'-C4'	2.38	107.27	102.64
2	B	1844	ADP	O2B-PB-O1B	2.32	119.78	110.68
2	A	1844	ADP	C4-C5-N7	-2.32	106.98	109.40
2	B	1844	ADP	O4'-C4'-C5'	-2.27	101.91	109.37
2	A	1844	ADP	PA-O3A-PB	-2.19	125.30	132.83
2	A	1844	ADP	O3B-PB-O2B	2.19	116.02	107.64
2	A	1844	ADP	O4'-C1'-C2'	2.09	109.98	106.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1843	ADP	C5'-O5'-PA-O2A
2	B	1844	ADP	C5'-O5'-PA-O3A
2	A	1843	ADP	O4'-C4'-C5'-O5'
2	A	1843	ADP	C3'-C4'-C5'-O5'
2	B	1844	ADP	O4'-C4'-C5'-O5'
2	B	1844	ADP	C3'-C4'-C5'-O5'
2	B	1843	ADP	C5'-O5'-PA-O1A
2	B	1844	ADP	C5'-O5'-PA-O1A
2	B	1843	ADP	C5'-O5'-PA-O3A

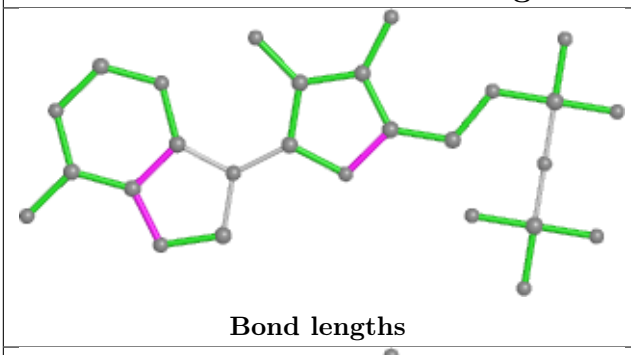
There are no ring outliers.

4 monomers are involved in 15 short contacts:

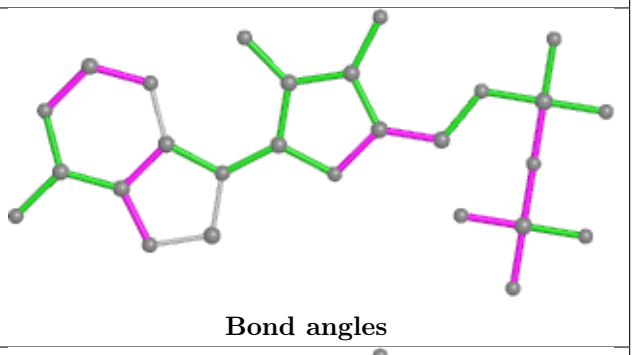
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1844	ADP	4	0
2	B	1843	ADP	6	0
2	A	1844	ADP	3	0
2	A	1843	ADP	2	0

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.

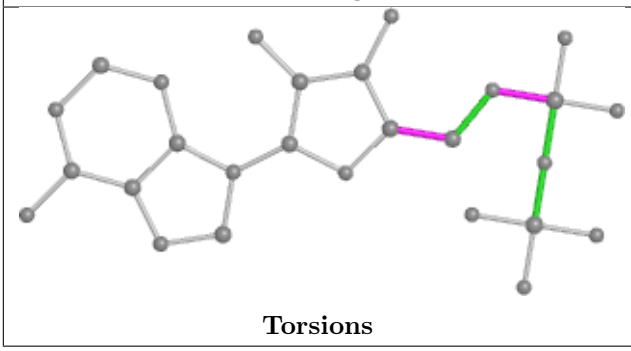
Ligand ADP B 1844



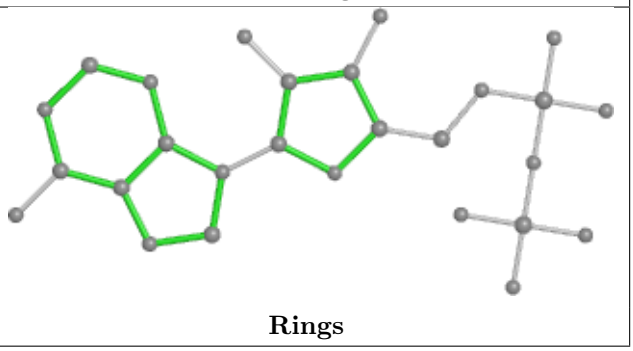
Bond lengths



Bond angles

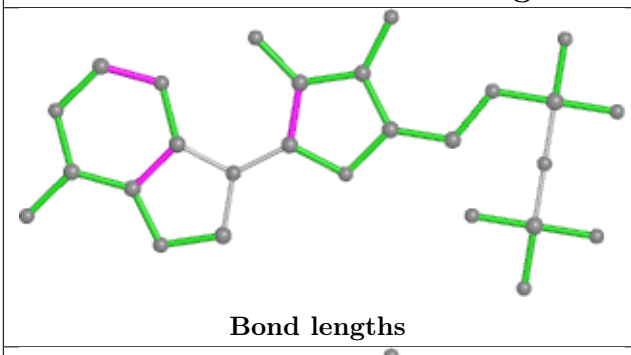


Torsions

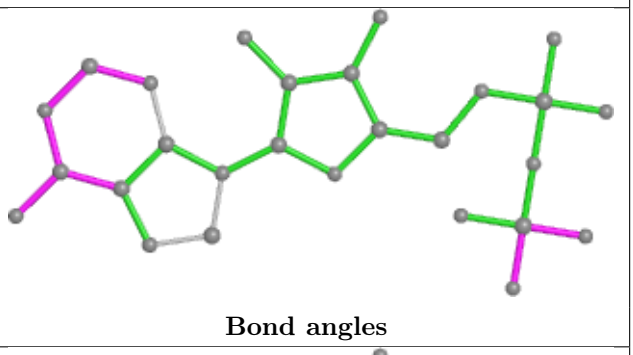


Rings

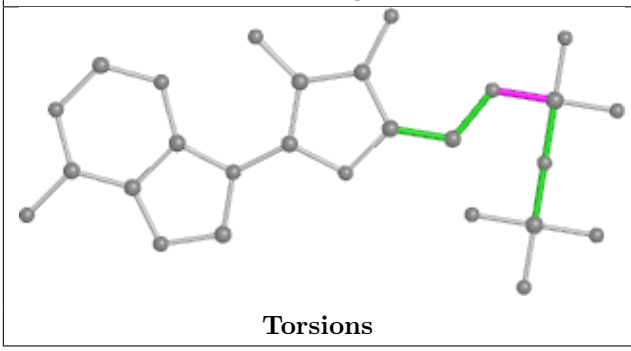
Ligand ADP B 1843



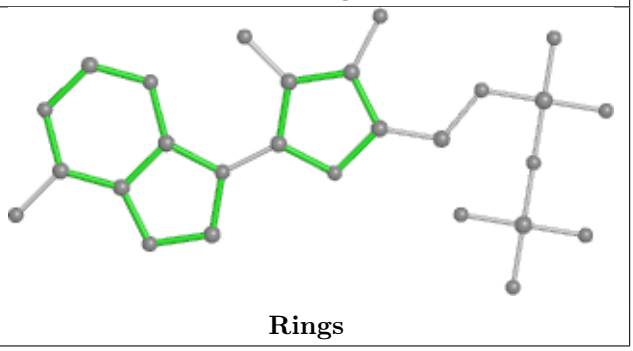
Bond lengths



Bond angles

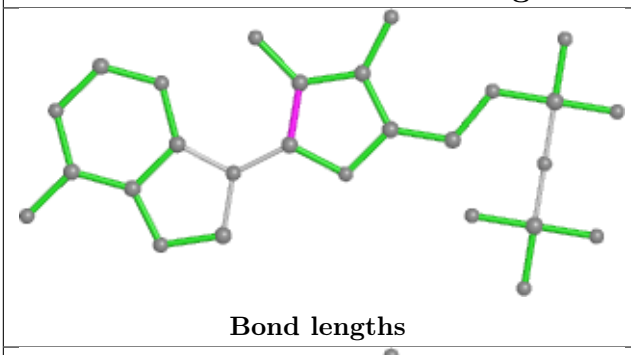


Torsions

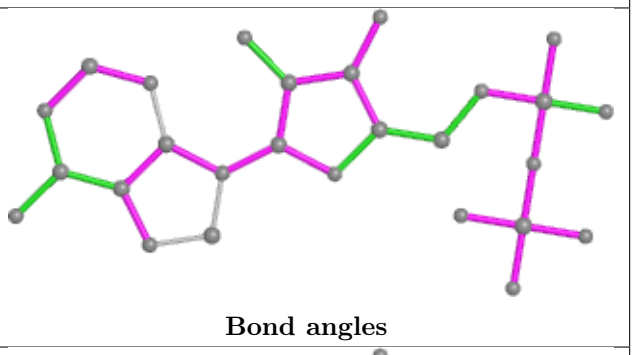


Rings

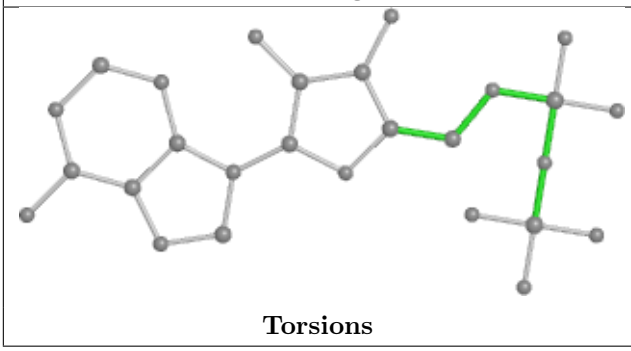
Ligand ADP A 1844



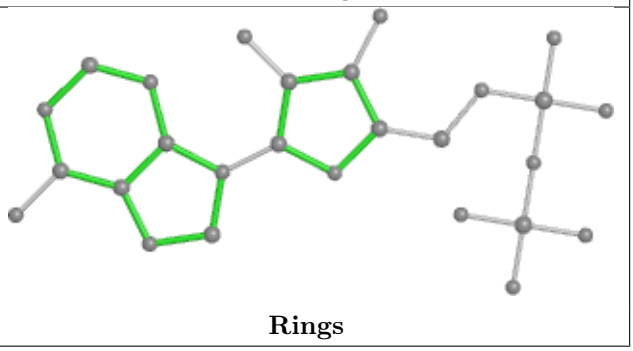
Bond lengths



Bond angles

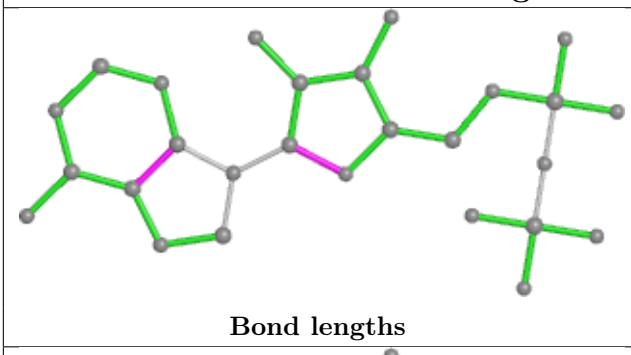


Torsions

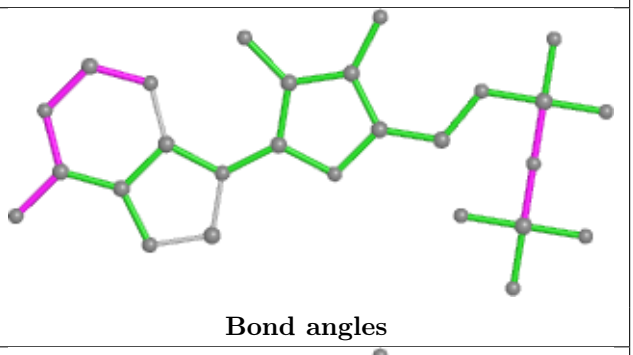


Rings

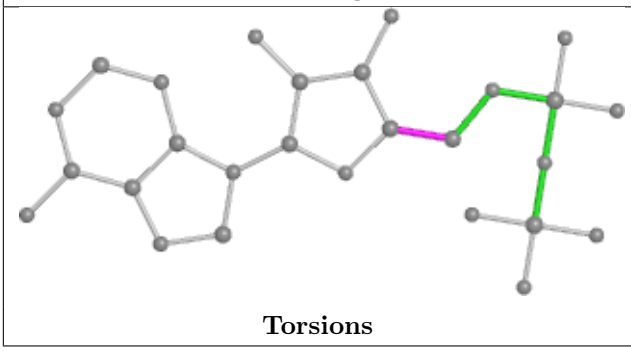
Ligand ADP A 1843



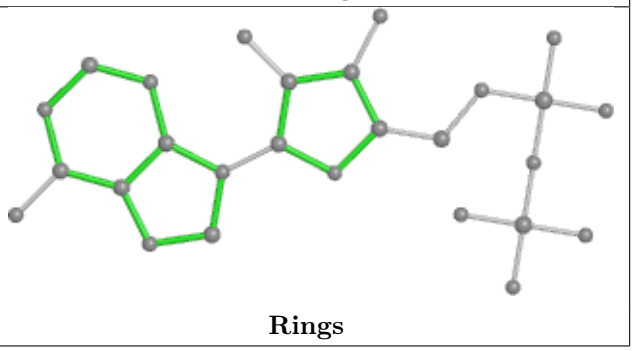
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	806/842 (95%)	-0.23	2 (0%) 95 87	38, 64, 92, 111	4 (0%)
1	B	835/842 (99%)	0.06	28 (3%) 45 19	40, 64, 97, 134	4 (0%)
All	All	1641/1684 (97%)	-0.09	30 (1%) 68 40	38, 64, 95, 134	8 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	TRP	4.1
1	B	180	ALA	3.9
1	B	206	VAL	3.4
1	B	253	GLY	3.2
1	B	241[A]	ARG	3.2
1	B	8	PRO	3.1
1	B	557	ASN	3.1
1	B	215	THR	3.1
1	B	217	HIS	3.0
1	B	569	HIS	2.9
1	A	650	VAL	2.8
1	B	560	PRO	2.7
1	B	563	ASP	2.7
1	B	333	PRO	2.6
1	B	247[A]	MET	2.6
1	B	212	PRO	2.6
1	B	244[A]	LYS	2.6
1	A	340	LYS	2.5
1	B	205	ASP	2.5
1	B	177	ARG	2.5
1	B	181	VAL	2.5
1	B	207	PRO	2.5
1	B	277	ARG	2.3
1	B	339	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	252	MET	2.3
1	B	340	LYS	2.3
1	B	200	LEU	2.2
1	B	245	LYS	2.1
1	B	211	LEU	2.1
1	B	210	GLU	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)

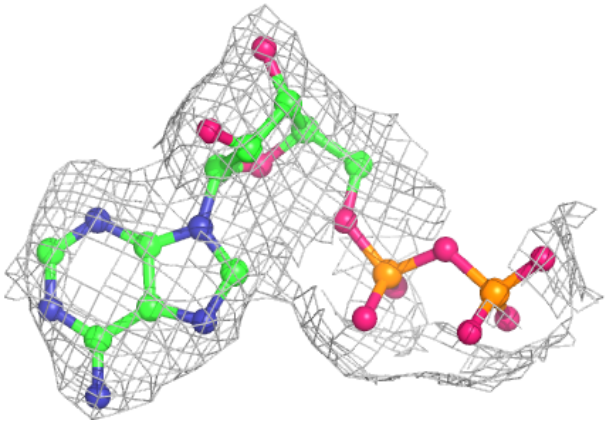
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

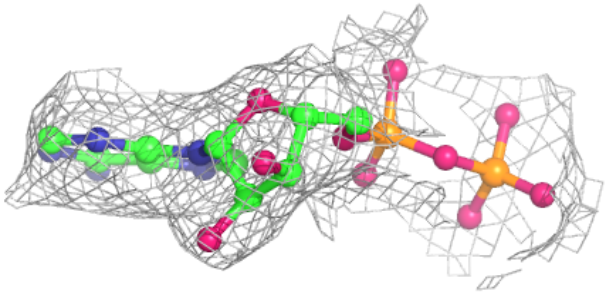
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1849[A]	5/5	0.73	0.38	89,90,90,91	5
4	SO4	B	1851[A]	5/5	0.76	0.31	98,98,100,100	5
4	SO4	A	1848[A]	5/5	0.86	0.14	93,93,94,95	5
5	PO4	B	1852[A]	5/5	0.89	0.27	85,86,86,86	5
4	SO4	B	1850[A]	5/5	0.90	0.17	80,81,82,82	5
4	SO4	B	1848[A]	5/5	0.92	0.19	95,95,95,95	5
4	SO4	A	1847[A]	5/5	0.94	0.18	87,88,88,88	5
2	ADP	A	1843	27/27	0.94	0.23	67,71,77,77	0
4	SO4	B	1849	5/5	0.94	0.18	93,94,95,96	0
2	ADP	B	1843	27/27	0.95	0.19	53,57,58,59	0
2	ADP	A	1844	27/27	0.97	0.18	31,47,51,51	0
2	ADP	B	1844	27/27	0.97	0.17	49,55,57,59	0
3	ZN	B	1845	1/1	0.97	0.19	44,44,44,44	1
3	ZN	B	1846	1/1	0.97	0.13	87,87,87,87	1
4	SO4	B	1847	5/5	0.98	0.26	90,91,91,91	0
3	ZN	A	1846	1/1	0.98	0.08	106,106,106,106	1
3	ZN	A	1845	1/1	0.98	0.10	80,80,80,80	1

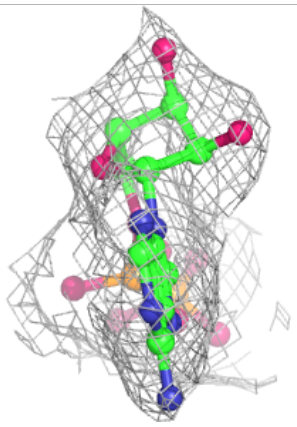
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1843:

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

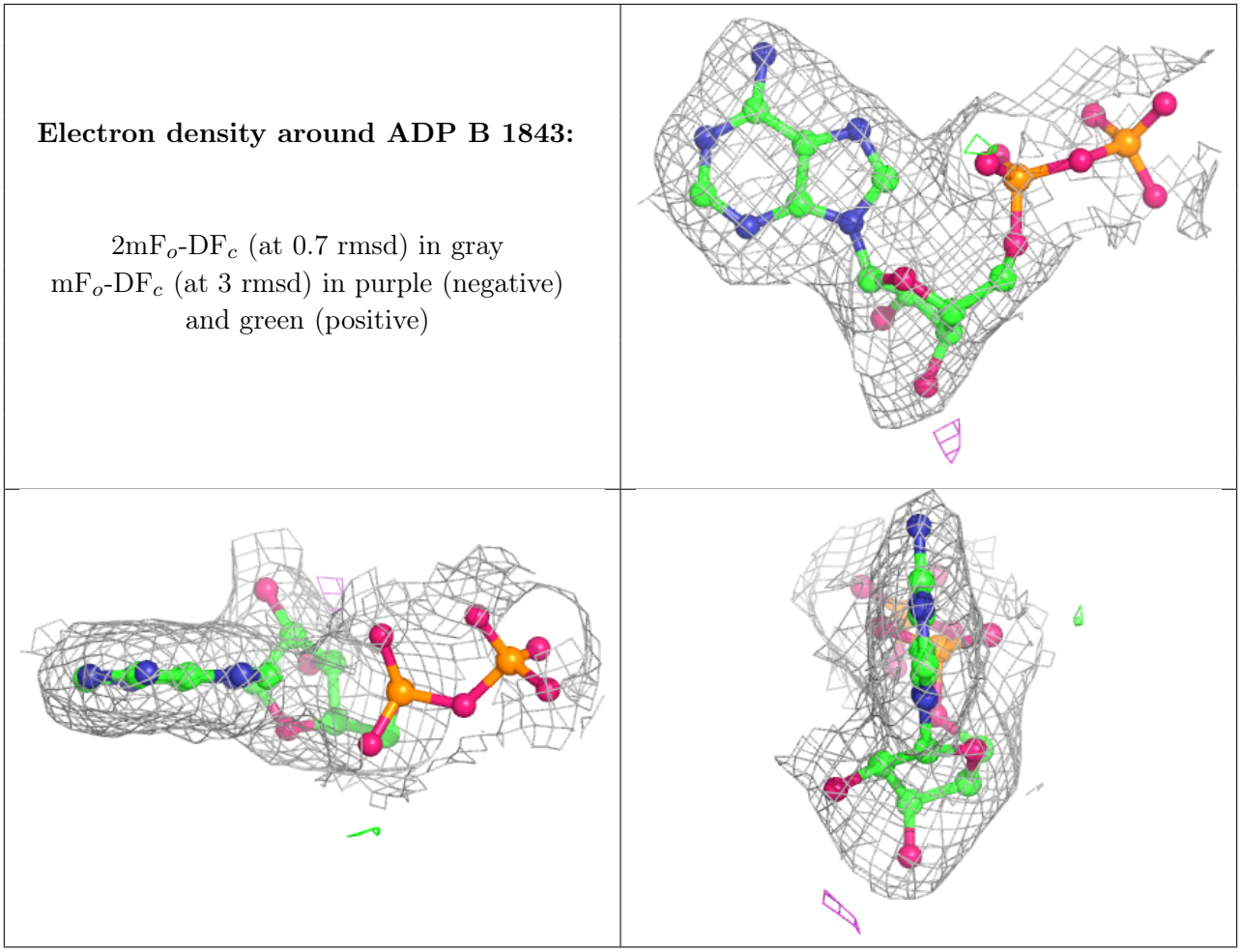






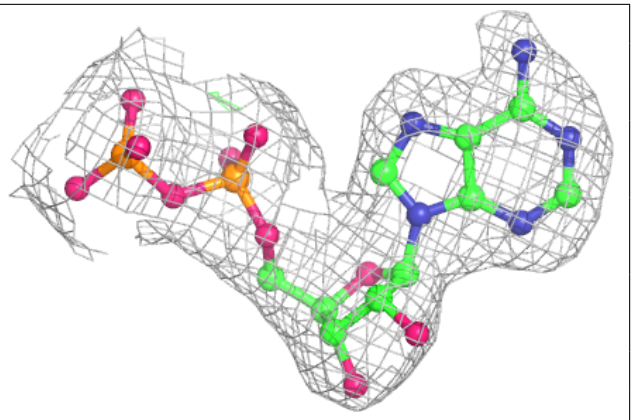
Electron density around ADP B 1843:

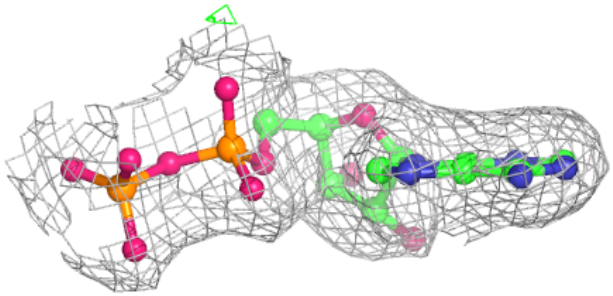
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

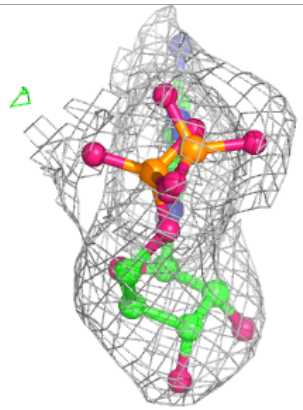


Electron density around ADP A 1844:

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

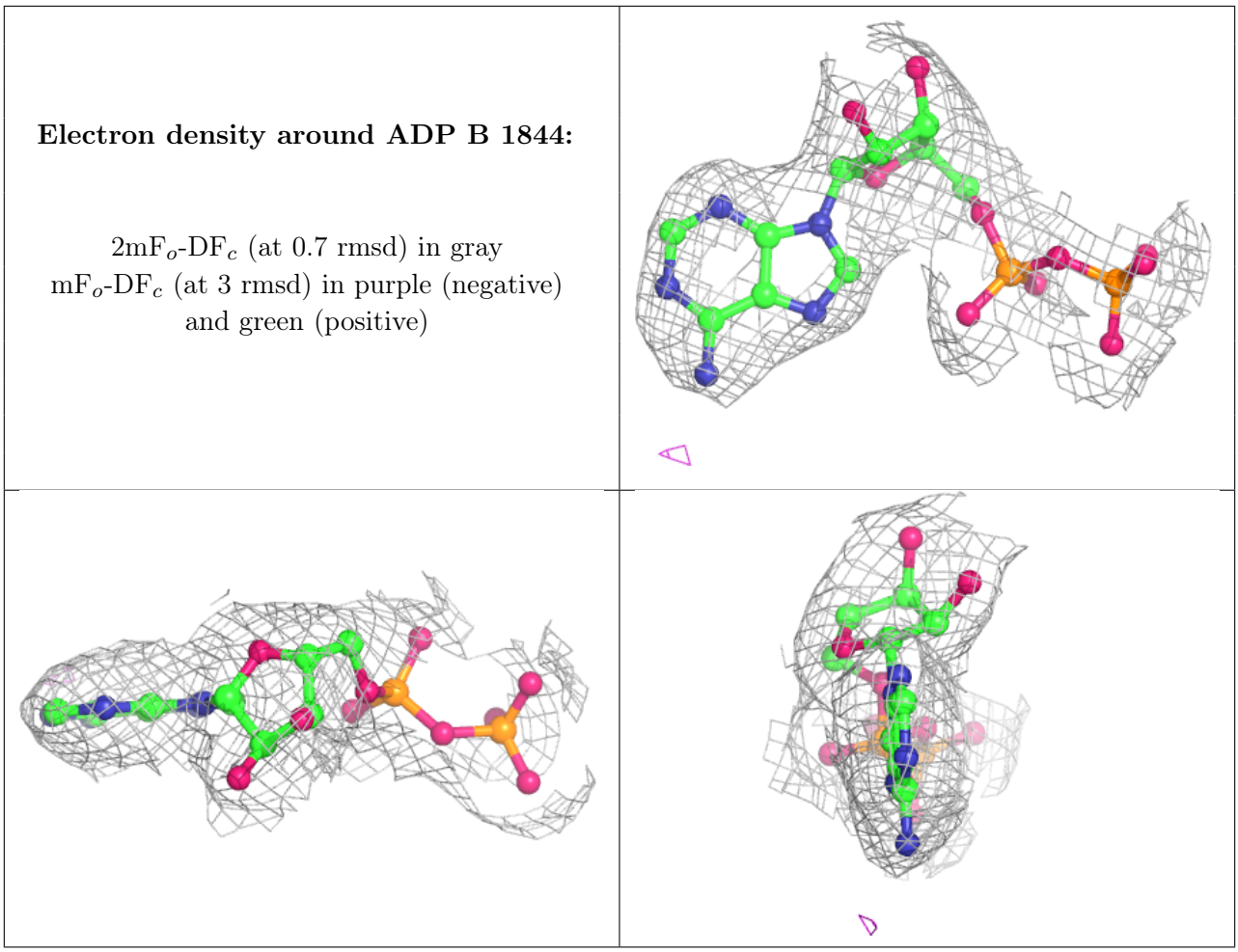






Electron density around ADP B 1844:

$2mF_o$-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.