



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2VF7
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 : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

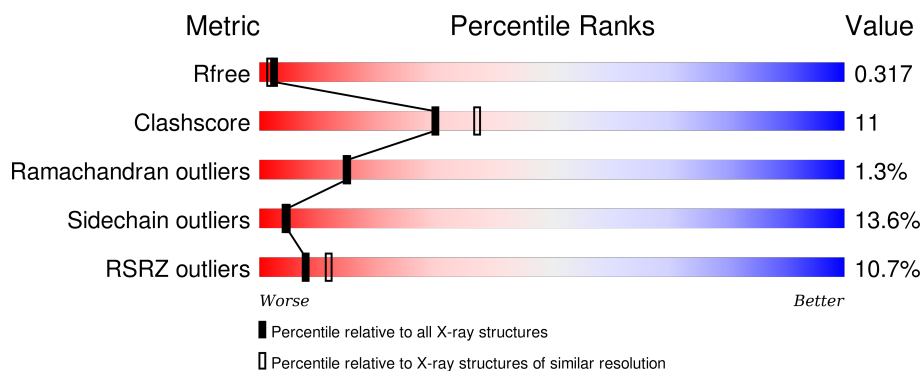
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	<div> <div>9%</div> <div>71%</div> <div>20%</div> <div>5%</div> <div>.</div> </div>
1	B	842	<div> <div>8%</div> <div>70%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	C	842	<div> <div>14%</div> <div>68%</div> <div>23%</div> <div>5%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19508 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.

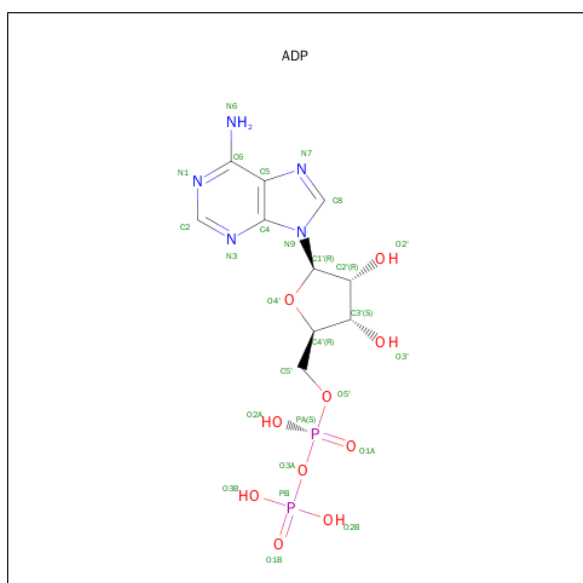
- Molecule 1 is a protein called EXCINUCLEASE ABC, SUBUNIT A..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	0	23	0
			6245	3918	1131	1177	19			
1	B	813	Total	C	N	O	S	0	26	0
			6240	3912	1134	1175	19			
1	C	814	Total	C	N	O	S	0	23	0
			6257	3930	1134	1174	19			

There are 3 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
C	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		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

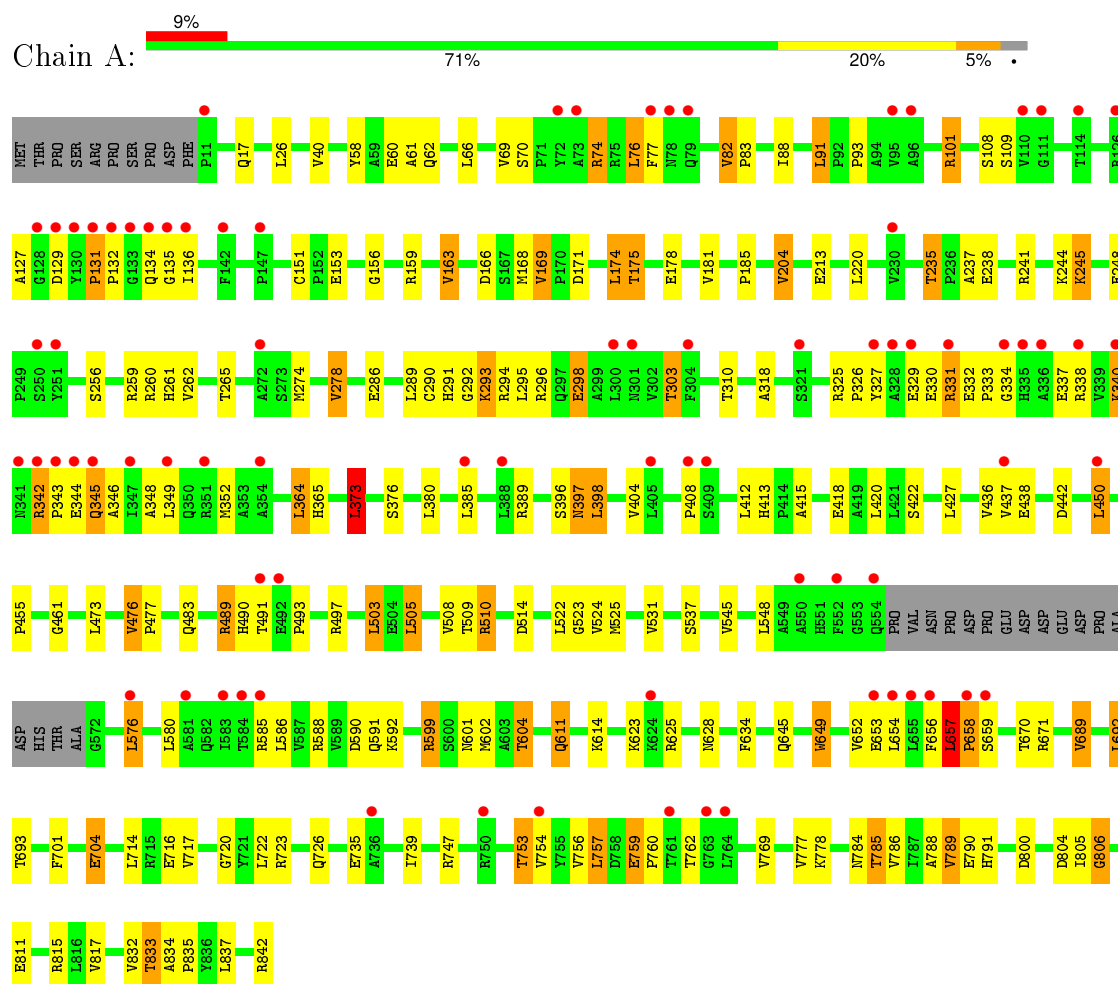
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	178	Total	O	0	0
			178	178		
5	B	230	Total	O	0	0
			230	230		
5	C	185	Total	O	0	0
			185	185		
5	G	2	Total	O	0	0
			2	2		
5	I	2	Total	O	0	0
			2	2		

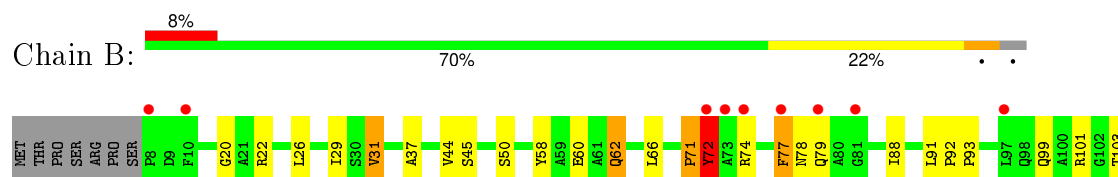
3 Residue-property plots

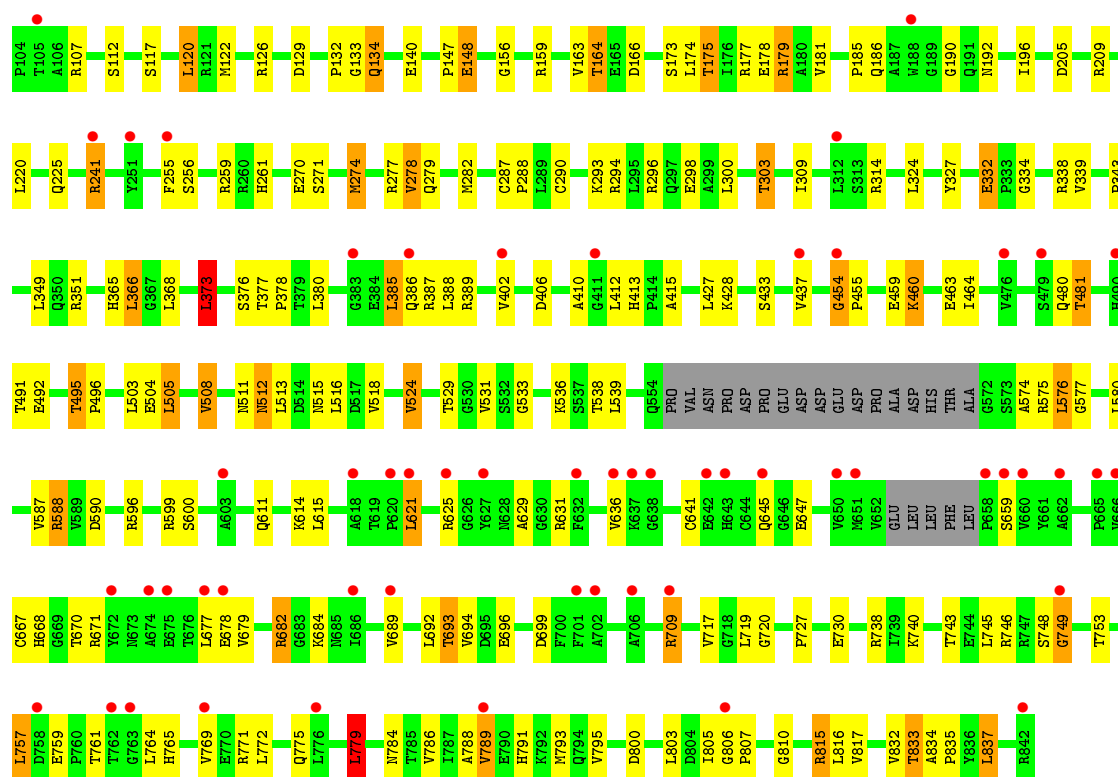
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

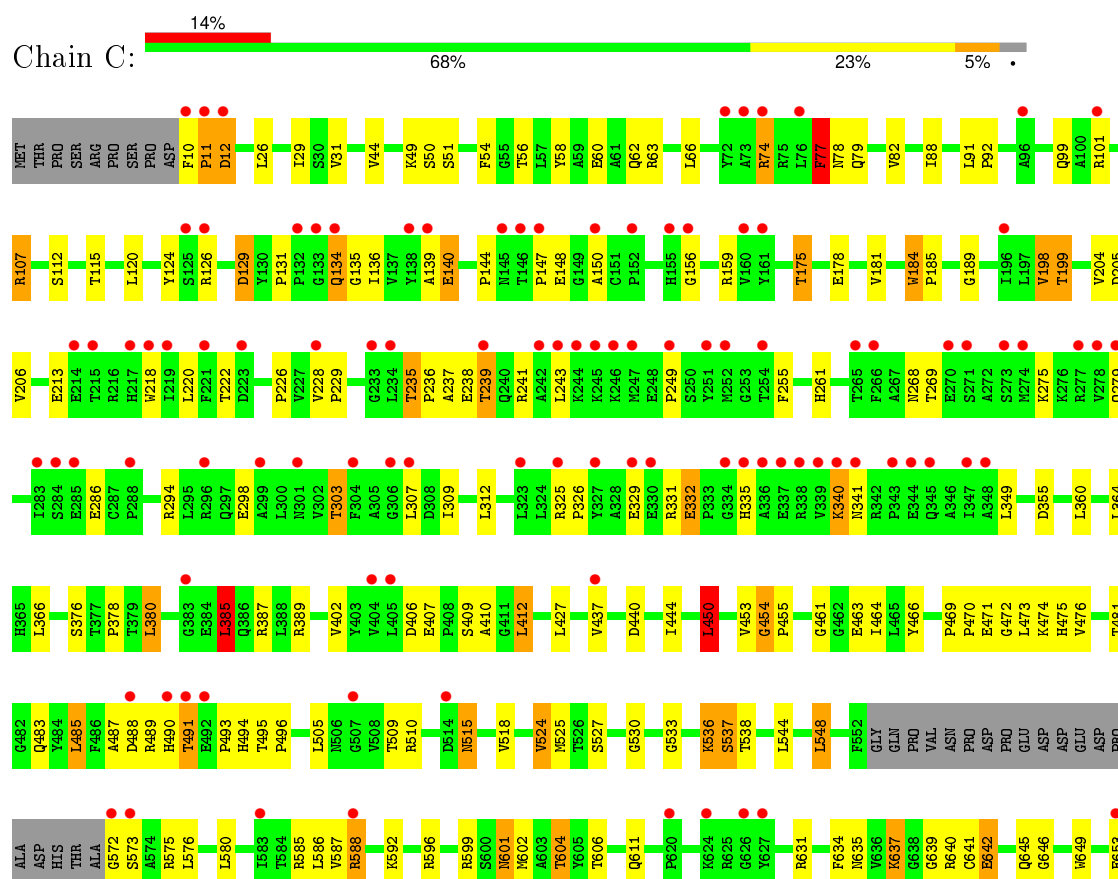


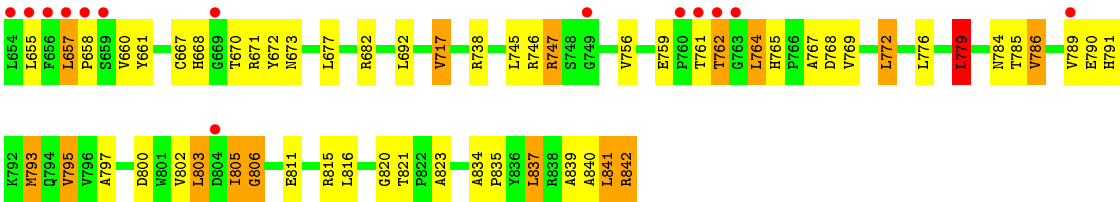
- Molecule 1: EXCINUCLEASE ABC, SUBUNIT A.





• Molecule 1: EXCINUCLEASE ABC, SUBUNIT A.





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.71Å 111.67Å 103.29Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 38.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.00-2.30) 95.0 (38.19-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.295 0.259 , 0.317	Depositor DCC
R_{free} test set	6451 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 127764 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19508	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.62	7/6375 (0.1%)	0.72	2/8662 (0.0%)
1	B	0.69	8/6376 (0.1%)	0.75	7/8661 (0.1%)
1	C	0.65	7/6395 (0.1%)	0.72	7/8689 (0.1%)
All	All	0.65	22/19146 (0.1%)	0.73	16/26012 (0.1%)

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	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	GLN	C-N	19.60	1.68	1.33
1	B	72	TYR	CE1-CZ	18.37	1.62	1.38
1	B	72	TYR	CG-CD1	15.35	1.59	1.39
1	A	330	GLU	CD-OE2	14.72	1.41	1.25
1	C	332	GLU	CD-OE1	10.20	1.36	1.25
1	B	72	TYR	CE2-CZ	10.19	1.51	1.38
1	B	678	GLU	CD-OE2	10.09	1.36	1.25
1	A	344	GLU	CD-OE2	10.03	1.36	1.25
1	A	344	GLU	CD-OE1	10.03	1.36	1.25
1	B	682	ARG	C-N	9.90	1.50	1.33
1	B	678	GLU	CD-OE1	8.72	1.35	1.25
1	B	682	ARG	NE-CZ	8.00	1.43	1.33
1	B	72	TYR	CG-CD2	7.96	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	GLN	CD-NE2	-7.75	1.13	1.32
1	C	340	LYS	CD-CE	7.40	1.69	1.51
1	C	332	GLU	CD-OE2	6.97	1.33	1.25
1	A	657	LEU	CG-CD2	6.67	1.76	1.51
1	A	330	GLU	CG-CD	6.60	1.61	1.51
1	C	129	ASP	CG-OD2	6.20	1.39	1.25
1	A	330	GLU	CD-OE1	5.93	1.32	1.25
1	A	657	LEU	CG-CD1	5.57	1.72	1.51
1	C	134	GLN	CG-CD	5.00	1.62	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	B	779	LEU	CA-CB-CG	7.79	133.23	115.30
1	B	385	LEU	CA-CB-CG	7.67	132.93	115.30
1	B	72	TYR	CD1-CG-CD2	7.00	125.61	117.90
1	C	485	LEU	CA-CB-CG	6.81	130.96	115.30
1	B	72	TYR	CG-CD2-CE2	-6.39	116.19	121.30
1	C	779	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	373	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	586	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	373	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	450	LEU	CA-CB-CG	5.34	127.59	115.30
1	C	134	GLN	CA-C-N	-5.23	105.75	116.20
1	C	385	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	682	ARG	CA-C-N	-5.18	105.83	116.20
1	C	380	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	772	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	HIS	Peptide
1	B	682	ARG	Mainchain

5.2 Too-close contacts

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	6245	0	6115	131	0
1	B	6240	0	6100	136	0
1	C	6257	0	6158	146	0
2	A	54	0	24	1	0
2	B	54	0	24	1	0
2	C	54	0	24	6	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	C	1	0	0	0	0
5	A	178	0	0	12	0
5	B	230	0	0	19	0
5	C	185	0	0	22	0
5	G	2	0	0	0	0
5	I	2	0	0	0	0
All	All	19508	0	18445	415	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 11.

All (415) 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:657:LEU:CD2	1:A:657:LEU:CG	1.76	1.62
1:C:134:GLN:C	1:C:135:GLY:N	1.68	1.43
1:C:184:TRP:HB2	1:C:185:PRO:HD2	1.27	1.14
1:C:657:LEU:HB3	1:C:658:PRO:HD2	1.39	1.04
2:C:1843:ADP:H8	5:C:2184:HOH:O	1.48	0.95
1:C:747:ARG:HD2	1:C:747:ARG:H	1.31	0.95
1:C:107:ARG:HE	1:C:378:PRO:HG2	1.31	0.92
1:B:366:LEU:HG	5:B:2137:HOH:O	1.68	0.91
1:C:184:TRP:HB2	1:C:185:PRO:CD	2.01	0.90
1:C:588[A]:ARG:HE	1:C:588[A]:ARG:H	1.18	0.89
1:B:377:THR:HA	1:B:380:LEU:HD13	1.56	0.87
1:A:175:THR:HG22	1:A:178:GLU:H	1.39	0.86
1:B:92:PRO:HG2	1:B:402:VAL:HG23	1.57	0.86
1:A:753:THR:HG23	1:A:784:ASN:ND2	1.92	0.84
1:B:524:VAL:HG13	1:B:800:ASP:HB2	1.59	0.84
1:C:765:HIS:HD2	1:C:767:ALA:H	1.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:HG23	1:C:239:THR:HG21	1.61	0.82
1:C:670:THR:HG21	1:C:677:LEU:HD11	1.62	0.81
1:A:649:TRP:HZ3	5:A:2140:HOH:O	1.63	0.80
1:C:175:THR:HG23	1:C:204:VAL:O	1.81	0.80
1:C:387:ARG:NH2	1:C:410:ALA:O	2.14	0.79
1:C:747:ARG:N	1:C:747:ARG:HD2	1.97	0.79
1:B:599:ARG:HG2	1:B:647:GLU:HG2	1.64	0.78
1:A:342:ARG:HG3	1:A:346:ALA:H	1.48	0.78
1:C:657:LEU:HB3	1:C:658:PRO:CD	2.13	0.78
1:A:163:VAL:HG21	1:A:168:MET:HE3	1.66	0.78
1:B:761:THR:HA	1:B:764:LEU:HD22	1.64	0.77
1:C:790:GLU:HG2	1:C:795:VAL:HG22	1.67	0.77
1:B:133:GLY:HA2	1:C:797:ALA:O	1.82	0.77
1:A:537:SER:HB3	2:A:1842:ADP:O2B	1.85	0.77
1:C:599:ARG:NH2	1:C:645:GLN:O	2.18	0.77
1:C:454:GLY:N	1:C:463:GLU:O	2.14	0.76
1:B:759:GLU:CG	1:B:791:HIS:HD2	2.00	0.74
1:B:290:CYS:SG	1:B:293:LYS:O	2.45	0.74
1:B:717:VAL:CG1	1:B:738:ARG:HB3	2.18	0.74
1:C:641:CYS:O	1:C:645:GLN:HA	1.86	0.73
1:A:657:LEU:CD2	1:A:657:LEU:CB	2.66	0.73
1:A:175:THR:HG21	5:A:2050:HOH:O	1.89	0.73
1:B:759:GLU:HG2	1:B:791:HIS:CD2	2.22	0.73
1:A:693:THR:HG23	1:A:720:GLY:O	1.90	0.72
1:B:481:THR:HG22	1:B:765:HIS:HE2	1.55	0.72
1:A:649:TRP:CZ3	5:A:2140:HOH:O	2.39	0.72
1:B:366:LEU:HD12	5:B:2118:HOH:O	1.88	0.72
1:C:834:ALA:HB3	1:C:835:PRO:HD3	1.72	0.71
1:A:248[A]:GLU:HG2	5:A:2073:HOH:O	1.91	0.71
1:B:386:GLN:HE22	1:B:406:ASP:H	1.39	0.70
1:B:759:GLU:CG	1:B:791:HIS:CD2	2.75	0.69
1:C:573:SER:HB2	5:C:2134:HOH:O	1.92	0.69
2:C:1843:ADP:C8	5:C:2184:HOH:O	2.32	0.69
1:B:156:GLY:O	1:B:294:ARG:HD2	1.93	0.69
1:C:440:ASP:O	1:C:444:ILE:HG12	1.92	0.69
1:A:524:VAL:HG13	1:A:800:ASP:HB2	1.75	0.68
1:A:340:LYS:HE3	1:A:340:LYS:H	1.59	0.68
1:A:735:GLU:O	1:A:739:ILE:HG13	1.93	0.68
1:C:453:VAL:O	1:C:454:GLY:O	2.11	0.67
1:B:511:ASN:HD22	1:B:538:THR:CG2	2.07	0.67
1:A:274:MET:HG3	5:A:2078:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG13	1:B:464:ILE:HD13	1.76	0.67
1:B:60:GLU:HG2	1:B:88:ILE:HD12	1.76	0.67
1:A:524:VAL:CG1	1:A:800:ASP:HB2	2.25	0.67
1:A:701:PHE:HD2	1:A:704:GLU:HG3	1.59	0.67
1:C:475:HIS:HB2	5:C:2115:HOH:O	1.95	0.67
1:A:175:THR:HG22	1:A:178:GLU:N	2.08	0.66
1:C:599:ARG:HE	1:C:635:ASN:HD22	1.43	0.66
1:B:122:MET:HG2	1:B:126[A]:ARG:HH12	1.60	0.66
1:C:66:LEU:HB3	1:C:74:ARG:HG2	1.77	0.66
1:A:523:GLY:H	1:A:785:THR:HG22	1.61	0.65
1:C:134:GLN:CA	1:C:135:GLY:N	2.58	0.65
1:A:293:LYS:HD3	1:A:310:THR:HG21	1.78	0.65
1:B:717:VAL:HG13	1:B:738:ARG:HB3	1.76	0.65
1:A:163:VAL:HG21	1:A:168:MET:CE	2.26	0.65
1:B:621:LEU:HD12	1:B:679:VAL:HG22	1.78	0.64
1:B:290:CYS:HB2	1:B:293:LYS:O	1.97	0.64
1:B:179[A]:ARG:NH2	1:B:185:PRO:O	2.31	0.64
1:C:226:PRO:HD2	1:C:255:PHE:HB3	1.79	0.64
1:C:717:VAL:HG13	1:C:738:ARG:HB3	1.78	0.64
1:A:156:GLY:O	1:A:294:ARG:HD2	1.96	0.64
1:C:235:THR:HG22	1:C:238:GLU:H	1.62	0.64
1:B:365:HIS:C	1:B:366:LEU:O	2.34	0.63
1:C:657:LEU:CB	1:C:658:PRO:HD2	2.24	0.63
1:A:61:ALA:HB2	1:A:91:LEU:HD13	1.79	0.63
1:A:455:PRO:HD2	1:A:461:GLY:HA2	1.81	0.63
1:C:144:PRO:HG2	1:C:294:ARG:HH21	1.63	0.62
1:B:693:THR:HG22	1:B:696:GLU:H	1.64	0.62
1:C:184:TRP:CB	1:C:185:PRO:HD2	2.18	0.62
1:C:129:ASP:HB2	1:C:303:THR:HG22	1.79	0.62
1:C:29:ILE:HD13	1:C:464:ILE:HD11	1.83	0.61
1:B:717:VAL:HG12	1:B:719:LEU:HG	1.83	0.61
1:B:511:ASN:HD22	1:B:538:THR:HG21	1.66	0.61
1:A:127:ALA:HB1	1:A:349:LEU:HD12	1.83	0.61
1:C:821:THR:HG22	1:C:823:ALA:H	1.66	0.61
1:C:44:VAL:CG1	5:C:2170:HOH:O	2.48	0.61
1:B:611:GLN:HA	1:B:614:LYS:HG2	1.83	0.60
1:B:20:GLY:O	1:B:22:ARG:NH1	2.34	0.60
1:C:811[A]:GLU:HG3	5:C:2081:HOH:O	2.00	0.60
1:B:576:LEU:HD13	1:B:580:LEU:HD11	1.82	0.60
1:A:759:GLU:OE2	1:A:790:GLU:OE2	2.19	0.60
1:B:71:PRO:HD2	1:B:72:TYR:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:GLY:N	1:C:815:ARG:O	2.33	0.60
1:B:62:GLN:O	1:B:66:LEU:HG	2.02	0.59
1:C:450:LEU:HD21	1:C:473:LEU:HD22	1.82	0.59
1:B:175:THR:HG22	1:B:178[A]:GLU:HG2	1.84	0.59
1:B:129:ASP:HB2	1:B:303:THR:HG22	1.84	0.59
1:C:115:THR:HB	5:C:2089:HOH:O	2.02	0.59
1:B:588:ARG:HH11	1:B:588:ARG:HB2	1.68	0.59
1:C:537:SER:HB2	2:C:1842:ADP:O3B	2.03	0.59
1:C:218:TRP:HA	1:C:222:THR:HG23	1.85	0.59
1:B:50:SER:HB3	5:B:2130:HOH:O	2.02	0.59
1:B:175:THR:HG23	1:B:177:ARG:H	1.66	0.58
1:A:93:PRO:HG2	1:B:93:PRO:HG2	1.84	0.58
1:A:413:HIS:HD2	1:A:415:ALA:H	1.51	0.58
1:B:745:LEU:HD11	1:B:775:GLN:HE21	1.68	0.58
1:B:373:LEU:HD23	1:B:373:LEU:H	1.66	0.58
1:B:140:GLU:HG3	1:B:148:GLU:HG3	1.85	0.58
1:A:545:VAL:CG2	1:A:756:VAL:HG21	2.32	0.58
1:C:841:LEU:O	1:C:842:ARG:C	2.40	0.58
1:C:670:THR:O	1:C:671:ARG:HB2	2.04	0.58
1:A:693:THR:HG21	5:A:2103:HOH:O	2.02	0.58
1:C:842:ARG:HB3	1:C:842:ARG:HH11	1.67	0.58
1:C:60:GLU:HG2	1:C:88:ILE:HD12	1.85	0.58
1:B:611:GLN:O	1:B:615:LEU:HD23	2.03	0.57
1:B:508:VAL:HG12	1:B:516:LEU:O	2.04	0.57
1:A:175:THR:HG23	1:A:204:VAL:O	2.04	0.57
5:B:2031:HOH:O	1:C:821:THR:HG23	2.05	0.57
1:A:652:VAL:C	1:A:654:LEU:H	2.07	0.57
1:B:689:VAL:O	1:B:692:LEU:HB2	2.05	0.57
1:B:209:ARG:NH1	5:B:2065:HOH:O	2.38	0.56
1:B:74:ARG:O	1:B:74:ARG:HG3	2.05	0.56
1:A:508:VAL:O	1:A:514:ASP:O	2.22	0.56
1:B:271:SER:HB3	1:B:274:MET:HB2	1.87	0.56
1:C:530:GLY:O	1:C:536:LYS:HE2	2.06	0.56
1:B:481:THR:HG22	1:B:765:HIS:NE2	2.19	0.56
1:B:134:GLN:HE22	1:B:298:GLU:HB2	1.71	0.56
1:B:185:PRO:HG3	1:B:261:HIS:NE2	2.21	0.56
1:C:409:SER:O	1:C:412:LEU:HB2	2.06	0.56
1:C:495:THR:HG23	1:C:496:PRO:HD2	1.87	0.56
1:A:159:ARG:NH1	1:A:286:GLU:HG3	2.21	0.56
1:A:524:VAL:HG13	1:A:800:ASP:CB	2.36	0.55
1:A:17:GLN:HB2	5:A:2003:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:N	1:A:326:PRO:HD2	2.21	0.55
1:B:670:THR:HG21	1:B:677:LEU:HD11	1.88	0.55
1:A:759:GLU:O	1:A:762:THR:HG23	2.05	0.55
2:C:1842:ADP:PA	5:C:2126:HOH:O	2.65	0.55
1:B:122:MET:HG2	1:B:126[A]:ARG:NH1	2.21	0.55
1:C:329:GLU:HG3	1:C:331:ARG:NH1	2.21	0.55
1:A:159:ARG:HH11	1:A:286:GLU:HG3	1.71	0.55
1:A:329:GLU:HB2	1:A:331:ARG:HD2	1.89	0.55
1:B:759:GLU:HG3	1:B:791:HIS:HD2	1.72	0.54
1:A:628:ASN:HB2	5:A:2129:HOH:O	2.07	0.54
1:A:657:LEU:O	1:A:658:PRO:C	2.46	0.54
1:C:49:LYS:HG2	2:C:1843:ADP:O1B	2.07	0.54
1:B:29:ILE:HD13	1:B:464:ILE:HD11	1.89	0.54
1:B:278:VAL:HG13	1:B:282:MET:CE	2.38	0.54
1:A:129:ASP:HB2	1:A:303:THR:HG22	1.90	0.54
1:B:764:LEU:HD13	5:B:2206:HOH:O	2.07	0.54
1:B:29:ILE:HB	1:B:464:ILE:HD12	1.89	0.54
1:A:398:LEU:HD22	5:A:2091:HOH:O	2.07	0.54
1:C:765:HIS:CD2	1:C:767:ALA:H	2.17	0.54
1:C:218:TRP:CD1	1:C:222:THR:HG21	2.43	0.54
1:C:745:LEU:N	1:C:747:ARG:HH21	2.07	0.53
1:A:483:GLN:HB3	1:A:489:ARG:HG3	1.89	0.53
1:A:168:MET:HE1	1:A:259:ARG:HA	1.91	0.53
1:C:134:GLN:C	1:C:135:GLY:CA	2.72	0.53
1:A:348:ALA:O	1:A:352:MET:HG3	2.08	0.53
1:B:791:HIS:CE1	5:B:2213:HOH:O	2.60	0.53
1:A:185:PRO:HG3	1:A:261:HIS:NE2	2.23	0.53
1:B:290:CYS:CB	1:B:293:LYS:O	2.57	0.53
1:A:342:ARG:NE	1:A:346:ALA:HB3	2.24	0.53
1:A:805:ILE:O	1:A:806:GLY:O	2.26	0.53
1:A:716[A]:GLU:OE2	1:A:778:LYS:NZ	2.39	0.53
1:A:576:LEU:HD12	1:A:580:LEU:HD11	1.90	0.53
1:A:503:LEU:HB2	1:A:522:LEU:HD21	1.90	0.52
1:A:804:ASP:OD1	1:A:833:THR:CG2	2.57	0.52
1:A:806:GLY:N	1:A:815:ARG:O	2.30	0.52
1:C:509:THR:HB	1:C:515:ASN:H	1.75	0.52
1:C:175:THR:HG22	1:C:178:GLU:H	1.74	0.52
1:A:497:ARG:NH2	1:A:777:VAL:HG13	2.25	0.52
1:A:757:LEU:O	1:A:788:ALA:HA	2.09	0.52
1:B:480:GLN:NE2	5:B:2149:HOH:O	2.43	0.52
1:A:373:LEU:H	1:A:373:LEU:HD23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:HH21	1:A:76:LEU:HD22	1.75	0.51
1:A:670:THR:O	1:A:671:ARG:HB2	2.09	0.51
1:C:54:PHE:HA	1:C:58:TYR:HB3	1.93	0.51
1:C:759:GLU:OE2	1:C:791:HIS:ND1	2.39	0.51
1:B:173:SER:HB3	5:B:2065:HOH:O	2.09	0.51
1:A:318:ALA:HA	1:A:364:LEU:HD11	1.93	0.51
1:C:185:PRO:HD3	1:C:261:HIS:CE1	2.46	0.51
1:B:717:VAL:HG11	1:B:738:ARG:HB3	1.90	0.51
1:C:790:GLU:OE2	1:C:795:VAL:HG21	2.11	0.51
1:A:604:THR:HG21	5:A:2123:HOH:O	2.10	0.51
1:B:117:SER:O	1:B:120:LEU:HD12	2.11	0.51
1:C:670:THR:HG22	1:C:672:TYR:H	1.76	0.51
1:A:689:VAL:O	1:A:692:LEU:HB2	2.12	0.51
1:B:511:ASN:HD22	1:B:538:THR:HG22	1.76	0.50
1:A:693:THR:CG2	1:A:720:GLY:O	2.57	0.50
1:B:387:ARG:NH2	1:B:410:ALA:O	2.45	0.50
1:C:802:VAL:N	1:C:820:GLY:O	2.43	0.50
1:C:385:LEU:HD12	1:C:385:LEU:C	2.32	0.50
1:A:599:ARG:NH2	1:A:645:GLN:O	2.38	0.50
1:A:753:THR:HG23	1:A:784:ASN:HD22	1.70	0.50
1:A:163:VAL:CG2	1:A:168:MET:HE3	2.38	0.50
1:C:44:VAL:HG12	5:C:2170:HOH:O	2.10	0.50
1:C:92:PRO:HG2	1:C:402:VAL:CG2	2.42	0.50
1:B:455:PRO:HD2	1:B:460:LYS:O	2.11	0.49
1:B:508:VAL:CG1	1:B:516:LEU:O	2.61	0.49
1:B:793:MET:CE	1:B:837:LEU:HG	2.42	0.49
1:C:175:THR:HG21	5:C:2010:HOH:O	2.12	0.49
1:B:512:ASN:HD21	1:B:810:GLY:C	2.15	0.49
1:A:235:THR:HG22	1:A:238:GLU:HG2	1.94	0.49
1:A:413:HIS:CD2	1:A:415:ALA:H	2.28	0.49
1:B:120:LEU:HD13	1:B:309:ILE:HD11	1.95	0.49
1:A:163:VAL:HG11	1:A:168:MET:HE1	1.94	0.49
1:B:748:SER:O	1:B:749:GLY:C	2.50	0.49
1:A:131:PRO:HB3	1:A:132:PRO:HD2	1.94	0.49
1:A:585:ARG:HB2	1:A:753:THR:HB	1.95	0.49
1:C:491:THR:HG21	5:C:2172:HOH:O	2.12	0.49
1:B:495:THR:HG23	5:B:2153:HOH:O	2.13	0.48
1:B:694:VAL:HB	1:B:720:GLY:HA2	1.94	0.48
1:C:49:LYS:HE2	1:C:437:VAL:CG2	2.44	0.48
1:C:510:ARG:HB3	1:C:572:GLY:HA2	1.94	0.48
1:A:804:ASP:OD1	1:A:833:THR:HG21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:HIS:HE1	1:B:833:THR:HB	1.77	0.48
1:C:793:MET:HG2	1:C:837:LEU:HA	1.94	0.48
1:B:164:THR:HG23	1:B:166:ASP:H	1.78	0.48
1:B:37:ALA:HA	1:B:428:LYS:HD2	1.96	0.48
1:A:523:GLY:H	1:A:785:THR:CG2	2.26	0.48
1:B:670:THR:O	1:B:671:ARG:HB2	2.13	0.48
1:C:634:PHE:O	1:C:646:GLY:HA3	2.14	0.48
1:B:225:GLN:HG2	1:B:255:PHE:O	2.14	0.48
1:C:518:VAL:HG13	1:C:803:LEU:HD21	1.96	0.48
1:B:834:ALA:HB3	1:B:835:PRO:HD3	1.96	0.48
1:C:601:ASN:ND2	1:C:604:THR:H	2.12	0.47
1:C:77:PHE:HB2	1:C:655:LEU:HG	1.95	0.47
1:C:406:ASP:HA	1:C:437:VAL:HG13	1.95	0.47
1:A:74:ARG:NH2	1:A:77:PHE:HA	2.29	0.47
1:A:689:VAL:HA	1:A:692:LEU:HD22	1.96	0.47
1:A:413:HIS:CE1	1:A:833:THR:HG22	2.49	0.47
1:A:74:ARG:HH22	1:A:77:PHE:HA	1.79	0.47
1:B:44:VAL:CG1	1:B:45:SER:N	2.76	0.47
1:C:576:LEU:HD13	1:C:580:LEU:HD11	1.95	0.47
1:B:757:LEU:O	1:B:788:ALA:HA	2.14	0.47
1:C:229:PRO:HB3	1:C:249:PRO:HG3	1.96	0.47
1:C:49:LYS:HE2	1:C:437:VAL:HG23	1.96	0.47
1:C:759:GLU:OE1	1:C:761:THR:HG22	2.14	0.47
1:B:327:TYR:HB3	1:B:349:LEU:HD22	1.96	0.47
1:A:290:CYS:O	1:A:292:GLY:N	2.45	0.47
1:B:743:THR:HG21	5:B:2070:HOH:O	2.14	0.47
1:C:185:PRO:HG2	1:C:189:GLY:C	2.34	0.47
1:B:179[A]:ARG:NH2	1:B:190:GLY:HA3	2.29	0.47
1:C:518:VAL:HG22	1:C:816:LEU:HD12	1.96	0.47
1:B:327:TYR:CD2	1:B:332:GLU:HG2	2.50	0.47
1:C:759:GLU:HB3	1:C:762:THR:HG22	1.97	0.47
1:C:150:ALA:HB1	1:C:156:GLY:CA	2.45	0.47
1:B:277:ARG:HD2	5:B:2090:HOH:O	2.14	0.47
1:B:590:ASP:OD2	1:B:590:ASP:N	2.43	0.47
1:C:199:THR:HG21	1:C:228:VAL:HB	1.97	0.46
1:B:179[A]:ARG:HH22	1:B:190:GLY:HA3	1.80	0.46
1:C:235:THR:HG23	1:C:237:ALA:H	1.81	0.46
1:A:611:GLN:O	1:A:614:LYS:HB3	2.16	0.46
1:C:139:ALA:O	1:C:140:GLU:HB2	2.13	0.46
1:B:163:VAL:HG21	1:B:259:ARG:HG3	1.96	0.46
1:C:525:MET:HG3	1:C:786:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:PRO:HG2	1:B:730:GLU:HG3	1.98	0.46
1:B:504:GLU:O	1:B:576:LEU:HA	2.16	0.46
1:A:505:LEU:HD22	1:A:508:VAL:HG22	1.97	0.46
1:B:775:GLN:O	1:B:779:LEU:HD22	2.16	0.46
1:A:171:ASP:HB3	1:A:174:LEU:HD22	1.98	0.46
1:C:466:TYR:OH	1:C:472:GLY:HA3	2.15	0.46
1:A:342:ARG:HE	1:A:346:ALA:HB3	1.81	0.46
1:B:278:VAL:HG13	1:B:282:MET:HE3	1.97	0.46
1:A:332:GLU:O	1:A:334:GLY:N	2.49	0.46
1:B:413:HIS:HD2	1:B:415:ALA:CB	2.29	0.46
1:A:753:THR:CG2	1:A:784:ASN:ND2	2.70	0.46
1:A:545:VAL:HG22	1:A:756:VAL:HG21	1.96	0.46
1:C:150:ALA:HB3	5:C:2045:HOH:O	2.15	0.45
1:B:492:GLU:HG2	5:B:2152:HOH:O	2.17	0.45
1:C:510:ARG:HG3	1:C:538:THR:HG23	1.99	0.45
1:A:293:LYS:HG2	1:A:293:LYS:H	1.50	0.45
1:C:77:PHE:O	1:C:79:GLN:N	2.49	0.45
1:C:776:LEU:O	1:C:779:LEU:HD22	2.17	0.45
1:C:667:CYS:O	1:C:668:HIS:HB2	2.16	0.45
1:B:29:ILE:HD13	1:B:464:ILE:CD1	2.46	0.45
1:B:779:LEU:O	1:B:784:ASN:HB2	2.16	0.45
1:A:408:PRO:HB2	1:A:420:LEU:HD11	1.98	0.45
1:B:177:ARG:NH1	1:B:205:ASP:OD1	2.50	0.45
1:C:325:ARG:HD2	5:C:2083:HOH:O	2.17	0.45
1:C:494:HIS:HB3	5:C:2122:HOH:O	2.15	0.45
1:B:377:THR:N	1:B:378:PRO:CD	2.80	0.45
1:C:481:THR:O	1:C:485:LEU:HD23	2.17	0.45
1:C:471:GLU:O	1:C:474:LYS:HE3	2.17	0.45
1:B:77:PHE:C	1:B:79:GLN:H	2.21	0.45
1:B:339:VAL:O	1:B:343:PRO:HG3	2.17	0.44
1:B:539:LEU:HD22	1:B:805:ILE:HD11	1.99	0.44
1:B:759:GLU:HG3	1:B:791:HIS:CD2	2.51	0.44
1:B:279:GLN:HA	1:B:282:MET:HG2	2.00	0.44
1:A:757:LEU:HB3	1:A:760:PRO:HG3	1.99	0.44
1:C:779:LEU:O	1:C:784:ASN:HB2	2.16	0.44
1:C:481:THR:OG1	1:C:765:HIS:HE1	2.00	0.44
1:A:163:VAL:CG2	1:A:168:MET:CE	2.95	0.44
1:C:120:LEU:O	1:C:124:TYR:HD1	2.00	0.44
1:C:764:LEU:HG	1:C:768:ASP:HB3	1.99	0.44
1:A:408:PRO:HD2	1:A:438:GLU:OE1	2.18	0.44
1:A:265:THR:HB	1:A:278:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:C	1:A:76:LEU:H	2.19	0.44
1:A:599:ARG:NH2	1:A:634:PHE:O	2.49	0.44
1:B:413:HIS:CD2	1:B:415:ALA:H	2.36	0.44
1:C:213:GLU:HG2	5:C:2059:HOH:O	2.17	0.44
1:B:454:GLY:N	1:B:463:GLU:O	2.32	0.44
1:C:360:LEU:O	1:C:364:LEU:HD23	2.17	0.44
1:C:131:PRO:HB2	1:C:134:GLN:HG3	1.99	0.43
1:C:51:SER:O	1:C:56:THR:HG23	2.18	0.43
1:B:148:GLU:HG2	1:B:148:GLU:H	1.51	0.43
1:A:476:VAL:HA	1:A:477:PRO:HD3	1.67	0.43
1:A:237:ALA:O	1:A:241[A]:ARG:HG3	2.17	0.43
1:A:657:LEU:H	1:A:657:LEU:HD23	1.83	0.43
1:A:58:TYR:HB2	1:A:404:VAL:HG21	2.01	0.43
1:A:274:MET:CG	5:A:2078:HOH:O	2.62	0.43
1:C:637:LYS:HB3	5:C:2144:HOH:O	2.18	0.43
1:A:135:GLY:O	1:A:136:ILE:HG13	2.18	0.43
1:B:92:PRO:HG2	1:B:402:VAL:CG2	2.37	0.43
1:B:533:GLY:O	2:B:1842:ADP:H5'2	2.18	0.43
1:C:839:ALA:O	1:C:842:ARG:HG3	2.18	0.43
1:C:524:VAL:HG22	1:C:800:ASP:OD2	2.19	0.43
1:C:840:ALA:HA	5:C:2182:HOH:O	2.19	0.43
1:C:660:VAL:HG12	1:C:661:TYR:H	1.84	0.43
1:A:602:MET:HE1	1:A:722:LEU:HD12	2.01	0.43
1:C:82:VAL:HG12	5:C:2016:HOH:O	2.18	0.43
1:C:159:ARG:NH2	1:C:286:GLU:HG3	2.34	0.43
1:A:156:GLY:HA2	1:A:294:ARG:O	2.19	0.42
1:C:115:THR:O	1:C:115:THR:HG22	2.19	0.42
1:B:505:LEU:HD22	1:B:574:ALA:HB1	2.01	0.42
1:B:709:ARG:HG3	1:B:746:ARG:CZ	2.49	0.42
1:C:332:GLU:CD	1:C:335:HIS:HD2	2.22	0.42
1:A:701:PHE:CD2	1:A:704:GLU:HG3	2.48	0.42
1:C:533:GLY:HA2	2:C:1842:ADP:O2A	2.20	0.42
1:C:150:ALA:CB	5:C:2045:HOH:O	2.66	0.42
1:B:529:THR:C	1:B:536:LYS:HD3	2.40	0.42
1:C:243:LEU:HD21	5:C:2056:HOH:O	2.19	0.42
1:A:40:VAL:HA	1:A:436:VAL:O	2.20	0.42
1:B:413:HIS:HD2	1:B:415:ALA:H	1.67	0.42
1:A:396:SER:O	1:A:397:ASN:HB2	2.20	0.42
1:A:327:TYR:HD2	1:A:349:LEU:HD21	1.84	0.42
1:A:497:ARG:HH22	1:A:777:VAL:HG13	1.83	0.42
1:A:296:ARG:HB3	1:A:298:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:LEU:HA	1:C:745:LEU:HD23	1.92	0.42
1:B:58:TYR:CZ	1:B:62:GLN:HG3	2.54	0.42
1:B:689:VAL:HA	1:B:692:LEU:HD13	2.01	0.42
1:A:262:VAL:HG22	5:A:2040:HOH:O	2.18	0.42
1:A:548:LEU:HD11	1:A:754:VAL:HG11	2.02	0.42
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.91	0.42
1:A:657:LEU:CD2	1:A:657:LEU:HG	2.20	0.42
1:C:670:THR:O	1:C:671:ARG:CB	2.68	0.42
1:B:147:PRO:O	1:B:296:ARG:NH1	2.51	0.42
1:B:807:PRO:HD3	1:B:815[A]:ARG:HD3	2.02	0.42
1:A:450:LEU:HD21	1:A:473:LEU:HD22	2.01	0.42
1:A:60:GLU:HG2	1:A:88:ILE:HD12	2.01	0.42
1:A:151:CYS:SG	1:A:289:LEU:HD23	2.60	0.42
1:C:747:ARG:H	1:C:747:ARG:CD	2.16	0.42
1:C:495:THR:CG2	1:C:496:PRO:HD2	2.50	0.42
1:B:495:THR:HA	1:B:496:PRO:HD3	1.77	0.41
1:A:66:LEU:HA	1:A:69:VAL:HG22	2.01	0.41
1:C:455:PRO:HD2	1:C:461:GLY:HA2	2.01	0.41
1:B:588:ARG:HB2	1:B:588:ARG:NH1	2.34	0.41
1:A:235:THR:HG22	1:A:238:GLU:CG	2.50	0.41
1:B:684:LYS:HE3	1:B:692:LEU:HD11	2.01	0.41
1:B:192:ASN:O	1:B:196:ILE:HG13	2.21	0.41
1:C:631:ARG:O	1:C:639:GLY:HA3	2.20	0.41
1:C:805:ILE:O	1:C:806:GLY:O	2.38	0.41
1:C:450:LEU:C	1:C:450:LEU:HD12	2.40	0.41
1:A:398:LEU:CD2	5:B:2010:HOH:O	2.68	0.41
1:C:611[A]:GLN:NE2	5:C:2141:HOH:O	2.53	0.41
1:A:169:VAL:HG22	1:A:169:VAL:O	2.20	0.41
1:A:602:MET:HE2	1:A:714:LEU:HD22	2.01	0.41
1:C:483:GLN:HA	1:C:487:ALA:HB3	2.02	0.41
1:B:186:GLN:HG3	5:B:2053:HOH:O	2.20	0.41
1:C:236:PRO:O	1:C:239:THR:HG22	2.20	0.41
1:B:641:CYS:HB2	1:B:667:CYS:HB3	2.03	0.41
1:C:640:ARG:NE	1:C:642:GLU:OE2	2.50	0.41
1:A:509:THR:O	1:A:510:ARG:HB2	2.20	0.41
1:C:544:LEU:O	1:C:548:LEU:HB2	2.20	0.41
1:C:469:PRO:HA	1:C:470:PRO:HD3	1.91	0.41
1:B:387:ARG:NH1	5:B:2126:HOH:O	2.53	0.41
1:C:92:PRO:HG2	1:C:402:VAL:HG23	2.01	0.41
1:B:433:SER:HB3	5:B:2006:HOH:O	2.19	0.41
1:A:723:ARG:HB2	1:A:726:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:CYS:HA	1:B:288:PRO:HD3	1.82	0.41
1:A:834:ALA:HB3	1:A:835:PRO:CD	2.51	0.41
1:B:368:LEU:HD13	1:B:388:LEU:HD23	2.03	0.41
1:A:602:MET:HG3	1:A:739:ILE:HD13	2.03	0.41
1:C:62:GLN:O	1:C:66:LEU:HG	2.20	0.41
1:B:413:HIS:CE1	1:B:833:THR:HB	2.56	0.41
1:C:601:ASN:ND2	1:C:604:THR:HB	2.35	0.41
1:C:63:ARG:HD2	1:C:82:VAL:HG13	2.03	0.41
1:B:241[A]:ARG:HB2	1:B:241[A]:ARG:CZ	2.50	0.41
1:C:50:SER:HB3	5:C:2034:HOH:O	2.21	0.41
1:B:693:THR:HG23	1:B:720:GLY:O	2.21	0.40
1:A:759:GLU:HG3	1:A:791:HIS:ND1	2.36	0.40
1:A:82:VAL:HG12	1:A:83:PRO:HD2	2.03	0.40
1:C:510:ARG:HG3	1:C:538:THR:CG2	2.52	0.40
1:C:779:LEU:HD23	1:C:779:LEU:C	2.41	0.40
1:B:334:GLY:O	1:B:338:ARG:HG3	2.21	0.40
1:A:804:ASP:OD1	1:A:833:THR:HG23	2.21	0.40
1:B:815[B]:ARG:HD2	5:B:2219:HOH:O	2.21	0.40
1:C:325:ARG:N	1:C:326:PRO:CD	2.85	0.40
1:C:649:TRP:CD1	1:C:661:TYR:HB3	2.56	0.40
1:C:11:PRO:HB2	1:C:12:ASP:H	1.58	0.40
1:C:488:ASP:O	1:C:488:ASP:CG	2.59	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	811/842 (96%)	748 (92%)	51 (6%)	12 (2%)	13	12
1	B	809/842 (96%)	748 (92%)	51 (6%)	10 (1%)	16	16
1	C	812/842 (96%)	756 (93%)	46 (6%)	10 (1%)	16	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2432/2526 (96%)	2252 (93%)	148 (6%)	32 (1%)	15	15

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	A	345	GLN
1	A	806	GLY
1	B	72	TYR
1	B	749	GLY
1	C	78	ASN
1	C	454	GLY
1	A	343	PRO
1	B	71	PRO
1	B	78	ASN
1	B	366	LEU
1	B	454	GLY
1	B	629	ALA
1	B	806	GLY
1	C	11	PRO
1	C	806	GLY
1	A	333	PRO
1	A	510	ARG
1	A	658	PRO
1	C	77	PHE
1	A	131	PRO
1	A	291	HIS
1	A	759	GLU
1	C	493	PRO
1	A	653	GLU
1	C	489	ARG
1	C	657	LEU
1	C	673	ASN
1	C	147	PRO
1	A	493	PRO
1	B	132	PRO
1	B	577	GLY

5.3.2 Protein sidechains ⓘ

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	658/683 (96%)	567 (86%)	91 (14%)	4	4
1	B	657/683 (96%)	571 (87%)	86 (13%)	5	5
1	C	659/683 (96%)	566 (86%)	93 (14%)	4	4
All	All	1974/2049 (96%)	1704 (86%)	270 (14%)	5	4

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	62	GLN
1	A	70	SER
1	A	74	ARG
1	A	76	LEU
1	A	82	VAL
1	A	91	LEU
1	A	101	ARG
1	A	108	SER
1	A	109	SER
1	A	134	GLN
1	A	153	GLU
1	A	163	VAL
1	A	166	ASP
1	A	169	VAL
1	A	174	LEU
1	A	175	THR
1	A	181	VAL
1	A	204	VAL
1	A	213[A]	GLU
1	A	220	LEU
1	A	235	THR
1	A	244[A]	LYS
1	A	245	LYS
1	A	256	SER
1	A	260	ARG
1	A	278	VAL
1	A	293	LYS
1	A	295	LEU
1	A	298	GLU

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Mol	Chain	Res	Type
1	A	303	THR
1	A	331	ARG
1	A	337	GLU
1	A	338	ARG
1	A	340	LYS
1	A	342	ARG
1	A	345	GLN
1	A	364	LEU
1	A	365	HIS
1	A	373	LEU
1	A	376	SER
1	A	380	LEU
1	A	385	LEU
1	A	389	ARG
1	A	397	ASN
1	A	398	LEU
1	A	412	LEU
1	A	418	GLU
1	A	422	SER
1	A	437	VAL
1	A	442[A]	ASP
1	A	450	LEU
1	A	476	VAL
1	A	489	ARG
1	A	491	THR
1	A	503	LEU
1	A	505	LEU
1	A	525	MET
1	A	531	VAL
1	A	576	LEU
1	A	588	ARG
1	A	590[A]	ASP
1	A	591[A]	GLN
1	A	592	LYS
1	A	599	ARG
1	A	601	ASN
1	A	604	THR
1	A	611	GLN
1	A	623	LYS
1	A	625	ARG
1	A	649	TRP
1	A	656	PHE

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Mol	Chain	Res	Type
1	A	657	LEU
1	A	659	SER
1	A	689	VAL
1	A	692	LEU
1	A	704	GLU
1	A	717	VAL
1	A	747	ARG
1	A	753	THR
1	A	757	LEU
1	A	769	VAL
1	A	785	THR
1	A	786	VAL
1	A	789	VAL
1	A	811[A]	GLU
1	A	817	VAL
1	A	832	VAL
1	A	833	THR
1	A	837	LEU
1	A	842	ARG
1	B	26	LEU
1	B	31	VAL
1	B	62	GLN
1	B	72	TYR
1	B	77	PHE
1	B	91	LEU
1	B	99[A]	GLN
1	B	101	ARG
1	B	103	THR
1	B	107	ARG
1	B	112	SER
1	B	120	LEU
1	B	134	GLN
1	B	148	GLU
1	B	159	ARG
1	B	164	THR
1	B	174	LEU
1	B	175	THR
1	B	179[A]	ARG
1	B	181	VAL
1	B	220	LEU
1	B	241[A]	ARG
1	B	256	SER

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Mol	Chain	Res	Type
1	B	274	MET
1	B	278	VAL
1	B	300	LEU
1	B	303	THR
1	B	314	ARG
1	B	324	LEU
1	B	332	GLU
1	B	351	ARG
1	B	373	LEU
1	B	376	SER
1	B	385	LEU
1	B	389	ARG
1	B	412	LEU
1	B	427	LEU
1	B	437	VAL
1	B	459[A]	GLU
1	B	460	LYS
1	B	481	THR
1	B	491	THR
1	B	495	THR
1	B	503	LEU
1	B	505	LEU
1	B	508	VAL
1	B	512	ASN
1	B	513	LEU
1	B	515	ASN
1	B	518	VAL
1	B	524	VAL
1	B	531	VAL
1	B	575	ARG
1	B	576	LEU
1	B	587	VAL
1	B	588	ARG
1	B	596	ARG
1	B	600	SER
1	B	621	LEU
1	B	625	ARG
1	B	631	ARG
1	B	636	VAL
1	B	645	GLN
1	B	659	SER
1	B	668	HIS

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Mol	Chain	Res	Type
1	B	693	THR
1	B	699	ASP
1	B	709	ARG
1	B	740	LYS
1	B	753	THR
1	B	757	LEU
1	B	769	VAL
1	B	771[A]	ARG
1	B	772	LEU
1	B	779	LEU
1	B	786	VAL
1	B	789	VAL
1	B	795	VAL
1	B	803	LEU
1	B	815[A]	ARG
1	B	815[B]	ARG
1	B	816	LEU
1	B	817	VAL
1	B	832	VAL
1	B	833	THR
1	B	837	LEU
1	C	10	PHE
1	C	12	ASP
1	C	26	LEU
1	C	31	VAL
1	C	74	ARG
1	C	77	PHE
1	C	91	LEU
1	C	99	GLN
1	C	101	ARG
1	C	107	ARG
1	C	112	SER
1	C	126	ARG
1	C	136	ILE
1	C	140	GLU
1	C	148	GLU
1	C	175	THR
1	C	181	VAL
1	C	184	TRP
1	C	198	VAL
1	C	199	THR
1	C	205	ASP

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Mol	Chain	Res	Type
1	C	206	VAL
1	C	220	LEU
1	C	235	THR
1	C	239	THR
1	C	241	ARG
1	C	268	ASN
1	C	269	THR
1	C	275	LYS
1	C	279	GLN
1	C	298	GLU
1	C	303	THR
1	C	307	LEU
1	C	309	ILE
1	C	312	LEU
1	C	340	LYS
1	C	341	ASN
1	C	349	LEU
1	C	355	ASP
1	C	366	LEU
1	C	376	SER
1	C	380	LEU
1	C	385	LEU
1	C	389	ARG
1	C	407	GLU
1	C	412	LEU
1	C	427	LEU
1	C	450	LEU
1	C	476	VAL
1	C	490	HIS
1	C	491	THR
1	C	505	LEU
1	C	515	ASN
1	C	524	VAL
1	C	527	SER
1	C	536	LYS
1	C	537	SER
1	C	548	LEU
1	C	575	ARG
1	C	585	ARG
1	C	586	LEU
1	C	587	VAL
1	C	588[A]	ARG

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Mol	Chain	Res	Type
1	C	588[B]	ARG
1	C	592	LYS
1	C	596[A]	ARG
1	C	601	ASN
1	C	602[A]	MET
1	C	604	THR
1	C	637	LYS
1	C	642	GLU
1	C	653	GLU
1	C	682	ARG
1	C	692	LEU
1	C	717	VAL
1	C	746	ARG
1	C	747	ARG
1	C	756	VAL
1	C	762	THR
1	C	764	LEU
1	C	769	VAL
1	C	772	LEU
1	C	779	LEU
1	C	785	THR
1	C	786	VAL
1	C	789	VAL
1	C	793	MET
1	C	795	VAL
1	C	803	LEU
1	C	805	ILE
1	C	837	LEU
1	C	841	LEU
1	C	842	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	134	GLN
1	A	192	ASN
1	A	345	GLN
1	A	397	ASN
1	A	413	HIS
1	A	591[A]	GLN
1	A	601	ASN

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Mol	Chain	Res	Type
1	A	628	ASN
1	A	784	ASN
1	A	827	GLN
1	B	134	GLN
1	B	192	ASN
1	B	291	HIS
1	B	335	HIS
1	B	386	GLN
1	B	413	HIS
1	B	511	ASN
1	B	512	ASN
1	B	551	HIS
1	B	635	ASN
1	B	645	GLN
1	B	773[A]	GLN
1	B	775	GLN
1	B	784	ASN
1	B	791	HIS
1	C	62	GLN
1	C	99	GLN
1	C	192	ASN
1	C	335	HIS
1	C	494	HIS
1	C	582	GLN
1	C	601	ASN
1	C	611[A]	GLN
1	C	628	ASN
1	C	635	ASN
1	C	643	HIS
1	C	673	ASN
1	C	765	HIS
1	C	775	GLN
1	C	819	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
2	ADP	A	1842	-	22,29,29	1.17	2 (9%)	27,45,45	1.95	3 (11%)
2	ADP	A	1843	-	22,29,29	1.00	1 (4%)	27,45,45	1.91	3 (11%)
2	ADP	B	1842	-	22,29,29	1.14	2 (9%)	27,45,45	1.77	4 (14%)
2	ADP	B	1843	-	22,29,29	1.08	2 (9%)	27,45,45	1.92	5 (18%)
2	ADP	C	1842	-	22,29,29	1.08	3 (13%)	27,45,45	2.14	2 (7%)
2	ADP	C	1843	4	22,29,29	1.16	2 (9%)	27,45,45	2.07	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1842	-	-	0/12/32/32	0/3/3/3
2	ADP	A	1843	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1842	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1843	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1842	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1843	4	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1842	ADP	C2-N3	2.01	1.35	1.32
2	B	1843	ADP	O4'-C1'	2.05	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1842	ADP	O4'-C1'	2.05	1.43	1.41
2	B	1842	ADP	O4'-C1'	2.15	1.43	1.41
2	C	1843	ADP	C2-N3	2.16	1.36	1.32
2	A	1842	ADP	O4'-C1'	2.60	1.44	1.41
2	A	1843	ADP	C5-C4	3.05	1.47	1.40
2	C	1842	ADP	C5-C4	3.07	1.47	1.40
2	A	1842	ADP	C5-C4	3.25	1.47	1.40
2	B	1843	ADP	C5-C4	3.27	1.47	1.40
2	B	1842	ADP	C5-C4	3.31	1.48	1.40
2	C	1843	ADP	C5-C4	3.74	1.48	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1842	ADP	N3-C2-N1	-8.07	122.71	128.89
2	A	1843	ADP	N3-C2-N1	-8.06	122.72	128.89
2	A	1842	ADP	N3-C2-N1	-7.78	122.94	128.89
2	B	1842	ADP	N3-C2-N1	-7.19	123.39	128.89
2	B	1843	ADP	N3-C2-N1	-6.92	123.59	128.89
2	C	1843	ADP	N3-C2-N1	-6.57	123.86	128.89
2	C	1843	ADP	PA-O3A-PB	-5.15	115.41	132.67
2	C	1842	ADP	C2'-C1'-N9	-4.97	106.70	114.29
2	A	1843	ADP	PA-O3A-PB	-3.67	120.34	132.67
2	B	1843	ADP	C2'-C1'-N9	-2.84	109.95	114.29
2	B	1843	ADP	C4-C5-N7	-2.67	107.02	109.48
2	A	1842	ADP	C2'-C1'-N9	-2.46	110.53	114.29
2	B	1843	ADP	PA-O3A-PB	-2.37	124.72	132.67
2	A	1842	ADP	C4-C5-N7	-2.09	107.56	109.48
2	B	1842	ADP	C2-N1-C6	2.00	122.35	118.77
2	B	1842	ADP	O3B-PB-O2B	2.13	115.48	107.38
2	B	1842	ADP	N6-C6-N1	2.17	123.87	119.20
2	B	1843	ADP	O3A-PA-O5'	2.20	108.78	102.94
2	A	1843	ADP	C2-N1-C6	2.36	122.99	118.77
2	C	1843	ADP	O4'-C1'-N9	2.53	113.40	108.10
2	C	1843	ADP	C2'-C1'-N9	3.78	120.06	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1842	ADP	1	0
2	B	1842	ADP	1	0
2	C	1842	ADP	3	0
2	C	1843	ADP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	815/842 (96%)	0.86	79 (9%) 10 14	43, 57, 70, 79	6 (0%)
1	B	813/842 (96%)	0.81	65 (7%) 15 21	42, 56, 70, 88	5 (0%)
1	C	814/842 (96%)	0.91	117 (14%) 3 5	42, 56, 69, 81	8 (0%)
All	All	2442/2526 (96%)	0.86	261 (10%) 8 12	42, 56, 70, 88	19 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	9.6
1	A	654	LEU	8.3
1	C	654	LEU	7.6
1	C	656	PHE	7.0
1	C	491	THR	6.7
1	C	655	LEU	5.9
1	A	341	ASN	5.9
1	A	347	ILE	5.8
1	B	674	ALA	5.6
1	C	624	LYS	5.6
1	A	656	PHE	5.6
1	B	73	ALA	5.5
1	C	247[A]	MET	5.4
1	C	152	PRO	5.3
1	B	72	TYR	5.3
1	C	340	LYS	5.3
1	A	72	TYR	5.2
1	C	246	LYS	5.1
1	B	749	GLY	5.0
1	B	651	MET	5.0
1	A	343	PRO	4.9
1	C	270	GLU	4.7
1	C	138	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	336	ALA	4.7
1	A	340	LYS	4.7
1	C	271	SER	4.6
1	B	637	LYS	4.6
1	A	77	PHE	4.6
1	A	653	GLU	4.5
1	C	11	PRO	4.5
1	B	8	PRO	4.4
1	C	133	GLY	4.4
1	C	344	GLU	4.4
1	C	337	GLU	4.3
1	C	161	TYR	4.3
1	A	79	GLN	4.2
1	B	650	VAL	4.2
1	A	335	HIS	4.1
1	B	632	PHE	4.1
1	B	636	VAL	4.0
1	C	341	ASN	4.0
1	C	284	SER	4.0
1	C	12	ASP	4.0
1	A	344	GLU	4.0
1	B	81	GLY	4.0
1	C	339	VAL	4.0
1	B	659	SER	3.9
1	A	131	PRO	3.8
1	C	132	PRO	3.8
1	B	10	PHE	3.8
1	C	572	GLY	3.8
1	C	274	MET	3.7
1	A	132	PRO	3.7
1	B	627	TYR	3.7
1	C	160	VAL	3.7
1	C	74	ARG	3.6
1	A	334	GLY	3.6
1	C	335	HIS	3.6
1	A	321	SER	3.6
1	C	490	HIS	3.6
1	A	554	GLN	3.5
1	B	677	LEU	3.5
1	C	345	GLN	3.5
1	A	128	GLY	3.5
1	C	243	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	702	ALA	3.4
1	B	77	PHE	3.4
1	C	219	ILE	3.4
1	C	266	PHE	3.4
1	B	660	VAL	3.4
1	C	218	TRP	3.3
1	C	126	ARG	3.3
1	A	659	SER	3.3
1	C	583	ILE	3.3
1	C	343	PRO	3.3
1	C	10	PHE	3.3
1	C	72	TYR	3.2
1	B	642	GLU	3.2
1	A	133	GLY	3.2
1	A	331	ARG	3.1
1	C	653	GLU	3.1
1	A	345	GLN	3.1
1	B	621	LEU	3.1
1	B	665	PRO	3.1
1	C	304	PHE	3.1
1	C	760	PRO	3.1
1	C	223	ASP	3.0
1	A	11	PRO	3.0
1	C	492	GLU	3.0
1	B	188	TRP	3.0
1	C	252	MET	3.0
1	C	307	LEU	3.0
1	A	342	ARG	2.9
1	A	583	ILE	2.9
1	B	638	GLY	2.8
1	C	146	THR	2.8
1	A	78	ASN	2.8
1	A	301	ASN	2.8
1	C	514[A]	ASP	2.8
1	B	709	ARG	2.8
1	A	230	VAL	2.8
1	A	126	ARG	2.8
1	C	134	GLN	2.8
1	B	643	HIS	2.7
1	A	655	LEU	2.7
1	B	701	PHE	2.7
1	A	354	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	408	PRO	2.7
1	A	550	ALA	2.7
1	C	761	THR	2.7
1	C	156	GLY	2.7
1	C	285	GLU	2.7
1	A	388	LEU	2.7
1	C	245	LYS	2.7
1	B	625	ARG	2.6
1	A	272	ALA	2.6
1	C	327	TYR	2.6
1	B	411	GLY	2.6
1	A	73	ALA	2.6
1	C	251	TYR	2.6
1	C	147	PRO	2.6
1	A	250	SER	2.6
1	C	507	GLY	2.6
1	C	763	GLY	2.6
1	B	666	VAL	2.6
1	C	329	GLU	2.6
1	C	125	SER	2.6
1	A	134	GLN	2.6
1	A	96	ALA	2.6
1	A	761	THR	2.6
1	C	573	SER	2.5
1	A	750	ARG	2.5
1	B	479	SER	2.5
1	B	658	PRO	2.5
1	A	585	ARG	2.5
1	B	241[A]	ARG	2.5
1	C	233	GLY	2.5
1	C	296	ARG	2.5
1	C	348	ALA	2.5
1	B	383	GLY	2.5
1	B	789	VAL	2.5
1	C	155	HIS	2.5
1	C	145	ASN	2.5
1	C	588[A]	ARG	2.5
1	B	454	GLY	2.5
1	B	678	GLU	2.5
1	C	669	GLY	2.5
1	C	249	PRO	2.5
1	B	758[A]	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	73	ALA	2.4
1	C	762	THR	2.4
1	C	658	PRO	2.4
1	A	329	GLU	2.4
1	B	706	ALA	2.4
1	C	139	ALA	2.4
1	C	659	SER	2.4
1	A	658	PRO	2.4
1	A	763	GLY	2.4
1	B	675	GLU	2.4
1	C	150	ALA	2.4
1	A	349	LEU	2.4
1	B	312	LEU	2.4
1	B	251	TYR	2.4
1	B	672	TYR	2.4
1	C	244	LYS	2.4
1	C	488	ASP	2.4
1	B	79	GLN	2.4
1	C	301	ASN	2.4
1	A	754	VAL	2.3
1	B	842	ARG	2.3
1	B	105	THR	2.3
1	C	288	PRO	2.3
1	C	306	GLY	2.3
1	A	251	TYR	2.3
1	C	347	ILE	2.3
1	B	620	PRO	2.3
1	A	552	PHE	2.3
1	C	96	ALA	2.3
1	B	763	GLY	2.3
1	A	492	GLU	2.3
1	C	657	LEU	2.3
1	B	476	VAL	2.3
1	A	736	ALA	2.3
1	C	242	ALA	2.3
1	C	234	LEU	2.3
1	C	620	PRO	2.3
1	B	689	VAL	2.3
1	A	338	ARG	2.3
1	A	136	ILE	2.2
1	C	273	SER	2.2
1	A	300	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	437	VAL	2.2
1	B	74	ARG	2.2
1	B	645	GLN	2.2
1	C	383	GLY	2.2
1	C	749	GLY	2.2
1	B	603	ALA	2.2
1	B	618	ALA	2.2
1	B	662	ALA	2.2
1	A	110	VAL	2.2
1	B	437	VAL	2.2
1	C	228	VAL	2.2
1	A	130	TYR	2.2
1	A	327	TYR	2.2
1	A	135	GLY	2.2
1	A	405	LEU	2.2
1	A	409	SER	2.2
1	C	239	THR	2.2
1	B	402	VAL	2.2
1	C	404	VAL	2.2
1	C	627	TYR	2.2
1	C	334	GLY	2.2
1	A	576	LEU	2.2
1	C	101	ARG	2.2
1	C	277	ARG	2.2
1	B	686	ILE	2.2
1	A	95	VAL	2.2
1	A	437	VAL	2.2
1	B	769	VAL	2.2
1	C	338	ARG	2.2
1	C	626	GLY	2.2
1	B	255	PHE	2.2
1	C	221	PHE	2.2
1	A	764	LEU	2.2
1	A	304	PHE	2.1
1	B	762	THR	2.1
1	A	351	ARG	2.1
1	C	196	ILE	2.1
1	C	278	VAL	2.1
1	A	584	THR	2.1
1	C	299	ALA	2.1
1	A	111	GLY	2.1
1	B	490	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	217	HIS	2.1
1	C	804	ASP	2.1
1	A	491	THR	2.1
1	C	215	THR	2.1
1	A	129	ASP	2.1
1	A	114	THR	2.1
1	A	385	LEU	2.1
1	B	97	LEU	2.1
1	B	386	GLN	2.1
1	C	279	GLN	2.1
1	A	624	LYS	2.1
1	B	776	LEU	2.1
1	A	581	ALA	2.1
1	A	147	PRO	2.1
1	C	254	THR	2.0
1	A	450	LEU	2.0
1	C	76	LEU	2.0
1	A	328	ALA	2.0
1	C	330	GLU	2.0
1	C	283	ILE	2.0
1	B	806	GLY	2.0
1	C	265	THR	2.0
1	C	405	LEU	2.0
1	C	214[A]	GLU	2.0
1	C	325	ARG	2.0
1	C	789	VAL	2.0
1	A	142	PHE	2.0
1	C	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	MG	C	1846	1/1	0.97	0.30	1.79	42,42,42,42	0
3	ZN	C	1844	1/1	0.71	0.17	0.03	70,70,70,70	1
3	ZN	A	1844	1/1	0.99	0.14	-0.33	59,59,59,59	1
2	ADP	C	1842	27/27	0.97	0.12	-0.39	48,55,56,57	1
2	ADP	A	1842	27/27	0.97	0.12	-0.53	43,55,56,57	0
2	ADP	B	1843	27/27	0.96	0.14	-0.90	46,50,58,59	0
2	ADP	C	1843	27/27	0.96	0.14	-1.00	39,45,56,57	0
3	ZN	B	1844	1/1	0.98	0.09	-1.02	71,71,71,71	0
3	ZN	B	1845	1/1	0.88	0.14	-1.08	59,59,59,59	1
2	ADP	B	1842	27/27	0.97	0.15	-1.40	35,40,42,43	0
2	ADP	A	1843	27/27	0.98	0.12	-1.96	36,39,45,47	0
3	ZN	C	1845	1/1	0.98	0.06	-3.28	66,66,66,66	1
3	ZN	A	1845	1/1	1.00	0.08	-4.61	55,55,55,55	0

6.5 Other polymers

There are no such residues in this entry.