



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:31 am BST

PDB ID : 6BNB
Title : Crystal structure of DDB1-CRBN-BRD4(BD1) complex bound to dBET57 PROTAC
Authors : Nowak, R.P.; DeAngelo, S.L.; Buckley, D.; Ishoey, M.; He, Z.; Zhang, T.; Bradner, J.E.; Fischer, E.S.
Deposited on : 2017-11-16
Resolution : 6.34 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

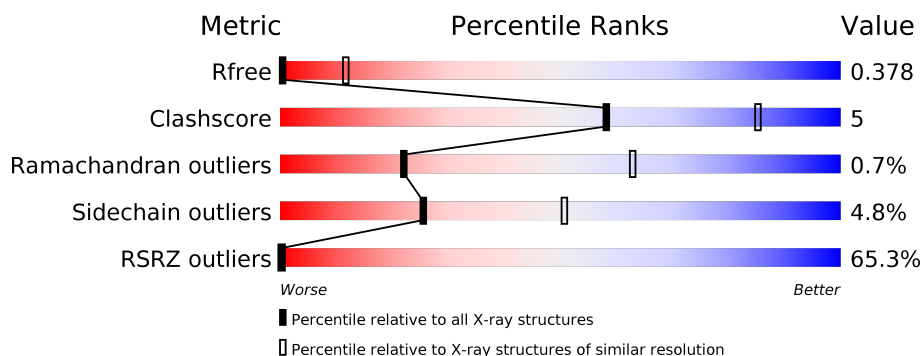
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.34 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	1009 (8.70-3.88)
Clashscore	141614	1058 (8.70-3.90)
Ramachandran outliers	138981	1006 (8.70-3.88)
Sidechain outliers	138945	1005 (8.70-3.84)
RSRZ outliers	127900	1018 (8.70-3.78)

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 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 $\leq 5\%$. 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	864	<div> <div>68%</div> <div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
2	B	463	<div> <div>39%</div> <div> <div>62%</div> <div>13%</div> <div>24%</div> </div> </div>
3	C	127	<div> <div>44%</div> <div> <div>84%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	0	0	0
			6128	3892	1024	1178	34			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q16531
A	-26	GLY	-	expression tag	UNP Q16531
A	-25	SER	-	expression tag	UNP Q16531
A	-24	SER	-	expression tag	UNP Q16531
A	-23	HIS	-	expression tag	UNP Q16531
A	-22	HIS	-	expression tag	UNP Q16531
A	-21	HIS	-	expression tag	UNP Q16531
A	-20	HIS	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	SER	-	expression tag	UNP Q16531
A	-16	ALA	-	expression tag	UNP Q16531
A	-15	ALA	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	ILE	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	MET	-	expression tag	UNP Q16531
A	-10	VAL	-	expression tag	UNP Q16531
A	-9	ASP	-	expression tag	UNP Q16531
A	-8	ALA	-	expression tag	UNP Q16531
A	-7	TYR	-	expression tag	UNP Q16531
A	-6	LYS	-	expression tag	UNP Q16531
A	-5	PRO	-	expression tag	UNP Q16531
A	-4	THR	-	expression tag	UNP Q16531
A	-3	LYS	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	351	Total	C	N	O	S	0	0	0
			2839	1812	488	515	24			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP Q96SW2
B	-19	GLY	-	expression tag	UNP Q96SW2
B	-18	SER	-	expression tag	UNP Q96SW2
B	-17	SER	-	expression tag	UNP Q96SW2
B	-16	HIS	-	expression tag	UNP Q96SW2
B	-15	HIS	-	expression tag	UNP Q96SW2
B	-14	HIS	-	expression tag	UNP Q96SW2
B	-13	HIS	-	expression tag	UNP Q96SW2
B	-12	HIS	-	expression tag	UNP Q96SW2
B	-11	HIS	-	expression tag	UNP Q96SW2
B	-10	SER	-	expression tag	UNP Q96SW2
B	-9	ALA	-	expression tag	UNP Q96SW2
B	-8	VAL	-	expression tag	UNP Q96SW2
B	-7	ASP	-	expression tag	UNP Q96SW2
B	-6	GLU	-	expression tag	UNP Q96SW2
B	-5	ASN	-	expression tag	UNP Q96SW2
B	-4	LEU	-	expression tag	UNP Q96SW2
B	-3	TYR	-	expression tag	UNP Q96SW2
B	-2	PHE	-	expression tag	UNP Q96SW2
B	-1	GLN	-	expression tag	UNP Q96SW2
B	0	GLY	-	expression tag	UNP Q96SW2
B	1	GLY	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	127	Total	C	N	O	S	Se	0	4	0
			1074	695	175	197	2	5			

There is a discrepancy between the modelled and reference sequences:

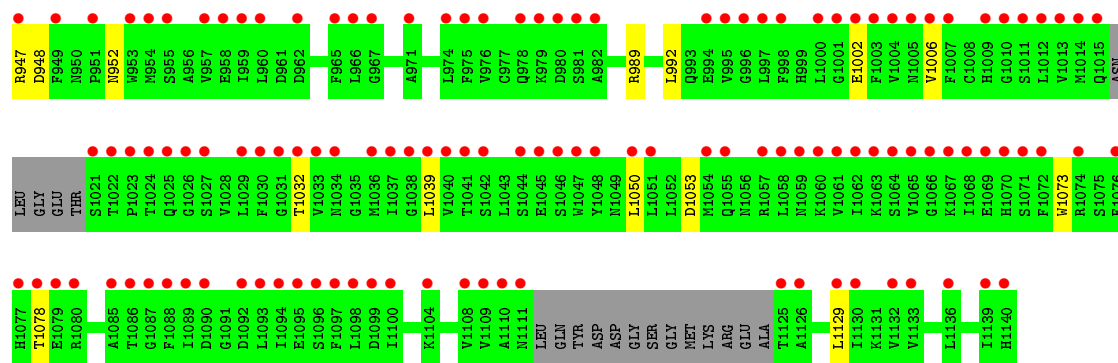
Chain	Residue	Modelled	Actual	Comment	Reference
C	43	MSE	THR	engineered mutation	UNP O60885

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

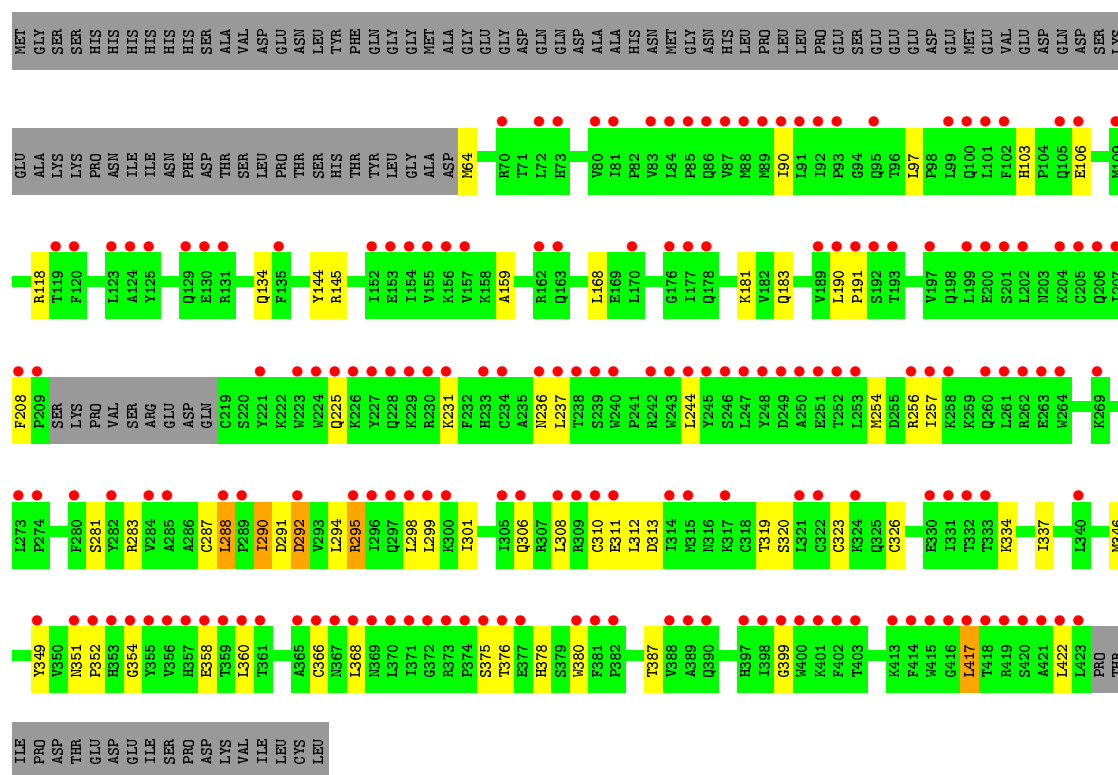
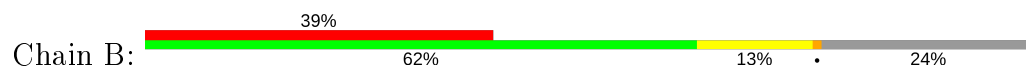
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 1: DNA damage-binding protein 1

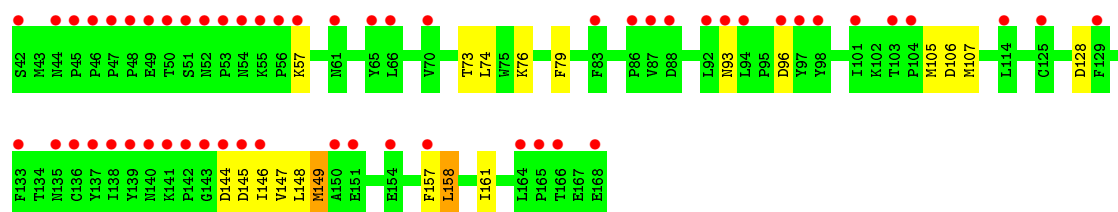
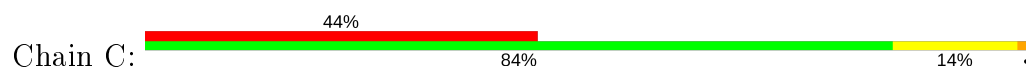




• Molecule 2: Protein cereblon



• Molecule 3: Bromodomain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	313.36Å 313.36Å 167.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.63 – 6.34 147.63 – 6.34	Depositor EDS
% Data completeness (in resolution range)	98.2 (147.63-6.34) 98.2 (147.63-6.34)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 6.20Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.337 , 0.381 0.337 , 0.378	Depositor DCC
R_{free} test set	415 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	465.5	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 568.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	10042	wwPDB-VP
Average B, all atoms (Å ²)	484.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.34	0/6237	0.51	0/8449
2	B	0.41	0/2905	0.57	0/3936
3	C	0.41	0/1115	0.55	0/1508
All	All	0.37	0/10257	0.53	0/13893

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6128	0	6031	36	0
2	B	2839	0	2832	44	0
3	C	1074	0	1064	17	0
4	B	1	0	0	0	0
All	All	10042	0	9927	95	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 5.

All (95) 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)
2:B:290:ILE:HD11	2:B:295:ARG:N	1.73	1.04
2:B:290:ILE:HG13	2:B:294:LEU:CB	1.92	0.99
2:B:290:ILE:HG13	2:B:294:LEU:HB3	1.45	0.95
3:C:79:PHE:HB3	3:C:149:MSE:CG	1.99	0.92
2:B:290:ILE:HD11	2:B:294:LEU:C	1.92	0.90
3:C:79:PHE:CG	3:C:149:MSE:HG3	2.12	0.85
3:C:79:PHE:CD1	3:C:149:MSE:HG3	2.13	0.84
3:C:79:PHE:HB3	3:C:149:MSE:HG3	1.63	0.80
2:B:290:ILE:HD11	2:B:295:ARG:CA	2.11	0.79
3:C:145:ASP:O	3:C:149:MSE:SE	2.52	0.77
2:B:290:ILE:HG13	2:B:294:LEU:HB2	1.66	0.76
3:C:79:PHE:CB	3:C:149:MSE:HG3	2.21	0.70
2:B:290:ILE:HD12	2:B:298:LEU:HD22	1.72	0.70
2:B:290:ILE:CD1	2:B:295:ARG:N	2.55	0.68
2:B:290:ILE:HD11	2:B:295:ARG:HA	1.76	0.67
2:B:290:ILE:CD1	2:B:295:ARG:HA	2.27	0.64
3:C:79:PHE:CD1	3:C:149:MSE:CG	2.81	0.63
3:C:105:MSE:HG3	3:C:106:ASP:N	2.12	0.63
2:B:290:ILE:CD1	2:B:295:ARG:CA	2.78	0.62
2:B:254:MET:HA	2:B:257:ILE:HD12	1.84	0.60
3:C:79:PHE:CB	3:C:149:MSE:CG	2.78	0.60
2:B:90:ILE:HB	2:B:295:ARG:HD3	1.83	0.60
1:A:118:THR:HB	1:A:134:ARG:HH22	1.66	0.60
2:B:290:ILE:CG1	2:B:294:LEU:CB	2.76	0.59
2:B:301:ILE:HG12	2:B:306:GLN:HB3	1.85	0.58
1:A:837:TYR:HB2	1:A:840:GLU:HB2	1.87	0.57
2:B:168:LEU:HD11	2:B:183:GLN:HB2	1.88	0.56
2:B:351:ASN:HB3	2:B:380:TRP:HZ2	1.72	0.54
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.90	0.54
2:B:290:ILE:CG1	2:B:294:LEU:HB3	2.29	0.53
2:B:168:LEU:HB2	2:B:181:LYS:HB3	1.90	0.53
2:B:281:SER:HB3	2:B:308:LEU:HD23	1.90	0.53
2:B:399:GLY:HA3	2:B:417:LEU:HA	1.89	0.53
2:B:360:LEU:HD23	2:B:417:LEU:HD12	1.90	0.53
2:B:323:CYS:HB3	2:B:326:CYS:HB2	1.90	0.52
1:A:331:SER:HB2	1:A:353:PHE:HB2	1.92	0.52
3:C:145:ASP:HA	3:C:148:LEU:HD12	1.92	0.52
1:A:387:LEU:HB2	1:A:715:VAL:HB	1.92	0.52
2:B:417:LEU:HB2	2:B:422:LEU:HD11	1.93	0.51
2:B:351:ASN:HB3	2:B:380:TRP:CZ2	2.46	0.50
3:C:105:MSE:HG3	3:C:106:ASP:H	1.76	0.50
1:A:948:ASP:HB2	1:A:992:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ARG:HD3	2:B:312:LEU:HD11	1.93	0.50
2:B:351:ASN:HB2	2:B:352:PRO:CD	2.42	0.50
1:A:362:MET:HB3	1:A:377:THR:HG22	1.93	0.50
3:C:79:PHE:HB3	3:C:149:MSE:HG2	1.89	0.50
1:A:791:LEU:HB3	1:A:805:HIS:HB3	1.93	0.50
1:A:305:LEU:HD22	1:A:336:LEU:HD22	1.93	0.49
1:A:366:ASP:HB3	1:A:370:GLN:HA	1.95	0.48
2:B:337:ILE:HG12	2:B:360:LEU:HD11	1.96	0.48
2:B:291:ASP:N	2:B:291:ASP:OD1	2.46	0.48
1:A:367:LEU:HD22	1:A:796:GLN:HB2	1.95	0.48
1:A:14:ALA:HB1	1:A:327:ARG:HD2	1.94	0.48
3:C:79:PHE:HB3	3:C:149:MSE:CB	2.44	0.48
2:B:346:MET:HG2	2:B:358:GLU:HB3	1.96	0.47
3:C:158:LEU:HA	3:C:161:ILE:HG22	1.96	0.47
1:A:273:LEU:HD11	1:A:283:LEU:HB2	1.97	0.47
2:B:349:TYR:HB3	2:B:380:TRP:CD1	2.50	0.47
1:A:761:LEU:HD12	1:A:802:LEU:HA	1.97	0.46
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.97	0.46
1:A:931:LEU:HG	1:A:947:ARG:HB3	1.96	0.46
1:A:123:ILE:HG21	1:A:168:LYS:HA	1.97	0.46
2:B:97:LEU:HB3	2:B:159:ALA:HB3	1.98	0.45
2:B:290:ILE:CG1	2:B:294:LEU:HB2	2.39	0.45
1:A:361:ASP:HA	1:A:1006:VAL:HG11	1.99	0.45
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.98	0.45
1:A:135:LEU:HD12	1:A:141:LYS:HZ3	1.82	0.44
2:B:417:LEU:HD13	2:B:422:LEU:HD21	1.99	0.44
1:A:269:SER:HA	1:A:285:LEU:HB2	2.00	0.44
3:C:73:THR:HA	3:C:76:LYS:HE2	1.99	0.44
2:B:291:ASP:O	2:B:292:ASP:C	2.56	0.43
3:C:144:ASP:HB2	3:C:147:VAL:HG23	2.00	0.43
1:A:333:LEU:HD12	1:A:351:GLU:HB2	2.00	0.43
1:A:756:ALA:HB1	1:A:801:VAL:HG21	2.01	0.43
1:A:177:THR:HG21	1:A:206:PRO:HD3	2.00	0.43
2:B:287:CYS:SG	2:B:288:LEU:N	2.91	0.43
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.54	0.42
2:B:64:MET:HG2	2:B:145:ARG:HB2	2.01	0.42
1:A:1002:GLU:HB3	1:A:1032:THR:HG21	2.01	0.42
1:A:952:ASN:HA	2:B:190:LEU:HD21	2.02	0.42
1:A:718:TYR:HB2	1:A:755:SER:HA	2.02	0.42
2:B:351:ASN:HB2	2:B:352:PRO:HD2	2.02	0.42
2:B:319:THR:HG21	2:B:334:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:GLU:HB2	2:B:256:ARG:HH12	1.84	0.41
2:B:298:LEU:HA	2:B:301:ILE:HD12	2.02	0.41
1:A:850:VAL:HB	1:A:862:ALA:H	1.85	0.41
1:A:723:LYS:HB2	1:A:736:LEU:HD12	2.01	0.41
1:A:886:SER:HA	1:A:911:ALA:H	1.86	0.41
1:A:879:LYS:HE2	1:A:892:GLU:HG2	2.03	0.41
1:A:847:ARG:HG2	1:A:865:GLU:HG2	2.03	0.40
3:C:74:LEU:HD21	3:C:157:PHE:HB2	2.03	0.40
2:B:208:PHE:HZ	2:B:231:LYS:HB2	1.87	0.40
1:A:258:ILE:HA	1:A:275:ASP:HA	2.03	0.40
1:A:848:ILE:HB	1:A:864:LYS:HB3	2.04	0.40
2:B:103:HIS:HB3	2:B:106:GLU:HB2	2.02	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	777/864 (90%)	738 (95%)	32 (4%)	7 (1%)	17	56
2	B	347/463 (75%)	312 (90%)	33 (10%)	2 (1%)	25	66
3	C	129/127 (102%)	124 (96%)	5 (4%)	0	100	100
All	All	1253/1454 (86%)	1174 (94%)	70 (6%)	9 (1%)	22	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	371	GLY
1	A	885	ASN
2	B	354	GLY
1	A	36	ASN

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Mol	Chain	Res	Type
1	A	340	SER
2	B	191	PRO
1	A	310	ILE
1	A	747	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	671/749 (90%)	650 (97%)	21 (3%)	40	62
2	B	316/416 (76%)	292 (92%)	24 (8%)	13	37
3	C	123/115 (107%)	115 (94%)	8 (6%)	17	42
All	All	1110/1280 (87%)	1057 (95%)	53 (5%)	25	51

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	54	GLU
1	A	80	LEU
1	A	92	LYS
1	A	102	THR
1	A	123	ILE
1	A	127	GLU
1	A	157	ILE
1	A	246	LEU
1	A	361	ASP
1	A	849	VAL
1	A	874	VAL
1	A	881	LEU
1	A	928	ARG
1	A	931	LEU
1	A	989	ARG
1	A	1039	LEU
1	A	1050	LEU

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Mol	Chain	Res	Type
1	A	1053	ASP
1	A	1078	THR
1	A	1129	LEU
2	B	118	ARG
2	B	134	GLN
2	B	144	TYR
2	B	225	GLN
2	B	236	ASN
2	B	237	LEU
2	B	244	LEU
2	B	283	ARG
2	B	288	LEU
2	B	290	ILE
2	B	292	ASP
2	B	295	ARG
2	B	299	LEU
2	B	310	CYS
2	B	311	GLU
2	B	313	ASP
2	B	320	SER
2	B	366	CYS
2	B	368	LEU
2	B	375	SER
2	B	376	THR
2	B	378	HIS
2	B	387	THR
2	B	417	LEU
3	C	57	LYS
3	C	93	ASN
3	C	96	ASP
3	C	107	MSE
3	C	128	ASP
3	C	146	ILE
3	C	149	MSE
3	C	158	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	374	GLN
1	A	392	ASN

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Mol	Chain	Res	Type
1	A	731	GLN
1	A	743	GLN
1	A	796	GLN
1	A	797	HIS
1	A	905	HIS
2	B	112	ASN
2	B	127	ASN
2	B	206	GLN
2	B	412	GLN
3	C	52	ASN
3	C	121	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	789/864 (91%)	3.63	588 (74%) 0 0	485, 485, 485, 485	0
2	B	351/463 (75%)	2.36	180 (51%) 0 1	484, 485, 485, 485	0
3	C	122/127 (96%)	2.13	56 (45%) 0 1	485, 485, 485, 485	0
All	All	1262/1454 (86%)	3.13	824 (65%) 0 0	484, 485, 485, 485	0

All (824) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	SER	19.0
1	A	1022	THR	14.0
1	A	90	GLU	11.3
1	A	787	GLU	10.8
1	A	161	GLU	10.7
1	A	1064	SER	10.6
1	A	1062	ILE	10.5
1	A	1066	GLY	10.4
1	A	20	THR	10.2
1	A	103	ARG	10.1
1	A	1065	VAL	9.7
1	A	91	TYR	9.6
1	A	165	ILE	9.4
1	A	739	ARG	9.3
1	A	196	SER	9.1
1	A	863	GLU	9.1
1	A	1063	LYS	9.0
1	A	215	GLU	9.0
1	A	1061	VAL	8.9
1	A	1011	SER	8.9
1	A	1023	PRO	8.9
1	A	757	SER	8.8
1	A	1067	LYS	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	1024	THR	8.6
1	A	19	VAL	8.5
1	A	307	GLU	8.5
1	A	164	VAL	8.5
1	A	100	ILE	8.4
2	B	372	GLY	8.4
1	A	723	LYS	8.3
1	A	24	THR	8.3
1	A	323	PHE	8.2
1	A	102	THR	8.1
1	A	785	GLU	8.1
2	B	355	TYR	8.0
1	A	195	VAL	8.0
1	A	108	VAL	7.9
3	C	48	PRO	7.8
1	A	217	SER	7.8
1	A	234	GLN	7.7
1	A	202	PHE	7.7
1	A	847	ARG	7.7
2	B	207	ILE	7.7
1	A	105	HIS	7.7
1	A	170	LEU	7.7
1	A	308	THR	7.7
1	A	32	LEU	7.6
1	A	311	ALA	7.6
1	A	107	ASN	7.6
1	A	122	GLY	7.6
1	A	853	TYR	7.6
1	A	141	LYS	7.6
1	A	160	GLU	7.5
1	A	200	LYS	7.5
1	A	235	GLU	7.5
1	A	236	SER	7.5
2	B	418	THR	7.5
2	B	420	SER	7.4
1	A	214	ALA	7.4
2	B	353	HIS	7.4
1	A	143	ILE	7.3
1	A	1026	GLY	7.3
1	A	154	ALA	7.2
1	A	197	LEU	7.2
2	B	421	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	176	PRO	7.1
1	A	1015	GLN	7.1
2	B	236	ASN	7.1
1	A	109	GLN	7.1
1	A	74	LYS	7.1
1	A	38	ARG	7.1
2	B	356	VAL	7.0
1	A	146	ASP	7.0
1	A	144	PRO	7.0
1	A	322	VAL	7.0
2	B	153	GLU	7.0
1	A	175	ALA	7.0
3	C	143	GLY	7.0
1	A	66	LEU	6.9
1	A	300	LEU	6.9
1	A	981	SER	6.9
1	A	302	VAL	6.9
1	A	131	ILE	6.9
2	B	357	HIS	6.8
1	A	813	ALA	6.8
2	B	208	PHE	6.8
2	B	422	LEU	6.8
1	A	740	ILE	6.7
1	A	106	GLY	6.7
2	B	381	PHE	6.7
1	A	56	GLY	6.7
1	A	31	LEU	6.7
1	A	149	ASN	6.7
1	A	133	LEU	6.7
2	B	248	TYR	6.6
2	B	416	GLY	6.6
1	A	75	ASP	6.6
1	A	33	ILE	6.6
1	A	152	LEU	6.6
1	A	753	ARG	6.6
1	A	383	LYS	6.5
1	A	201	GLU	6.5
3	C	145	ASP	6.5
1	A	714	THR	6.4
1	A	104	ALA	6.4
1	A	57	MET	6.4
2	B	237	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	155	PHE	6.3
1	A	360	VAL	6.3
1	A	156	ASN	6.2
2	B	209	PRO	6.2
3	C	104	PRO	6.2
1	A	213	GLU	6.2
1	A	715	VAL	6.2
1	A	957	VAL	6.2
1	A	220	ILE	6.2
1	A	163	HIS	6.2
1	A	23	PHE	6.2
1	A	101	ILE	6.2
1	A	301	ARG	6.2
1	A	752	LEU	6.2
1	A	786	VAL	6.1
1	A	725	CYS	6.1
1	A	1014	MET	6.1
1	A	99	ASP	6.1
1	A	811	GLU	6.1
1	A	212	VAL	6.1
1	A	150	LYS	6.1
3	C	66	LEU	6.1
1	A	120	ILE	6.1
1	A	1068	ILE	6.1
1	A	736	LEU	6.1
1	A	177	THR	6.0
1	A	142	VAL	6.0
1	A	89	LEU	6.0
2	B	371	ILE	5.9
1	A	179	CYS	5.9
1	A	147	ARG	5.9
1	A	862	ALA	5.9
1	A	967	GLY	5.9
1	A	140	PHE	5.9
1	A	858	LEU	5.9
1	A	809	GLN	5.9
1	A	1093	LEU	5.9
1	A	158	ARG	5.8
1	A	312	GLU	5.8
1	A	40	GLU	5.8
1	A	1070	HIS	5.8
1	A	1059	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	5.8
1	A	1005	ASN	5.8
1	A	864	LYS	5.8
2	B	354	GLY	5.8
1	A	248	ILE	5.8
1	A	58	TYR	5.8
1	A	151	GLU	5.8
1	A	1139	ILE	5.7
1	A	92	LYS	5.7
1	A	76	LEU	5.7
1	A	324	VAL	5.7
1	A	153	LYS	5.7
1	A	180	PHE	5.7
1	A	966	LEU	5.7
1	A	216	ALA	5.7
1	A	722	ARG	5.7
1	A	354	THR	5.6
2	B	415	TRP	5.6
1	A	1094	ILE	5.6
3	C	45	PRO	5.6
1	A	30	ASN	5.6
1	A	923	VAL	5.6
3	C	87	VAL	5.6
1	A	738	SER	5.6
1	A	1058	LEU	5.6
1	A	1097	PHE	5.6
1	A	849	VAL	5.5
2	B	205	CYS	5.5
1	A	1088	PHE	5.5
1	A	1025	GLN	5.5
1	A	232	ILE	5.5
1	A	198	ARG	5.5
1	A	1096	SER	5.4
1	A	206	PRO	5.4
1	A	810	ASN	5.4
1	A	784	GLU	5.4
1	A	751	ALA	5.4
1	A	178	ILE	5.4
1	A	852	GLN	5.4
1	A	733	PHE	5.4
1	A	67	PHE	5.4
1	A	130	MET	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	724	ILE	5.3
1	A	1010	GLY	5.3
1	A	93	GLN	5.3
1	A	230	ILE	5.3
1	A	789	HIS	5.3
1	A	716	PRO	5.3
1	A	812	TYR	5.3
1	A	1055	GLN	5.3
1	A	792	LEU	5.3
1	A	1051	LEU	5.2
2	B	414	PHE	5.2
1	A	838	PRO	5.2
1	A	735	VAL	5.2
1	A	788	VAL	5.2
1	A	332	GLN	5.2
1	A	713	ARG	5.2
2	B	154	ILE	5.1
1	A	148	ASP	5.1
3	C	139	TYR	5.1
1	A	1047	TRP	5.1
1	A	229	ALA	5.1
1	A	306	GLY	5.1
2	B	351	ASN	5.1
1	A	712	ILE	5.1
3	C	44	ASN	5.1
1	A	157	ILE	5.1
2	B	417	LEU	5.1
2	B	243	TRP	5.1
1	A	39	LEU	5.0
1	A	261	HIS	5.0
1	A	64	MET	5.0
1	A	272	LEU	5.0
2	B	423	LEU	5.0
1	A	1109	VAL	5.0
1	A	327	ARG	5.0
3	C	51[A]	SER	5.0
1	A	237	ILE	5.0
2	B	373	ARG	5.0
2	B	102	PHE	5.0
3	C	47	PRO	5.0
1	A	720	SER	5.0
1	A	1079	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	352	PRO	4.9
1	A	842	GLU	4.9
1	A	194	GLU	4.9
1	A	865	GLU	4.9
1	A	317	LEU	4.9
1	A	314	LEU	4.9
1	A	734	GLY	4.9
1	A	783	GLY	4.9
1	A	231	ILE	4.9
1	A	793	ILE	4.9
1	A	166	ASP	4.9
3	C	42	SER	4.9
2	B	162	ARG	4.9
1	A	192	THR	4.8
2	B	85	PRO	4.8
2	B	100	GLN	4.8
1	A	1012	LEU	4.8
1	A	732	CYS	4.8
1	A	790	ASN	4.8
1	A	207	TRP	4.8
1	A	87	CYS	4.8
1	A	273	LEU	4.8
1	A	247	ALA	4.8
1	A	233	GLY	4.8
1	A	55	VAL	4.8
1	A	191	LYS	4.8
1	A	368	GLU	4.8
1	A	310	ILE	4.8
1	A	741	GLU	4.8
2	B	397	HIS	4.8
1	A	848	ILE	4.8
1	A	1027	SER	4.8
1	A	37	THR	4.8
3	C	98	TYR	4.8
1	A	1140	HIS	4.7
2	B	400	TRP	4.7
1	A	65	GLU	4.7
1	A	60	LYS	4.7
2	B	131	ARG	4.7
1	A	356	LEU	4.7
2	B	91	LEU	4.7
1	A	721	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	238	THR	4.7
1	A	259	VAL	4.7
1	A	253	ILE	4.7
2	B	93	PRO	4.7
3	C	49	GLU	4.6
1	A	1072	PHE	4.6
1	A	836	VAL	4.6
1	A	167	VAL	4.6
1	A	240	HIS	4.6
1	A	931	LEU	4.6
1	A	979	LYS	4.6
3	C	142	PRO	4.6
1	A	392	ASN	4.6
1	A	86	ALA	4.6
3	C	144	ASP	4.6
3	C	140	ASN	4.6
1	A	132	GLY	4.6
1	A	1090	ASP	4.6
1	A	351	GLU	4.6
1	A	814	LEU	4.6
1	A	218	MET	4.6
1	A	353	PHE	4.6
1	A	35	LYS	4.5
1	A	859	GLN	4.5
1	A	361	ASP	4.5
2	B	197	VAL	4.5
1	A	17	GLY	4.5
1	A	922	LEU	4.5
1	A	882	ALA	4.5
1	A	382	PHE	4.5
1	A	808	LEU	4.5
2	B	201	SER	4.5
1	A	1001	GLY	4.5
1	A	199	GLU	4.5
2	B	130	GLU	4.5
1	A	376	VAL	4.5
1	A	381	ALA	4.5
2	B	377	GLU	4.4
1	A	336	LEU	4.4
1	A	63	VAL	4.4
2	B	227	TYR	4.4
3	C	70	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	370	LEU	4.4
1	A	49	LEU	4.4
1	A	915	LYS	4.4
1	A	1108	VAL	4.4
1	A	839	GLU	4.4
1	A	363	CYS	4.4
1	A	1002	GLU	4.4
1	A	183	GLN	4.4
1	A	221	ALA	4.4
1	A	730	SER	4.4
1	A	974	LEU	4.4
1	A	315	THR	4.4
3	C	50	THR	4.4
1	A	193	TYR	4.4
1	A	358	PRO	4.4
2	B	322	CYS	4.3
1	A	370	GLN	4.3
1	A	1003	PHE	4.3
1	A	1030	PHE	4.3
2	B	239	SER	4.3
2	B	331	ILE	4.3
1	A	260	CYS	4.3
1	A	881	LEU	4.3
1	A	54	GLU	4.3
1	A	77	LEU	4.3
1	A	297	LEU	4.3
1	A	726	TYR	4.3
1	A	352	THR	4.3
1	A	1054	MET	4.2
1	A	280	LEU	4.2
1	A	219	VAL	4.2
1	A	874	VAL	4.2
2	B	264	TRP	4.2
1	A	309	SER	4.2
1	A	328	LEU	4.2
1	A	11	LYS	4.2
1	A	387	LEU	4.2
2	B	101	LEU	4.2
1	A	168	LYS	4.2
3	C	133	PHE	4.2
1	A	84	TYR	4.2
1	A	121	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1006	VAL	4.2
2	B	360	LEU	4.2
1	A	841	ALA	4.2
2	B	369	ASN	4.2
1	A	801	VAL	4.1
1	A	325	GLY	4.1
1	A	1	MET	4.1
1	A	61	ILE	4.1
1	A	758	THR	4.1
1	A	285	LEU	4.1
1	A	1000	LEU	4.1
1	A	1074	ARG	4.1
1	A	303	GLU	4.1
1	A	389	ILE	4.1
1	A	851	PHE	4.1
1	A	914	LEU	4.1
3	C	154	GLU	4.1
1	A	287	LYS	4.1
3	C	150	ALA	4.1
2	B	190	LEU	4.1
1	A	1060	LYS	4.1
1	A	1029	LEU	4.1
1	A	1041	THR	4.1
2	B	368	LEU	4.1
3	C	129	PHE	4.1
2	B	305	ILE	4.0
2	B	230	ARG	4.0
2	B	374	PRO	4.0
2	B	376	THR	4.0
1	A	791	LEU	4.0
1	A	274	GLY	4.0
3	C	136	CYS	4.0
1	A	211	ASN	4.0
1	A	1089	ILE	4.0
2	B	401	LYS	4.0
1	A	1080	ARG	4.0
1	A	10	GLN	4.0
1	A	390	ILE	4.0
1	A	737	SER	4.0
1	A	807	PHE	4.0
1	A	42	TYR	4.0
1	A	871	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	93	ASN	4.0
2	B	90	ILE	4.0
1	A	369	ARG	4.0
1	A	238	THR	3.9
2	B	200	GLU	3.9
1	A	891	TYR	3.9
1	A	377	THR	3.9
1	A	1007	PHE	3.9
2	B	256	ARG	3.9
1	A	843	PRO	3.9
1	A	867	LYS	3.9
1	A	902	GLU	3.9
1	A	908	ASN	3.9
1	A	250	PRO	3.9
1	A	975	PHE	3.9
1	A	889	ARG	3.9
1	A	962	ASP	3.9
2	B	402	PHE	3.9
1	A	70	LYS	3.9
1	A	880	LEU	3.9
1	A	334	VAL	3.8
2	B	249	ASP	3.8
3	C	114	LEU	3.8
1	A	21	GLY	3.8
1	A	375	LEU	3.8
1	A	88	ILE	3.8
1	A	362	MET	3.8
1	A	910	MET	3.8
1	A	850	VAL	3.8
1	A	1040	VAL	3.8
2	B	299	LEU	3.8
1	A	835	MET	3.8
1	A	1132	VAL	3.8
1	A	803	HIS	3.8
2	B	152	ILE	3.8
1	A	286	GLU	3.8
1	A	1004	VAL	3.8
1	A	806	GLN	3.8
1	A	932	LEU	3.8
2	B	84	LEU	3.8
2	B	156	LYS	3.8
2	B	88	MET	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	146	ILE	3.7
2	B	273	LEU	3.7
3	C	97	TYR	3.7
2	B	86	GLN	3.7
2	B	92	ILE	3.7
2	B	413	LYS	3.7
3	C	168	GLU	3.7
3	C	56	PRO	3.7
1	A	43	VAL	3.7
2	B	332	THR	3.7
2	B	247	LEU	3.7
1	A	976	VAL	3.7
1	A	1057	ARG	3.7
2	B	206	GLN	3.7
1	A	62	ALA	3.7
1	A	110	ASP	3.7
1	A	173	CYS	3.7
1	A	953	TRP	3.7
2	B	359	THR	3.7
1	A	209	GLN	3.7
1	A	879	LYS	3.7
2	B	367	ASN	3.6
2	B	306	GLN	3.6
1	A	710	LEU	3.6
2	B	419	ARG	3.6
1	A	245	TYR	3.6
1	A	782	PHE	3.6
1	A	367	LEU	3.6
1	A	899	LEU	3.6
1	A	5	TYR	3.6
2	B	193	THR	3.6
1	A	239	TYR	3.6
1	A	227	GLY	3.6
1	A	69	PRO	3.6
2	B	204	LYS	3.6
2	B	119	THR	3.6
1	A	181	VAL	3.5
1	A	1045	GLU	3.5
1	A	305	LEU	3.5
1	A	816	LEU	3.5
2	B	284	VAL	3.5
3	C	165	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1129	LEU	3.5
1	A	919	ASP	3.5
1	A	994	GLU	3.5
1	A	1013	VAL	3.5
1	A	1095	GLU	3.5
1	A	162	LEU	3.5
1	A	333	LEU	3.5
1	A	1031	GLY	3.5
1	A	299	ASP	3.5
1	A	246	LEU	3.5
1	A	997	LEU	3.5
1	A	1033	VAL	3.5
1	A	890	LEU	3.5
1	A	1136	LEU	3.5
1	A	854	SER	3.5
1	A	258	ILE	3.5
1	A	2	SER	3.5
3	C	103[A]	THR	3.5
1	A	9	ALA	3.5
1	A	59	GLY	3.4
1	A	819	CYS	3.4
1	A	341	ASN	3.4
2	B	366	CYS	3.4
1	A	860	THR	3.4
1	A	276	MET	3.4
2	B	258	LYS	3.4
3	C	54	ASN	3.4
2	B	288	LEU	3.4
1	A	378	CYS	3.4
1	A	321	VAL	3.4
2	B	199	LEU	3.4
2	B	349	TYR	3.4
1	A	12	PRO	3.4
1	A	271	TYR	3.4
1	A	920	PHE	3.4
1	A	866	VAL	3.4
1	A	916	THR	3.4
1	A	926	LEU	3.4
1	A	388	ARG	3.4
1	A	844	LYS	3.4
2	B	380	TRP	3.4
2	B	252	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	391	ARG	3.3
1	A	1046	SER	3.3
2	B	81	ILE	3.3
2	B	135	PHE	3.3
1	A	79	ILE	3.3
1	A	145	LEU	3.3
1	A	877	ASN	3.3
2	B	375	SER	3.3
1	A	1069	GLU	3.3
2	B	189	VAL	3.3
3	C	157	PHE	3.3
1	A	833	THR	3.3
2	B	390	GLN	3.3
1	A	384	GLU	3.3
1	A	1039	LEU	3.3
1	A	951	PRO	3.3
2	B	229	LYS	3.3
1	A	313	CYS	3.3
1	A	36	ASN	3.3
2	B	106	GLU	3.3
2	B	250	ALA	3.3
1	A	78	PHE	3.3
1	A	1078	THR	3.3
3	C	135	ASN	3.3
1	A	756	ALA	3.3
1	A	364	VAL	3.2
1	A	1077	HIS	3.2
2	B	398	ILE	3.2
1	A	339	ASP	3.2
1	A	68	ARG	3.2
1	A	1092	ASP	3.2
1	A	982	ALA	3.2
1	A	277	GLU	3.2
1	A	830	ILE	3.2
1	A	821	LEU	3.2
1	A	873	MET	3.2
2	B	324	LYS	3.2
1	A	372	GLN	3.2
1	A	279	ARG	3.2
1	A	139	LEU	3.2
1	A	34	ALA	3.2
1	A	949	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	120	PHE	3.2
1	A	190	VAL	3.2
1	A	4	ASN	3.2
1	A	371	GLY	3.2
1	A	1042	SER	3.2
1	A	16	ASN	3.2
2	B	224	TRP	3.2
1	A	41	ILE	3.2
1	A	837	TYR	3.2
1	A	18	CYS	3.2
2	B	289	PRO	3.2
1	A	829	PHE	3.1
1	A	907	ASN	3.1
2	B	225	GLN	3.1
3	C	52	ASN	3.1
1	A	794	ILE	3.1
2	B	315	MET	3.1
1	A	347	VAL	3.1
1	A	998	PHE	3.1
2	B	242	ARG	3.1
1	A	304	LEU	3.1
2	B	257	ILE	3.1
1	A	917	LYS	3.1
1	A	188	ARG	3.1
1	A	252	ILE	3.1
1	A	930	VAL	3.1
1	A	13	THR	3.1
1	A	929	SER	3.1
1	A	903	CYS	3.1
1	A	804	ALA	3.1
1	A	845	GLN	3.1
3	C	88	ASP	3.1
2	B	388	VAL	3.1
2	B	399	GLY	3.1
1	A	320	GLY	3.0
1	A	80	LEU	3.0
1	A	921	ILE	3.0
1	A	995	VAL	3.0
1	A	1126	ALA	3.0
2	B	389	ALA	3.0
1	A	338	VAL	3.0
2	B	157	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	876	PHE	3.0
1	A	283	LEU	3.0
1	A	805	HIS	3.0
3	C	53	PRO	3.0
2	B	73	HIS	3.0
1	A	918	GLY	3.0
3	C	166	THR	3.0
1	A	15	VAL	3.0
1	A	1098	LEU	3.0
1	A	82	ALA	3.0
2	B	253	LEU	3.0
1	A	872	SER	3.0
1	A	980	ASP	3.0
2	B	330	GLU	3.0
2	B	155	VAL	3.0
1	A	978	GLN	3.0
1	A	44	VAL	3.0
1	A	831	VAL	3.0
2	B	262	ARG	3.0
2	B	263	GLU	3.0
2	B	285	ALA	3.0
2	B	308	LEU	3.0
3	C	55	LYS	3.0
2	B	178	GLN	3.0
2	B	321	LEU	3.0
1	A	861	VAL	3.0
2	B	231	LYS	3.0
2	B	170	LEU	3.0
1	A	226	PHE	2.9
1	A	228	GLY	2.9
2	B	382	PRO	2.9
1	A	284	LEU	2.9
1	A	912	LEU	2.9
2	B	191	PRO	2.9
1	A	834	ALA	2.9
2	B	240	TRP	2.9
3	C	101	ILE	2.9
3	C	151	GLU	2.9
1	A	374	GLN	2.9
2	B	340	LEU	2.9
1	A	208	LYS	2.9
1	A	174	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	298	LEU	2.9
1	A	913	TYR	2.9
1	A	996	GLY	2.9
2	B	202	LEU	2.9
1	A	909	ILE	2.9
1	A	893	TRP	2.9
1	A	820	LYS	2.9
2	B	251	GLU	2.9
2	B	311	GLU	2.9
1	A	72	GLU	2.8
1	A	85	ASN	2.8
1	A	331	SER	2.8
1	A	359	ILE	2.8
1	A	281	PHE	2.8
1	A	945	ILE	2.8
2	B	105	GLN	2.8
1	A	947	ARG	2.8
2	B	300	LYS	2.8
2	B	361	THR	2.8
1	A	959	ILE	2.8
1	A	1111	ASN	2.8
2	B	123	LEU	2.8
3	C	164	LEU	2.8
2	B	129	GLN	2.8
1	A	960	LEU	2.8
1	A	169	PHE	2.8
1	A	1133	VAL	2.7
1	A	241	ASN	2.7
1	A	1110	ALA	2.7
2	B	221	TYR	2.7
1	A	1050	LEU	2.7
1	A	50	ARG	2.7
1	A	954	MET	2.7
2	B	261	LEU	2.7
1	A	946	ALA	2.7
3	C	65	TYR	2.7
2	B	309	ARG	2.6
1	A	203	ASN	2.6
1	A	115	PRO	2.6
1	A	127	GLU	2.6
1	A	296	THR	2.6
1	A	126	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	70	ARG	2.6
1	A	257	THR	2.6
1	A	1071	SER	2.6
1	A	799	PHE	2.6
1	A	47	GLU	2.6
1	A	349	ALA	2.6
1	A	1037	ILE	2.6
1	A	717	LEU	2.6
2	B	228	GLN	2.6
1	A	840	GLU	2.5
1	A	1032	THR	2.5
2	B	223	TRP	2.5
3	C	46	PRO	2.5
1	A	205	GLY	2.5
2	B	365	ALA	2.5
1	A	278	GLY	2.5
2	B	176	GLY	2.5
1	A	73	SER	2.5
1	A	350	MET	2.5
1	A	135	LEU	2.5
1	A	817	VAL	2.5
2	B	83	VAL	2.5
2	B	244	LEU	2.5
1	A	52	VAL	2.5
1	A	1086	THR	2.5
2	B	403	THR	2.5
1	A	171	TYR	2.5
1	A	123	ILE	2.5
2	B	89	MET	2.5
1	A	98	ILE	2.5
2	B	297	GLN	2.5
1	A	911	ALA	2.5
2	B	95	GLN	2.5
1	A	1125	THR	2.5
2	B	280	PHE	2.4
1	A	316	TYR	2.4
2	B	296	ILE	2.4
1	A	797	HIS	2.4
3	C	57	LYS	2.4
1	A	885	ASN	2.4
2	B	310	CYS	2.4
1	A	955	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	163	GLN	2.4
2	B	358	GLU	2.4
1	A	1009	HIS	2.4
3	C	94	LEU	2.4
2	B	282	TYR	2.4
1	A	729	VAL	2.4
1	A	719	GLU	2.4
1	A	883	SER	2.4
2	B	333	THR	2.4
1	A	728	GLU	2.4
2	B	99	LEU	2.4
2	B	72	LEU	2.4
1	A	965	PHE	2.4
1	A	117	GLU	2.3
3	C	83	PHE	2.3
3	C	125	CYS	2.3
1	A	875	GLU	2.3
1	A	1100	ILE	2.3
1	A	1104	LYS	2.3
2	B	234	CYS	2.3
1	A	28	ASP	2.3
1	A	138	GLY	2.3
2	B	274	PRO	2.3
1	A	1048	TYR	2.3
2	B	177	ILE	2.3
1	A	210	GLU	2.3
1	A	927	MET	2.3
1	A	828	TYR	2.3
1	A	1034	ASN	2.3
1	A	796	GLN	2.3
1	A	1036	MET	2.3
1	A	1130	ILE	2.3
3	C	138	ILE	2.3
2	B	245	TYR	2.3
1	A	182	TYR	2.3
2	B	233	HIS	2.3
1	A	25	SER	2.3
2	B	246	SER	2.3
3	C	137	TYR	2.3
1	A	1076	PHE	2.3
1	A	118	THR	2.2
1	A	249	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	125	TYR	2.2
3	C	141	LYS	2.2
1	A	128	CYS	2.2
1	A	764	SER	2.2
2	B	226	LYS	2.2
1	A	818	SER	2.2
1	A	48	GLY	2.2
1	A	342	GLU	2.2
3	C	86	PRO	2.2
1	A	1099	ASP	2.2
1	A	1087	GLY	2.2
2	B	80	VAL	2.2
2	B	292	ASP	2.2
3	C	61	ASN	2.2
1	A	795	ASP	2.1
1	A	892	GLU	2.1
2	B	260	GLN	2.1
2	B	109	MET	2.1
1	A	124	ILE	2.1
2	B	87	VAL	2.1
2	B	314	ILE	2.1
3	C	92	LEU	2.1
1	A	134	ARG	2.1
1	A	326	SER	2.1
1	A	904	ASN	2.1
1	A	1038	GLY	2.1
2	B	192	SER	2.1
2	B	124	ALA	2.1
1	A	760	ALA	2.1
1	A	1085	ALA	2.1
1	A	222	VAL	2.1
1	A	29	LEU	2.1
1	A	755	SER	2.1
1	A	884	ILE	2.1
3	C	96	ASP	2.1
1	A	282	MET	2.1
1	A	53	LYS	2.1
2	B	295	ARG	2.0
1	A	971	ALA	2.0
1	A	958	GLU	2.0
2	B	269	LYS	2.0
1	A	365	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	942	PHE	2.0
2	B	317	LYS	2.0
1	A	1044	SER	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	B	501	1/1	0.85	0.25	465,465,465,465	0

6.5 Other polymers [i](#)

There are no such residues in this entry.