



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:07 PM UTC

PDB ID : 6BNB / pdb_00006bnb
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

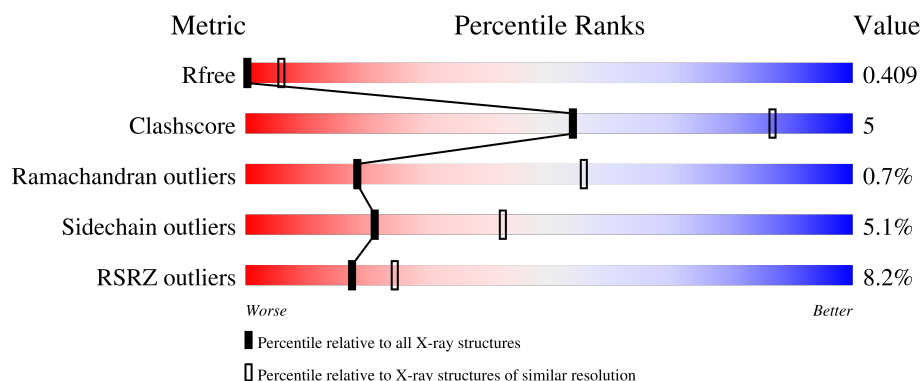
1 Overall quality at a glance

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}	180053	1154 (8.50-4.00)
Clashscore	190562	1016 (8.60-4.02)
Ramachandran outliers	187476	1042 (8.50-4.00)
Sidechain outliers	187428	1007 (8.50-4.00)
RSRZ outliers	180081	1147 (8.50-4.00)

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 $\leq 5\%$. 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	 7% 80% 11% 9%
2	B	463	 7% 62% 13% 24%
3	C	127	 10% 82% 15%

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

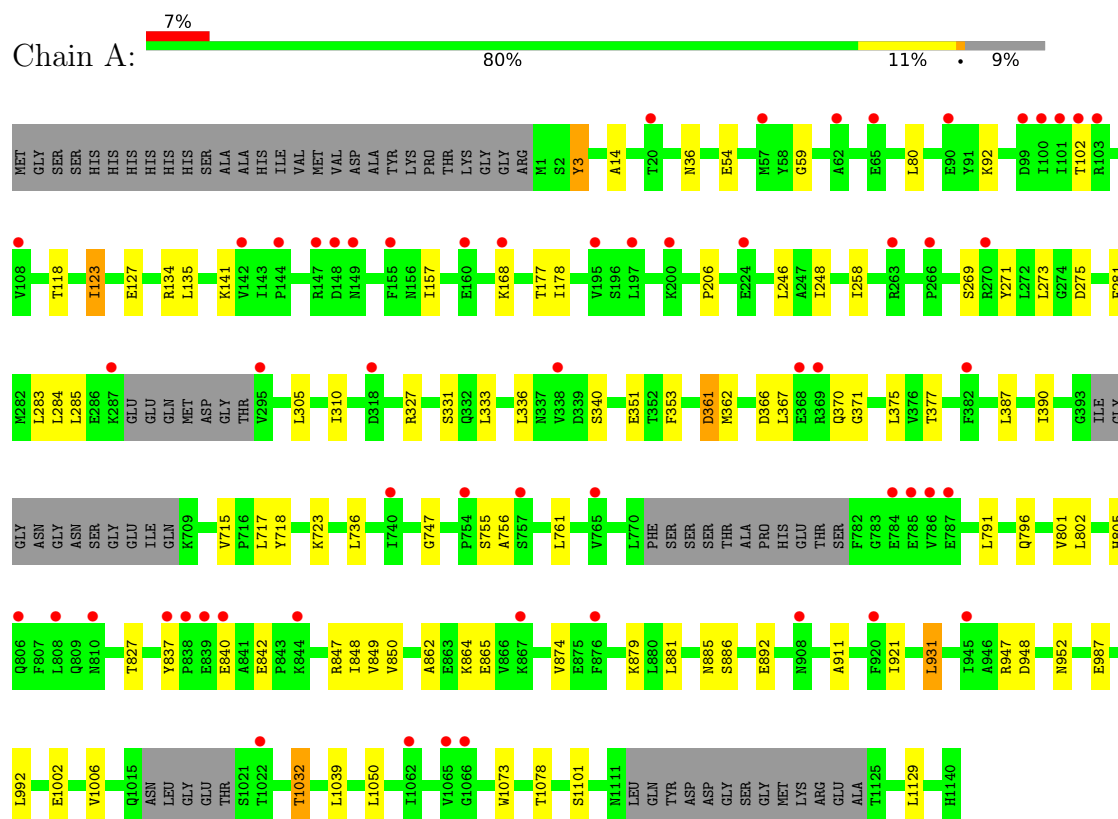
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

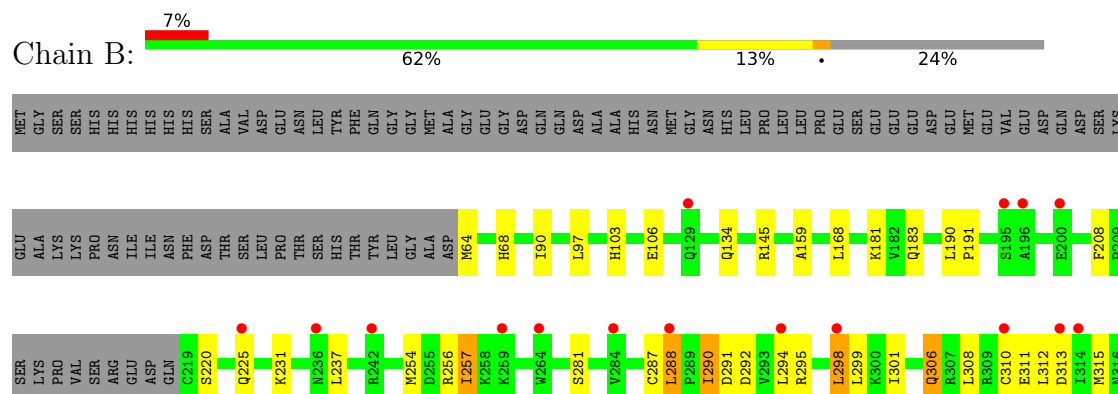
3 Residue-property plots

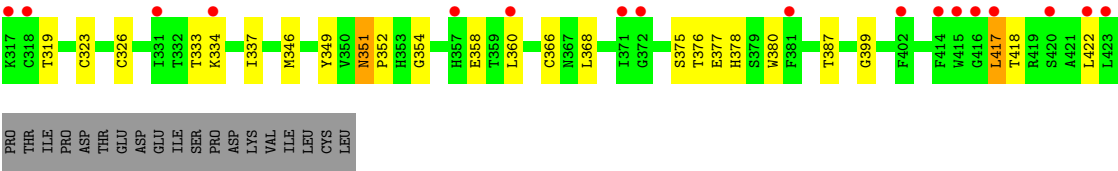
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA damage-binding protein 1

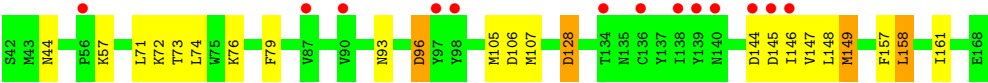
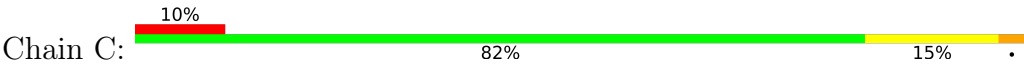


• Molecule 2: Protein cereblon





● 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 0.339 , 0.409	Depositor DCC
R_{free} test set	417 reflections (4.57%)	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)	0.36 , 641.9	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

5.1 Standard geometry

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	0.68	0/6237	1.06	4/8449 (0.0%)
2	B	0.76	0/2905	1.21	7/3936 (0.2%)
3	C	0.79	0/1115	1.24	2/1508 (0.1%)
All	All	0.72	0/10257	1.13	13/13893 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	ASN	CA-CB-CG	7.61	120.21	112.60
1	A	1032	THR	CA-C-N	5.66	128.22	120.46
1	A	1032	THR	C-N-CA	5.66	128.22	120.46
3	C	44	ASN	N-CA-CB	5.65	117.63	110.23
3	C	96	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	1101	SER	CA-C-N	5.41	126.85	120.09
1	A	1101	SER	C-N-CA	5.41	126.85	120.09
2	B	220	SER	CA-C-N	5.37	127.42	120.44
2	B	220	SER	C-N-CA	5.37	127.42	120.44
2	B	418	THR	CA-C-N	5.32	127.41	120.28
2	B	418	THR	C-N-CA	5.32	127.41	120.28
2	B	68	HIS	CA-C-N	5.18	124.89	119.92
2	B	68	HIS	C-N-CA	5.18	124.89	119.92

There are no chirality outliers.

There are no planarity outliers.

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	6128	0	6031	37	0
2	B	2839	0	2832	45	0
3	C	1074	0	1064	18	0
4	B	1	0	0	0	0
All	All	10042	0	9927	98	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 (98) 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
2:B:290:ILE:HD11	2:B:294:LEU:C	1.92	0.94
3:C:79:PHE:HB3	3:C:149:MSE:CG	1.99	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:362:MET:HE3	1:A:375:LEU:HD11	1.92	0.51
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
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
2:B:291:ASP:O	2:B:292:ASP:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:105:MSE:HE3	3:C:128:ASP:CG	2.42	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
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
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
2:B:312:LEU:HA	2:B:315:MET:HE3	2.02	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:135:LEU:HD12	1:A:141:LYS:HZ3	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%)	14	50
2	B	347/463 (75%)	312 (90%)	33 (10%)	2 (1%)	21	59
3	C	129/127 (102%)	124 (96%)	5 (4%)	0	100	100
All	All	1253/1454 (86%)	1174 (94%)	70 (6%)	9 (1%)	18	56

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
1	A	340	SER
2	B	191	PRO
1	A	310	ILE
1	A	747	GLY

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	671/749 (90%)	646 (96%)	25 (4%)	30	51
2	B	316/416 (76%)	295 (93%)	21 (7%)	15	37
3	C	123/115 (107%)	112 (91%)	11 (9%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1110/1280 (87%)	1053 (95%)	57 (5%)	21	42

All (57) 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	178	ILE
1	A	246	LEU
1	A	248	ILE
1	A	284	LEU
1	A	361	ASP
1	A	390	ILE
1	A	827	THR
1	A	849	VAL
1	A	874	VAL
1	A	881	LEU
1	A	921	ILE
1	A	931	LEU
1	A	987	GLU
1	A	1039	LEU
1	A	1050	LEU
1	A	1078	THR
1	A	1129	LEU
2	B	134	GLN
2	B	225	GLN
2	B	237	LEU
2	B	257	ILE
2	B	288	LEU
2	B	290	ILE
2	B	298	LEU
2	B	299	LEU
2	B	306	GLN
2	B	310	CYS
2	B	311	GLU
2	B	313	ASP

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Mol	Chain	Res	Type
2	B	333	THR
2	B	366	CYS
2	B	368	LEU
2	B	375	SER
2	B	376	THR
2	B	377	GLU
2	B	378	HIS
2	B	387	THR
2	B	417	LEU
3	C	57	LYS
3	C	71	LEU
3	C	72[A]	LYS
3	C	72[B]	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	234	GLN
1	A	241	ASN
1	A	262	ASN
1	A	343	GLN
1	A	355	ASN
1	A	370	GLN
1	A	392	ASN
1	A	731	GLN
1	A	790	ASN
1	A	796	GLN
1	A	797	HIS
1	A	806	GLN
1	A	852	GLN
1	A	905	HIS
1	A	964	ASN
1	A	978	GLN
1	A	1025	GLN

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Mol	Chain	Res	Type
1	A	1059	ASN
1	A	1070	HIS
2	B	112	ASN
2	B	163	GLN
2	B	173	GLN
2	B	179	GLN
2	B	198	GLN
2	B	206	GLN
2	B	236	ASN
2	B	260	GLN
2	B	306	GLN
2	B	412	GLN
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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	789/864 (91%)	0.42	58 (7%)	20 26	485, 485, 485, 485	0
2	B	351/463 (75%)	0.62	33 (9%)	14 21	484, 485, 485, 485	0
3	C	122/127 (96%)	0.64	13 (10%)	11 18	312, 485, 485, 485	4 (3%)
All	All	1262/1454 (86%)	0.50	104 (8%)	17 24	312, 485, 485, 485	4 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	ILE	6.5
1	A	844	LYS	6.1
2	B	372	GLY	5.7
1	A	810	ASN	5.5
3	C	146	ILE	4.9
2	B	422	LEU	4.7
1	A	786	VAL	4.6
3	C	139	TYR	4.5
1	A	784	GLU	4.4
3	C	97	TYR	4.4
1	A	142	VAL	4.3
1	A	838	PRO	4.1
1	A	785	GLU	4.0
1	A	1065	VAL	4.0
1	A	787	GLU	4.0
2	B	415	TRP	4.0
2	B	318	CYS	3.8
1	A	806	GLN	3.8
3	C	144	ASP	3.7
2	B	314	ILE	3.7
1	A	382	PHE	3.6
2	B	417	LEU	3.6
1	A	147	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	145	ASP	3.6
2	B	420	SER	3.4
2	B	381	PHE	3.4
1	A	369	ARG	3.4
1	A	295	VAL	3.4
1	A	102	THR	3.4
2	B	294	LEU	3.3
2	B	317	LYS	3.3
1	A	839	GLU	3.3
2	B	129	GLN	3.3
2	B	288	LEU	3.2
2	B	195	SER	3.1
1	A	270	ARG	3.1
2	B	225	GLN	3.1
2	B	264	TRP	3.1
1	A	1022	THR	3.0
2	B	334	LYS	3.0
3	C	138	ILE	3.0
2	B	414	PHE	3.0
1	A	266	PRO	3.0
1	A	1066	GLY	3.0
1	A	740	ILE	3.0
1	A	62	ALA	3.0
1	A	945	ILE	2.9
1	A	287	LYS	2.9
1	A	808	LEU	2.9
3	C	87	VAL	2.8
3	C	140	ASN	2.8
1	A	195	VAL	2.8
1	A	103	ARG	2.8
2	B	371	ILE	2.7
1	A	197	LEU	2.7
2	B	310	CYS	2.7
1	A	920	PHE	2.7
3	C	56	PRO	2.6
1	A	160	GLU	2.6
2	B	423	LEU	2.6
1	A	100	ILE	2.6
2	B	200	GLU	2.6
1	A	908	ASN	2.5
1	A	155	PHE	2.5
1	A	65	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	90	VAL	2.5
1	A	148	ASP	2.5
1	A	144	PRO	2.5
1	A	90	GLU	2.5
2	B	284	VAL	2.4
2	B	357	HIS	2.4
2	B	313	ASP	2.4
2	B	236	ASN	2.4
1	A	263	ARG	2.4
3	C	136	CYS	2.4
2	B	331	ILE	2.4
1	A	108	VAL	2.4
3	C	134	THR	2.3
1	A	765	VAL	2.3
1	A	867	LYS	2.3
3	C	98	TYR	2.3
1	A	99	ASP	2.3
1	A	200	LYS	2.3
2	B	416	GLY	2.2
2	B	298	LEU	2.2
1	A	318	ASP	2.2
1	A	837	TYR	2.2
1	A	876	PHE	2.2
1	A	168	LYS	2.2
2	B	402	PHE	2.2
1	A	149	ASN	2.1
1	A	20	THR	2.1
1	A	754	PRO	2.1
2	B	196	ALA	2.1
2	B	360	LEU	2.1
1	A	757	SER	2.1
1	A	840	GLU	2.1
1	A	57	MET	2.0
1	A	368	GLU	2.0
1	A	1062	ILE	2.0
1	A	224	GLU	2.0
1	A	338	VAL	2.0
2	B	259	LYS	2.0
2	B	242	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	ZN	B	501	1/1	0.99	0.09	465,465,465,465	0

6.5 Other polymers [i](#)

There are no such residues in this entry.