



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:58 PM EDT

PDB ID : 3HVE / pdb_00003hve
Title : Structures of SPOP-Substrate Complexes: Insights into Molecular Architectures of BTB-Cul3 Ubiquitin Ligases: GigaxoninBTB/3-box
Authors : Zhuang, M.; Schulman, B.A.
Deposited on : 2009-06-16
Resolution : 2.80 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

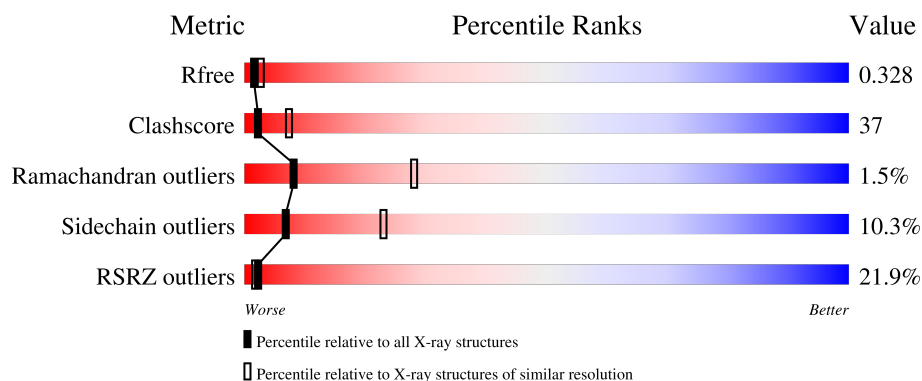
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

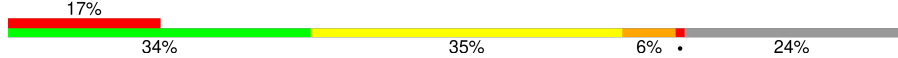
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	256	
2	B	256	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3049 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 Gigaxonin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1636	1050	279	296	6	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9H2C0
A	0	SER	-	expression tag	UNP Q9H2C0

- Molecule 2 is a protein called Gigaxonin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	Se	0	0	0
			1413	900	245	257	6	5			

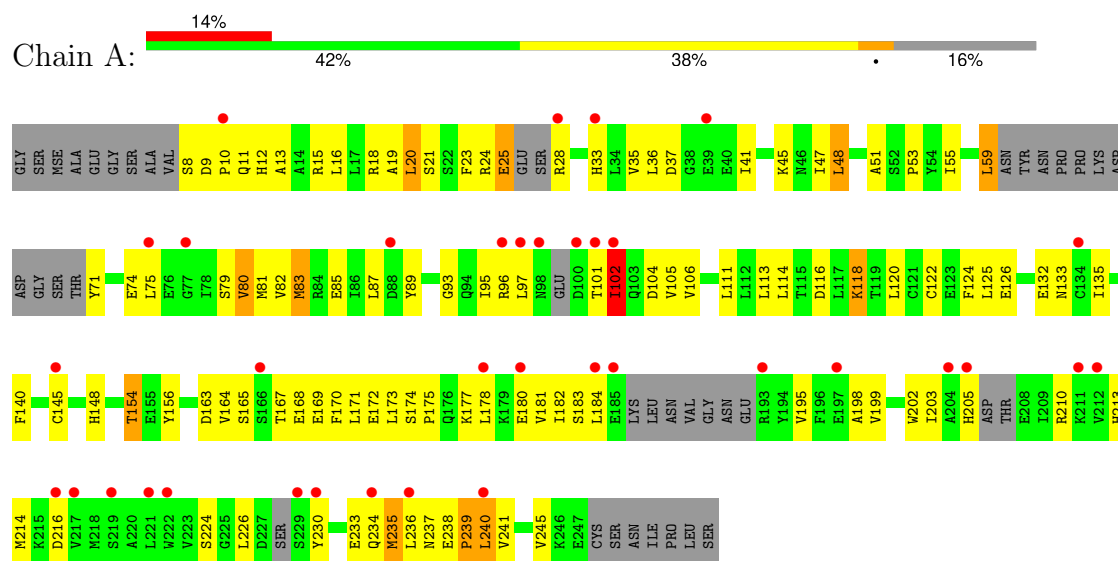
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q9H2C0
B	0	SER	-	expression tag	UNP Q9H2C0

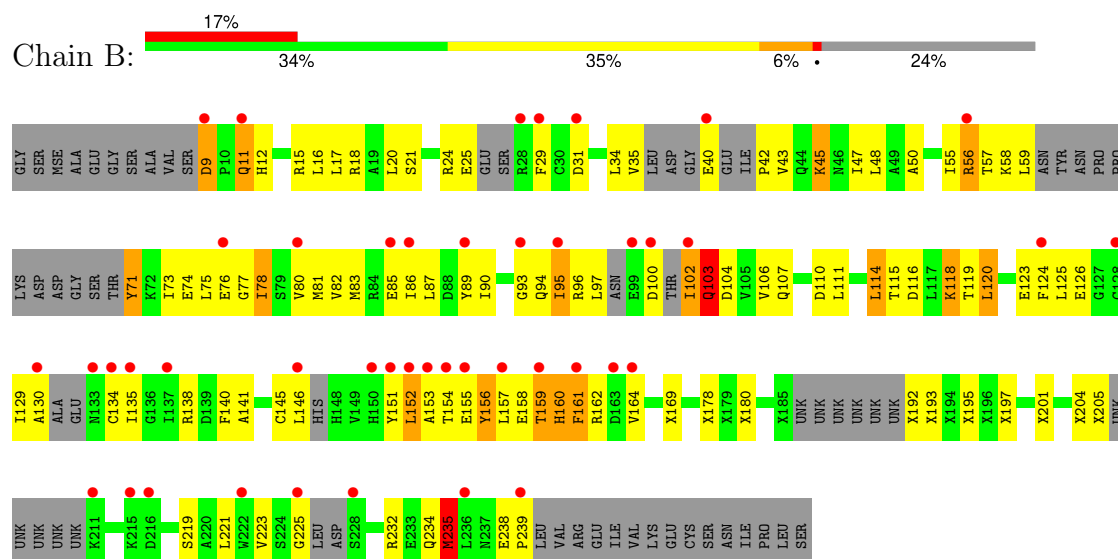
3 Residue-property plots [i](#)

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

• Molecule 1: Gigaxonin



• Molecule 2: Gigaxonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.48Å 55.60Å 120.60Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	88.0 (50.00-2.80) 91.0 (50.00-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.302 , 0.333 0.297 , 0.328	Depositor DCC
R_{free} test set	693 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3049	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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](#)

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	0.76	5/1656 (0.3%)	1.10	10/2238 (0.4%)
2	B	0.54	1/1247 (0.1%)	1.09	10/1668 (0.6%)
All	All	0.67	6/2903 (0.2%)	1.10	20/3906 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	VAL	C-O	-6.64	1.16	1.24
1	A	235	MSE	SE-CE	-6.52	1.75	1.95
2	B	235	MSE	CG-SE	-5.89	1.77	1.95
1	A	83	MSE	SE-CE	-5.58	1.78	1.95
1	A	81	MSE	CA-CB	5.36	1.62	1.53
1	A	235	MSE	CG-SE	-5.35	1.79	1.95

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ALA	N-CA-C	-8.94	104.43	114.62
1	A	240	LEU	N-CA-C	-8.15	102.37	111.82
2	B	156	TYR	N-CA-C	-7.89	103.61	113.55
2	B	114	LEU	N-CA-C	-7.51	98.33	109.15
2	B	11	GLN	CB-CA-C	-7.26	102.22	111.22
2	B	78	ILE	N-CA-C	-7.11	97.27	108.86
1	A	23	PHE	CB-CA-C	-6.91	102.72	111.22
2	B	76	GLU	N-CA-C	6.62	120.06	107.75
2	B	77	GLY	N-CA-C	6.48	125.77	114.76
1	A	133	ASN	N-CA-C	-6.44	103.96	112.72
2	B	89	TYR	N-CA-C	-6.41	104.30	111.28
2	B	43	VAL	N-CA-C	6.21	116.10	108.53
1	A	154	THR	N-CA-C	-6.07	104.59	111.14
1	A	23	PHE	N-CA-C	-5.88	104.72	112.72
2	B	159	THR	N-CA-C	5.79	120.36	113.12
1	A	135	ILE	N-CA-C	-5.51	105.35	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ASN	CB-CA-C	-5.30	104.70	111.22
2	B	45	LYS	N-CA-C	5.21	119.97	111.37
1	A	156	TYR	N-CA-C	-5.20	105.50	111.07
1	A	89	TYR	N-CA-C	-5.08	105.64	111.07

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	1636	0	1547	108	0
2	B	1413	0	1238	125	0
All	All	3049	0	2785	213	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 37.

All (213) 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:75:LEU:HD13	2:B:83:MSE:CE	1.74	1.18
2:B:238:GLU:HB2	2:B:239:PRO:HD2	1.27	1.16
2:B:75:LEU:HD13	2:B:83:MSE:HE1	1.32	1.06
2:B:238:GLU:CB	2:B:239:PRO:HD2	1.78	1.06
2:B:75:LEU:CD1	2:B:83:MSE:HE3	1.91	1.00
1:A:172:GLU:HA	1:A:210:ARG:HH22	1.26	0.97
1:A:95:ILE:CG1	1:A:97:LEU:HD11	1.94	0.96
2:B:75:LEU:CD1	2:B:83:MSE:CE	2.46	0.94
1:A:75:LEU:CD1	1:A:83:MSE:CE	2.47	0.92
1:A:75:LEU:CD1	1:A:83:MSE:HE1	2.01	0.91
1:A:203:ILE:HD12	1:A:214:MSE:HE2	1.52	0.89
1:A:75:LEU:HD12	1:A:83:MSE:HE3	1.52	0.89
1:A:95:ILE:HG23	1:A:97:LEU:HD13	1.55	0.89
1:A:75:LEU:HD12	1:A:83:MSE:CE	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:SER:HA	2:B:94:GLN:CD	1.99	0.87
2:B:95:ILE:HD12	2:B:95:ILE:H	1.38	0.87
1:A:95:ILE:HG13	1:A:97:LEU:CD1	2.04	0.86
1:A:8:SER:HA	2:B:94:GLN:NE2	1.91	0.86
2:B:75:LEU:HD12	2:B:83:MSE:HE3	1.57	0.85
2:B:35:VAL:CG1	2:B:74:GLU:HA	2.07	0.84
1:A:28:ARG:NH1	2:B:59:LEU:HD13	1.92	0.84
1:A:28:ARG:HH11	2:B:59:LEU:HD13	1.43	0.84
1:A:95:ILE:HG13	1:A:97:LEU:HD11	1.60	0.84
1:A:21:SER:O	1:A:24:ARG:HG3	1.79	0.81
1:A:9:ASP:H	2:B:94:GLN:HE21	1.25	0.80
1:A:20:LEU:HG	1:A:47:ILE:HD11	1.63	0.80
1:A:95:ILE:HG12	1:A:97:LEU:HD11	1.64	0.80
2:B:35:VAL:HG12	2:B:74:GLU:HA	1.65	0.79
1:A:45:LYS:HG2	1:A:59:LEU:HD21	1.68	0.76
1:A:93:GLY:HA2	2:B:12:HIS:ND1	2.02	0.74
2:B:126:GLU:HG3	2:B:152:LEU:HD22	1.70	0.74
1:A:28:ARG:HH11	2:B:59:LEU:CD1	2.00	0.74
1:A:36:LEU:HD11	1:A:75:LEU:HD12	1.70	0.71
1:A:230:TYR:O	1:A:234:GLN:HG3	1.90	0.71
1:A:75:LEU:CD1	1:A:83:MSE:HE3	2.18	0.71
2:B:115:THR:HG23	2:B:116:ASP:H	1.56	0.70
2:B:20:LEU:HD13	2:B:47:ILE:HD11	1.73	0.70
2:B:238:GLU:CB	2:B:239:PRO:CD	2.66	0.70
1:A:241:VAL:O	1:A:245:VAL:HG23	1.91	0.69
2:B:100:ASP:HA	2:B:102:ILE:HD12	1.73	0.69
2:B:104:ASP:HA	2:B:107:GLN:HB3	1.75	0.68
1:A:95:ILE:CG1	1:A:97:LEU:CD1	2.66	0.68
1:A:167:THR:HG22	1:A:169:GLU:H	1.59	0.68
1:A:102:ILE:HD13	1:A:124:PHE:HE2	1.56	0.68
1:A:95:ILE:HG23	1:A:97:LEU:CD1	2.23	0.68
2:B:204:UNK:O	2:B:205:UNK:CB	2.41	0.67
1:A:11:GLN:O	1:A:15:ARG:HB2	1.95	0.67
2:B:238:GLU:CG	2:B:239:PRO:HD2	2.24	0.66
2:B:160:HIS:N	2:B:160:HIS:CD2	2.64	0.66
1:A:75:LEU:HD13	1:A:83:MSE:HE1	1.78	0.66
2:B:219:SER:O	2:B:223:VAL:HG23	1.96	0.66
1:A:36:LEU:HG	1:A:75:LEU:HB2	1.78	0.65
2:B:118:LYS:NZ	2:B:118:LYS:HB3	2.12	0.65
2:B:129:ILE:O	2:B:130:ALA:HB2	1.95	0.65
2:B:129:ILE:O	2:B:130:ALA:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:OG	1:A:82:VAL:HG23	1.97	0.64
1:A:9:ASP:OD2	1:A:15:ARG:NH1	2.32	0.63
2:B:102:ILE:HD12	2:B:102:ILE:N	2.14	0.63
2:B:103:GLN:H	2:B:103:GLN:NE2	1.95	0.63
1:A:45:LYS:CG	1:A:59:LEU:HD21	2.29	0.63
1:A:126:GLU:OE1	1:A:148:HIS:HD2	1.81	0.63
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.64	0.63
1:A:203:ILE:HD12	1:A:214:MSE:CE	2.25	0.62
1:A:37:ASP:OD2	1:A:80:VAL:HG23	2.00	0.62
2:B:130:ALA:O	2:B:134:CYS:HB3	2.00	0.61
1:A:48:LEU:HD22	1:A:55:ILE:HG13	1.83	0.61
1:A:177:LYS:O	1:A:181:VAL:HG23	2.01	0.60
1:A:238:GLU:C	1:A:240:LEU:H	2.09	0.60
2:B:11:GLN:O	2:B:15:ARG:HG3	2.00	0.60
2:B:159:THR:HB	2:B:160:HIS:HD2	1.67	0.60
2:B:238:GLU:HG3	2:B:239:PRO:HG2	1.84	0.60
2:B:104:ASP:HA	2:B:107:GLN:CB	2.32	0.60
1:A:180:GLU:O	1:A:183:SER:HB3	2.03	0.59
1:A:203:ILE:CD1	1:A:214:MSE:HE2	2.28	0.59
1:A:132:GLU:HA	1:A:167:THR:HG21	1.84	0.59
2:B:85:GLU:OE1	2:B:97:LEU:HD11	2.02	0.59
1:A:95:ILE:HG13	1:A:97:LEU:HD12	1.82	0.59
2:B:141:ALA:HA	2:B:146:LEU:HD12	1.84	0.59
2:B:238:GLU:O	2:B:239:PRO:C	2.45	0.58
1:A:12:HIS:CD2	2:B:93:GLY:HA2	2.38	0.58
2:B:82:VAL:O	2:B:85:GLU:HB2	2.04	0.58
1:A:102:ILE:HD13	1:A:124:PHE:CE2	2.37	0.57
1:A:96:ARG:C	1:A:97:LEU:HD12	2.29	0.57
1:A:59:LEU:HD23	2:B:29:PHE:CE2	2.40	0.57
2:B:160:HIS:O	2:B:164:VAL:HG23	2.05	0.57
1:A:79:SER:HG	1:A:82:VAL:HG23	1.68	0.57
2:B:78:ILE:HD11	2:B:111:LEU:HD23	1.85	0.57
1:A:12:HIS:CG	2:B:93:GLY:HA2	2.39	0.56
1:A:35:VAL:HB	1:A:74:GLU:HA	1.87	0.56
1:A:182:ILE:HD11	1:A:199:VAL:HG22	1.88	0.56
2:B:78:ILE:CD1	2:B:111:LEU:HD23	2.35	0.56
1:A:173:LEU:HG	1:A:174:SER:N	2.21	0.56
1:A:102:ILE:CD1	1:A:124:PHE:HE2	2.18	0.56
1:A:97:LEU:HD12	1:A:97:LEU:N	2.21	0.56
2:B:96:ARG:HG3	2:B:96:ARG:O	2.06	0.55
1:A:173:LEU:HG	1:A:174:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:HD12	2:B:95:ILE:N	2.16	0.55
1:A:122:CYS:O	1:A:126:GLU:HG3	2.06	0.55
2:B:135:ILE:HD12	2:B:169:UNK:CB	2.37	0.55
1:A:173:LEU:HD23	1:A:178:LEU:HB2	1.87	0.55
2:B:104:ASP:O	2:B:107:GLN:HB3	2.08	0.54
1:A:8:SER:CA	2:B:94:GLN:NE2	2.68	0.54
2:B:161:PHE:HE2	2:B:195:UNK:HA	1.72	0.54
2:B:234:GLN:O	2:B:238:GLU:HB3	2.08	0.53
1:A:178:LEU:HD23	1:A:178:LEU:C	2.33	0.53
1:A:9:ASP:N	2:B:94:GLN:HE21	2.01	0.53
2:B:34:LEU:HD12	2:B:73:ILE:O	2.09	0.53
2:B:103:GLN:HA	2:B:140:PHE:CZ	2.44	0.52
1:A:168:GLU:O	1:A:172:GLU:HG2	2.09	0.52
1:A:8:SER:HA	2:B:94:GLN:CG	2.39	0.52
2:B:197:UNK:O	2:B:201:UNK:N	2.42	0.52
1:A:95:ILE:CG2	1:A:97:LEU:CD1	2.88	0.51
1:A:105:VAL:HG12	1:A:105:VAL:O	2.10	0.51
2:B:138:ARG:HB2	2:B:153:ALA:HB1	1.91	0.51
2:B:78:ILE:CG2	2:B:82:VAL:HB	2.39	0.51
2:B:100:ASP:HA	2:B:102:ILE:CD1	2.40	0.51
1:A:36:LEU:HD21	1:A:83:MSE:HE2	1.92	0.51
2:B:86:ILE:O	2:B:90:ILE:HG13	2.11	0.51
1:A:235:MSE:C	1:A:237:ASN:H	2.19	0.50
2:B:11:GLN:O	2:B:11:GLN:HG3	2.11	0.50
2:B:160:HIS:C	2:B:162:ARG:N	2.69	0.50
2:B:115:THR:HG23	2:B:116:ASP:N	2.24	0.50
2:B:159:THR:HB	2:B:160:HIS:CD2	2.47	0.49
2:B:154:THR:O	2:B:158:GLU:HB3	2.12	0.49
1:A:18:ARG:O	1:A:21:SER:HB3	2.12	0.49
1:A:132:GLU:N	1:A:132:GLU:CD	2.70	0.49
2:B:80:VAL:HG23	2:B:81:MSE:N	2.27	0.49
2:B:192:UNK:O	2:B:195:UNK:N	2.46	0.49
2:B:118:LYS:HB3	2:B:118:LYS:HZ3	1.77	0.49
2:B:86:ILE:HG21	2:B:114:LEU:HD11	1.94	0.49
1:A:13:ALA:HB2	2:B:17:LEU:CD2	2.43	0.49
1:A:36:LEU:CG	1:A:75:LEU:HB2	2.43	0.48
2:B:35:VAL:HG13	2:B:74:GLU:HA	1.92	0.48
1:A:93:GLY:CA	2:B:12:HIS:ND1	2.76	0.48
1:A:171:LEU:C	1:A:173:LEU:H	2.21	0.48
2:B:238:GLU:CG	2:B:239:PRO:CD	2.90	0.48
1:A:59:LEU:HD23	2:B:29:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:HB2	2:B:17:LEU:HD23	1.96	0.47
1:A:16:LEU:O	1:A:19:ALA:HB3	2.14	0.47
2:B:118:LYS:NZ	2:B:118:LYS:CB	2.76	0.47
2:B:160:HIS:N	2:B:160:HIS:HD2	2.10	0.47
2:B:160:HIS:O	2:B:162:ARG:N	2.48	0.47
2:B:9:ASP:C	2:B:11:GLN:H	2.23	0.47
1:A:102:ILE:O	1:A:106:VAL:HG23	2.15	0.47
2:B:102:ILE:HD11	2:B:124:PHE:HE2	1.80	0.46
1:A:51:ALA:HB2	2:B:16:LEU:CD1	2.46	0.46
2:B:9:ASP:C	2:B:11:GLN:N	2.74	0.46
2:B:81:MSE:O	2:B:85:GLU:HG2	2.15	0.46
2:B:160:HIS:C	2:B:162:ARG:H	2.23	0.46
2:B:21:SER:O	2:B:24:ARG:HG3	2.15	0.46
2:B:178:UNK:C	2:B:180:UNK:N	2.77	0.46
1:A:51:ALA:HB2	2:B:16:LEU:HD11	1.97	0.46
2:B:57:THR:O	2:B:57:THR:HG22	2.16	0.46
2:B:238:GLU:HG3	2:B:239:PRO:CG	2.45	0.46
1:A:10:PRO:C	1:A:12:HIS:H	2.24	0.45
2:B:35:VAL:CG1	2:B:74:GLU:CA	2.88	0.45
2:B:96:ARG:C	2:B:97:LEU:HG	2.41	0.45
2:B:221:LEU:O	2:B:225:GLY:N	2.46	0.45
2:B:34:LEU:H	2:B:42:PRO:N	2.15	0.45
2:B:59:LEU:HD23	2:B:71:TYR:CE1	2.52	0.45
1:A:24:ARG:C	1:A:25:GLU:CG	2.88	0.45
1:A:172:GLU:HA	1:A:210:ARG:NH2	2.10	0.45
1:A:238:GLU:CB	1:A:239:PRO:HD2	2.46	0.45
1:A:111:LEU:C	1:A:111:LEU:HD13	2.42	0.44
2:B:11:GLN:O	2:B:11:GLN:CG	2.64	0.44
2:B:93:GLY:O	2:B:94:GLN:HG3	2.17	0.44
2:B:145:CYS:SG	2:B:145:CYS:O	2.76	0.44
2:B:151:TYR:CD1	2:B:151:TYR:C	2.96	0.44
1:A:238:GLU:C	1:A:240:LEU:N	2.75	0.44
2:B:118:LYS:HB3	2:B:118:LYS:HZ2	1.83	0.44
2:B:232:ARG:O	2:B:235:MSE:HB2	2.18	0.43
2:B:238:GLU:HG3	2:B:239:PRO:CD	2.48	0.43
2:B:157:LEU:HD12	2:B:164:VAL:HG11	2.00	0.43
1:A:213:HIS:O	1:A:216:ASP:N	2.52	0.43
2:B:102:ILE:C	2:B:104:ASP:N	2.77	0.43
1:A:101:THR:O	1:A:102:ILE:C	2.62	0.43
2:B:192:UNK:O	2:B:193:UNK:C	2.64	0.43
2:B:31:ASP:OD1	2:B:45:LYS:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ARG:HH11	2:B:56:ARG:CG	2.31	0.42
2:B:58:LYS:O	2:B:59:LEU:HB3	2.19	0.42
1:A:235:MSE:C	1:A:237:ASN:N	2.77	0.42
1:A:224:SER:C	1:A:226:LEU:H	2.26	0.42
1:A:125:LEU:HD11	1:A:140:PHE:CE2	2.54	0.42
2:B:130:ALA:C	2:B:134:CYS:HB3	2.45	0.42
2:B:160:HIS:CD2	2:B:160:HIS:H	2.35	0.42
2:B:9:ASP:O	2:B:11:GLN:N	2.53	0.42
1:A:37:ASP:CG	1:A:80:VAL:HG23	2.45	0.42
2:B:102:ILE:HG22	2:B:106:VAL:HG23	2.02	0.42
2:B:34:LEU:O	2:B:40:GLU:HA	2.19	0.42
2:B:31:ASP:CG	2:B:45:LYS:HE3	2.45	0.41
2:B:130:ALA:H	2:B:134:CYS:HB3	1.85	0.41
2:B:119:THR:O	2:B:123:GLU:HG3	2.19	0.41
2:B:120:LEU:HD12	2:B:120:LEU:HA	1.88	0.41
1:A:114:LEU:O	1:A:118:LYS:HB2	2.19	0.41
1:A:180:GLU:HG3	1:A:181:VAL:N	2.35	0.41
1:A:238:GLU:O	1:A:240:LEU:N	2.53	0.41
2:B:129:ILE:HG21	2:B:156:TYR:CG	2.56	0.41
1:A:101:THR:O	1:A:104:ASP:HB2	2.19	0.41
1:A:165:SER:HA	1:A:170:PHE:CD2	2.56	0.41
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.85	0.41
2:B:48:LEU:CD2	2:B:55:ILE:HD13	2.50	0.41
1:A:19:ALA:CB	2:B:50:ALA:HB1	2.51	0.41
1:A:53:PRO:HD2	1:A:113:LEU:O	2.20	0.41
1:A:182:ILE:HD11	1:A:199:VAL:CG2	2.50	0.41
1:A:182:ILE:HG23	1:A:195:VAL:HG11	2.03	0.41
2:B:15:ARG:O	2:B:18:ARG:HB3	2.20	0.41
1:A:33:HIS:HA	1:A:41:ILE:O	2.20	0.41
1:A:163:ASP:O	1:A:164:VAL:C	2.64	0.40
1:A:205:HIS:O	1:A:210:ARG:N	2.50	0.40
2:B:104:ASP:CA	2:B:107:GLN:HB3	2.47	0.40
1:A:83:MSE:O	1:A:87:LEU:N	2.48	0.40
1:A:37:ASP:HB2	1:A:80:VAL:CG2	2.51	0.40
1:A:175:PRO:HB3	1:A:202:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	202/256 (79%)	176 (87%)	23 (11%)	3 (2%)	8	28
2	B	140/256 (55%)	121 (86%)	17 (12%)	2 (1%)	9	30
All	All	342/512 (67%)	297 (87%)	40 (12%)	5 (2%)	8	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
2	B	161	PHE
2	B	103	GLN
1	A	102	ILE
1	A	239	PRO

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	162/222 (73%)	148 (91%)	14 (9%)	10	31
2	B	129/179 (72%)	113 (88%)	16 (12%)	4	16
All	All	291/401 (73%)	261 (90%)	30 (10%)	7	23

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU

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Mol	Chain	Res	Type
1	A	25	GLU
1	A	48	LEU
1	A	59	LEU
1	A	71	TYR
1	A	85	GLU
1	A	102	ILE
1	A	116	ASP
1	A	118	LYS
1	A	120	LEU
1	A	145	CYS
1	A	154	THR
1	A	184	LEU
1	A	233	GLU
2	B	9	ASP
2	B	25	GLU
2	B	56	ARG
2	B	71	TYR
2	B	87	LEU
2	B	95	ILE
2	B	102	ILE
2	B	103	GLN
2	B	110	ASP
2	B	118	LYS
2	B	120	LEU
2	B	125	LEU
2	B	152	LEU
2	B	155	GLU
2	B	160	HIS
2	B	235	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	133	ASN
1	A	148	HIS
1	A	150	HIS
1	A	160	HIS
1	A	234	GLN
1	A	237	ASN
2	B	11	GLN
2	B	94	GLN

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Mol	Chain	Res	Type
2	B	103	GLN
2	B	143	HIS
2	B	160	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	211/256 (82%)	0.94	36 (17%) 4 3	39, 71, 113, 136	0
2	B	155/256 (60%)	1.49	44 (28%) 1 1	45, 100, 137, 144	0
All	All	366/512 (71%)	1.17	80 (21%) 2 2	39, 84, 134, 144	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	100	ASP	7.5
2	B	155	GLU	6.4
2	B	85	GLU	5.0
1	A	229	SER	4.9
1	A	98	ASN	4.8
2	B	222	TRP	4.4
2	B	236	LEU	4.4
1	A	134	CYS	4.2
2	B	86	ILE	4.2
2	B	153	ALA	4.1
1	A	185	GLU	3.8
2	B	102	ILE	3.8
2	B	130	ALA	3.7
1	A	217	VAL	3.5
2	B	163	ASP	3.5
2	B	150	HIS	3.5
2	B	134	CYS	3.4
1	A	102	ILE	3.4
1	A	222	TRP	3.2
1	A	211	LYS	3.2
1	A	10	PRO	3.2
2	B	128	CYS	3.1
2	B	40	GLU	3.1
1	A	166	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	80	VAL	3.0
2	B	137	ILE	3.0
2	B	225	GLY	2.9
2	B	76	GLU	2.9
2	B	29	PHE	2.8
2	B	159	THR	2.8
1	A	101	THR	2.8
2	B	154	THR	2.7
2	B	99	GLU	2.7
2	B	95	ILE	2.6
1	A	205	HIS	2.6
2	B	135	ILE	2.6
2	B	211	LYS	2.6
1	A	100	ASP	2.6
2	B	93	GLY	2.6
2	B	215	LYS	2.6
1	A	234	GLN	2.6
1	A	77	GLY	2.5
2	B	133	ASN	2.5
1	A	145	CYS	2.5
1	A	216	ASP	2.5
1	A	193	ARG	2.5
1	A	230	TYR	2.4
1	A	178	LEU	2.4
1	A	180	GLU	2.4
2	B	89	TYR	2.4
1	A	221	LEU	2.4
1	A	75	LEU	2.3
2	B	157	LEU	2.3
2	B	124	PHE	2.3
1	A	240	LEU	2.3
2	B	28	ARG	2.3
2	B	164	VAL	2.3
1	A	197	GLU	2.2
1	A	204	ALA	2.2
1	A	236	LEU	2.2
2	B	56	ARG	2.2
1	A	96	ARG	2.2
2	B	151	TYR	2.2
2	B	152	LEU	2.2
2	B	11	GLN	2.2
2	B	31	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	2.1
1	A	212	VAL	2.1
1	A	97	LEU	2.1
1	A	184	LEU	2.1
2	B	146	LEU	2.1
1	A	88	ASP	2.1
2	B	228	SER	2.1
2	B	9	ASP	2.1
1	A	219	SER	2.0
1	A	33	HIS	2.0
2	B	161	PHE	2.0
2	B	216	ASP	2.0
2	B	239	PRO	2.0
1	A	39	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.