



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 12:18 AM EDT

PDB ID : 3HU6
Title : Structures of SPOP-Substrate Complexes: Insights into Molecular Architectures of BTB-Cul3 Ubiquitin Ligases: SPOPMATHx/BTB/3-box-PucSBC 1
Authors : Zhuang, M.; Schulman, B.A.
Deposited on : 2009-06-13
Resolution : 2.70 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
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

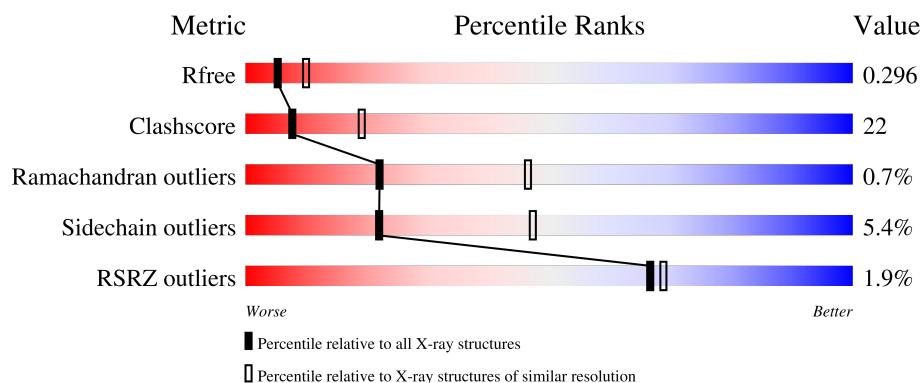
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	312	<div> <div>2%</div> <div>58%</div> <div>29%</div> <div>9%</div> </div>
1	B	312	<div> <div>2%</div> <div>55%</div> <div>32%</div> <div>10%</div> </div>
2	C	7	<div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
2	D	7	<div> <div>86%</div> <div>14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4690 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 Speckle-type POZ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2227	1423	374	409	21			
1	B	282	Total	C	N	O	S	0	0	0
			2231	1426	372	413	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP O43791
A	27	SER	-	expression tag	UNP O43791
A	140	GLY	ASP	engineered mutation	UNP O43791
A	330	THR	-	linker	UNP O43791
A	331	ASP	-	linker	UNP O43791
A	332	VAL	-	linker	UNP O43791
A	333	LEU	-	linker	UNP O43791
A	334	GLU	-	linker	UNP O43791
A	335	THR	-	linker	UNP O43791
A	336	SER	-	linker	UNP O43791
A	337	GLY	-	linker	UNP O43791
B	26	GLY	-	expression tag	UNP O43791
B	27	SER	-	expression tag	UNP O43791
B	140	GLY	ASP	engineered mutation	UNP O43791
B	330	THR	-	linker	UNP O43791
B	331	ASP	-	linker	UNP O43791
B	332	VAL	-	linker	UNP O43791
B	333	LEU	-	linker	UNP O43791
B	334	GLU	-	linker	UNP O43791
B	335	THR	-	linker	UNP O43791
B	336	SER	-	linker	UNP O43791
B	337	GLY	-	linker	UNP O43791

- Molecule 2 is a protein called Puckered.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			40	23	6	11			
2	D	6	Total	C	N	O	0	0	0
			38	22	6	10			

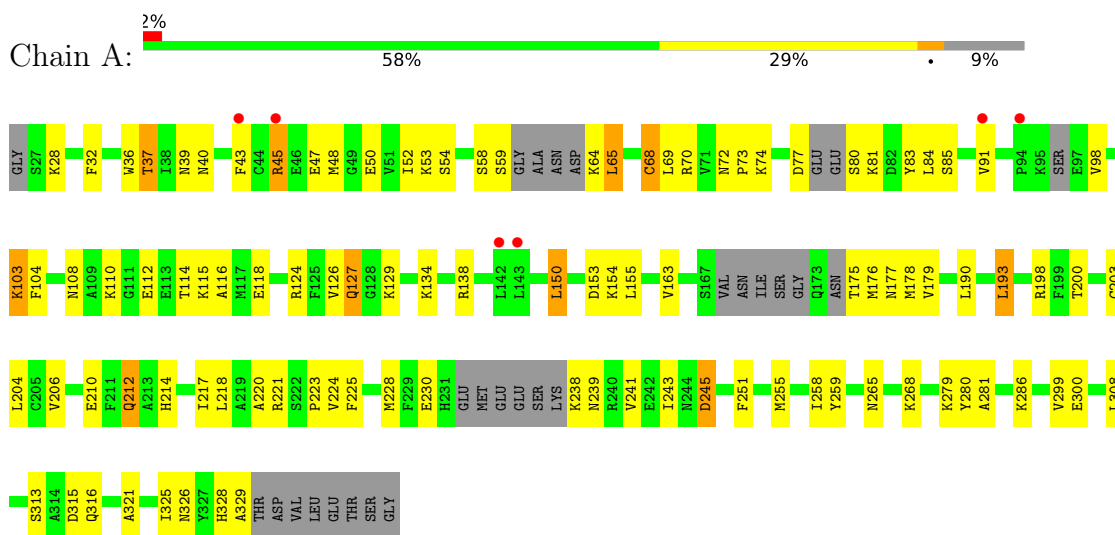
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	84	Total	O	0	0
			84	84		
3	C	2	Total	O	0	0
			2	2		

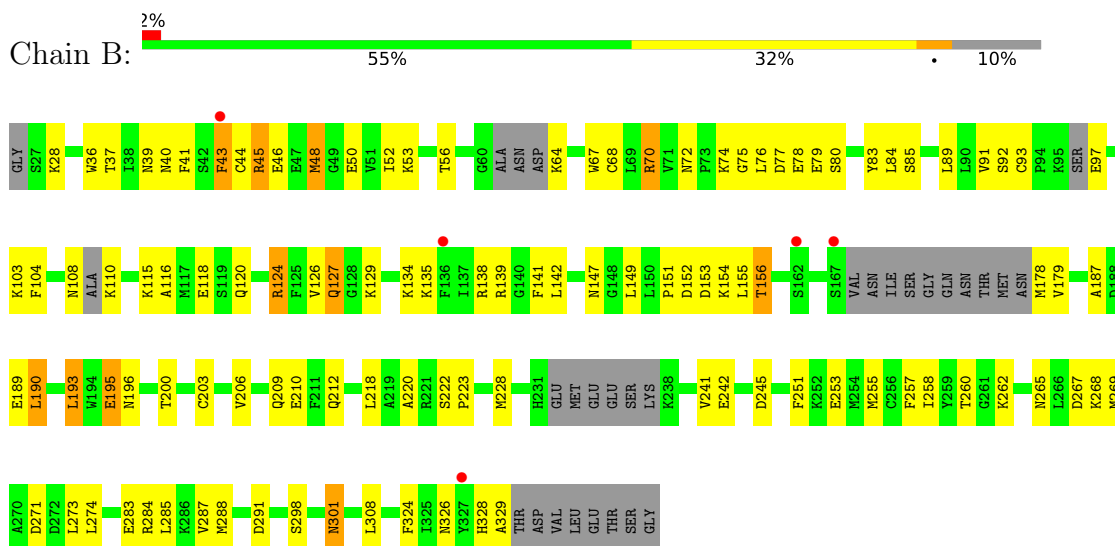
3 Residue-property plots [i](#)

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: Speckle-type POZ protein



• Molecule 1: Speckle-type POZ protein




• Molecule 2: Puckered





- Molecule 2: Puckered

Chain D:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.74Å 107.74Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-2.70) 93.4 (49.81-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.296 0.242 , 0.296	Depositor DCC
R_{free} test set	1211 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.908	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	0.44	0/2264	0.65	0/3042
1	B	0.44	0/2269	0.64	0/3048
2	C	0.55	0/39	0.80	0/52
2	D	0.64	0/37	0.77	0/49
All	All	0.44	0/4609	0.65	0/6191

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	2227	0	2188	103	0
1	B	2231	0	2197	113	0
2	C	40	0	36	2	0
2	D	38	0	31	0	0
3	A	68	0	0	15	1
3	B	84	0	0	15	1
3	C	2	0	0	0	0
All	All	4690	0	4452	197	1

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 22.

All (197) 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:265:ASN:HD22	1:A:268:LYS:HE2	1.41	0.85
1:A:77:ASP:C	1:A:80:SER:HA	2.02	0.79
1:A:221:ARG:HG2	1:A:258:ILE:HG23	1.64	0.79
1:B:44:CYS:HB2	1:B:46:GLU:OE1	1.84	0.78
1:B:78:GLU:HA	3:B:368:HOH:O	1.82	0.77
1:B:284:ARG:HG2	1:B:288:MET:HE2	1.66	0.77
1:B:92:SER:HA	1:B:127:GLN:NE2	2.00	0.77
1:A:193:LEU:CD1	1:B:220:ALA:HB2	2.18	0.73
1:B:40:ASN:HB3	1:B:43:PHE:HB2	1.68	0.73
1:A:48:MET:HG2	3:A:350:HOH:O	1.89	0.72
1:A:220:ALA:HB2	1:B:193:LEU:HD13	1.69	0.72
1:A:50:GLU:HG3	3:A:20:HOH:O	1.88	0.72
1:A:28:LYS:HE2	1:B:28:LYS:HD2	1.71	0.71
1:A:114:THR:HB	3:A:370:HOH:O	1.90	0.71
1:B:45:ARG:CB	1:B:45:ARG:HH11	2.04	0.71
1:B:45:ARG:HH11	1:B:45:ARG:HB2	1.55	0.71
1:B:139:ARG:HH11	1:B:139:ARG:HB3	1.56	0.70
1:A:193:LEU:HD11	1:B:220:ALA:HB2	1.72	0.69
1:A:83:TYR:CE1	1:A:138:ARG:HG2	2.28	0.69
1:A:217:ILE:O	1:A:221:ARG:HB2	1.92	0.69
1:B:41:PHE:CZ	1:B:84:LEU:HD21	2.27	0.69
1:B:92:SER:HA	1:B:127:GLN:HE22	1.56	0.68
1:B:139:ARG:HB3	1:B:139:ARG:NH1	2.08	0.68
1:B:262:LYS:HE2	3:B:395:HOH:O	1.94	0.68
1:A:190:LEU:HD11	1:B:190:LEU:HD11	1.75	0.67
1:B:40:ASN:HA	1:B:153:ASP:OD2	1.95	0.67
1:A:103:LYS:HG2	1:A:118:GLU:HB3	1.75	0.66
1:A:70:ARG:HH12	2:C:101:THR:HG21	1.59	0.66
1:A:228:MET:HE3	1:A:241:VAL:HG11	1.77	0.65
1:A:70:ARG:NH1	2:C:101:THR:HG21	2.12	0.65
1:B:79:GLU:HG2	1:B:135:LYS:HZ2	1.62	0.65
1:B:218:LEU:HD21	1:B:255:MET:HE1	1.80	0.64
1:B:110:LYS:N	3:B:7:HOH:O	2.31	0.64
1:B:329:ALA:HA	3:B:354:HOH:O	1.97	0.63
1:A:177:ASN:O	1:A:178:MET:HB2	1.98	0.62
1:A:190:LEU:CD1	1:B:190:LEU:HD11	2.29	0.61
1:B:41:PHE:HZ	1:B:84:LEU:HD21	1.61	0.61
1:A:108:ASN:HD21	1:A:112:GLU:HB2	1.65	0.61
1:B:269:MET:HE2	1:B:273:LEU:HD22	1.81	0.61
1:B:89:LEU:HD12	1:B:129:LYS:O	2.01	0.61
1:A:220:ALA:HB2	1:B:193:LEU:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:MET:SD	1:B:52:ILE:HG21	2.41	0.60
1:A:279:LYS:HD3	1:A:279:LYS:O	2.02	0.60
1:B:56:THR:HA	1:B:67:TRP:O	2.01	0.60
1:A:175:THR:HG22	1:B:37:THR:HB	1.84	0.59
1:B:103:LYS:HG3	1:B:118:GLU:HB3	1.84	0.59
1:B:283:GLU:O	1:B:287:VAL:HG23	2.02	0.59
1:A:74:LYS:O	1:A:81:LYS:HA	2.03	0.58
1:A:85:SER:HB3	1:A:134:LYS:O	2.03	0.58
1:A:91:VAL:O	1:A:127:GLN:NE2	2.36	0.58
1:B:120:GLN:NE2	1:B:120:GLN:H	2.01	0.58
1:B:228:MET:HE1	1:B:241:VAL:HG21	1.86	0.58
1:B:104:PHE:O	1:B:116:ALA:HA	2.04	0.57
1:A:190:LEU:HD11	1:B:190:LEU:CD1	2.35	0.57
1:A:176:MET:HE1	3:A:363:HOH:O	2.04	0.57
1:B:253:GLU:HG2	1:B:269:MET:HE2	1.86	0.57
1:B:40:ASN:CB	1:B:43:PHE:HB2	2.33	0.57
1:A:108:ASN:ND2	1:A:112:GLU:HB2	2.20	0.56
1:B:245:ASP:N	1:B:245:ASP:OD1	2.34	0.56
1:B:39:ASN:OD1	1:B:154:LYS:HE2	2.06	0.56
1:A:40:ASN:HB3	1:A:43:PHE:HD2	1.71	0.55
1:A:218:LEU:HD21	1:A:255:MET:HE1	1.87	0.55
1:A:223:PRO:HD2	1:A:281:ALA:HB3	1.88	0.55
1:B:48:MET:HG3	3:B:368:HOH:O	2.07	0.55
1:B:92:SER:O	1:B:93:CYS:HB3	2.05	0.55
1:B:284:ARG:HG2	1:B:288:MET:CE	2.36	0.54
1:B:115:LYS:HE2	1:B:141:PHE:CE2	2.42	0.54
1:A:243:ILE:HD12	1:A:243:ILE:N	2.23	0.54
1:B:83:TYR:CE1	1:B:138:ARG:HG2	2.43	0.54
1:A:321:ALA:O	1:A:325:ILE:HG13	2.06	0.54
1:A:103:LYS:CG	1:A:118:GLU:HB3	2.37	0.54
1:A:316:GLN:CB	1:B:179:VAL:HG13	2.38	0.54
1:B:79:GLU:HG2	1:B:135:LYS:NZ	2.22	0.54
1:A:193:LEU:HD13	1:B:220:ALA:HB2	1.88	0.54
1:A:40:ASN:HA	1:A:153:ASP:OD2	2.09	0.53
1:A:64:LYS:C	3:A:348:HOH:O	2.45	0.53
1:A:245:ASP:N	1:A:245:ASP:OD1	2.40	0.53
1:B:67:TRP:O	1:B:68:CYS:HB3	2.08	0.53
1:B:271:ASP:HB2	1:B:308:LEU:HD21	1.90	0.53
1:B:37:THR:HG23	1:B:156:THR:OG1	2.07	0.53
1:B:48:MET:SD	1:B:48:MET:O	2.67	0.52
1:A:286:LYS:NZ	1:A:313:SER:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:HB3	1:B:179:VAL:HG13	1.91	0.52
1:A:73:PRO:HA	1:A:84:LEU:HD13	1.91	0.52
1:B:257:PHE:HA	1:B:262:LYS:O	2.09	0.52
1:A:245:ASP:OD2	1:A:279:LYS:HE3	2.10	0.52
1:A:47:GLU:HB3	3:A:359:HOH:O	2.11	0.51
1:A:110:LYS:HD2	1:A:112:GLU:OE1	2.10	0.51
1:B:187:ALA:O	1:B:260:THR:HG22	2.10	0.51
1:A:238:LYS:HG3	1:A:238:LYS:O	2.10	0.51
1:B:76:LEU:HD23	1:B:134:LYS:HE2	1.91	0.51
1:B:120:GLN:NE2	1:B:120:GLN:N	2.58	0.51
1:B:218:LEU:HD23	1:B:258:ILE:HG21	1.92	0.51
1:A:200:THR:HG21	1:A:212:GLN:HB3	1.93	0.51
1:B:200:THR:HG21	1:B:212:GLN:HB2	1.93	0.51
1:A:238:LYS:O	1:A:239:ASN:HB2	2.11	0.51
1:B:45:ARG:HB2	1:B:45:ARG:NH1	2.24	0.51
1:A:48:MET:HE3	3:A:350:HOH:O	2.10	0.50
1:A:225:PHE:HD2	1:A:228:MET:HE2	1.76	0.50
1:B:91:VAL:O	1:B:127:GLN:NE2	2.44	0.50
1:B:178:MET:CB	3:B:381:HOH:O	2.59	0.50
1:B:179:VAL:N	3:B:381:HOH:O	2.45	0.50
1:A:65:LEU:CD2	1:A:98:VAL:HG21	2.42	0.50
1:A:50:GLU:N	3:A:20:HOH:O	2.41	0.49
1:A:214:HIS:HD2	1:A:259:TYR:OH	1.95	0.49
1:B:74:LYS:C	3:B:391:HOH:O	2.51	0.49
1:B:265:ASN:HB3	1:B:268:LYS:HE2	1.94	0.49
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.78	0.49
1:A:77:ASP:O	1:A:80:SER:HA	2.12	0.49
1:B:301:ASN:HD22	1:B:301:ASN:C	2.16	0.49
1:B:46:GLU:HA	1:B:50:GLU:OE1	2.13	0.49
1:B:178:MET:HB3	3:B:381:HOH:O	2.12	0.48
1:B:36:TRP:HH2	1:B:52:ILE:O	1.97	0.48
1:B:70:ARG:HD2	3:B:369:HOH:O	2.13	0.48
1:A:39:ASN:OD1	1:A:154:LYS:HD3	2.14	0.48
1:B:45:ARG:O	1:B:45:ARG:HG2	2.13	0.48
1:B:139:ARG:HH11	1:B:139:ARG:CB	2.26	0.48
1:A:114:THR:CB	3:A:370:HOH:O	2.57	0.47
1:A:40:ASN:HB3	1:A:43:PHE:CD2	2.50	0.47
1:A:218:LEU:HD21	1:A:255:MET:CE	2.44	0.47
1:B:228:MET:HE1	1:B:241:VAL:CG2	2.44	0.47
1:A:69:LEU:HD22	1:A:104:PHE:HE1	1.79	0.46
1:B:298:SER:HA	1:B:324:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:O	1:B:209:GLN:HB2	2.16	0.46
1:A:47:GLU:HG3	3:A:358:HOH:O	2.15	0.46
1:A:47:GLU:HA	1:A:74:LYS:HG3	1.98	0.46
1:B:142:LEU:HA	1:B:149:LEU:HD12	1.98	0.46
1:B:301:ASN:ND2	1:B:301:ASN:H	2.14	0.46
1:A:218:LEU:HD23	1:A:258:ILE:HG21	1.99	0.45
1:A:39:ASN:HA	1:A:154:LYS:HG2	1.97	0.45
1:A:28:LYS:CE	1:B:28:LYS:HD2	2.44	0.45
1:A:72:ASN:HB2	1:A:85:SER:OG	2.15	0.45
1:B:228:MET:HE1	1:B:241:VAL:HG11	1.99	0.45
1:A:329:ALA:HB3	3:A:349:HOH:O	2.16	0.45
1:B:77:ASP:HB3	3:B:387:HOH:O	2.15	0.45
1:A:98:VAL:O	1:A:124:ARG:HA	2.17	0.45
1:A:221:ARG:NH1	1:B:189:GLU:OE1	2.49	0.45
1:B:178:MET:C	3:B:359:HOH:O	2.54	0.45
1:B:142:LEU:HD11	1:B:155:LEU:HD13	1.99	0.45
1:B:203:CYS:SG	1:B:210:GLU:HG2	2.57	0.45
1:A:179:VAL:HB	1:B:291:ASP:HB3	1.99	0.45
1:A:224:VAL:O	1:A:228:MET:HG3	2.17	0.44
1:B:253:GLU:HB3	1:B:269:MET:HE1	1.99	0.44
1:A:73:PRO:HA	1:A:84:LEU:CD1	2.47	0.44
1:A:316:GLN:CD	1:B:179:VAL:HG13	2.37	0.44
1:B:126:VAL:H	1:B:129:LYS:HB3	1.83	0.44
1:A:52:ILE:O	1:A:52:ILE:HG13	2.18	0.44
1:A:47:GLU:C	3:A:20:HOH:O	2.56	0.44
1:B:75:GLY:HA3	1:B:80:SER:O	2.17	0.44
1:A:238:LYS:N	3:A:19:HOH:O	2.51	0.43
1:B:108:ASN:OD1	1:B:108:ASN:C	2.56	0.43
1:B:262:LYS:CE	3:B:395:HOH:O	2.61	0.43
1:B:326:ASN:C	1:B:328:HIS:H	2.21	0.43
1:A:36:TRP:CE2	1:A:54:SER:CB	3.02	0.43
1:B:274:LEU:HD12	1:B:274:LEU:O	2.18	0.43
1:A:175:THR:HA	1:B:37:THR:O	2.18	0.43
1:A:221:ARG:CG	1:A:258:ILE:HG23	2.39	0.43
1:A:37:THR:HA	1:A:155:LEU:O	2.18	0.43
1:A:53:LYS:HG2	1:A:70:ARG:HG2	2.01	0.43
1:A:198:ARG:O	1:A:214:HIS:HE1	2.02	0.43
1:B:53:LYS:HE3	1:B:68:CYS:SG	2.59	0.43
1:B:206:VAL:HG21	1:B:251:PHE:CD2	2.54	0.43
1:B:298:SER:H	1:B:301:ASN:HD21	1.66	0.43
1:A:300:GLU:CB	3:A:380:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:O	1:B:46:GLU:C	2.57	0.42
1:B:200:THR:HG21	1:B:212:GLN:CB	2.48	0.42
1:A:47:GLU:CB	3:A:359:HOH:O	2.66	0.42
1:B:284:ARG:NH1	1:B:288:MET:HE1	2.35	0.42
1:A:68:CYS:HB3	1:A:91:VAL:CG2	2.49	0.42
1:B:74:LYS:HG2	1:B:139:ARG:NE	2.35	0.42
1:B:115:LYS:HD3	1:B:115:LYS:HA	1.90	0.42
1:B:178:MET:HG2	3:B:381:HOH:O	2.19	0.42
1:A:138:ARG:HB3	1:A:138:ARG:NH1	2.35	0.42
1:A:126:VAL:O	1:A:127:GLN:C	2.58	0.42
1:B:257:PHE:CE1	1:B:288:MET:CE	3.02	0.41
1:A:126:VAL:H	1:A:129:LYS:HB3	1.84	0.41
1:A:150:LEU:HA	1:A:154:LYS:O	2.21	0.41
1:A:203:CYS:SG	1:A:210:GLU:HG2	2.61	0.41
1:B:178:MET:CG	3:B:381:HOH:O	2.69	0.41
1:A:176:MET:SD	1:B:52:ILE:CG2	3.08	0.41
1:B:72:ASN:HB2	1:B:85:SER:HB2	2.02	0.41
1:B:97:GLU:OE2	1:B:124:ARG:NE	2.48	0.41
1:A:65:LEU:HD22	1:A:98:VAL:HG21	2.02	0.41
1:B:147:ASN:N	1:B:147:ASN:ND2	2.68	0.41
1:A:279:LYS:HD2	1:A:280:TYR:CE1	2.56	0.41
1:B:151:PRO:O	1:B:152:ASP:HB2	2.20	0.41
1:A:206:VAL:HG21	1:A:251:PHE:CD2	2.56	0.41
1:A:32:PHE:HE1	1:A:163:VAL:HG23	1.86	0.41
1:A:326:ASN:C	1:A:328:HIS:H	2.25	0.40
1:A:115:LYS:HD3	1:A:115:LYS:HA	1.87	0.40
1:A:36:TRP:CE2	1:A:54:SER:HB2	2.55	0.40
1:A:70:ARG:HE	1:A:70:ARG:HB3	1.76	0.40
1:B:222:SER:HA	1:B:223:PRO:HD3	1.86	0.40
1:A:103:LYS:HD3	1:A:116:ALA:HB1	2.03	0.40
1:B:64:LYS:HE3	1:B:178:MET:CE	2.51	0.40
1:B:285:LEU:HA	1:B:288:MET:HE3	2.03	0.40
1:A:58:SER:OG	1:A:59:SER:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:HOH:O	3:B:22:HOH:O[3_554]	2.06	0.14

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	271/312 (87%)	242 (89%)	28 (10%)	1 (0%)	34	60
1	B	270/312 (86%)	244 (90%)	23 (8%)	3 (1%)	14	34
2	C	4/7 (57%)	4 (100%)	0	0	100	100
2	D	4/7 (57%)	4 (100%)	0	0	100	100
All	All	549/638 (86%)	494 (90%)	51 (9%)	4 (1%)	22	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	GLN
1	B	195	GLU
1	A	127	GLN
1	B	48	MET

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	237/271 (88%)	223 (94%)	14 (6%)	19	43
1	B	239/271 (88%)	227 (95%)	12 (5%)	24	51
2	C	5/7 (71%)	5 (100%)	0	100	100
2	D	4/7 (57%)	4 (100%)	0	100	100
All	All	485/556 (87%)	459 (95%)	26 (5%)	22	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	45	ARG
1	A	65	LEU
1	A	68	CYS
1	A	103	LYS
1	A	150	LEU
1	A	193	LEU
1	A	204	LEU
1	A	212	GLN
1	A	230	GLU
1	A	245	ASP
1	A	299	VAL
1	A	308	LEU
1	A	315	ASP
1	B	43	PHE
1	B	45	ARG
1	B	70	ARG
1	B	124	ARG
1	B	156	THR
1	B	190	LEU
1	B	193	LEU
1	B	195	GLU
1	B	196	ASN
1	B	242	GLU
1	B	267	ASP
1	B	301	ASN

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	147	ASN
1	A	165	GLN
1	A	209	GLN
1	A	212	GLN
1	A	214	HIS
1	A	265	ASN
1	A	320	GLN
1	A	328	HIS
1	B	120	GLN
1	B	127	GLN
1	B	147	ASN

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Mol	Chain	Res	Type
1	B	301	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 monosaccharides 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 [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	284/312 (91%)	0.10	6 (2%) 63 65	34, 58, 92, 107	5 (1%)
1	B	282/312 (90%)	0.14	5 (1%) 68 70	32, 58, 86, 100	5 (1%)
2	C	6/7 (85%)	-0.37	0 100 100	49, 50, 55, 56	0
2	D	6/7 (85%)	-0.19	0 100 100	48, 52, 63, 71	0
All	All	578/638 (90%)	0.11	11 (1%) 66 69	32, 58, 89, 107	10 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	TYR	4.3
1	A	43	PHE	4.2
1	A	45	ARG	3.7
1	B	43	PHE	3.5
1	B	136	PHE	3.4
1	B	162	SER	2.6
1	A	142	LEU	2.4
1	A	91	VAL	2.3
1	B	167	SER	2.3
1	A	143	LEU	2.3
1	A	94	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.