



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:10 AM UTC

PDB ID : 5WAK / pdb_00005wak
Title : Crystal Structure of a Suz12-Rbbp4 Binary Complex
Authors : Chen, S.; Jiao, L.; Liu, X.
Deposited on : 2017-06-26
Resolution : 3.20 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
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

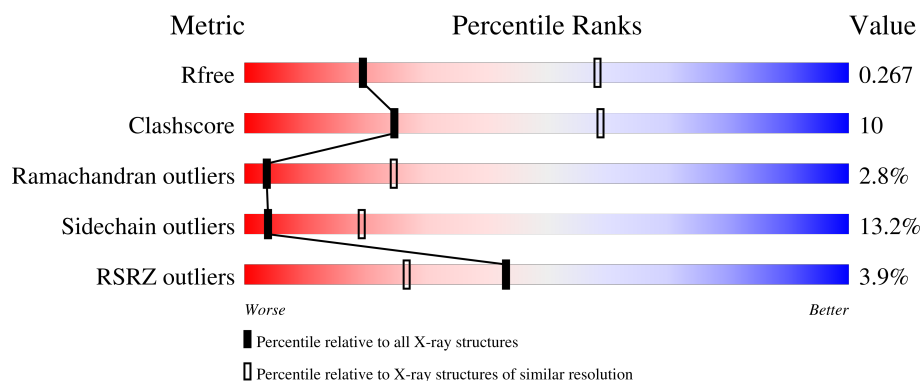
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	439	
2	B	478	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4766 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 Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3128	1971	533	614	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q09028
A	-12	SER	-	expression tag	UNP Q09028
A	-11	HIS	-	expression tag	UNP Q09028
A	-10	HIS	-	expression tag	UNP Q09028
A	-9	HIS	-	expression tag	UNP Q09028
A	-8	HIS	-	expression tag	UNP Q09028
A	-7	HIS	-	expression tag	UNP Q09028
A	-6	HIS	-	expression tag	UNP Q09028
A	-5	LEU	-	expression tag	UNP Q09028
A	-4	VAL	-	expression tag	UNP Q09028
A	-3	PRO	-	expression tag	UNP Q09028
A	-2	ARG	-	expression tag	UNP Q09028
A	-1	GLY	-	expression tag	UNP Q09028
A	0	SER	-	expression tag	UNP Q09028

- Molecule 2 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1637	1047	305	274	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	546	TRP	-	expression tag	UNP Q15022
B	547	SER	-	expression tag	UNP Q15022

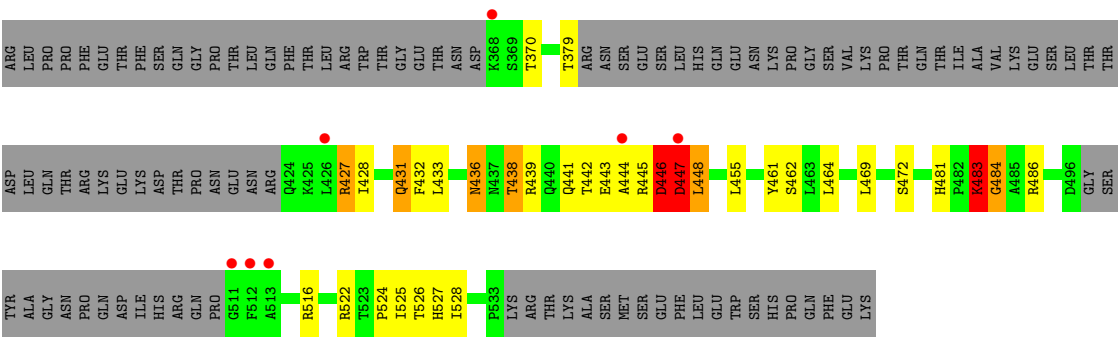
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Chain	Residue	Modelled	Actual	Comment	Reference
B	548	HIS	-	expression tag	UNP Q15022
B	549	PRO	-	expression tag	UNP Q15022
B	550	GLN	-	expression tag	UNP Q15022
B	551	PHE	-	expression tag	UNP Q15022
B	552	GLU	-	expression tag	UNP Q15022
B	553	LYS	-	expression tag	UNP Q15022

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.98Å 107.70Å 107.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 3.20 28.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	73.6 (28.76-3.20) 73.5 (28.76-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 3.17Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.178 , 0.251 0.194 , 0.267	Depositor DCC
R_{free} test set	797 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k 0.027 for -l,-k,-h 0.019 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4766	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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	0.85	2/3214 (0.1%)	1.34	20/4382 (0.5%)
2	B	0.94	0/1672	1.46	22/2240 (1.0%)
All	All	0.88	2/4886 (0.0%)	1.38	42/6622 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	MET	SD-CE	-6.17	1.64	1.79
1	A	210	VAL	CA-C	5.78	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	447	ASP	CA-CB-CG	9.17	121.77	112.60
1	A	209	ALA	N-CA-C	-8.90	98.54	110.55
1	A	248	ASP	CA-C-N	7.62	132.79	120.60
1	A	248	ASP	C-N-CA	7.62	132.79	120.60
2	B	446	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	33	ASP	N-CA-C	-7.33	104.48	113.50
2	B	85	LEU	N-CA-C	-7.30	103.97	114.12
1	A	364	PRO	CA-C-N	7.13	130.55	120.28
1	A	364	PRO	C-N-CA	7.13	130.55	120.28
2	B	86	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	250	GLN	N-CA-C	-6.71	104.39	112.58
1	A	12	VAL	N-CA-C	-6.26	104.75	110.82
2	B	242	SER	CA-C-N	6.24	132.93	121.70
2	B	242	SER	C-N-CA	6.24	132.93	121.70
2	B	105	LEU	CA-C-N	6.19	128.44	120.70
2	B	105	LEU	C-N-CA	6.19	128.44	120.70
2	B	147	GLU	CA-C-N	5.78	129.42	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	147	GLU	C-N-CA	5.78	129.42	121.33
1	A	272	HIS	N-CA-C	5.62	116.78	108.86
2	B	84	GLU	CA-C-N	5.61	131.04	122.23
2	B	84	GLU	C-N-CA	5.61	131.04	122.23
2	B	85	LEU	CA-C-N	5.52	128.22	120.28
2	B	85	LEU	C-N-CA	5.52	128.22	120.28
1	A	271	ALA	N-CA-C	5.49	116.94	111.07
1	A	88	ASN	CA-C-N	5.37	127.79	120.54
1	A	88	ASN	C-N-CA	5.37	127.79	120.54
2	B	461	TYR	CA-C-N	5.24	127.25	120.44
2	B	461	TYR	C-N-CA	5.24	127.25	120.44
2	B	102	THR	CA-C-N	5.20	127.20	120.44
2	B	102	THR	C-N-CA	5.20	127.20	120.44
1	A	294	ALA	N-CA-C	-5.19	106.20	112.54
1	A	96	SER	CA-C-N	5.16	130.99	121.70
1	A	96	SER	C-N-CA	5.16	130.99	121.70
2	B	370	THR	CA-C-N	5.13	128.56	120.97
2	B	370	THR	C-N-CA	5.13	128.56	120.97
2	B	436	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	134	PRO	CA-C-N	5.11	127.13	120.28
1	A	134	PRO	C-N-CA	5.11	127.13	120.28
1	A	90	ASP	CA-CB-CG	5.11	117.70	112.60
2	B	104	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	214	GLY	CA-C-N	5.01	127.69	120.38
1	A	214	GLY	C-N-CA	5.01	127.69	120.38

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	3128	0	2965	66	0
2	B	1637	0	1676	40	0
3	B	1	0	0	0	0
All	All	4766	0	4641	92	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 10.

All (92) 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:239:HIS:HD2	1:A:241:SER:H	1.34	0.75
1:A:119:ILE:HG23	1:A:159:SER:HA	1.69	0.71
1:A:198:ASP:HA	1:A:229:VAL:HG13	1.71	0.71
1:A:97:HIS:HD2	2:B:526:THR:H	1.37	0.71
2:B:431:GLN:HG2	2:B:441:GLN:CG	2.24	0.68
1:A:229:VAL:HB	1:A:248:ASP:OD2	1.94	0.67
1:A:298:VAL:HB	1:A:313:PHE:HB2	1.77	0.67
1:A:210:VAL:HG13	1:A:212:LYS:HE2	1.77	0.67
1:A:36:MET:HG2	2:B:528:ILE:HG13	1.81	0.63
1:A:95:ALA:HB3	2:B:528:ILE:HD13	1.81	0.63
2:B:483:LYS:H	2:B:484:GLY:HA3	1.65	0.62
2:B:431:GLN:HG2	2:B:441:GLN:HG2	1.81	0.62
2:B:481:HIS:O	2:B:484:GLY:HA3	2.00	0.60
2:B:427:ARG:HA	2:B:445:ARG:HA	1.84	0.60
1:A:380:PHE:HA	1:A:391:CYS:O	2.02	0.59
1:A:315:SER:HB2	1:A:345:TRP:HH2	1.68	0.58
1:A:305:ASN:HB3	2:B:138:LEU:HD21	1.84	0.58
1:A:48:GLN:NE2	1:A:131:ARG:HA	2.19	0.58
2:B:431:GLN:HG2	2:B:441:GLN:HG3	1.86	0.57
1:A:210:VAL:N	1:A:211:PRO:HD3	2.19	0.57
1:A:357:GLU:O	1:A:360:GLU:HB2	2.06	0.56
1:A:50:LEU:HG	1:A:67:VAL:HG23	1.89	0.54
1:A:210:VAL:HG22	1:A:212:LYS:HZ1	1.71	0.54
1:A:315:SER:HB2	1:A:345:TRP:CH2	2.42	0.54
1:A:16:VAL:HG12	2:B:103:ARG:HH21	1.72	0.54
2:B:445:ARG:C	2:B:447:ASP:H	2.15	0.54
1:A:328:HIS:CD2	1:A:387:PRO:HA	2.44	0.53
1:A:354:GLN:HG2	2:B:124:ARG:HD3	1.90	0.53
2:B:427:ARG:HB3	2:B:445:ARG:HG3	1.89	0.53
1:A:48:GLN:HE22	1:A:131:ARG:HA	1.73	0.52
2:B:112:HIS:HA	2:B:115:LEU:HD12	1.92	0.52
1:A:92:GLN:HG2	1:A:93:PHE:H	1.75	0.51
1:A:153:ASP:HB3	1:A:156:LYS:HB2	1.94	0.50
2:B:194:LYS:HG2	2:B:244:MET:SD	2.52	0.50
2:B:483:LYS:N	2:B:484:GLY:HA3	2.27	0.50
1:A:28:THR:N	1:A:29:PRO:HD2	2.26	0.50
1:A:210:VAL:HG12	1:A:210:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:HG2	1:A:410:ASN:HB2	1.94	0.49
1:A:294:ALA:HA	1:A:319:GLU:HG2	1.95	0.48
1:A:71:HIS:HA	1:A:126:GLU:HB3	1.95	0.48
1:A:236:HIS:HE1	1:A:238:LEU:HB3	1.79	0.48
2:B:447:ASP:CG	2:B:448:LEU:H	2.22	0.48
1:A:249:ASP:HB3	1:A:251:LYS:HB2	1.96	0.47
1:A:144:THR:HG22	1:A:145:PRO:HD2	1.96	0.47
1:A:317:LYS:HD2	2:B:106:ILE:O	2.14	0.47
1:A:352:GLU:HB3	2:B:124:ARG:HD2	1.96	0.47
1:A:393:VAL:HG12	1:A:399:MET:HG3	1.96	0.47
1:A:313:PHE:CZ	1:A:347:LEU:HD22	2.50	0.46
1:A:92:GLN:HG2	1:A:93:PHE:N	2.31	0.46
2:B:191:VAL:HG13	2:B:247:SER:HB3	1.98	0.46
1:A:115:ILE:HD12	2:B:526:THR:HG23	1.98	0.46
1:A:302:ASP:HB2	1:A:310:LEU:HD11	1.98	0.45
2:B:100:LEU:O	2:B:104:ASN:HB2	2.16	0.45
1:A:126:GLU:O	1:A:145:PRO:HD3	2.15	0.45
2:B:92:LYS:HB3	2:B:93:PRO:HD3	1.98	0.45
2:B:110:PHE:CE1	2:B:115:LEU:HD11	2.52	0.45
1:A:178:LYS:HD3	1:A:198:ASP:HB2	1.99	0.45
1:A:313:PHE:HZ	1:A:347:LEU:HD22	1.82	0.45
1:A:144:THR:CG2	1:A:145:PRO:HD2	2.47	0.44
1:A:239:HIS:CD2	1:A:241:SER:H	2.24	0.44
1:A:31:LEU:HD21	2:B:115:LEU:HG	1.99	0.44
1:A:150:LEU:HB3	1:A:169:PRO:HB3	1.99	0.44
2:B:87:LEU:HD12	2:B:87:LEU:H	1.82	0.44
1:A:195:SER:O	1:A:202:ILE:HA	2.18	0.44
2:B:93:PRO:HA	2:B:96:ILE:HD12	1.98	0.44
1:A:42:TRP:CD2	1:A:72:THR:HG22	2.53	0.43
1:A:342:LEU:HB3	1:A:370:HIS:HB3	2.00	0.43
2:B:444:ALA:C	2:B:446:ASP:H	2.25	0.43
1:A:200:HIS:HA	1:A:230:VAL:HG23	2.01	0.43
2:B:193:HIS:HE1	2:B:247:SER:HB2	1.84	0.43
1:A:16:VAL:HG11	2:B:103:ARG:HD3	2.01	0.43
1:A:39:ALA:O	2:B:524:PRO:HA	2.19	0.43
1:A:138:CYS:HA	1:A:154:TYR:CE2	2.54	0.43
1:A:241:SER:HB3	1:A:258:ARG:HG3	2.01	0.43
1:A:397:ASN:HB2	2:B:522:ARG:HD3	2.00	0.43
2:B:111:LEU:HB2	2:B:114:THR:HG23	2.00	0.43
1:A:373:HIS:NE2	1:A:400:GLN:HG3	2.34	0.42
1:A:48:GLN:HE22	1:A:132:TYR:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:CG1	2:B:103:ARG:HH21	2.31	0.42
1:A:151:VAL:HG23	1:A:173:LEU:HD11	2.01	0.42
1:A:275:GLU:H	1:A:275:GLU:CD	2.28	0.42
2:B:90:PHE:CE2	2:B:432:PHE:HD2	2.38	0.42
1:A:141:ALA:HB2	1:A:185:TRP:CZ2	2.55	0.42
2:B:447:ASP:CG	2:B:448:LEU:N	2.77	0.42
1:A:92:GLN:CG	1:A:93:PHE:H	2.31	0.42
2:B:483:LYS:N	2:B:484:GLY:CA	2.84	0.41
1:A:56:PRO:HG2	1:A:59:LYS:HB2	2.01	0.41
1:A:393:VAL:CG1	1:A:399:MET:HG3	2.51	0.41
2:B:102:THR:O	2:B:106:ILE:HD12	2.20	0.41
1:A:129:ARG:HH11	1:A:131:ARG:HH11	1.69	0.40
1:A:342:LEU:HD13	1:A:402:TRP:HZ2	1.86	0.40
2:B:92:LYS:O	2:B:96:ILE:HG13	2.22	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	388/439 (88%)	359 (92%)	21 (5%)	8 (2%)	5	31
2	B	184/478 (38%)	154 (84%)	22 (12%)	8 (4%)	2	16
All	All	572/917 (62%)	513 (90%)	43 (8%)	16 (3%)	4	25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	PHE
1	A	315	SER
1	A	214	GLY
2	B	438	THR

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Mol	Chain	Res	Type
2	B	446	ASP
1	A	208	SER
2	B	119	SER
2	B	436	ASN
2	B	483	LYS
1	A	166	GLU
2	B	244	MET
1	A	319	GLU
2	B	243	HIS
2	B	484	GLY
1	A	211	PRO
1	A	210	VAL

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	352/388 (91%)	319 (91%)	33 (9%)	8	33
2	B	184/442 (42%)	146 (79%)	38 (21%)	1	7
All	All	536/830 (65%)	465 (87%)	71 (13%)	4	19

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	15	ARG
1	A	25	LYS
1	A	111	VAL
1	A	116	GLU
1	A	119	ILE
1	A	121	ILE
1	A	126	GLU
1	A	143	LYS
1	A	156	LYS
1	A	160	LYS

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Mol	Chain	Res	Type
1	A	166	GLU
1	A	173	LEU
1	A	179	GLU
1	A	186	ASN
1	A	200	HIS
1	A	221	THR
1	A	227	THR
1	A	252	LEU
1	A	264	LYS
1	A	279	LEU
1	A	289	LEU
1	A	307	LYS
1	A	312	SER
1	A	317	LYS
1	A	322	GLN
1	A	347	LEU
1	A	349	LYS
1	A	365	GLU
1	A	395	GLU
1	A	400	GLN
1	A	403	GLN
1	A	410	ASN
2	B	85	LEU
2	B	86	PHE
2	B	91	GLU
2	B	105	LEU
2	B	106	ILE
2	B	109	ILE
2	B	128	LYS
2	B	139	SER
2	B	145	LYS
2	B	149	GLU
2	B	195	LYS
2	B	196	ARG
2	B	199	VAL
2	B	243	HIS
2	B	244	MET
2	B	249	SER
2	B	250	LEU
2	B	379	THR
2	B	427	ARG
2	B	428	ILE

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Mol	Chain	Res	Type
2	B	431	GLN
2	B	433	LEU
2	B	438	THR
2	B	439	ARG
2	B	442	THR
2	B	443	GLU
2	B	447	ASP
2	B	448	LEU
2	B	455	LEU
2	B	462	SER
2	B	464	LEU
2	B	469	LEU
2	B	472	SER
2	B	483	LYS
2	B	486	ARG
2	B	516	ARG
2	B	525	ILE
2	B	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	48	GLN
1	A	88	ASN
1	A	97	HIS
1	A	122	ASN
1	A	136	ASN
1	A	239	HIS
1	A	267	HIS
1	A	328	HIS
1	A	354	GLN
1	A	400	GLN
1	A	403	GLN
1	A	410	ASN
2	B	95	GLN
2	B	122	ASN
2	B	193	HIS
2	B	435	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

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	392/439 (89%)	-0.11	9 (2%) 61 41	23, 64, 134, 176	0
2	B	196/478 (41%)	0.35	14 (7%) 22 14	29, 79, 141, 170	0
All	All	588/917 (64%)	0.05	23 (3%) 43 27	23, 69, 136, 176	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	250	LEU	5.3
2	B	189	VAL	4.9
1	A	95	ALA	4.8
2	B	512	PHE	4.2
2	B	447	ASP	4.1
2	B	513	ALA	3.2
1	A	93	PHE	3.0
1	A	198	ASP	3.0
1	A	111	VAL	3.0
2	B	106	ILE	2.9
2	B	368	LYS	2.9
2	B	83	HIS	2.8
2	B	511	GLY	2.8
2	B	104	ASN	2.7
2	B	426	LEU	2.6
1	A	8	PHE	2.4
2	B	249	SER	2.4
2	B	149	GLU	2.3
1	A	97	HIS	2.2
1	A	144	THR	2.2
1	A	146	SER	2.1
1	A	158	PRO	2.1
2	B	444	ALA	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
3	ZN	B	1001	1/1	1.00	0.02	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.