



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:32 am BST

PDB ID : 6BRO
Title : Crystal structure of ASK1-D3 ubiquitin ligase form1
Authors : Shabek, N.; Zheng, N.
Deposited on : 2017-11-30
Resolution : 2.50 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 : 2.11
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

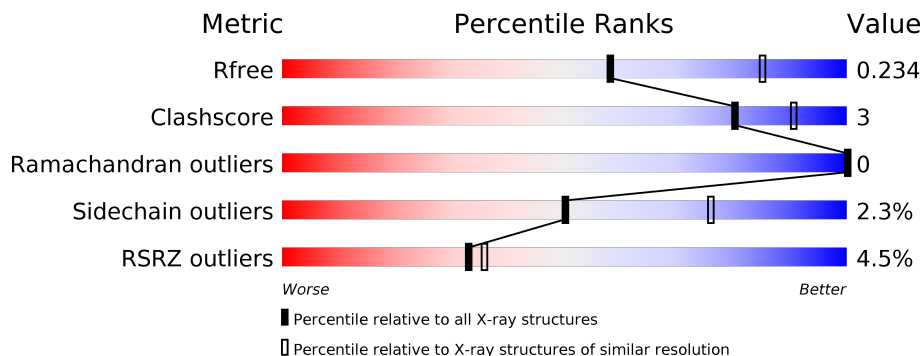
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	B	688	 2% 83% 6% • 11%
1	D	688	 4% 82% 6% • 11%
2	A	160	 6% 60% 13% • 27%
2	C	160	 9% 63% 9% • 27%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11832 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 F-box/LRR-repeat MAX2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	614	Total	C	N	O	S	0	0	0
			4766	3034	837	865	30			
1	D	610	Total	C	N	O	S	0	0	0
			4728	3011	827	861	29			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	509	GLU	-	cloning artifact	UNP Q5VMP0
B	510	ASN	-	cloning artifact	UNP Q5VMP0
B	511	LEU	-	cloning artifact	UNP Q5VMP0
B	512	TYR	-	cloning artifact	UNP Q5VMP0
B	513	PHE	-	cloning artifact	UNP Q5VMP0
B	514	GLN	-	cloning artifact	UNP Q5VMP0
B	515	SER	-	cloning artifact	UNP Q5VMP0
D	509	GLU	-	cloning artifact	UNP Q5VMP0
D	510	ASN	-	cloning artifact	UNP Q5VMP0
D	511	LEU	-	cloning artifact	UNP Q5VMP0
D	512	TYR	-	cloning artifact	UNP Q5VMP0
D	513	PHE	-	cloning artifact	UNP Q5VMP0
D	514	GLN	-	cloning artifact	UNP Q5VMP0
D	515	SER	-	cloning artifact	UNP Q5VMP0

- Molecule 2 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	117	Total	C	N	O	S	0	0	0
			934	590	152	188	4			
2	C	117	Total	C	N	O	S	0	0	0
			938	594	152	188	4			

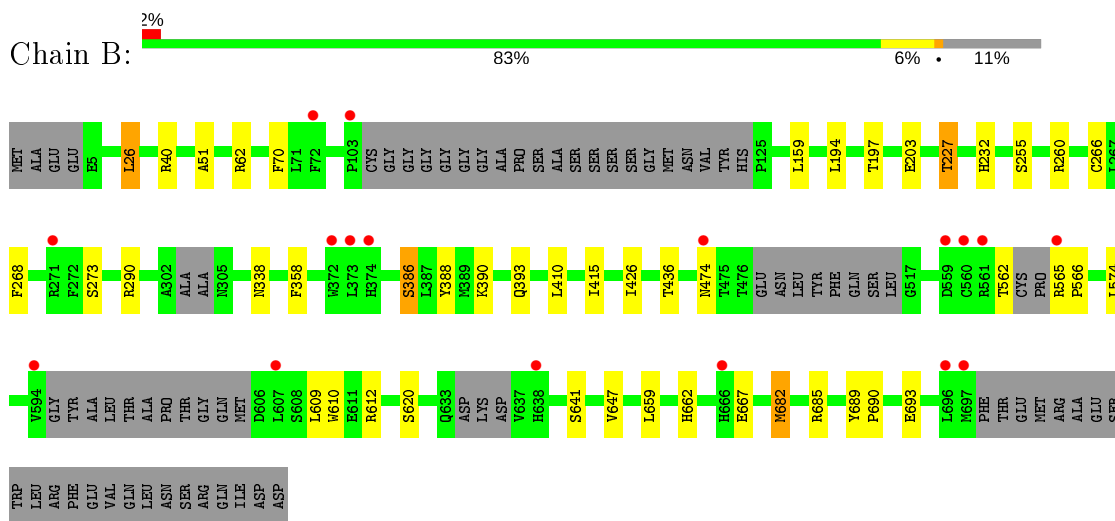
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	232	Total 232	O 232	0	0
3	A	21	Total 21	O 21	0	0
3	D	187	Total 187	O 187	0	0
3	C	26	Total 26	O 26	0	0

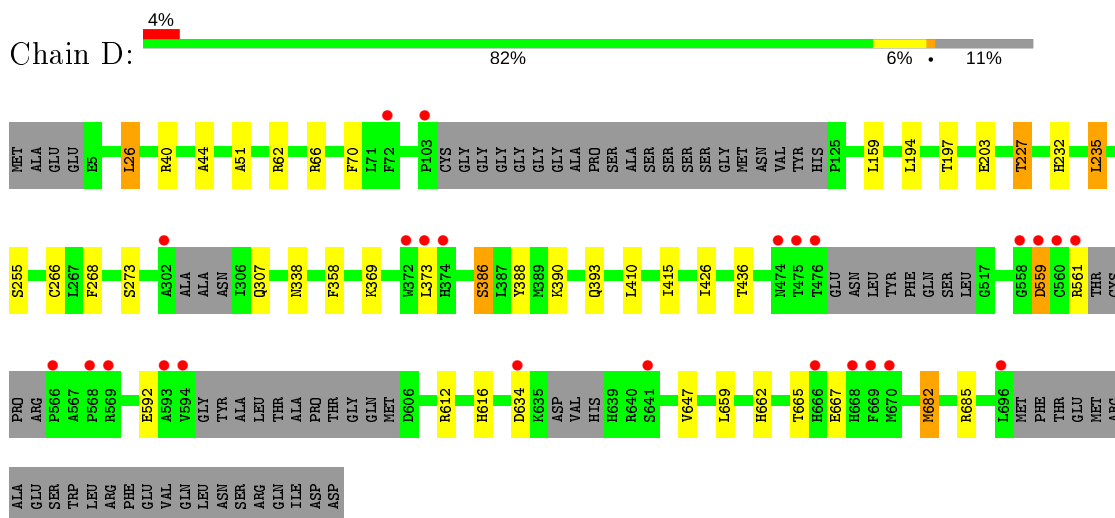
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: F-box/LRR-repeat MAX2 homolog

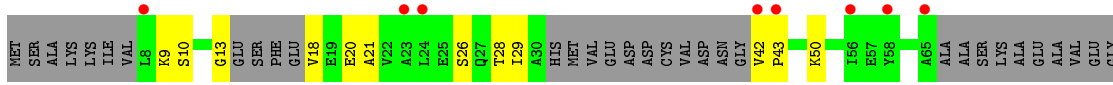


- Molecule 1: F-box/LRR-repeat MAX2 homolog

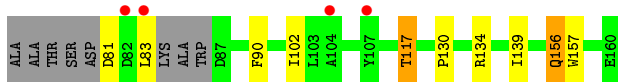
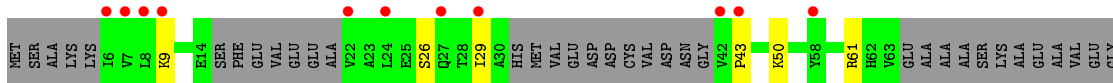


- Molecule 2: SKP1-like protein 1A





• Molecule 2: SKP1-like protein 1A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.73 Å 79.73 Å 153.44 Å 90.00° 128.59° 90.00°	Depositor
Resolution (Å)	119.93 – 2.50 48.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (119.93-2.50) 98.6 (48.39-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.51 Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.234 0.203 , 0.234	Depositor DCC
R_{free} test set	3700 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.138 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11832	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	B	0.56	0/4874	0.74	1/6627 (0.0%)
1	D	0.55	0/4835	0.75	4/6574 (0.1%)
2	A	0.53	0/944	0.72	0/1272
2	C	0.51	0/947	0.74	0/1275
All	All	0.55	0/11600	0.74	5/15748 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	B	26	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	373	LEU	CA-CB-CG	5.11	127.05	115.30
1	D	26	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	66	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	B	4766	0	4784	23	0
1	D	4728	0	4740	22	0
2	A	934	0	929	12	0
2	C	938	0	936	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	0	0	0
3	B	232	0	0	0	0
3	C	26	0	0	0	0
3	D	187	0	0	1	0
All	All	11832	0	11389	61	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 3.

All (61) 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:A:102:ILE:HG12	2:A:117:THR:HG23	1.53	0.90
2:C:102:ILE:HG12	2:C:117:THR:HG23	1.54	0.89
2:A:134:ARG:HG3	2:A:139:ILE:HB	1.73	0.70
2:C:134:ARG:HG3	2:C:139:ILE:HB	1.73	0.69
1:B:70:PHE:HB2	2:A:157:TRP:CH2	2.30	0.67
1:B:565:ARG:HD3	1:B:566:PRO:HD2	1.78	0.65
1:D:647:VAL:HG11	1:D:667:GLU:HG3	1.78	0.64
1:B:647:VAL:HG11	1:B:667:GLU:HG3	1.78	0.63
1:D:410:LEU:O	1:D:436:THR:HG23	2.00	0.61
1:B:410:LEU:O	1:B:436:THR:HG23	2.01	0.61
1:D:70:PHE:HB2	2:C:157:TRP:CH2	2.37	0.60
2:A:28:THR:HG21	2:A:107:TYR:O	2.02	0.59
1:B:40:ARG:HG2	2:A:130:PRO:HD3	1.86	0.58
1:D:159:LEU:HD13	1:D:194:LEU:HG	1.89	0.55
1:D:40:ARG:HG2	2:C:130:PRO:HD3	1.87	0.54
1:B:159:LEU:HD13	1:B:194:LEU:HG	1.89	0.54
1:B:266:CYS:HB2	1:B:268:PHE:CE2	2.43	0.53
1:B:609:LEU:HD23	1:B:612:ARG:HH11	1.75	0.52
1:D:266:CYS:HB2	1:D:268:PHE:CE2	2.44	0.52
1:B:562:THR:HA	1:B:565:ARG:N	2.26	0.50
1:D:662:HIS:HA	1:D:685:ARG:O	2.11	0.50
1:B:662:HIS:HA	1:B:685:ARG:O	2.11	0.49
1:D:203:GLU:HG2	1:D:232:HIS:HB2	1.94	0.49
1:B:203:GLU:HG2	1:B:232:HIS:HB2	1.95	0.49
2:C:9:LYS:HB2	2:C:43:PRO:HA	1.96	0.48
1:D:665:THR:HG22	1:D:667:GLU:H	1.78	0.48
1:B:62:ARG:HH12	2:A:156:GLN:HG3	1.79	0.48
1:B:358:PHE:HD1	1:B:386:SER:HB3	1.79	0.48
2:A:9:LYS:HB2	2:A:43:PRO:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:ARG:HH22	2:C:90:PHE:HB2	1.79	0.46
1:B:388:TYR:HE1	1:B:390:LYS:HG2	1.80	0.46
1:D:358:PHE:HD1	1:D:386:SER:HB3	1.79	0.46
2:A:26:SER:HB3	2:A:29:ILE:HD12	1.98	0.45
1:B:566:PRO:HD3	1:B:610:TRP:CH2	2.51	0.45
2:A:20:GLU:HG2	2:A:21:ALA:H	1.80	0.45
2:C:26:SER:HB3	2:C:29:ILE:HD12	1.97	0.45
1:D:369:LYS:HE3	3:D:969:HOH:O	2.16	0.45
1:D:559:ASP:HB2	1:D:561:ARG:HH21	1.82	0.44
1:D:388:TYR:HE1	1:D:390:LYS:HG2	1.81	0.44
2:C:61:ARG:NH2	2:C:90:PHE:HB2	2.33	0.44
1:D:227:THR:HG21	1:D:255:SER:HB3	2.00	0.44
2:A:102:ILE:HG12	2:A:117:THR:CG2	2.37	0.44
1:B:474:ASN:N	1:B:474:ASN:OD1	2.51	0.43
1:B:415:ILE:HD11	1:B:426:ILE:HD11	2.01	0.42
1:D:338:ASN:HD21	1:D:393:GLN:HE22	1.68	0.42
2:A:10:SER:HB3	2:A:13:GLY:H	1.85	0.42
1:B:659:LEU:O	1:B:682:MET:HA	2.19	0.42
1:D:659:LEU:O	1:D:682:MET:HA	2.20	0.42
1:D:62:ARG:HH12	2:C:156:GLN:HG3	1.83	0.42
1:B:260:ARG:HH22	1:B:290:ARG:CZ	2.33	0.41
1:B:227:THR:HG21	1:B:255:SER:HB3	2.01	0.41
1:D:415:ILE:HD11	1:D:426:ILE:HD11	2.03	0.41
1:B:338:ASN:HD21	1:B:393:GLN:HE22	1.67	0.41
1:D:659:LEU:HB3	1:D:682:MET:HG3	2.03	0.41
1:B:26:LEU:HD22	1:B:51:ALA:HA	2.03	0.41
1:D:44:ALA:O	2:C:134:ARG:HD2	2.21	0.41
1:D:26:LEU:HD22	1:D:51:ALA:HA	2.03	0.41
2:C:102:ILE:HG12	2:C:117:THR:CG2	2.38	0.41
1:D:612:ARG:O	1:D:616:HIS:HB2	2.21	0.41
1:B:689:TYR:HA	1:B:690:PRO:HA	1.85	0.40
2:A:42:VAL:N	2:A:43:PRO:HD3	2.36	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	B	600/688 (87%)	587 (98%)	13 (2%)	0	100	100
1	D	596/688 (87%)	584 (98%)	12 (2%)	0	100	100
2	A	109/160 (68%)	106 (97%)	3 (3%)	0	100	100
2	C	107/160 (67%)	105 (98%)	2 (2%)	0	100	100
All	All	1412/1696 (83%)	1382 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	518/575 (90%)	509 (98%)	9 (2%)	60	82
1	D	513/575 (89%)	503 (98%)	10 (2%)	57	80
2	A	104/137 (76%)	100 (96%)	4 (4%)	33	58
2	C	106/137 (77%)	101 (95%)	5 (5%)	26	49
All	All	1241/1424 (87%)	1213 (98%)	28 (2%)	50	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	THR
1	B	227	THR
1	B	273	SER
1	B	386	SER
1	B	574	LEU
1	B	620	SER
1	B	641	SER
1	B	682	MET

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Mol	Chain	Res	Type
1	B	693	GLU
2	A	18	VAL
2	A	50	LYS
2	A	117	THR
2	A	149	GLU
1	D	197	THR
1	D	227	THR
1	D	235	LEU
1	D	273	SER
1	D	307	GLN
1	D	386	SER
1	D	559	ASP
1	D	592	GLU
1	D	634	ASP
1	D	682	MET
2	C	50	LYS
2	C	81	ASP
2	C	83	LEU
2	C	117	THR
2	C	156	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	HIS
1	B	374	HIS
1	B	393	GLN
2	A	95	GLN
1	D	393	GLN

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](#)

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	B	614/688 (89%)	-0.11	17 (2%) 53 56	20, 29, 65, 107	0
1	D	610/688 (88%)	-0.11	25 (4%) 37 40	21, 31, 71, 108	0
2	A	117/160 (73%)	0.44	9 (7%) 13 13	24, 52, 104, 112	0
2	C	117/160 (73%)	0.60	15 (12%) 3 3	28, 56, 113, 119	0
All	All	1458/1696 (85%)	-0.01	66 (4%) 33 36	20, 31, 89, 119	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	372	TRP	6.3
2	C	7	VAL	5.8
1	D	696	LEU	4.9
1	D	560	CYS	4.7
1	B	696	LEU	4.6
2	C	42	VAL	4.5
1	D	634	ASP	4.4
1	D	373	LEU	4.4
1	B	373	LEU	4.4
2	C	43	PRO	4.1
1	B	697	MET	4.1
2	C	6	ILE	3.8
2	A	42	VAL	3.6
1	B	561	ARG	3.5
1	D	666	HIS	3.5
1	B	560	CYS	3.4
1	D	568	PRO	3.4
1	B	559	ASP	3.4
2	C	8	LEU	3.4
1	B	638	HIS	3.4
1	D	476	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	474	ASN	3.3
2	C	83	LEU	3.2
1	D	559	ASP	3.2
2	A	24	LEU	3.2
1	D	566	PRO	3.2
1	B	72	PHE	3.1
1	D	569	ARG	3.1
1	B	565	ARG	3.1
1	D	594	VAL	3.1
2	C	24	LEU	3.1
2	A	8	LEU	2.9
1	D	558	GLY	2.9
1	B	594	VAL	2.9
1	B	666	HIS	2.8
2	C	82	ASP	2.8
1	D	593	ALA	2.7
1	D	72	PHE	2.6
1	B	372	TRP	2.6
2	C	104	ALA	2.5
2	C	9	LYS	2.5
2	A	23	ALA	2.5
2	C	107	TYR	2.5
1	D	668	HIS	2.5
1	D	669	PHE	2.4
2	A	43	PRO	2.4
2	C	22	VAL	2.3
1	B	271	ARG	2.3
1	B	103	PRO	2.3
1	D	302	ALA	2.3
1	D	641	SER	2.3
2	C	58	TYR	2.2
2	A	111	LYS	2.2
1	D	670	MET	2.2
1	D	374	HIS	2.2
1	D	561	ARG	2.2
1	D	474	ASN	2.1
1	B	607	LEU	2.1
2	A	65	ALA	2.1
2	A	58	TYR	2.1
2	A	56	ILE	2.1
2	C	29	ILE	2.1
1	D	103	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	374	HIS	2.0
1	D	475	THR	2.0
2	C	27	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.