



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:07 PM UTC

PDB ID : 5GS2 / pdb_00005gs2
Title : Crystal structure of diabody complex with reepbody and MBP
Authors : Kim, J.H.; Song, D.H.; Youn, S.J.; Kim, J.W.; Cho, G.; Lee, H.; Lee, J.O.
Deposited on : 2016-08-13
Resolution : 3.59 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

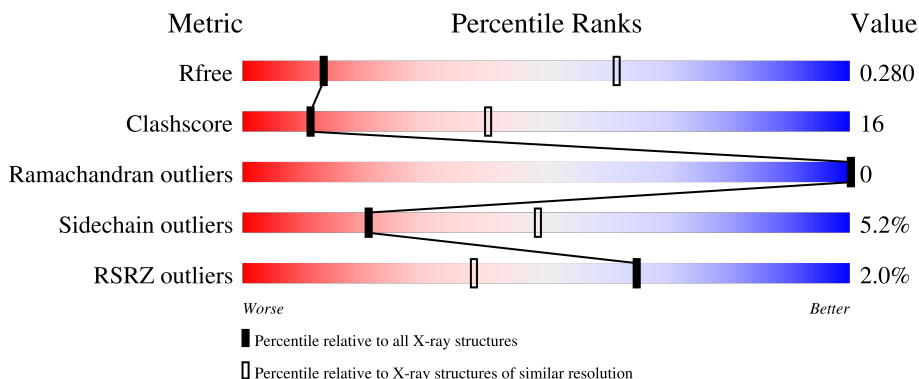
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 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	367	% 75% 24% .
2	D	233	3% 65% 25% 6% .
3	H	239	4% 66% 21% 8% .
4	B	273	% 69% 26% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8503 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	4	0
			2874	1855	466	547	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	ASN	ARG	engineered mutation	UNP P0AEX9

- Molecule 2 is a protein called anti-repebody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	226	Total	C	N	O	S	0	2	0
			1733	1091	283	352	7			

- Molecule 3 is a protein called anti-MBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	231	Total	C	N	O	S	0	4	0
			1791	1130	304	349	8			

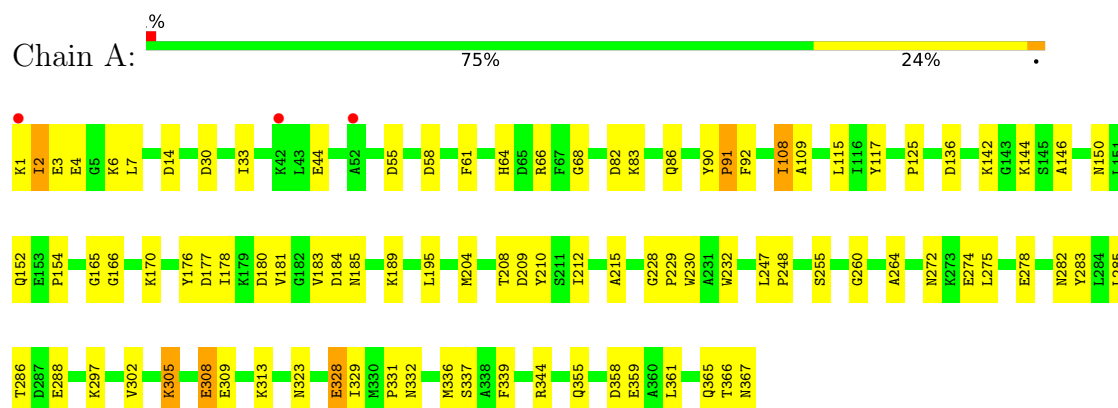
- Molecule 4 is a protein called repebody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	268	Total	C	N	O	S	0	0	0
			2105	1336	354	411	4			

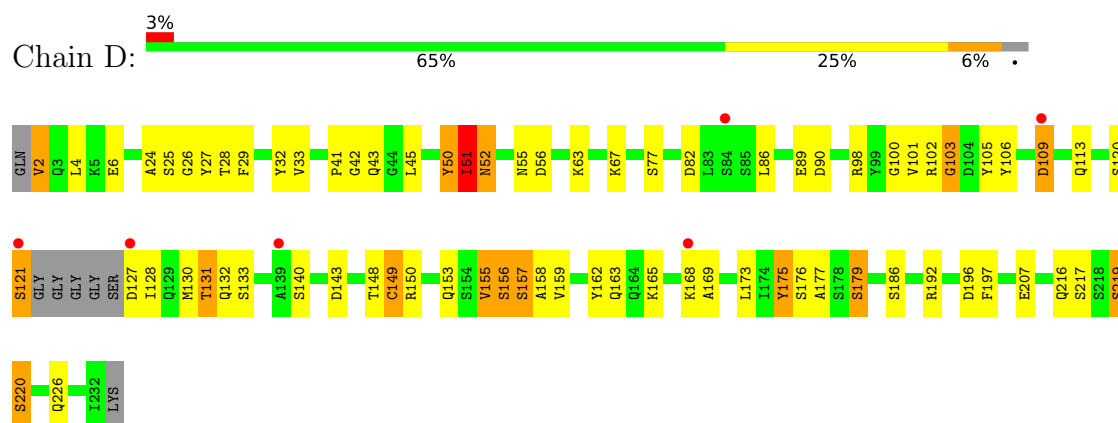
3 Residue-property plots [i](#)

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.

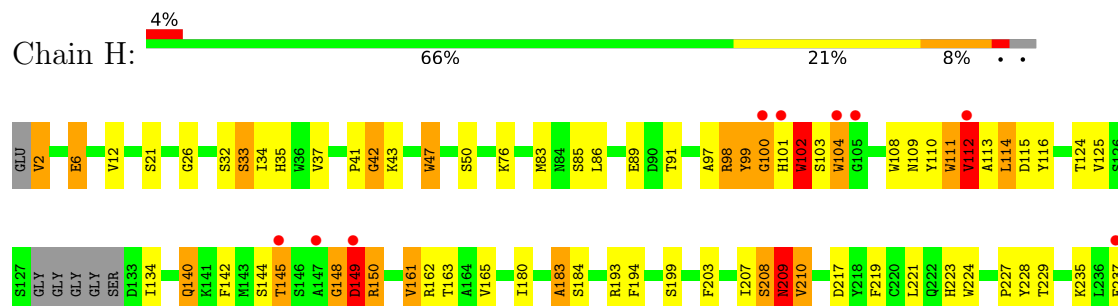
• Molecule 1: Maltose-binding periplasmic protein



• Molecule 2: anti-repebody



• Molecule 3: anti-MBP



ILE
LYS

● Molecule 4: repebody



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	278.83Å 278.83Å 132.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.11 – 3.59 44.11 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.11-3.59) 96.4 (44.11-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.217 , 0.278 0.221 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (8.69%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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

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	0.50	0/2955	0.75	8/4007 (0.2%)
2	D	0.65	1/1778 (0.1%)	1.06	13/2409 (0.5%)
3	H	0.76	4/1851 (0.2%)	1.35	25/2518 (1.0%)
4	B	0.82	14/2143 (0.7%)	0.93	12/2921 (0.4%)
All	All	0.68	19/8727 (0.2%)	1.01	58/11855 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
3	H	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	243	ASN	N-CA	15.02	1.70	1.46
4	B	244	LEU	N-CA	10.49	1.59	1.46
4	B	243	ASN	CA-C	-9.94	1.41	1.53
3	H	184	SER	N-CA	-7.79	1.36	1.46
4	B	120	GLN	CA-C	7.69	1.63	1.52
4	B	120	GLN	N-CA	-7.30	1.38	1.46
4	B	242	LEU	N-CA	7.03	1.54	1.46
4	B	244	LEU	CA-CB	-6.63	1.42	1.53
3	H	41	PRO	CA-CB	6.59	1.63	1.53
3	H	184	SER	CA-C	6.49	1.60	1.53
4	B	63	PRO	N-CD	6.24	1.56	1.47
4	B	119	ASN	N-CA	-6.14	1.36	1.46
4	B	243	ASN	CA-CB	-6.12	1.46	1.54
4	B	242	LEU	CA-C	-6.06	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	177	ALA	N-CA	6.03	1.53	1.46
4	B	62	LEU	CA-C	-5.76	1.46	1.52
4	B	119	ASN	CA-C	5.73	1.60	1.53
3	H	41	PRO	N-CA	-5.53	1.40	1.47
4	B	246	PRO	N-CD	5.35	1.55	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	209	ASN	N-CA-C	-22.26	73.75	109.59
3	H	208	SER	N-CA-C	19.33	136.18	111.24
2	D	50	TYR	N-CA-C	-16.37	82.89	108.76
3	H	184	SER	N-CA-C	15.90	134.67	109.39
3	H	111	TRP	N-CA-C	13.63	130.61	111.52
2	D	42	GLY	N-CA-C	11.89	129.36	114.37
3	H	101	HIS	N-CA-C	11.60	128.05	108.67
3	H	150	ARG	N-CA-C	10.85	128.23	112.94
3	H	209	ASN	CB-CA-C	10.80	128.82	109.38
3	H	150	ARG	N-CA-CB	-10.52	93.63	110.98
3	H	210	VAL	N-CA-C	-10.28	93.27	108.89
2	D	179	SER	N-CA-C	10.08	124.68	109.25
1	A	91	PRO	CB-CA-C	-10.01	96.33	111.44
1	A	92	PHE	N-CA-CB	-9.83	95.56	109.91
3	H	183	ALA	N-CA-C	-9.26	93.21	108.67
3	H	100	GLY	N-CA-C	-8.91	93.74	112.45
3	H	110	TYR	CB-CA-C	8.40	123.72	109.53
3	H	149	ASP	CB-CA-C	-8.23	95.71	110.36
3	H	148	GLY	N-CA-C	-8.19	93.76	113.18
2	D	51	ILE	N-CA-CB	-8.15	97.78	111.23
3	H	42	GLY	N-CA-C	7.65	131.32	113.18
2	D	103	GLY	N-CA-C	-7.49	95.42	113.18
3	H	112	VAL	N-CA-C	7.34	119.66	109.45
4	B	126	ASP	N-CA-C	-7.29	94.28	107.98
4	B	243	ASN	CA-C-O	7.25	128.41	120.80
3	H	184	SER	CB-CA-C	-6.98	100.77	112.00
3	H	208	SER	CB-CA-C	-6.93	99.43	110.86
4	B	62	LEU	N-CA-C	-6.92	93.37	108.74
4	B	234	HIS	N-CA-CB	-6.90	100.25	110.88
2	D	177	ALA	CB-CA-C	-6.63	100.52	110.06
1	A	108	ILE	N-CA-C	6.44	117.79	111.67
2	D	177	ALA	N-CA-C	6.41	123.34	113.28
3	H	102	TRP	N-CA-CB	-6.39	98.67	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	243	ASN	CB-CA-C	6.27	127.33	114.10
2	D	41	PRO	N-CA-C	-6.07	101.12	110.95
4	B	233	GLN	CB-CA-C	6.01	120.39	110.90
1	A	91	PRO	CA-C-N	5.91	128.45	120.65
1	A	91	PRO	C-N-CA	5.91	128.45	120.65
1	A	283	TYR	N-CA-C	5.90	120.50	113.12
2	D	52	ASN	CB-CA-C	5.86	116.53	109.85
4	B	120	GLN	N-CA-C	-5.84	105.97	112.57
2	D	219	SER	N-CA-CB	-5.83	101.79	110.71
4	B	207	LEU	N-CA-C	5.64	117.87	109.25
2	D	51	ILE	N-CA-C	-5.63	97.64	109.34
3	H	113	ALA	N-CA-C	-5.58	96.67	107.44
4	B	95	ASN	CB-CA-C	-5.42	100.38	109.48
1	A	108	ILE	CB-CA-C	-5.37	105.46	111.80
3	H	47	TRP	CB-CA-C	-5.37	102.20	110.26
2	D	43	GLN	N-CA-CB	5.34	120.24	111.31
4	B	119	ASN	CA-CB-CG	-5.32	107.28	112.60
2	D	41	PRO	CB-CA-C	5.30	118.60	111.71
3	H	100	GLY	CA-C-N	5.29	130.77	123.04
3	H	100	GLY	C-N-CA	5.29	130.77	123.04
3	H	99	TYR	N-CA-C	5.29	119.65	111.56
4	B	243	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	283	TYR	N-CA-CB	-5.21	102.45	110.42
3	H	149	ASP	N-CA-C	5.17	117.74	110.14
4	B	245	ASP	N-CA-C	-5.11	98.52	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	220	SER	Peptide
3	H	104	TRP	Peptide

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	2874	0	2871	63	0
2	D	1733	0	1677	71	0
3	H	1791	0	1697	90	3
4	B	2105	0	2123	65	3
All	All	8503	0	8368	275	3

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 16.

All (275) 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)
4:B:243:ASN:N	4:B:243:ASN:CA	1.70	1.50
3:H:149:ASP:O	3:H:208:SER:O	1.53	1.27
3:H:99:TYR:CD1	3:H:112:VAL:HG12	1.70	1.24
3:H:149:ASP:CB	3:H:210:VAL:CG2	2.22	1.18
3:H:149:ASP:HB2	3:H:210:VAL:CB	1.74	1.17
3:H:149:ASP:HB3	3:H:210:VAL:HG23	1.27	1.12
3:H:149:ASP:CB	3:H:210:VAL:HG23	1.84	1.06
3:H:149:ASP:HB2	3:H:210:VAL:HB	1.30	1.05
2:D:175:TYR:CE1	2:D:179:SER:OG	2.08	1.04
3:H:149:ASP:CB	3:H:210:VAL:HB	1.86	1.03
3:H:149:ASP:CB	3:H:210:VAL:CB	2.36	1.02
3:H:149:ASP:HB3	3:H:210:VAL:CG2	1.88	1.00
3:H:149:ASP:OD2	3:H:210:VAL:CB	2.10	1.00
3:H:115:ASP:OD1	3:H:116:TYR:CD1	2.16	0.98
3:H:149:ASP:CG	3:H:210:VAL:HB	1.91	0.95
2:D:52:ASN:O	2:D:56:ASP:CG	2.11	0.93
3:H:115:ASP:OD1	3:H:116:TYR:N	2.02	0.92
3:H:99:TYR:CD2	3:H:100:GLY:O	2.22	0.92
3:H:115:ASP:OD1	3:H:116:TYR:CG	2.23	0.92
4:B:41:ASN:O	4:B:64:ASN:ND2	2.02	0.91
4:B:61:TYR:C	4:B:62:LEU:HD23	1.95	0.91
2:D:103:GLY:HA2	4:B:171:SER:HB2	1.51	0.90
3:H:193:ARG:HD2	3:H:209:ASN:O	1.71	0.90
2:D:175:TYR:CD1	2:D:179:SER:OG	2.22	0.89
3:H:149:ASP:OD2	3:H:210:VAL:HG11	1.70	0.88
2:D:165:LYS:NZ	2:D:207:GLU:O	2.09	0.85
2:D:162:TYR:OH	3:H:114:LEU:HD12	1.77	0.85
3:H:149:ASP:OD2	3:H:210:VAL:CG1	2.24	0.84
3:H:42:GLY:O	3:H:43:LYS:HD3	1.78	0.82
3:H:149:ASP:CG	3:H:210:VAL:CB	2.54	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:149:ASP:OD2	3:H:210:VAL:HG21	1.80	0.81
3:H:148:GLY:HA2	3:H:209:ASN:OD1	1.82	0.79
3:H:149:ASP:OD2	3:H:210:VAL:HB	1.80	0.79
3:H:149:ASP:OD2	3:H:210:VAL:CG2	2.31	0.79
4:B:43:ILE:HD12	4:B:62:LEU:HD13	1.65	0.77
3:H:99:TYR:CG	3:H:112:VAL:HG12	2.20	0.77
1:A:166:GLY:HA2	1:A:185:ASN:HD21	1.49	0.76
3:H:149:ASP:CG	3:H:210:VAL:CG2	2.59	0.75
4:B:61:TYR:O	4:B:62:LEU:HD23	1.87	0.74
4:B:243:ASN:N	4:B:243:ASN:C	2.44	0.73
4:B:243:ASN:N	4:B:243:ASN:CB	2.52	0.72
1:A:189[B]:LYS:NZ	1:A:358:ASP:OD1	2.22	0.72
2:D:175:TYR:HE1	2:D:179:SER:CB	2.03	0.72
3:H:149:ASP:HB2	3:H:210:VAL:N	2.06	0.71
3:H:91:THR:HG23	3:H:124:THR:HA	1.73	0.70
3:H:99:TYR:CD1	3:H:112:VAL:CG1	2.64	0.69
1:A:4:GLU:HA	1:A:272:ASN:HD21	1.56	0.69
3:H:103:SER:O	3:H:104:TRP:HB3	1.90	0.69
3:H:149:ASP:CG	3:H:210:VAL:HG21	2.18	0.69
4:B:115:VAL:HG22	4:B:139:TYR:HD2	1.57	0.69
3:H:35:HIS:ND1	3:H:50[B]:SER:OG	2.22	0.69
3:H:149:ASP:C	3:H:150:ARG:HG3	2.16	0.68
2:D:101:VAL:HA	2:D:105:TYR:O	1.94	0.68
1:A:108:ILE:HD13	1:A:285:LEU:HD21	1.75	0.67
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.77	0.67
2:D:105:TYR:OH	2:D:109:ASP:OD1	2.08	0.67
4:B:43:ILE:HD12	4:B:62:LEU:CD1	2.26	0.66
2:D:140:SER:OG	2:D:143:ASP:OD2	2.11	0.66
2:D:89:GLU:OE1	2:D:89:GLU:N	2.27	0.65
3:H:149:ASP:HB2	3:H:210:VAL:CG2	2.04	0.65
1:A:184:ASP:HB3	1:A:365:GLN:NE2	2.13	0.64
1:A:365:GLN:C	1:A:367:ASN:H	2.04	0.64
1:A:1:LYS:NZ	1:A:2:ILE:O	2.31	0.64
1:A:91:PRO:HG2	2:D:219:SER:HB3	1.80	0.64
4:B:185:GLN:HG2	4:B:209:HIS:HB2	1.79	0.64
2:D:52:ASN:O	2:D:56:ASP:OD1	2.16	0.64
3:H:99:TYR:CE1	3:H:112:VAL:HA	2.33	0.63
3:H:42:GLY:C	3:H:43:LYS:HD3	2.22	0.63
2:D:120:SER:OG	2:D:121:SER:N	2.30	0.62
2:D:175:TYR:HE1	2:D:179:SER:HB2	1.64	0.62
2:D:175:TYR:CE1	2:D:179:SER:CB	2.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:MET:HE3	2:D:149:CYS:SG	2.39	0.62
1:A:90:TYR:OH	1:A:308:GLU:HG2	2.00	0.62
2:D:55:ASN:HB2	2:D:56:ASP:HA	1.81	0.62
3:H:102:TRP:HZ3	3:H:111:TRP:HB2	1.62	0.62
1:A:165:GLY:O	1:A:185:ASN:ND2	2.33	0.62
3:H:32:SER:HA	3:H:100:GLY:HA2	1.82	0.62
3:H:99:TYR:CE2	3:H:100:GLY:O	2.53	0.61
2:D:51:ILE:HG12	2:D:56:ASP:OD2	2.01	0.61
4:B:213:LEU:HB3	4:B:248:SER:HB2	1.82	0.60
3:H:149:ASP:CB	3:H:210:VAL:HG21	2.29	0.60
4:B:23:LYS:HD2	4:B:30:SER:O	2.01	0.60
4:B:242:LEU:HD23	4:B:243:ASN:HB2	1.84	0.60
2:D:63:LYS:NZ	3:H:89:GLU:OE1	2.35	0.59
1:A:355:GLN:HB3	1:A:359:GLU:HB2	1.83	0.59
3:H:144:SER:HA	3:H:237:GLU:HB2	1.85	0.59
3:H:149:ASP:HB2	3:H:210:VAL:CA	2.31	0.59
1:A:64:HIS:HE1	1:A:260:GLY:HA2	1.66	0.59
1:A:64:HIS:CE1	1:A:260:GLY:HA2	2.37	0.59
1:A:152:GLN:HG2	1:A:209:ASP:HB3	1.85	0.59
3:H:102:TRP:CZ3	3:H:111:TRP:HB2	2.37	0.59
4:B:30:SER:OG	4:B:31:VAL:N	2.36	0.58
4:B:62:LEU:N	4:B:63:PRO:CD	2.66	0.58
2:D:6:GLU:O	2:D:113:GLN:NE2	2.36	0.58
1:A:184:ASP:HB3	1:A:365:GLN:CD	2.28	0.58
1:A:150:ASN:ND2	1:A:210:TYR:HB2	2.19	0.58
1:A:68:GLY:HA3	1:A:332:ASN:O	2.03	0.57
3:H:161:VAL:HG23	3:H:224:TRP:HB2	1.87	0.57
4:B:61:TYR:O	4:B:62:LEU:CD2	2.52	0.57
1:A:309:GLU:OE1	2:D:192:ARG:NH2	2.37	0.57
4:B:115:VAL:HG22	4:B:139:TYR:CD2	2.40	0.57
1:A:4:GLU:HA	1:A:272:ASN:ND2	2.18	0.57
2:D:163:GLN:NE2	2:D:165:LYS:HD3	2.20	0.57
2:D:67:LYS:NZ	2:D:90:ASP:OD2	2.33	0.56
2:D:217:SER:OG	3:H:111:TRP:HA	2.04	0.56
1:A:142:LYS:HB2	1:A:144:LYS:HG2	1.87	0.56
2:D:32:TYR:HD1	2:D:100:GLY:HA2	1.71	0.56
1:A:1:LYS:HB2	1:A:55:ASP:HB3	1.87	0.56
4:B:215:ASN:HB2	4:B:217:TRP:NE1	2.21	0.56
3:H:140:GLN:HG3	3:H:142:PHE:O	2.06	0.56
2:D:33:VAL:HG11	2:D:50:TYR:CD2	2.41	0.56
2:D:150:ARG:NH2	2:D:196:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG12	1:A:183:VAL:HG22	1.88	0.55
1:A:150:ASN:HD22	1:A:210:TYR:HB2	1.72	0.55
2:D:131:THR:O	2:D:149:CYS:HA	2.06	0.55
2:D:128:ILE:HG21	2:D:216:GLN:HG3	1.90	0.54
1:A:282:ASN:O	1:A:286:THR:HG21	2.07	0.54
1:A:288:GLU:CD	1:A:288:GLU:H	2.15	0.54
4:B:230:TRP:HE3	4:B:231:ILE:HD13	1.73	0.54
2:D:132:GLN:HG2	2:D:149:CYS:HB2	1.89	0.54
4:B:219:CYS:HA	4:B:224:ILE:HG21	1.89	0.54
2:D:127:ASP:CG	2:D:128:ILE:H	2.16	0.54
3:H:162:ARG:O	3:H:163:THR:HG22	2.08	0.54
3:H:99:TYR:CG	3:H:100:GLY:O	2.60	0.54
1:A:82:ASP:O	1:A:86:GLN:HG3	2.07	0.53
2:D:52:ASN:N	2:D:56:ASP:OD1	2.42	0.53
4:B:23:LYS:HD3	4:B:31:VAL:HG12	1.89	0.53
2:D:32:TYR:CD1	2:D:100:GLY:HA2	2.44	0.53
4:B:242:LEU:C	4:B:243:ASN:CA	2.71	0.53
2:D:157:SER:OG	2:D:192:ARG:NH1	2.39	0.53
4:B:67:TYR:HD1	4:B:89:TYR:HB2	1.73	0.52
3:H:6:GLU:HA	3:H:21:SER:O	2.09	0.52
2:D:168:LYS:HD2	2:D:169:ALA:H	1.73	0.52
1:A:361:LEU:O	1:A:365:GLN:NE2	2.43	0.51
4:B:95:ASN:O	4:B:119:ASN:OD1	2.28	0.51
1:A:7:LEU:HA	1:A:58:ASP:OD2	2.10	0.51
2:D:33:VAL:HG22	2:D:52:ASN:HB2	1.92	0.51
3:H:149:ASP:HB2	3:H:210:VAL:HG23	1.74	0.51
1:A:328:GLU:OE1	3:H:102:TRP:HA	2.10	0.51
3:H:34:ILE:HD13	3:H:98:ARG:HA	1.92	0.51
2:D:127:ASP:CG	2:D:128:ILE:N	2.69	0.51
3:H:97:ALA:HB1	3:H:114:LEU:HB3	1.93	0.51
1:A:90:TYR:CD1	1:A:305:LYS:HG3	2.47	0.50
2:D:101:VAL:HB	2:D:106:TYR:CE1	2.47	0.50
3:H:148:GLY:HA2	3:H:209:ASN:CG	2.36	0.50
4:B:62:LEU:HD23	4:B:62:LEU:N	2.22	0.50
1:A:183:VAL:HG23	1:A:365:GLN:HG3	1.93	0.50
2:D:103:GLY:HA2	4:B:171:SER:CB	2.34	0.50
3:H:149:ASP:HB2	3:H:210:VAL:H	1.77	0.49
1:A:90:TYR:CE1	1:A:305:LYS:HG3	2.47	0.49
2:D:220:SER:OG	3:H:109:ASN:ND2	2.45	0.49
1:A:247:LEU:HD12	1:A:323:ASN:HD21	1.76	0.49
2:D:216:GLN:C	2:D:216:GLN:CD	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:115:ASP:CG	3:H:116:TYR:N	2.70	0.49
3:H:199:SER:HA	3:H:203:PHE:HE1	1.78	0.49
2:D:155:VAL:HG23	2:D:156:SER:O	2.12	0.49
4:B:9:ILE:HD12	4:B:28:LYS:HZ3	1.77	0.49
4:B:62:LEU:N	4:B:63:PRO:HD3	2.27	0.49
2:D:155:VAL:HG11	2:D:216:GLN:HG3	1.95	0.49
4:B:111:LEU:HD12	4:B:132:LEU:HD22	1.93	0.49
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.94	0.49
2:D:51:ILE:HG23	2:D:51:ILE:O	2.13	0.49
3:H:98:ARG:O	3:H:98:ARG:HG2	2.13	0.49
1:A:228:GLY:HA3	1:A:230:TRP:CH2	2.48	0.48
4:B:186:LEU:O	4:B:210:ILE:HA	2.14	0.48
3:H:227:PRO:O	3:H:229:THR:HG23	2.13	0.48
4:B:8:PRO:HA	4:B:33:ASP:O	2.13	0.48
4:B:227:LEU:O	4:B:231:ILE:HG12	2.12	0.48
1:A:177:ASP:OD2	1:A:180:ASP:HB2	2.12	0.48
4:B:48:ALA:HB3	4:B:70:LEU:HD23	1.94	0.48
2:D:29:PHE:CD2	2:D:77:SER:HA	2.49	0.48
2:D:98:ARG:HH21	2:D:109:ASP:CG	2.21	0.48
2:D:157:SER:N	2:D:192:ARG:NH1	2.62	0.47
2:D:163:GLN:HB2	2:D:173:LEU:HD11	1.95	0.47
1:A:189[B]:LYS:NZ	1:A:358:ASP:CG	2.72	0.47
1:A:66:ARG:NH1	1:A:337:SER:HA	2.29	0.47
1:A:176:TYR:CE2	1:A:331:PRO:HB3	2.49	0.47
1:A:365:GLN:C	1:A:367:ASN:N	2.72	0.47
2:D:216:GLN:O	2:D:216:GLN:OE1	2.32	0.47
3:H:149:ASP:H	3:H:210:VAL:H	1.63	0.47
1:A:66:ARG:HH12	1:A:337:SER:HA	1.79	0.47
3:H:162:ARG:O	3:H:163:THR:CG2	2.63	0.47
4:B:9:ILE:HA	4:B:12:ILE:HD12	1.96	0.47
4:B:226:TYR:HA	4:B:229:ARG:HD3	1.96	0.46
2:D:192:ARG:HD2	2:D:197:PHE:CE2	2.50	0.46
4:B:67:TYR:CD1	4:B:89:TYR:HB2	2.50	0.46
2:D:2:VAL:HA	2:D:25:SER:O	2.15	0.46
4:B:9:ILE:HD12	4:B:28:LYS:NZ	2.30	0.46
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.97	0.46
1:A:44:GLU:HB2	1:A:66:ARG:HD2	1.98	0.46
2:D:132:GLN:H	2:D:226:GLN:HE22	1.62	0.46
1:A:1:LYS:HG3	1:A:2:ILE:N	2.31	0.46
2:D:52:ASN:C	2:D:56:ASP:CG	2.81	0.45
1:A:248:PRO:O	1:A:255:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:TYR:CD1	2:D:175:TYR:O	2.69	0.45
4:B:4:THR:O	4:B:4:THR:OG1	2.21	0.45
4:B:9:ILE:HG12	4:B:35:VAL:HG11	1.97	0.45
4:B:79:SER:HB3	4:B:82:LYS:NZ	2.31	0.45
4:B:100:LEU:HA	4:B:100:LEU:HD23	1.70	0.45
1:A:212:ILE:HA	1:A:215:ALA:HB3	1.98	0.45
2:D:101:VAL:HB	2:D:106:TYR:HE1	1.81	0.45
4:B:18:PHE:HD1	4:B:53:ILE:HD13	1.82	0.45
4:B:43:ILE:CD1	4:B:62:LEU:CD1	2.95	0.45
1:A:33:ILE:HG12	1:A:275:LEU:HD13	1.98	0.45
4:B:184:LYS:HA	4:B:207:LEU:HA	1.98	0.44
4:B:190:ASP:OD1	4:B:214:ASN:ND2	2.48	0.44
4:B:103:GLY:HA2	4:B:106:ASP:OD1	2.17	0.44
3:H:194:PHE:CD1	3:H:207:ILE:HG12	2.53	0.44
1:A:208:THR:HG23	1:A:212:ILE:HG23	1.99	0.44
2:D:130:MET:SD	2:D:216:GLN:HB2	2.58	0.44
3:H:102:TRP:HZ3	3:H:111:TRP:CB	2.30	0.44
1:A:154:PRO:HD3	1:A:344:ARG:HB3	1.99	0.44
1:A:170:LYS:HB2	1:A:180:ASP:OD1	2.18	0.44
3:H:98:ARG:NH1	3:H:100:GLY:HA3	2.32	0.44
4:B:41:ASN:C	4:B:64:ASN:ND2	2.74	0.44
4:B:215:ASN:HB2	4:B:217:TRP:CE2	2.52	0.43
3:H:163:THR:O	3:H:163:THR:OG1	2.33	0.43
4:B:14:PRO:HD2	4:B:57:GLN:O	2.19	0.43
3:H:12:VAL:O	3:H:125:VAL:HA	2.18	0.43
1:A:30:ASP:OD1	1:A:30:ASP:N	2.52	0.43
4:B:61:TYR:C	4:B:63:PRO:CD	2.91	0.43
3:H:149:ASP:C	3:H:208:SER:O	2.50	0.43
4:B:121:LEU:HA	4:B:121:LEU:HD23	1.79	0.43
3:H:35:HIS:NE2	3:H:99:TYR:HB2	2.33	0.43
3:H:2:VAL:HA	3:H:26:GLY:HA3	2.01	0.43
4:B:146:GLN:O	4:B:169:LEU:HA	2.18	0.43
4:B:219:CYS:HB3	4:B:261:VAL:HG21	2.01	0.43
2:D:133:SER:HB2	2:D:148:THR:OG1	2.18	0.43
2:D:4:LEU:HD23	2:D:24:ALA:HA	2.01	0.42
3:H:165:VAL:HG11	3:H:203:PHE:CD1	2.55	0.42
2:D:45:LEU:HD11	3:H:219:PHE:CZ	2.54	0.42
4:B:91:ILE:HG23	4:B:115:VAL:HB	2.01	0.42
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.02	0.42
3:H:217:ASP:HB2	3:H:235:LYS:HG3	2.01	0.42
1:A:274:GLU:O	1:A:278:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:TYR:HE2	4:B:147:SER:HB3	1.85	0.42
2:D:162:TYR:CZ	3:H:114:LEU:HD12	2.52	0.42
3:H:33:SER:OG	3:H:99:TYR:HD2	2.02	0.42
3:H:223:HIS:HB2	3:H:228:TYR:CZ	2.54	0.42
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.92	0.42
2:D:33:VAL:HG11	2:D:50:TYR:HD2	1.84	0.42
2:D:159:VAL:HG21	2:D:197:PHE:CD1	2.55	0.42
3:H:145:THR:HG21	3:H:210:VAL:HG21	2.01	0.42
4:B:65:VAL:HG11	4:B:68:LEU:HB2	2.02	0.42
1:A:14:ASP:O	1:A:297:LYS:HD3	2.20	0.42
3:H:33:SER:HG	3:H:99:TYR:HD2	1.67	0.41
3:H:103:SER:HA	3:H:108:TRP:HA	2.00	0.41
1:A:109:ALA:CB	1:A:302:VAL:HA	2.50	0.41
3:H:199:SER:HA	3:H:203:PHE:CE1	2.55	0.41
4:B:41:ASN:C	4:B:64:ASN:HD22	2.28	0.41
4:B:44:ASP:OD1	4:B:44:ASP:N	2.44	0.41
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.41
1:A:183:VAL:O	1:A:361:LEU:HB3	2.20	0.41
2:D:175:TYR:O	2:D:175:TYR:HD1	2.04	0.41
3:H:180:ILE:CG2	3:H:183:ALA:O	2.68	0.41
1:A:336:MET:HA	1:A:339:PHE:HB3	2.02	0.41
2:D:156:SER:O	2:D:158:ALA:N	2.54	0.41
2:D:176:SER:O	2:D:176:SER:OG	2.28	0.41
3:H:99:TYR:C	3:H:100:GLY:O	2.55	0.41
1:A:55:ASP:OD1	1:A:55:ASP:N	2.54	0.40
1:A:184:ASP:OD1	1:A:184:ASP:C	2.64	0.40
1:A:195:LEU:CD1	1:A:204:MET:HE1	2.50	0.40
2:D:128:ILE:CD1	2:D:153:GLN:HB2	2.51	0.40
3:H:99:TYR:HE1	3:H:112:VAL:HA	1.81	0.40
4:B:23:LYS:O	4:B:23:LYS:HG3	2.20	0.40
1:A:117:TYR:CE2	1:A:125:PRO:HD3	2.57	0.40
3:H:207:ILE:CG2	3:H:210:VAL:HG22	2.51	0.40
4:B:146:GLN:HG2	4:B:168:GLN:HB2	2.03	0.40
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.57	0.40
2:D:27:TYR:HB2	4:B:270:LYS:HE2	2.03	0.40
2:D:28:THR:HG23	4:B:270:LYS:HE3	2.03	0.40
1:A:115:LEU:HB2	1:A:247:LEU:HD23	2.04	0.40
3:H:102:TRP:HZ3	3:H:111:TRP:CG	2.40	0.40
4:B:21:THR:HG21	4:B:48:ALA:HB2	2.03	0.40
4:B:87:LEU:HD12	4:B:87:LEU:HA	1.96	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:150:ARG:CD	4:B:64:ASN:OD1[8_555]	1.68	0.52
3:H:150:ARG:CG	4:B:64:ASN:OD1[8_555]	1.92	0.28
3:H:150:ARG:CB	4:B:64:ASN:OD1[8_555]	1.94	0.26

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	369/367 (100%)	349 (95%)	20 (5%)	0	100	100
2	D	224/233 (96%)	204 (91%)	20 (9%)	0	100	100
3	H	231/239 (97%)	213 (92%)	18 (8%)	0	100	100
4	B	266/273 (97%)	242 (91%)	24 (9%)	0	100	100
All	All	1090/1112 (98%)	1008 (92%)	82 (8%)	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	A	298/294 (101%)	287 (96%)	11 (4%)	30	56
2	D	195/196 (100%)	181 (93%)	14 (7%)	13	40
3	H	194/194 (100%)	178 (92%)	16 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	245/249 (98%)	238 (97%)	7 (3%)	37	60
All	All	932/933 (100%)	884 (95%)	48 (5%)	21	48

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	GLU
1	A	6	LYS
1	A	83	LYS
1	A	178	ILE
1	A	305	LYS
1	A	308	GLU
1	A	313	LYS
1	A	328	GLU
1	A	329	ILE
1	A	366	THR
2	D	2	VAL
2	D	51	ILE
2	D	82	ASP
2	D	86	LEU
2	D	102	ARG
2	D	109	ASP
2	D	121	SER
2	D	131	THR
2	D	149	CYS
2	D	155	VAL
2	D	156	SER
2	D	157	SER
2	D	175	TYR
2	D	186	SER
3	H	2	VAL
3	H	6	GLU
3	H	33	SER
3	H	76	LYS
3	H	85	SER
3	H	98	ARG
3	H	102	TRP
3	H	112	VAL
3	H	114	LEU
3	H	134	ILE
3	H	140	GLN

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Mol	Chain	Res	Type
3	H	145	THR
3	H	149	ASP
3	H	161	VAL
3	H	209	ASN
3	H	221	LEU
4	B	11	GLN
4	B	28	LYS
4	B	31	VAL
4	B	62	LEU
4	B	96	GLN
4	B	174	GLU
4	B	184	LYS

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	49	GLN
1	A	118	ASN
1	A	152	GLN
1	A	185	ASN
2	D	164	GLN
3	H	77	ASN
3	H	170	GLN
3	H	185	ASN
3	H	211	GLN
4	B	64	ASN
4	B	119	ASN
4	B	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	367/367 (100%)	-0.09	3 (0%) 82 58	40, 93, 140, 166	4 (1%)
2	D	226/233 (96%)	0.01	6 (2%) 56 32	54, 82, 119, 133	2 (0%)
3	H	231/239 (96%)	0.06	9 (3%) 43 24	41, 81, 125, 153	4 (1%)
4	B	268/273 (98%)	0.03	4 (1%) 72 44	59, 93, 140, 183	0
All	All	1092/1112 (98%)	-0.01	22 (2%) 65 38	40, 87, 135, 183	10 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	4	THR	5.4
3	H	149	ASP	3.3
3	H	104	TRP	3.3
2	D	139	ALA	2.9
3	H	147	ALA	2.9
4	B	31	VAL	2.7
2	D	168	LYS	2.7
3	H	100	GLY	2.7
2	D	127	ASP	2.6
4	B	5	VAL	2.6
4	B	271	CYS	2.5
3	H	145	THR	2.5
3	H	237	GLU	2.4
1	A	52	ALA	2.4
2	D	84	SER	2.4
1	A	42[A]	LYS	2.4
3	H	105	GLY	2.2
2	D	121	SER	2.1
3	H	112	VAL	2.1
3	H	101	HIS	2.1
1	A	1	LYS	2.1
2	D	109	ASP	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.