



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:06 PM EDT

PDB ID : 6T1W / pdb_00006t1w
Title : Structure of E. coli BamA in complex with lipoprotein RcsF
Authors : Letoquart, J.; Remaut, H.; Collet, J.F.
Deposited on : 2019-10-07
Resolution : 3.79 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

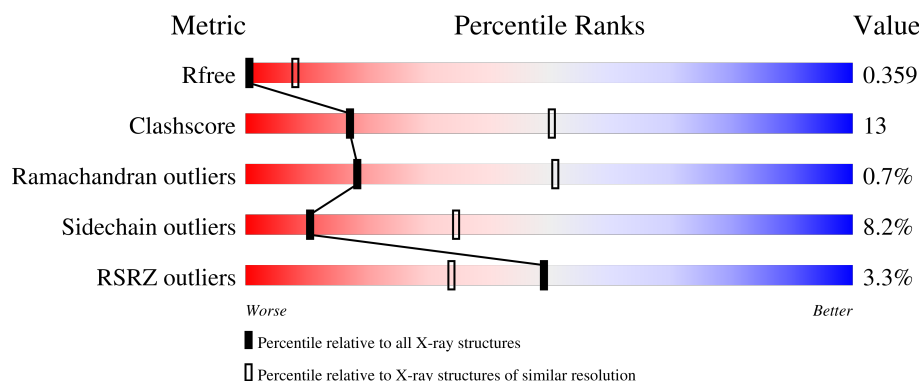
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	810	
1	B	810	
2	C	134	
2	D	134	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10838 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	0	0
			5991	3780	1004	1191	16			
1	B	466	Total	C	N	O	S	0	0	0
			3661	2318	595	736	12			

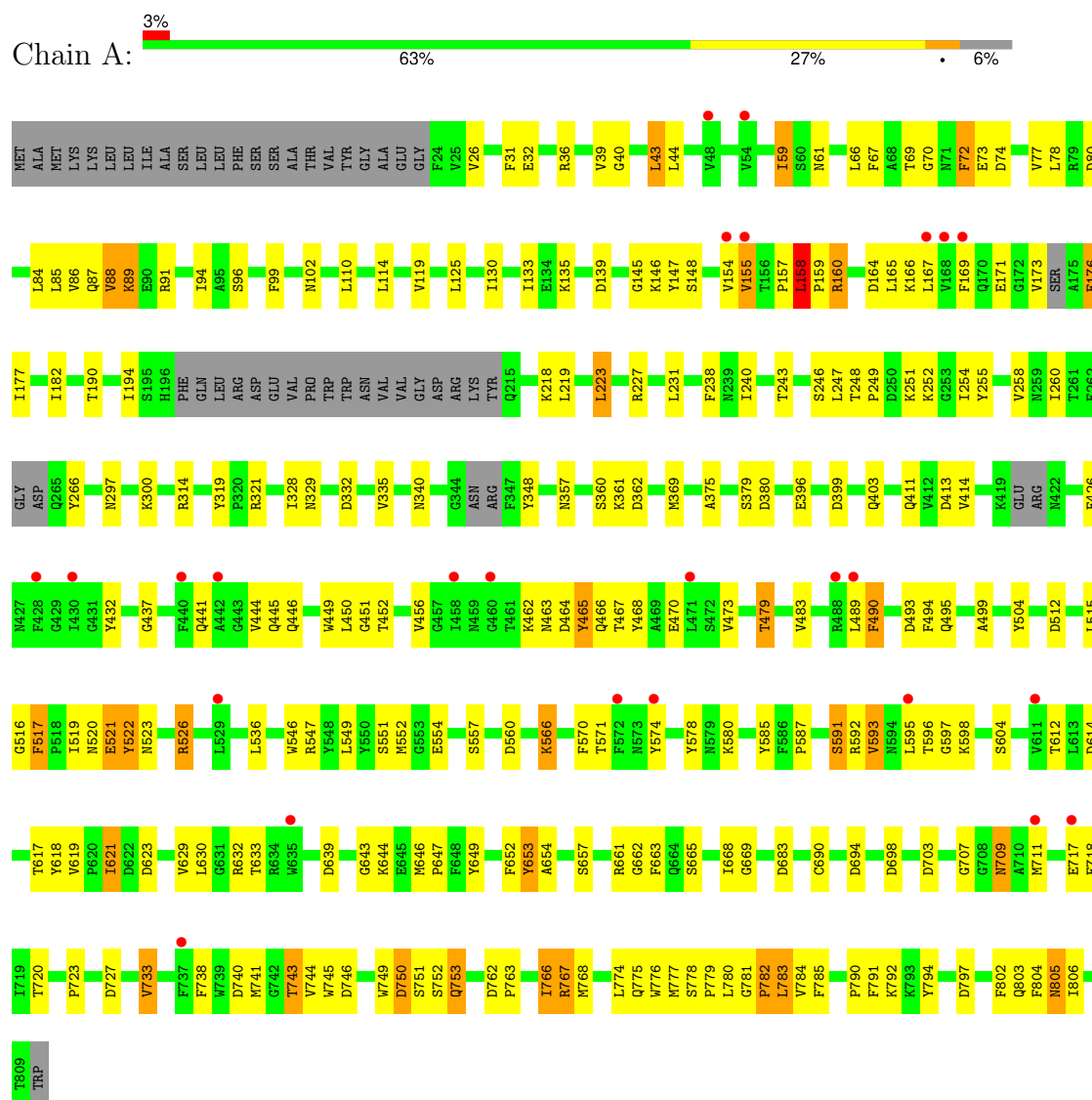
- Molecule 2 is a protein called Outer membrane lipoprotein RcsF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	S	0	0	0
			589	358	107	118	6			
2	D	81	Total	C	N	O	S	0	0	0
			597	364	108	119	6			

3 Residue-property plots

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: Outer membrane protein assembly factor BamA



- Molecule 1: Outer membrane protein assembly factor BamA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.84Å 142.53Å 116.42Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	48.58 – 3.79 48.58 – 3.79	Depositor EDS
% Data completeness (in resolution range)	73.4 (48.58-3.79) 73.3 (48.58-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.281 , 0.317 0.312 , 0.359	Depositor DCC
R_{free} test set	973 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	161.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 193.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10838	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	0.84	1/6122 (0.0%)	1.31	52/8297 (0.6%)
1	B	0.76	0/3762	1.27	30/5114 (0.6%)
2	C	0.96	2/597 (0.3%)	1.42	5/807 (0.6%)
2	D	0.91	1/605 (0.2%)	1.40	5/818 (0.6%)
All	All	0.82	4/11086 (0.0%)	1.31	92/15036 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	766	ILE	CA-C	-6.35	1.45	1.52
2	D	85	ILE	CA-CB	6.06	1.58	1.53
2	C	85	ILE	CA-CB	5.37	1.57	1.53
2	C	79	GLN	CD-OE1	5.11	1.33	1.23

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	660	VAL	N-CA-CB	9.55	122.20	112.65
2	C	84	SER	CA-C-N	8.93	125.87	120.24
2	C	84	SER	C-N-CA	8.93	125.87	120.24
2	D	84	SER	CA-C-N	8.53	125.62	120.24
2	D	84	SER	C-N-CA	8.53	125.62	120.24
1	A	494	PHE	CA-CB-CG	8.25	122.05	113.80
1	B	657	SER	CA-C-N	8.08	131.45	120.38
1	B	657	SER	C-N-CA	8.08	131.45	120.38
1	A	783	LEU	N-CA-C	7.74	120.83	109.07
1	B	735	THR	CB-CA-C	-7.72	97.68	110.19
1	A	61	ASN	N-CA-C	-7.63	102.78	112.93
1	A	657	SER	CA-C-N	7.58	130.77	120.54
1	A	657	SER	C-N-CA	7.58	130.77	120.54
1	A	522	TYR	N-CA-C	-7.46	104.79	114.04
1	B	517	PHE	CA-CB-CG	7.30	121.10	113.80
2	C	98	LYS	N-CA-C	-7.28	104.20	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	98	LYS	N-CA-C	-7.15	104.37	113.23
1	A	782	PRO	CB-CA-C	-6.98	100.65	110.63
1	A	709	ASN	CA-CB-CG	6.85	119.45	112.60
1	B	434	THR	N-CA-C	-6.73	105.06	113.28
1	A	176	GLU	CB-CG-CD	6.64	123.90	112.60
1	A	465	TYR	N-CA-C	6.64	121.33	111.04
2	D	99	MET	N-CA-C	-6.60	105.22	113.28
1	A	490	PHE	N-CA-C	6.60	118.97	109.14
1	B	772	ILE	N-CA-C	6.58	117.96	108.48
1	A	740	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	694	ASP	CA-CB-CG	6.41	119.01	112.60
1	B	733	VAL	N-CA-CB	6.41	121.48	111.99
1	B	732	SER	CB-CA-C	-6.38	100.41	110.94
1	A	751	SER	CA-C-N	6.35	129.08	120.44
1	A	751	SER	C-N-CA	6.35	129.08	120.44
1	B	659	THR	N-CA-C	6.26	124.13	110.80
1	A	139	ASP	CA-CB-CG	6.22	118.82	112.60
2	C	99	MET	N-CA-C	-6.21	105.70	113.28
1	A	177	ILE	N-CA-C	6.21	116.00	108.06
1	B	782	PRO	CB-CA-C	6.18	118.29	111.56
1	B	694	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	723	PRO	N-CA-C	6.05	121.93	113.53
1	A	413	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	463	ASN	CA-CB-CG	5.96	118.56	112.60
1	B	723	PRO	N-CA-C	5.95	121.81	113.53
1	A	479	THR	CA-C-N	5.94	128.91	120.53
1	A	479	THR	C-N-CA	5.94	128.91	120.53
1	B	771	GLY	CA-C-N	5.92	131.24	123.06
1	B	771	GLY	C-N-CA	5.92	131.24	123.06
1	B	490	PHE	N-CA-C	5.85	118.30	109.41
1	A	375	ALA	CA-C-N	5.77	129.30	120.82
1	A	375	ALA	C-N-CA	5.77	129.30	120.82
1	A	80	ASP	N-CA-C	-5.68	101.33	110.14
1	B	643	GLY	N-CA-C	-5.68	107.90	115.40
1	A	155	VAL	CA-C-N	5.67	128.36	120.65
1	A	155	VAL	C-N-CA	5.67	128.36	120.65
1	B	789	GLN	CB-CA-C	5.64	116.12	109.47
1	A	643	GLY	N-CA-C	-5.62	107.98	115.40
1	A	135	LYS	CA-C-N	5.62	126.18	119.94
1	A	135	LYS	C-N-CA	5.62	126.18	119.94
1	A	521	GLU	N-CA-CB	5.62	119.99	110.49
1	A	750	ASP	CA-C-N	5.62	127.81	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	750	ASP	C-N-CA	5.62	127.81	120.28
1	A	733	VAL	N-CA-C	5.60	116.01	108.17
1	A	746	ASP	CA-CB-CG	-5.57	107.03	112.60
2	C	85	ILE	N-CA-CB	5.52	113.98	110.50
1	A	779	PRO	CA-C-N	5.50	128.42	120.38
1	A	779	PRO	C-N-CA	5.50	128.42	120.38
2	D	85	ILE	N-CA-CB	5.46	113.94	110.50
1	A	164	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	520	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	72	PHE	N-CA-C	5.41	117.23	108.41
1	A	74	ASP	CA-CB-CG	5.41	118.00	112.60
1	B	790	PRO	CA-C-N	5.38	127.92	120.29
1	B	790	PRO	C-N-CA	5.38	127.92	120.29
1	A	380	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	648	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	639	ASP	CA-C-N	5.25	125.33	120.34
1	A	639	ASP	C-N-CA	5.25	125.33	120.34
1	B	717	GLU	CB-CA-C	-5.19	100.74	109.50
1	A	36	ARG	CA-C-N	5.15	129.96	123.10
1	A	36	ARG	C-N-CA	5.15	129.96	123.10
1	B	783	LEU	N-CA-C	-5.12	101.36	109.76
1	A	464	ASP	N-CA-C	-5.09	105.19	111.40
1	B	736	SER	N-CA-C	5.08	117.85	109.72
1	B	685	ASP	CA-C-N	5.08	130.88	121.94
1	B	685	ASP	C-N-CA	5.08	130.88	121.94
1	A	797	ASP	CA-CB-CG	5.08	117.67	112.60
1	B	523	ASN	CA-CB-CG	5.07	117.67	112.60
1	B	727	ASP	CA-C-N	5.07	127.32	120.38
1	B	727	ASP	C-N-CA	5.07	127.32	120.38
1	A	743	THR	CA-C-N	5.03	129.95	122.71
1	A	743	THR	C-N-CA	5.03	129.95	122.71
1	A	727	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	158	LEU	CA-C-N	-5.01	114.50	120.11
1	A	158	LEU	C-N-CA	-5.01	114.50	120.11

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	5991	0	5715	182	1
1	B	3661	0	3383	75	0
2	C	589	0	579	15	0
2	D	597	0	590	17	0
All	All	10838	0	10267	266	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 13.

All (266) 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:566:LYS:HD2	1:A:566:LYS:O	1.31	1.22
1:A:462:LYS:CD	1:A:467:THR:HG22	1.76	1.15
1:B:488:ARG:NH1	2:D:81:SER:HA	1.60	1.14
1:A:462:LYS:HD3	1:A:467:THR:HG22	1.15	1.11
1:A:158:LEU:HB3	1:A:159:PRO:HD2	1.35	1.09
1:A:632:ARG:HD3	2:C:116:PRO:HB3	1.33	1.06
1:A:462:LYS:HD3	1:A:467:THR:CG2	1.85	1.04
1:A:566:LYS:O	1:A:566:LYS:CD	2.05	1.03
1:A:219:LEU:O	1:A:219:LEU:HD12	1.58	1.03
1:A:157:PRO:C	1:A:158:LEU:HD23	1.86	1.00
1:A:146:LYS:HE2	1:A:173:VAL:HG22	1.45	0.99
1:B:632:ARG:HD2	2:D:116:PRO:HB3	1.41	0.98
1:B:479:THR:HG22	1:B:480:VAL:H	1.28	0.98
1:A:157:PRO:O	1:A:158:LEU:HD22	1.61	0.97
1:A:783:LEU:HD13	1:A:806:ILE:HG13	1.45	0.96
1:A:110:LEU:HD21	1:A:169:PHE:CZ	2.02	0.93
1:A:632:ARG:HD3	2:C:116:PRO:CB	1.97	0.93
1:A:40:GLY:HA2	1:A:43:LEU:HD23	1.50	0.91
1:A:557:SER:HB3	1:A:560:ASP:OD1	1.70	0.91
1:A:157:PRO:C	1:A:158:LEU:CD2	2.43	0.91
1:A:158:LEU:HB3	1:A:159:PRO:CD	2.01	0.89
1:B:462:LYS:HD3	1:B:467:THR:HB	1.52	0.89
1:A:157:PRO:O	1:A:158:LEU:CD2	2.24	0.86
1:B:488:ARG:HH12	2:D:81:SER:HA	1.40	0.86
1:B:479:THR:CG2	1:B:480:VAL:H	1.89	0.85
1:B:488:ARG:HH11	2:D:81:SER:HA	1.40	0.83
1:B:479:THR:HG22	1:B:480:VAL:N	1.92	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:LYS:HE2	2:C:94:ILE:HD11	1.63	0.80
1:A:146:LYS:HE2	1:A:173:VAL:CG2	2.13	0.79
1:A:219:LEU:CD1	1:A:223:LEU:HD23	2.12	0.79
1:A:750:ASP:OD2	1:A:753:GLN:HB2	1.84	0.78
1:A:125:LEU:CD2	1:A:165:LEU:HD12	2.13	0.78
2:D:90:LYS:HE2	2:D:94:ILE:HD11	1.64	0.78
1:A:219:LEU:HD13	1:A:223:LEU:HD23	1.67	0.77
1:A:155:VAL:O	1:A:155:VAL:HG12	1.86	0.76
1:A:462:LYS:CD	1:A:467:THR:CG2	2.55	0.75
1:A:783:LEU:HD12	1:A:784:VAL:H	1.50	0.75
1:A:462:LYS:HD2	1:A:467:THR:HG22	1.69	0.75
1:A:632:ARG:NH2	1:A:661:ARG:NH1	2.37	0.73
1:A:652:PHE:HB3	1:A:711:MET:HE3	1.69	0.73
1:A:467:THR:OG1	1:A:493:ASP:HB3	1.90	0.71
1:B:441:GLN:HE21	1:B:461:THR:HG23	1.55	0.71
1:A:465:TYR:HD1	1:A:466:GLN:H	1.37	0.71
1:A:767:ARG:HD2	1:A:794:TYR:HD2	1.56	0.70
1:B:478:PHE:HB3	1:B:483:VAL:HG13	1.73	0.70
1:A:630:LEU:HB3	1:A:717:GLU:HB2	1.74	0.69
1:A:73:GLU:HG3	1:A:91:ARG:HA	1.75	0.68
2:C:95:ASN:O	2:C:99:MET:HG2	1.93	0.68
1:B:770:ALA:HB3	1:B:791:PHE:CE1	2.28	0.68
1:A:450:LEU:O	1:A:450:LEU:HG	1.94	0.67
1:A:125:LEU:CD2	1:A:165:LEU:CD1	2.72	0.67
1:A:154:VAL:HB	1:A:166:LYS:HB3	1.75	0.67
1:A:99:PHE:HE1	1:A:167:LEU:HD12	1.59	0.67
1:B:630:LEU:HB3	1:B:717:GLU:HB2	1.77	0.66
1:A:247:LEU:HD21	1:A:254:ILE:HG12	1.77	0.66
1:A:247:LEU:CD2	1:A:254:ILE:HG12	2.25	0.66
1:A:536:LEU:HD11	1:A:649:TYR:CE1	2.30	0.66
1:A:77:VAL:O	1:A:78:LEU:HD23	1.96	0.65
1:A:125:LEU:HD22	1:A:165:LEU:HD12	1.78	0.65
1:A:805:ASN:HB3	2:C:113:SER:CB	2.27	0.65
1:A:125:LEU:HD22	1:A:165:LEU:CD1	2.27	0.65
1:B:738:PHE:CE2	1:B:773:ALA:HB2	2.33	0.64
1:A:805:ASN:HB3	2:C:113:SER:HB2	1.79	0.64
1:B:475:ASN:H	1:B:485:LEU:HB3	1.62	0.64
1:B:479:THR:CG2	1:B:480:VAL:N	2.57	0.64
1:A:632:ARG:NH2	1:A:717:GLU:OE1	2.31	0.64
1:B:766:ILE:HG21	1:B:768:MET:HE2	1.79	0.63
1:B:468:TYR:HE1	1:B:490:PHE:HB2	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HG	1:B:450:LEU:O	1.97	0.63
1:A:227:ARG:HG2	1:A:238:PHE:HE2	1.64	0.63
1:A:246:SER:O	1:A:247:LEU:HD23	2.00	0.61
1:A:557:SER:HB3	1:A:560:ASP:CG	2.24	0.61
1:A:102:ASN:HA	1:A:171:GLU:OE2	2.00	0.61
1:A:574:TYR:CZ	1:A:597:GLY:HA3	2.36	0.60
1:B:488:ARG:HH12	2:D:81:SER:CA	2.13	0.60
1:A:357:ASN:HD21	1:A:362:ASP:CG	2.09	0.60
1:B:766:ILE:HG21	1:B:768:MET:CE	2.31	0.60
1:A:99:PHE:CE1	1:A:167:LEU:HD12	2.38	0.59
1:A:176:GLU:O	1:A:254:ILE:HB	2.02	0.59
1:A:566:LYS:HD2	1:A:566:LYS:C	2.24	0.58
1:B:488:ARG:HH11	2:D:82:PRO:HD3	1.68	0.58
1:A:711:MET:HG3	1:A:744:VAL:HG22	1.84	0.58
1:A:467:THR:HG1	1:A:493:ASP:HB3	1.67	0.58
1:B:439:SER:HB2	1:B:441:GLN:HE22	1.69	0.57
1:B:520:ASN:HB3	1:B:523:ASN:HD22	1.67	0.57
1:B:571:THR:HG21	1:B:598:LYS:HD3	1.85	0.57
1:A:519:ILE:HD11	1:B:627:TRP:CZ3	2.39	0.57
1:A:571:THR:HG21	1:A:598:LYS:HD3	1.85	0.57
1:B:591:SER:HB3	1:B:617:THR:HG23	1.85	0.57
1:B:782:PRO:HG2	2:D:111:VAL:O	2.05	0.57
1:B:743:THR:OG1	1:B:766:ILE:HA	2.06	0.56
1:A:468:TYR:HE1	1:A:490:PHE:HB2	1.71	0.56
1:A:566:LYS:CD	1:A:566:LYS:C	2.79	0.55
1:A:591:SER:HB3	1:A:617:THR:HG23	1.87	0.55
1:A:782:PRO:HD3	2:C:110:GLU:HB3	1.89	0.55
1:A:445:GLN:HE21	2:C:86:PRO:HG2	1.71	0.55
1:B:467:THR:HG22	1:B:493:ASP:HB3	1.90	0.54
1:B:522:TYR:HE1	1:B:578:TYR:CE2	2.26	0.54
2:D:69:VAL:HG21	2:D:96:ALA:HB2	1.89	0.54
1:A:155:VAL:HG22	1:A:165:LEU:HG	1.88	0.54
1:A:465:TYR:HD2	1:A:499:ALA:HA	1.72	0.54
2:C:69:VAL:HG21	2:C:96:ALA:HB2	1.89	0.54
1:A:632:ARG:HH22	1:A:661:ARG:NH1	2.04	0.54
1:A:147:TYR:HE2	1:A:254:ILE:HD11	1.73	0.53
1:A:247:LEU:HD23	1:A:254:ILE:HA	1.89	0.53
1:A:632:ARG:NH2	1:A:661:ARG:HH12	2.07	0.53
1:B:531:TYR:CD1	1:B:570:PHE:HD1	2.27	0.53
1:A:432:TYR:HA	1:A:437:GLY:O	2.08	0.53
1:A:662:GLY:O	1:A:790:PRO:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:GLN:HA	1:A:783:LEU:O	2.08	0.53
1:A:190:THR:O	1:A:194:ILE:HG12	2.09	0.53
1:A:85:LEU:HG	1:A:86:VAL:N	2.23	0.52
1:A:70:GLY:HA2	1:A:91:ARG:HH21	1.74	0.52
1:A:768:MET:HB2	1:A:791:PHE:CE2	2.44	0.52
1:A:632:ARG:HH22	1:A:661:ARG:CZ	2.23	0.52
1:A:158:LEU:HD23	1:A:158:LEU:N	2.23	0.52
1:A:547:ARG:HH22	1:A:749:TRP:HE3	1.58	0.52
1:A:783:LEU:HD21	1:A:785:PHE:HE1	1.75	0.52
1:A:778:SER:OG	1:A:780:LEU:HD12	2.09	0.52
1:A:248:THR:HB	1:A:249:PRO:HD2	1.92	0.51
1:A:653:TYR:CD2	1:A:707:GLY:HA3	2.45	0.51
1:A:632:ARG:CD	2:C:116:PRO:HB3	2.23	0.51
1:A:319:TYR:HB3	1:A:321:ARG:HH11	1.75	0.51
1:B:668:ILE:HG23	1:B:767:ARG:HD3	1.92	0.51
1:B:785:PHE:O	1:B:785:PHE:CD1	2.63	0.51
1:A:32:GLU:HG3	1:A:85:LEU:HD11	1.91	0.51
1:B:738:PHE:HE2	1:B:773:ALA:HB2	1.75	0.51
1:A:781:GLY:HA2	2:C:110:GLU:CD	2.36	0.51
1:B:732:SER:HB2	1:B:777:MET:HB2	1.92	0.51
1:A:227:ARG:HG3	1:A:240:ILE:HD12	1.92	0.51
1:A:158:LEU:CB	1:A:159:PRO:CD	2.85	0.51
1:B:478:PHE:HB2	1:B:485:LEU:HB2	1.93	0.50
1:B:659:THR:O	1:B:740:ASP:OD2	2.29	0.50
1:A:69:THR:HG21	1:A:72:PHE:CE1	2.47	0.50
1:A:99:PHE:HD1	1:A:167:LEU:HB2	1.77	0.50
1:B:456:VAL:HG12	1:B:473:VAL:HG22	1.94	0.50
1:A:72:PHE:CD2	1:A:88:VAL:HB	2.48	0.49
1:A:99:PHE:CG	1:A:110:LEU:HD23	2.46	0.49
1:A:114:LEU:HB3	1:A:119:VAL:HG13	1.94	0.49
1:A:711:MET:CG	1:A:744:VAL:HG22	2.42	0.49
1:B:784:VAL:CG2	1:B:805:ASN:HB3	2.43	0.49
1:A:176:GLU:OE1	1:A:252:LYS:HB2	2.13	0.49
1:A:456:VAL:HG12	1:A:473:VAL:HG22	1.95	0.49
1:A:711:MET:HB2	1:A:744:VAL:HG13	1.94	0.49
1:B:470:GLU:OE2	2:D:82:PRO:HG3	2.13	0.49
1:A:148:SER:N	1:A:251:LYS:HB3	2.27	0.49
1:A:782:PRO:HG3	2:C:111:VAL:O	2.13	0.49
1:A:446:GLN:HB3	1:A:449:TRP:HB2	1.95	0.48
1:A:621:ILE:CD1	1:A:718:PHE:HE1	2.25	0.48
1:B:446:GLN:HB3	1:B:449:TRP:HB2	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLY:HA2	1:A:43:LEU:CD2	2.35	0.48
1:A:767:ARG:HD2	1:A:794:TYR:CD2	2.44	0.48
1:A:803:GLN:O	1:A:804:PHE:HB3	2.13	0.48
1:A:774:LEU:O	1:A:784:VAL:HA	2.13	0.48
1:A:66:LEU:O	1:A:69:THR:HG22	2.14	0.48
1:A:158:LEU:CD2	1:A:158:LEU:N	2.72	0.48
1:B:283:GLU:O	1:B:286:GLN:NE2	2.47	0.48
1:B:653:TYR:CD2	1:B:707:GLY:HA3	2.48	0.48
1:A:536:LEU:HD21	1:A:649:TYR:CD1	2.48	0.48
1:B:717:GLU:HG2	1:B:738:PHE:HB3	1.96	0.47
2:C:105:LEU:HB2	2:C:129:LEU:HD11	1.95	0.47
1:A:552:MET:HA	1:A:644:LYS:HE2	1.96	0.47
1:A:110:LEU:HD21	1:A:169:PHE:HZ	1.72	0.47
1:A:745:TRP:CE2	1:A:763:PRO:HB3	2.49	0.47
1:B:592:ARG:HH12	2:D:121:GLN:NE2	2.12	0.47
2:D:105:LEU:HB2	2:D:129:LEU:HD11	1.96	0.47
1:A:504:TYR:OH	1:A:649:TYR:HA	2.14	0.47
1:A:776:TRP:HD1	1:A:777:MET:H	1.63	0.47
1:B:475:ASN:O	1:B:484:SER:HA	2.13	0.47
1:A:94:ILE:HD11	1:A:125:LEU:HB2	1.97	0.47
1:B:621:ILE:CD1	1:B:718:PHE:HE1	2.27	0.47
1:A:361:LYS:HG2	1:A:451:GLY:HA3	1.96	0.46
1:A:426:PHE:HD1	1:A:444:VAL:HG23	1.79	0.46
1:A:570:PHE:H	1:A:604:SER:HB3	1.79	0.46
1:B:552:MET:HA	1:B:644:LYS:HE2	1.96	0.46
1:B:576:TRP:HE1	1:B:578:TYR:HD1	1.62	0.46
1:A:783:LEU:HD13	1:A:806:ILE:CG1	2.32	0.46
1:A:158:LEU:CB	1:A:159:PRO:HD2	2.25	0.46
1:A:246:SER:HB2	1:A:255:TYR:HB2	1.96	0.46
1:B:613:LEU:HB2	1:B:635:TRP:HB2	1.97	0.46
1:A:717:GLU:HG2	1:A:738:PHE:HB3	1.96	0.46
1:A:743:THR:OG1	1:A:766:ILE:HA	2.15	0.46
1:A:462:LYS:HD3	1:A:467:THR:HG21	1.91	0.45
1:A:783:LEU:CD1	1:A:784:VAL:H	2.25	0.45
1:A:551:SER:HB3	1:A:644:LYS:HA	1.99	0.45
1:B:587:PRO:HG2	1:B:618:TYR:CZ	2.52	0.45
1:A:125:LEU:HD21	1:A:165:LEU:CD1	2.46	0.45
1:A:26:VAL:HG21	1:A:84:LEU:HD22	1.98	0.45
1:A:587:PRO:HG2	1:A:618:TYR:CZ	2.52	0.45
1:B:570:PHE:H	1:B:604:SER:HB3	1.81	0.45
1:B:435:GLU:OE1	1:B:805:ASN:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:CD2	1:A:254:ILE:CG1	2.95	0.45
1:A:59:ILE:HD13	1:A:78:LEU:CD2	2.47	0.44
1:B:518:PRO:HG2	2:D:90:LYS:HE3	1.99	0.44
1:A:148:SER:O	1:A:251:LYS:CE	2.65	0.44
1:A:182:ILE:CG2	1:A:260:ILE:HD12	2.47	0.44
1:A:465:TYR:O	1:A:495:GLN:NE2	2.50	0.44
1:B:515:LEU:O	1:B:515:LEU:HD12	2.18	0.44
1:B:488:ARG:HH11	2:D:82:PRO:CD	2.30	0.44
2:D:56:GLU:HA	2:D:59:VAL:HG23	1.99	0.44
1:A:72:PHE:N	1:A:72:PHE:CD1	2.84	0.44
1:A:523:ASN:ND2	1:A:578:TYR:HD2	2.16	0.44
1:A:238:PHE:CE1	1:A:260:ILE:HG23	2.52	0.44
1:A:515:LEU:HB3	1:A:517:PHE:HE1	1.83	0.44
1:A:632:ARG:HH21	1:A:661:ARG:HH12	1.65	0.44
1:A:647:PRO:HB3	1:A:649:TYR:CE1	2.52	0.44
1:B:467:THR:CG2	1:B:493:ASP:HB3	2.48	0.44
1:A:147:TYR:H	1:A:251:LYS:HB2	1.83	0.43
1:A:219:LEU:O	1:A:219:LEU:CD1	2.48	0.43
1:A:783:LEU:HD12	1:A:805:ASN:O	2.19	0.43
1:A:593:VAL:HA	1:A:614:ASP:O	2.17	0.43
1:A:663:PHE:CG	1:A:668:ILE:HD11	2.53	0.43
1:A:77:VAL:O	1:A:78:LEU:CD2	2.64	0.43
1:A:297:ASN:HB3	1:A:300:LYS:HD2	2.01	0.43
1:B:617:THR:O	1:B:630:LEU:HD12	2.19	0.43
1:B:297:ASN:HB3	1:B:300:LYS:HD2	2.01	0.43
1:A:546:TRP:HA	1:A:549:LEU:HD12	2.00	0.43
1:A:762:ASP:HA	1:A:763:PRO:HD3	1.93	0.43
1:A:632:ARG:HH21	1:A:661:ARG:NH1	2.15	0.43
1:A:130:ILE:HA	1:A:133:ILE:HD12	2.01	0.43
1:A:266:TYR:OH	1:A:328:ILE:HG23	2.17	0.43
1:A:328:ILE:HA	1:A:335:VAL:HG22	2.01	0.43
1:A:654:ALA:HB3	1:A:668:ILE:HB	2.01	0.43
1:A:669:GLY:H	1:A:767:ARG:NH2	2.17	0.43
1:A:784:VAL:O	1:A:804:PHE:CB	2.67	0.43
1:A:73:GLU:N	1:A:89:LYS:O	2.51	0.42
1:B:647:PRO:HB3	1:B:649:TYR:CE1	2.54	0.42
1:A:148:SER:O	1:A:251:LYS:HE3	2.20	0.42
1:B:286:GLN:HE21	1:B:286:GLN:HB3	1.61	0.42
2:C:56:GLU:HA	2:C:59:VAL:HG23	2.01	0.42
1:A:348:TYR:HB2	1:A:411:GLN:HG2	2.02	0.42
1:B:551:SER:HB3	1:B:644:LYS:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:MET:HE1	1:A:709:ASN:HA	2.01	0.42
1:B:477:TYR:HB2	1:B:482:GLY:HA2	2.01	0.42
1:B:654:ALA:HB3	1:B:668:ILE:HB	2.01	0.42
1:A:86:VAL:HG12	1:A:88:VAL:HG12	2.00	0.42
1:A:243:THR:HG22	1:A:258:VAL:HG23	2.02	0.42
1:B:454:TYR:CD1	1:B:475:ASN:HB2	2.55	0.42
1:A:426:PHE:CD1	1:A:444:VAL:HG23	2.54	0.42
1:A:741:MET:HA	1:A:767:ARG:O	2.19	0.42
1:B:632:ARG:HD2	2:D:116:PRO:CB	2.31	0.42
1:B:477:TYR:O	1:B:477:TYR:CG	2.73	0.41
1:A:783:LEU:HG	1:A:784:VAL:N	2.34	0.41
1:A:520:ASN:C	1:A:522:TYR:H	2.29	0.41
1:B:431:GLY:HA3	1:B:806:ILE:O	2.20	0.41
1:B:729:TYR:HD1	1:B:729:TYR:HA	1.79	0.41
1:A:516:GLY:HA2	1:A:526:ARG:HA	2.03	0.41
1:A:72:PHE:HD2	1:A:88:VAL:HB	1.84	0.41
1:A:40:GLY:O	1:A:43:LEU:HG	2.21	0.41
1:A:147:TYR:HB2	1:A:251:LYS:HA	2.02	0.41
1:A:785:PHE:CD2	1:A:802:PHE:CE2	3.09	0.41
1:B:741:MET:SD	1:B:768:MET:CE	3.08	0.41
1:A:85:LEU:HD21	1:A:87:GLN:HG2	2.03	0.41
1:A:595:LEU:HD23	1:A:596:THR:N	2.36	0.41
1:A:617:THR:O	1:A:630:LEU:HD12	2.21	0.41
1:B:592:ARG:HH22	2:D:121:GLN:HE22	1.68	0.41
1:B:776:TRP:HD1	1:B:777:MET:N	2.19	0.41
1:A:85:LEU:HD23	1:A:87:GLN:HG3	2.02	0.41
1:B:535:SER:HB2	1:B:566:LYS:HG2	2.03	0.41
1:A:314:ARG:HA	1:A:379:SER:HB3	2.02	0.40
1:B:767:ARG:HD2	1:B:767:ARG:N	2.36	0.40
2:C:91:ARG:HA	2:C:94:ILE:HD12	2.03	0.40
1:A:31:PHE:CE2	1:A:39:VAL:HG13	2.56	0.40
1:A:784:VAL:O	1:A:804:PHE:HB2	2.21	0.40
1:A:783:LEU:CG	1:A:784:VAL:N	2.84	0.40
1:B:328:ILE:HA	1:B:335:VAL:HG22	2.03	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)
1:A:160:ARG:O	1:A:698:ASP:OD2[4_446]	2.17	0.03

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	749/810 (92%)	685 (92%)	61 (8%)	3 (0%)	30	62
1	B	462/810 (57%)	419 (91%)	41 (9%)	2 (0%)	30	62
2	C	78/134 (58%)	70 (90%)	6 (8%)	2 (3%)	4	27
2	D	79/134 (59%)	70 (89%)	7 (9%)	2 (2%)	4	28
All	All	1368/1888 (72%)	1244 (91%)	115 (8%)	9 (1%)	18	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	GLY
1	A	160	ARG
2	C	100	LYS
2	C	117	GLY
2	D	100	LYS
1	A	158	LEU
1	B	519	ILE
2	D	117	GLY
1	B	482	GLY

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	646/688 (94%)	591 (92%)	55 (8%)	10	33
1	B	389/688 (56%)	354 (91%)	35 (9%)	9	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	66/111 (60%)	63 (96%)	3 (4%)	24	48
2	D	67/111 (60%)	64 (96%)	3 (4%)	24	48
All	All	1168/1598 (73%)	1072 (92%)	96 (8%)	10	35

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LEU
1	A	59	ILE
1	A	67	PHE
1	A	88	VAL
1	A	89	LYS
1	A	96	SER
1	A	158	LEU
1	A	218	LYS
1	A	223	LEU
1	A	231	LEU
1	A	329	ASN
1	A	332	ASP
1	A	340	ASN
1	A	360	SER
1	A	369	MET
1	A	396	GLU
1	A	399	ASP
1	A	403	GLN
1	A	414	VAL
1	A	441	GLN
1	A	452	THR
1	A	470	GLU
1	A	479	THR
1	A	483	VAL
1	A	489	LEU
1	A	512	ASP
1	A	517	PHE
1	A	521	GLU
1	A	526	ARG
1	A	554	GLU
1	A	566	LYS
1	A	580	LYS
1	A	585	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	591	SER
1	A	592	ARG
1	A	593	VAL
1	A	612	THR
1	A	619	VAL
1	A	621	ILE
1	A	623	ASP
1	A	629	VAL
1	A	633	THR
1	A	653	TYR
1	A	665	SER
1	A	683	ASP
1	A	690	CYS
1	A	703	ASP
1	A	720	THR
1	A	733	VAL
1	A	752	SER
1	A	753	GLN
1	A	767	ARG
1	A	792	LYS
1	A	805	ASN
1	B	286	GLN
1	B	321	ARG
1	B	329	ASN
1	B	332	ASP
1	B	340	ASN
1	B	489	LEU
1	B	500	ASP
1	B	517	PHE
1	B	519	ILE
1	B	521	GLU
1	B	523	ASN
1	B	578	TYR
1	B	580	LYS
1	B	585	TYR
1	B	591	SER
1	B	593	VAL
1	B	595	LEU
1	B	619	VAL
1	B	621	ILE
1	B	623	ASP
1	B	629	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	632	ARG
1	B	633	THR
1	B	639	ASP
1	B	653	TYR
1	B	665	SER
1	B	683	ASP
1	B	690	CYS
1	B	720	THR
1	B	729	TYR
1	B	733	VAL
1	B	749	TRP
1	B	762	ASP
1	B	774	LEU
1	B	795	ASP
2	C	90	LYS
2	C	95	ASN
2	C	104	VAL
2	D	90	LYS
2	D	95	ASN
2	D	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	244	GLN
1	A	357	ASN
1	A	411	GLN
1	A	422	ASN
1	A	445	GLN
1	A	448	ASN
1	A	466	GLN
1	A	492	ASN
1	A	523	ASN
1	A	538	ASN
1	A	677	HIS
1	A	709	ASN
1	A	731	ASN
1	A	801	GLN
1	B	286	GLN
1	B	441	GLN
1	B	520	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	523	ASN
1	B	533	HIS
1	B	538	ASN
1	B	561	GLN
1	B	677	HIS
1	B	731	ASN
2	C	78	ASN
2	C	121	GLN
2	D	95	ASN
2	D	121	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 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	761/810 (93%)	-0.10	25 (3%) 49 34	49, 160, 295, 300	0
1	B	466/810 (57%)	0.05	19 (4%) 41 30	101, 227, 277, 300	0
2	C	80/134 (59%)	-0.08	1 (1%) 75 53	102, 206, 283, 296	0
2	D	81/134 (60%)	-0.07	1 (1%) 76 54	188, 254, 297, 300	0
All	All	1388/1888 (73%)	-0.05	46 (3%) 49 34	49, 202, 293, 300	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	LEU	7.4
1	B	471	LEU	6.2
1	B	593	VAL	4.3
1	B	739	TRP	4.3
1	A	48	VAL	4.0
1	A	458	ILE	3.7
1	B	611	VAL	3.7
1	B	685	ASP	3.6
1	A	489	LEU	3.5
2	C	111	VAL	3.5
1	A	460	GLY	3.4
1	A	430	ILE	3.3
1	B	296	TYR	3.3
1	B	684	PRO	3.2
1	A	529	LEU	3.1
1	A	428	PHE	3.0
1	B	458	ILE	3.0
1	B	428	PHE	3.0
1	A	635	TRP	2.9
1	A	711	MET	2.8
1	A	440	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	574	TYR	2.8
1	A	611	VAL	2.7
1	A	169	PHE	2.7
1	A	168	VAL	2.7
1	A	595	LEU	2.6
2	D	114	GLY	2.6
1	B	599	VAL	2.5
1	B	525	LEU	2.4
1	A	54	VAL	2.3
1	A	572	PHE	2.3
1	A	574	TYR	2.3
1	B	613	LEU	2.3
1	A	167	LEU	2.3
1	B	529	LEU	2.2
1	A	717	GLU	2.2
1	B	597	GLY	2.2
1	B	716	LEU	2.2
1	A	442	ALA	2.2
1	A	737	PHE	2.2
1	B	456	VAL	2.2
1	A	155	VAL	2.1
1	B	444	VAL	2.1
1	A	488	ARG	2.1
1	B	770	ALA	2.0
1	A	154	VAL	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.