



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 01:55 PM EDT

PDB ID : 5I5F
Title : Salmonella global domain 191
Authors : Dong, C.; Dong, H.
Deposited on : 2016-02-15
Resolution : 1.84 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

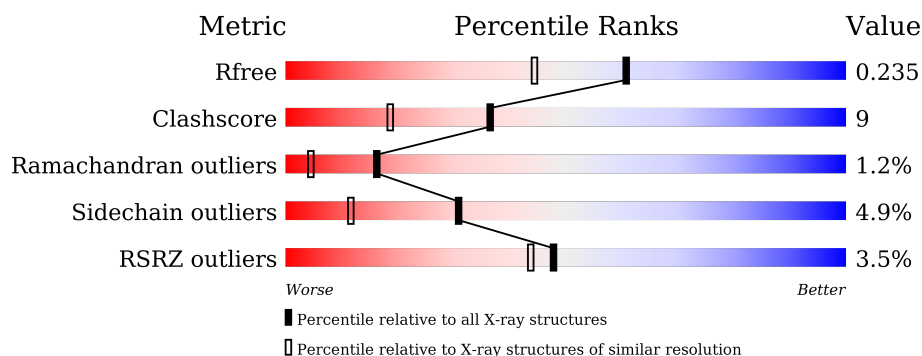
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	91344	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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. 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	586	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>10%</div> <div>••</div> <div>42%</div> </div> </div>
1	B	586	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>9%</div> <div>••</div> <div>42%</div> </div> </div>
1	C	586	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>9%</div> <div>•</div> <div>42%</div> </div> </div>
1	D	586	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>8%</div> <div>•</div> <div>42%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11684 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 Inner membrane protein YejM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			
1	B	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			
1	C	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			
1	D	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			

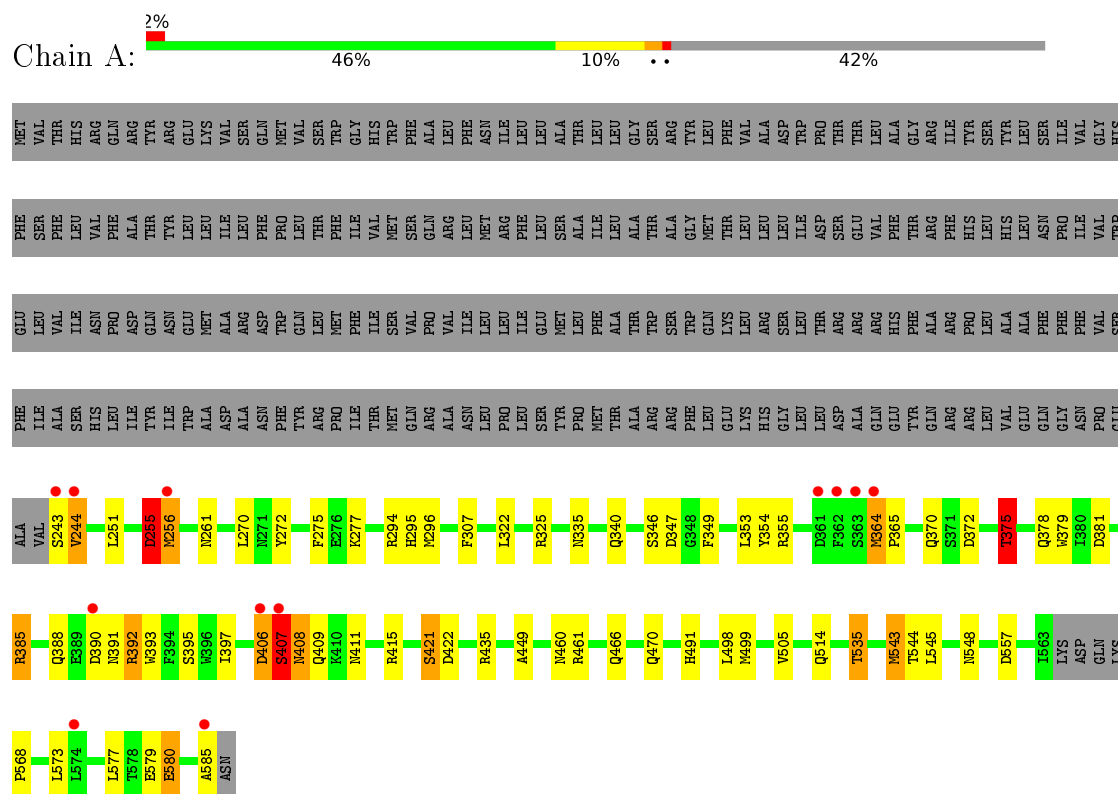
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	285	Total	O	0	0
			285	285		
2	B	187	Total	O	0	0
			187	187		
2	C	253	Total	O	0	0
			253	253		
2	D	235	Total	O	0	0
			235	235		

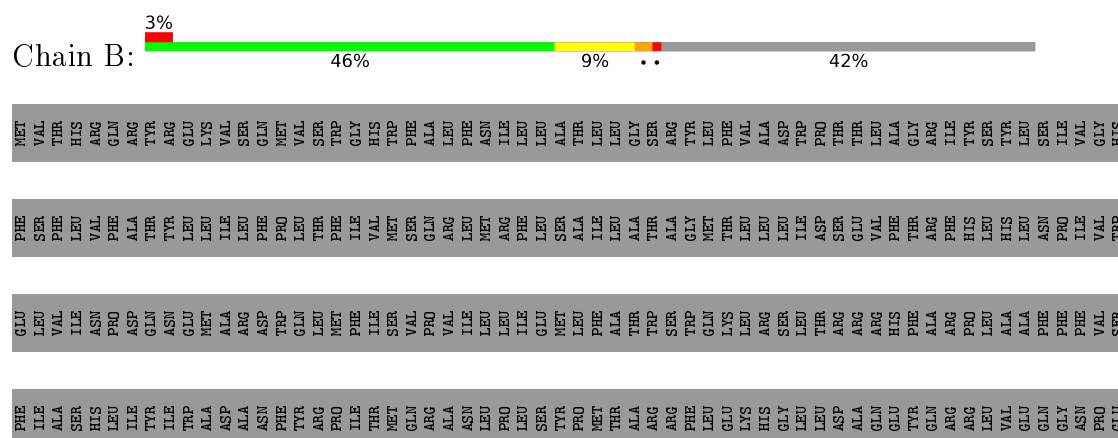
3 Residue-property plots [i](#)

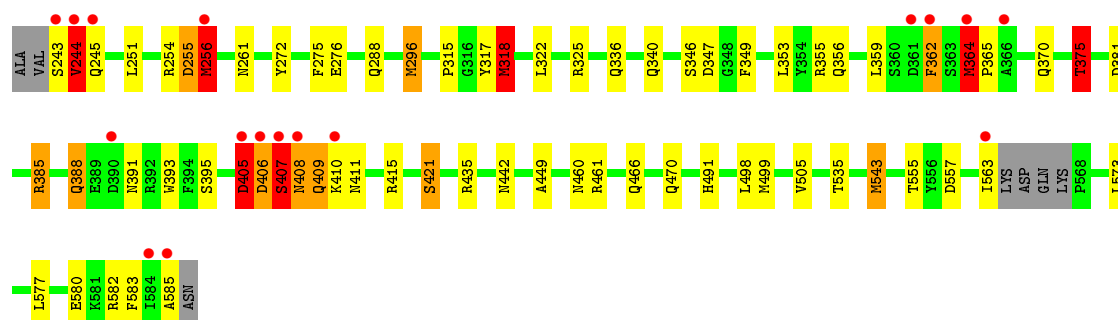
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Inner membrane protein YejM

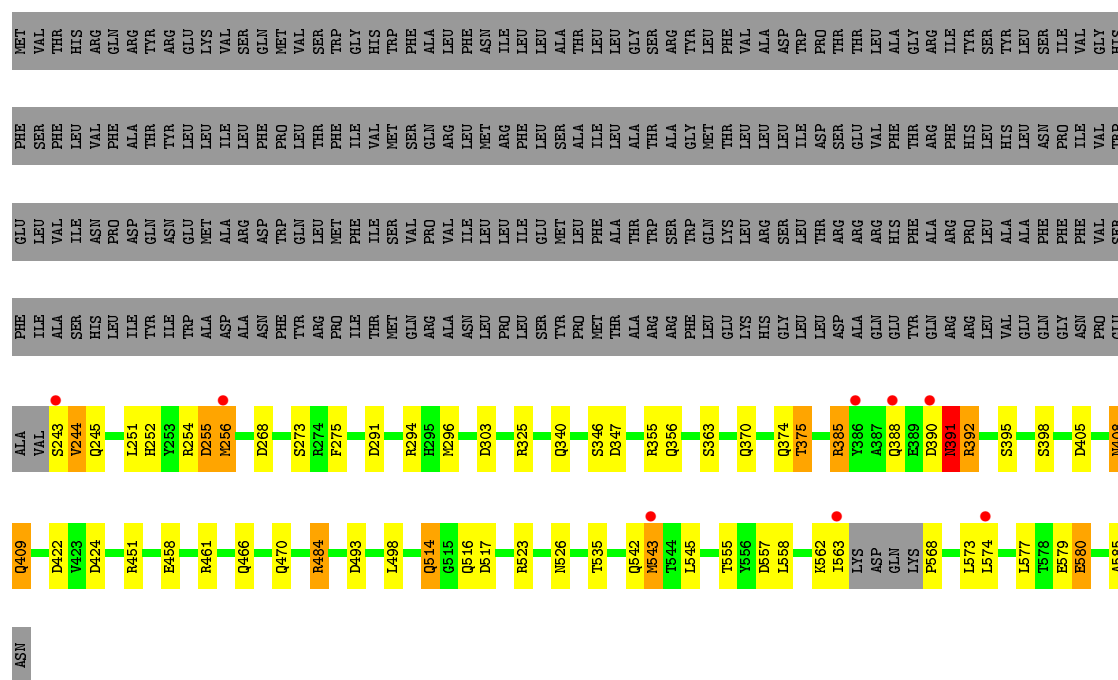


• Molecule 1: Inner membrane protein YejM

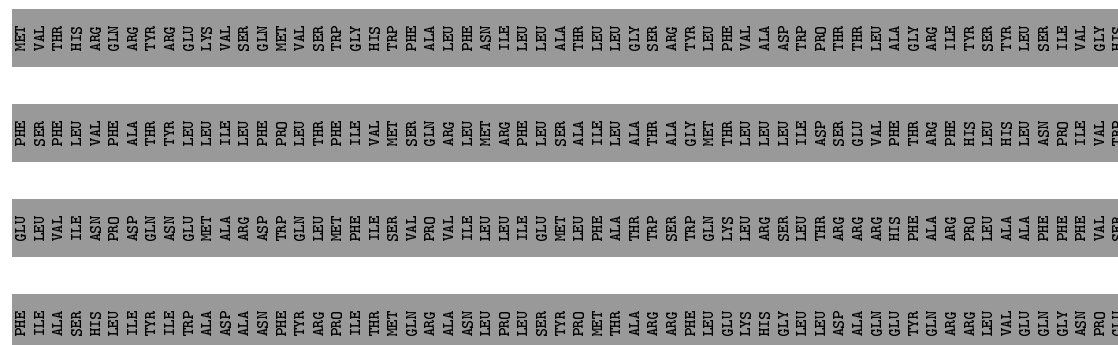


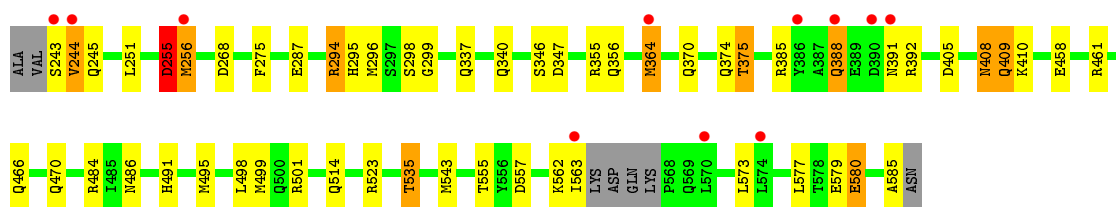


• Molecule 1: Inner membrane protein YejM



• Molecule 1: Inner membrane protein YejM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.57Å 195.88Å 70.09Å 90.00° 95.75° 90.00°	Depositor
Resolution (Å)	65.70 – 1.84 65.70 – 1.84	Depositor EDS
% Data completeness (in resolution range)	86.2 (65.70-1.84) 86.2 (65.70-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.244 0.171 , 0.235	Depositor DCC
R_{free} test set	5005 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.911	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	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	0.97	EDS
Total number of atoms	11684	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.82 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.8717e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	1.28	11/2744 (0.4%)	1.09	22/3738 (0.6%)
1	B	1.71	12/2744 (0.4%)	1.57	26/3738 (0.7%)
1	C	1.34	6/2744 (0.2%)	1.17	25/3738 (0.7%)
1	D	1.19	6/2744 (0.2%)	1.24	20/3738 (0.5%)
All	All	1.40	35/10976 (0.3%)	1.28	93/14952 (0.6%)

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
1	B	0	4
1	C	0	1
1	D	0	2
All	All	0	7

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	ASP	C-N	-49.91	0.19	1.34
1	B	317	TYR	C-N	-42.27	0.36	1.34
1	C	255	ASP	C-N	-33.40	0.57	1.34
1	B	256	MET	C-N	-31.93	0.75	1.33
1	A	255	ASP	C-N	-31.48	0.61	1.34
1	C	256	MET	C-N	-29.24	0.80	1.33
1	D	256	MET	C-N	-29.21	0.80	1.33
1	D	364	MET	C-N	-15.19	1.05	1.34
1	D	255	ASP	C-N	-13.43	1.03	1.34
1	B	498	LEU	C-N	-13.16	1.03	1.34
1	A	256	MET	C-N	-10.96	1.13	1.33
1	A	421	SER	CB-OG	-10.62	1.28	1.42
1	A	498	LEU	C-N	-9.73	1.11	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	SER	CB-OG	-8.41	1.31	1.42
1	D	498	LEU	C-N	-8.13	1.15	1.34
1	A	395	SER	CB-OG	-7.92	1.31	1.42
1	B	296	MET	C-N	-7.17	1.17	1.34
1	B	276	GLU	CD-OE2	-6.99	1.18	1.25
1	B	395	SER	CB-OG	-6.28	1.34	1.42
1	D	299	GLY	N-CA	6.25	1.55	1.46
1	B	318	MET	C-N	-6.17	1.19	1.34
1	A	307	PHE	CG-CD2	5.95	1.47	1.38
1	A	375	THR	CB-CG2	-5.93	1.32	1.52
1	D	298	SER	CB-OG	5.88	1.49	1.42
1	C	395	SER	CB-OG	-5.72	1.34	1.42
1	B	272	TYR	CE1-CZ	5.71	1.46	1.38
1	A	580	GLU	CD-OE1	-5.54	1.19	1.25
1	A	272	TYR	CE1-CZ	5.49	1.45	1.38
1	B	405	ASP	CB-CG	5.46	1.63	1.51
1	A	296	MET	C-N	-5.34	1.21	1.34
1	C	424	ASP	N-CA	5.23	1.56	1.46
1	C	398	SER	CB-OG	5.21	1.49	1.42
1	B	375	THR	CB-CG2	-5.19	1.35	1.52
1	C	493	ASP	N-CA	5.12	1.56	1.46
1	A	354	TYR	CZ-OH	5.08	1.46	1.37

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	MET	O-C-N	-42.37	51.18	123.20
1	B	317	TYR	O-C-N	-28.15	77.65	122.70
1	B	255	ASP	CA-C-N	-25.95	60.10	117.20
1	D	255	ASP	C-N-CA	-24.42	60.64	121.70
1	B	256	MET	CA-C-N	23.88	163.96	116.20
1	D	255	ASP	CA-C-N	-20.92	71.18	117.20
1	B	255	ASP	C-N-CA	-20.33	70.87	121.70
1	B	317	TYR	CA-C-N	20.20	161.65	117.20
1	B	317	TYR	C-N-CA	20.16	172.11	121.70
1	C	256	MET	O-C-N	-19.19	90.58	123.20
1	B	256	MET	C-N-CA	17.28	158.59	122.30
1	C	256	MET	CA-C-N	16.99	150.19	116.20
1	D	256	MET	C-N-CA	16.88	157.74	122.30
1	D	256	MET	O-C-N	-14.40	98.72	123.20
1	C	256	MET	C-N-CA	13.82	151.33	122.30
1	D	256	MET	CA-C-N	12.28	140.75	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	A	385	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	B	296	MET	O-C-N	-9.72	107.15	122.70
1	D	364	MET	O-C-N	-8.88	104.23	121.10
1	C	255	ASP	O-C-N	8.67	136.57	122.70
1	A	256	MET	C-N-CA	8.23	139.59	122.30
1	D	255	ASP	O-C-N	8.20	135.81	122.70
1	A	385	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	255	ASP	O-C-N	-7.66	110.45	122.70
1	A	256	MET	O-C-N	-7.30	110.78	123.20
1	C	255	ASP	CA-C-N	-7.26	101.22	117.20
1	A	296	MET	O-C-N	-7.25	111.10	122.70
1	C	543	MET	O-C-N	7.20	134.21	122.70
1	D	296	MET	O-C-N	-7.18	111.21	122.70
1	C	392	ARG	CG-CD-NE	6.90	126.30	111.80
1	B	461	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	406	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	D	294	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	294	ARG	CD-NE-CZ	6.67	132.94	123.60
1	D	364	MET	CA-C-N	6.57	135.50	117.10
1	C	296	MET	O-C-N	-6.57	112.19	122.70
1	D	385	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	542	GLN	O-C-N	-6.48	112.33	122.70
1	C	347	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	347	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	C	385	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	268	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	498	LEU	C-N-CA	6.22	137.25	121.70
1	B	385	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	451	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	461	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	254	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	254	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	347	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	347	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	256	MET	CA-C-N	5.84	127.88	116.20
1	B	276	GLU	OE1-CD-OE2	-5.83	116.31	123.30
1	B	245	GLN	N-CA-C	5.80	126.67	111.00
1	B	415	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	303	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	523	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	543	MET	CA-C-N	-5.66	104.75	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	MET	CA-C-N	5.65	129.64	117.20
1	D	347	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	385	ARG	CG-CD-NE	-5.57	100.10	111.80
1	C	391	ASN	CA-C-N	5.53	129.37	117.20
1	A	347	ASP	CB-CG-OD1	5.51	123.25	118.30
1	C	405	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	498	LEU	C-N-CA	5.41	135.23	121.70
1	A	498	LEU	C-N-CA	5.40	135.21	121.70
1	A	372	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	268	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	557	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	461	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	277	LYS	CB-CG-CD	5.30	125.37	111.60
1	C	523	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	296	MET	CA-C-N	5.20	128.63	117.20
1	A	325	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	318	MET	O-C-N	-5.18	114.41	122.70
1	C	254	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	244	VAL	N-CA-C	-5.17	97.04	111.00
1	C	514	GLN	CB-CG-CD	5.16	125.01	111.60
1	D	405	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	276	GLU	CG-CD-OE1	5.13	128.56	118.30
1	A	461	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	347	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	364	MET	C-N-CD	5.07	139.05	128.40
1	A	294	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	461	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	364	MET	C-N-CD	5.05	139.00	128.40
1	A	557	ASP	CB-CG-OD1	5.04	122.83	118.30
1	D	385	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	422	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	557	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	461	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	580	GLU	CG-CD-OE2	5.00	128.31	118.30
1	C	254	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	255	ASP	Mainchain
1	B	256	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	B	318	MET	Mainchain
1	B	407	SER	Peptide
1	C	391	ASN	Peptide
1	D	255	ASP	Mainchain
1	D	364	MET	Mainchain

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	2681	0	2580	76	1
1	B	2681	0	2579	47	0
1	C	2681	0	2581	48	0
1	D	2681	0	2581	32	0
2	A	285	0	0	23	1
2	B	187	0	0	16	0
2	C	253	0	0	21	0
2	D	235	0	0	11	0
All	All	11684	0	10321	199	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 9.

All (199) 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:C:255:ASP:CA	1:C:256:MET:N	1.72	1.48
1:C:255:ASP:C	1:C:256:MET:CA	1.76	1.48
1:A:255:ASP:C	1:A:256:MET:CA	1.86	1.44
1:A:255:ASP:CA	1:A:256:MET:N	1.81	1.42
1:C:255:ASP:O	1:C:256:MET:N	1.69	1.24
1:A:255:ASP:O	1:A:256:MET:N	1.71	1.23
1:A:270:LEU:HB3	2:A:605:HOH:O	1.39	1.22
1:C:543:MET:HE2	1:C:545:LEU:HB2	1.32	1.09
1:C:526:ASN:HB2	2:C:617:HOH:O	1.52	1.08
1:A:543:MET:CE	1:A:544:THR:C	2.35	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:580:GLU:HB3	2:D:789:HOH:O	1.66	0.94
1:B:411:ASN:HA	2:B:730:HOH:O	1.70	0.92
1:D:255:ASP:OD1	1:D:256:MET:N	2.02	0.91
1:C:255:ASP:O	1:C:256:MET:CA	2.13	0.90
1:D:555:THR:HG22	1:D:563:ILE:HD12	1.56	0.87
1:A:543:MET:HE2	1:A:544:THR:CA	2.05	0.86
1:B:555:THR:HB	2:B:612:HOH:O	1.74	0.86
1:A:406:ASP:HA	1:A:407:SER:CB	2.07	0.85
1:A:543:MET:CE	1:A:544:THR:N	2.42	0.83
1:C:255:ASP:O	1:C:256:MET:HA	1.78	0.82
1:A:543:MET:HE2	1:A:544:THR:C	2.00	0.82
1:C:255:ASP:C	1:C:256:MET:HA	1.98	0.81
1:C:558:LEU:HD13	2:C:827:HOH:O	1.81	0.80
1:C:543:MET:CE	1:C:545:LEU:HB2	2.12	0.80
1:A:408:ASN:HB2	2:A:716:HOH:O	1.81	0.79
1:C:255:ASP:CB	1:C:256:MET:N	2.45	0.79
1:C:422:ASP:HB2	2:C:735:HOH:O	1.84	0.78
1:A:255:ASP:CB	1:A:256:MET:N	2.47	0.76
1:A:388:GLN:HG2	2:A:703:HOH:O	1.87	0.74
1:A:543:MET:HE2	1:A:544:THR:N	2.03	0.74
1:B:555:THR:HG22	2:B:654:HOH:O	1.89	0.73
1:A:408:ASN:CB	2:A:716:HOH:O	2.36	0.73
1:A:543:MET:HE3	1:A:544:THR:N	2.01	0.73
1:A:406:ASP:HA	1:A:407:SER:HB3	1.71	0.72
1:A:460:ASN:HB2	2:A:654:HOH:O	1.89	0.72
1:C:579:GLU:HG2	2:C:638:HOH:O	1.90	0.72
1:A:407:SER:H	1:A:408:ASN:CG	1.95	0.70
1:A:378:GLN:CD	2:A:615:HOH:O	2.30	0.70
1:C:458:GLU:OE1	2:C:601:HOH:O	2.09	0.68
1:B:385:ARG:NH1	2:B:604:HOH:O	2.26	0.68
1:B:406:ASP:CB	1:B:407:SER:HA	2.24	0.68
1:A:255:ASP:O	1:A:256:MET:CA	2.30	0.68
1:A:568:PRO:HD2	2:A:862:HOH:O	1.94	0.67
1:A:255:ASP:C	1:A:256:MET:N	0.61	0.66
1:C:256:MET:HE3	2:C:770:HOH:O	1.96	0.66
1:A:340:GLN:HE22	1:A:388:GLN:H	1.46	0.64
1:A:255:ASP:C	1:A:256:MET:HA	2.10	0.64
1:B:555:THR:CB	2:B:612:HOH:O	2.39	0.63
1:A:243:SER:O	2:A:601:HOH:O	2.16	0.63
1:A:411:ASN:HA	2:A:789:HOH:O	1.97	0.63
1:A:543:MET:HE1	1:A:544:THR:C	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:GLN:HB3	2:C:710:HOH:O	1.99	0.62
1:A:535:THR:HG21	2:A:834:HOH:O	1.99	0.62
1:C:255:ASP:C	1:C:256:MET:N	0.57	0.62
1:A:255:ASP:O	1:A:256:MET:HA	2.00	0.61
1:B:543:MET:HG2	2:B:774:HOH:O	2.01	0.61
1:B:421:SER:HB3	1:D:374:GLN:HE21	1.66	0.60
1:A:460:ASN:CB	2:A:654:HOH:O	2.47	0.60
1:B:406:ASP:CG	1:B:407:SER:HA	2.22	0.60
1:B:244:VAL:O	1:B:583:PHE:O	2.20	0.59
1:B:406:ASP:HB3	1:B:407:SER:HA	1.83	0.59
1:B:364:MET:HB3	1:B:365:PRO:HD3	1.83	0.59
1:D:484:ARG:HE	1:D:486:ASN:HD21	1.48	0.59
1:C:363:SER:OG	1:D:287:GLU:HA	2.03	0.59
1:C:543:MET:CE	1:C:555:THR:OG1	2.51	0.59
1:B:364:MET:HB3	1:B:365:PRO:CD	2.34	0.58
1:B:325:ARG:HD3	1:B:356:GLN:O	2.04	0.57
1:B:244:VAL:HB	1:B:585:ALA:HB3	1.87	0.57
1:B:256:MET:HG2	1:B:256:MET:O	2.04	0.57
1:A:381:ASP:OD1	1:A:385:ARG:HD3	2.04	0.57
1:A:244:VAL:HB	1:A:585:ALA:HB3	1.87	0.56
1:C:458:GLU:O	2:C:602:HOH:O	2.18	0.56
1:B:406:ASP:OD1	1:B:408:ASN:N	2.38	0.55
1:D:244:VAL:HB	1:D:585:ALA:HB3	1.87	0.55
1:D:256:MET:O	1:D:256:MET:HG2	2.07	0.55
1:B:340:GLN:HE22	1:B:388:GLN:H	1.54	0.55
1:A:407:SER:HB2	1:B:288:GLN:HA	1.89	0.55
1:D:408:ASN:OD1	1:D:408:ASN:N	2.39	0.55
1:B:364:MET:CB	1:B:365:PRO:CD	2.86	0.54
1:D:340:GLN:HE22	1:D:388:GLN:H	1.56	0.54
1:D:555:THR:CG2	1:D:563:ILE:HD12	2.34	0.54
1:C:392:ARG:NH2	2:C:603:HOH:O	2.27	0.54
1:C:244:VAL:HB	1:C:585:ALA:HB3	1.89	0.54
1:D:355:ARG:HB2	2:D:687:HOH:O	2.08	0.54
1:B:381:ASP:HB3	2:B:604:HOH:O	2.06	0.54
1:A:568:PRO:CG	2:A:862:HOH:O	2.55	0.54
1:A:543:MET:CE	1:A:544:THR:CA	2.76	0.53
1:C:385:ARG:HG3	2:C:740:HOH:O	2.08	0.53
1:D:579:GLU:CD	2:D:621:HOH:O	2.47	0.53
1:A:256:MET:O	1:A:256:MET:HG2	2.08	0.53
1:B:408:ASN:O	1:B:410:LYS:N	2.42	0.52
1:A:435:ARG:HD3	2:A:682:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ARG:HD3	1:C:356:GLN:HG2	1.92	0.52
1:C:408:ASN:N	1:C:408:ASN:OD1	2.43	0.52
1:A:460:ASN:CG	2:A:654:HOH:O	2.48	0.52
1:A:355:ARG:HB2	2:A:690:HOH:O	2.10	0.51
1:A:548:ASN:HB3	2:A:635:HOH:O	2.11	0.51
1:C:273:SER:HB2	2:C:708:HOH:O	2.10	0.51
1:C:555:THR:HG23	1:C:563:ILE:HB	1.93	0.51
1:A:421:SER:HB3	1:C:374:GLN:HE21	1.76	0.50
1:A:261:ASN:HD22	1:A:393:TRP:H	1.59	0.50
1:A:543:MET:CE	1:A:545:LEU:N	2.74	0.50
1:A:378:GLN:NE2	2:A:615:HOH:O	2.44	0.49
1:A:579:GLU:HG2	2:A:838:HOH:O	2.13	0.49
1:A:466:GLN:HE21	1:A:470:GLN:NE2	2.10	0.49
1:A:243:SER:OG	1:A:244:VAL:N	2.46	0.49
1:B:582:ARG:HD2	2:B:615:HOH:O	2.11	0.49
1:A:364:MET:HB3	1:A:365:PRO:CD	2.43	0.49
1:A:406:ASP:HA	1:A:407:SER:OG	2.11	0.48
1:A:335:ASN:ND2	2:A:606:HOH:O	2.32	0.48
1:D:458:GLU:O	2:D:601:HOH:O	2.20	0.48
1:A:256:MET:HG2	1:A:392:ARG:HH22	1.79	0.48
1:C:466:GLN:HE21	1:C:470:GLN:HE21	1.61	0.48
1:B:555:THR:HG23	1:B:563:ILE:HB	1.96	0.48
1:B:499:MET:HE1	1:B:505:VAL:HG21	1.96	0.47
1:B:442:ASN:O	2:B:601:HOH:O	2.20	0.47
1:C:568:PRO:CB	2:C:805:HOH:O	2.61	0.47
1:A:543:MET:HB2	1:A:543:MET:HE3	1.53	0.47
1:D:370:GLN:HE21	1:D:375:THR:HG22	1.79	0.47
1:A:568:PRO:CD	2:A:862:HOH:O	2.54	0.47
1:B:582:ARG:NE	2:B:615:HOH:O	2.48	0.47
1:D:256:MET:O	1:D:256:MET:CG	2.62	0.47
1:A:514:GLN:OE1	2:A:603:HOH:O	2.20	0.47
1:C:568:PRO:HA	2:C:805:HOH:O	2.14	0.47
1:A:346:SER:OG	1:A:375:THR:HG21	2.15	0.47
1:C:243:SER:OG	1:C:244:VAL:N	2.47	0.47
1:C:355:ARG:HB2	2:C:696:HOH:O	2.14	0.47
1:B:296:MET:CE	2:B:772:HOH:O	2.63	0.46
1:A:408:ASN:OD1	2:A:602:HOH:O	2.20	0.46
1:D:294:ARG:NE	2:D:607:HOH:O	2.43	0.46
1:C:580:GLU:HB3	2:C:799:HOH:O	2.15	0.46
1:B:370:GLN:HE21	1:B:375:THR:HG22	1.80	0.46
1:A:390:ASP:HB2	2:A:703:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:HB2	1:A:415:ARG:HH22	1.81	0.46
1:C:568:PRO:CA	2:C:805:HOH:O	2.63	0.46
1:D:243:SER:OG	1:D:244:VAL:N	2.49	0.46
1:A:466:GLN:HE21	1:A:470:GLN:HE21	1.64	0.46
1:A:543:MET:C	1:A:543:MET:CE	2.84	0.46
1:C:370:GLN:HE21	1:C:375:THR:HG22	1.80	0.46
1:D:514:GLN:NE2	2:D:613:HOH:O	2.49	0.46
1:D:466:GLN:HE21	1:D:470:GLN:NE2	2.13	0.46
1:D:340:GLN:HB2	2:D:602:HOH:O	2.16	0.45
1:A:295:HIS:NE2	1:A:491:HIS:HD2	2.14	0.45
1:B:359:LEU:HD22	1:B:362:PHE:CE2	2.51	0.45
1:A:370:GLN:HE21	1:A:375:THR:HG22	1.81	0.45
1:A:406:ASP:CA	1:A:407:SER:CB	2.85	0.45
1:D:408:ASN:O	1:D:410:LYS:N	2.49	0.45
1:B:466:GLN:HE21	1:B:470:GLN:NE2	2.15	0.45
1:D:256:MET:HA	1:D:337:GLN:HE22	1.82	0.45
1:A:543:MET:HE2	1:A:545:LEU:N	2.32	0.45
1:D:466:GLN:HE21	1:D:470:GLN:HE21	1.65	0.45
1:C:466:GLN:HE21	1:C:470:GLN:NE2	2.13	0.44
1:D:243:SER:OG	1:D:245:GLN:N	2.50	0.44
1:D:501:ARG:HD3	2:D:746:HOH:O	2.17	0.44
1:B:315:PRO:O	1:B:318:MET:HB2	2.17	0.44
1:D:557:ASP:HB2	2:D:627:HOH:O	2.17	0.44
1:B:466:GLN:HE21	1:B:470:GLN:HE21	1.64	0.44
1:A:499:MET:HE1	1:A:505:VAL:HG21	2.00	0.44
1:D:388:GLN:OE1	2:D:602:HOH:O	2.21	0.44
1:D:495:MET:O	1:D:499:MET:HG2	2.18	0.44
1:A:379:TRP:CG	1:A:397:ILE:HD11	2.53	0.43
1:C:346:SER:OG	1:C:375:THR:HG21	2.18	0.43
1:B:243:SER:OG	1:B:244:VAL:N	2.52	0.43
1:B:261:ASN:HD22	1:B:393:TRP:H	1.67	0.43
1:A:543:MET:HE1	1:A:545:LEU:N	2.33	0.43
1:C:243:SER:OG	1:C:245:GLN:N	2.51	0.43
1:C:291:ASP:OD2	1:C:484:ARG:NH2	2.52	0.43
1:C:563:ILE:C	2:C:781:HOH:O	2.56	0.43
1:C:568:PRO:N	2:C:616:HOH:O	2.51	0.43
1:C:574:LEU:HB2	2:C:823:HOH:O	2.19	0.43
1:C:543:MET:HE3	1:C:555:THR:OG1	2.17	0.43
1:A:408:ASN:ND2	1:A:408:ASN:N	2.67	0.43
1:A:406:ASP:HB2	1:A:415:ARG:NH2	2.33	0.43
1:B:256:MET:HB3	2:B:775:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:ASN:ND2	2:C:617:HOH:O	2.51	0.42
1:A:322:LEU:HD21	1:A:353:LEU:HA	2.01	0.42
1:C:252:HIS:HB2	2:C:645:HOH:O	2.19	0.42
1:B:349:PHE:O	1:B:355:ARG:NH1	2.52	0.42
1:B:256:MET:O	1:B:256:MET:CG	2.66	0.42
1:A:295:HIS:NE2	1:A:491:HIS:CD2	2.87	0.42
1:B:435:ARG:HD3	2:B:627:HOH:O	2.19	0.42
1:D:346:SER:OG	1:D:375:THR:HG21	2.19	0.42
1:B:346:SER:OG	1:B:375:THR:HG21	2.20	0.42
1:C:516:GLN:O	1:C:517:ASP:C	2.58	0.42
1:B:336:GLN:HG3	2:B:725:HOH:O	2.19	0.41
1:B:460:ASN:ND2	2:B:618:HOH:O	2.51	0.41
1:D:295:HIS:NE2	1:D:491:HIS:HD2	2.18	0.41
1:A:449:ALA:O	1:A:491:HIS:HE1	2.03	0.41
1:B:322:LEU:HD21	1:B:353:LEU:HA	2.02	0.41
1:A:543:MET:C	1:A:543:MET:HE2	2.40	0.41
1:B:315:PRO:O	1:B:318:MET:CB	2.68	0.41
1:C:543:MET:HE1	1:C:555:THR:OG1	2.21	0.41
1:A:349:PHE:O	1:A:355:ARG:NH1	2.54	0.41
1:B:405:ASP:O	1:B:406:ASP:CB	2.69	0.41
1:A:346:SER:OG	1:A:375:THR:CG2	2.68	0.41
1:A:256:MET:O	1:A:256:MET:CG	2.68	0.41
1:B:582:ARG:CD	2:B:615:HOH:O	2.68	0.41
1:B:449:ALA:O	1:B:491:HIS:HE1	2.05	0.40
1:D:535:THR:HG21	2:D:793:HOH:O	2.21	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:256:MET:SD	2:A:864:HOH:O[1_455]	2.15	0.05

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	335/586 (57%)	316 (94%)	16 (5%)	3 (1%)	21	7
1	B	335/586 (57%)	311 (93%)	18 (5%)	6 (2%)	11	2
1	C	335/586 (57%)	319 (95%)	13 (4%)	3 (1%)	21	7
1	D	335/586 (57%)	321 (96%)	10 (3%)	4 (1%)	16	4
All	All	1340/2344 (57%)	1267 (95%)	57 (4%)	16 (1%)	16	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	MET
1	B	406	ASP
1	B	409	GLN
1	C	409	GLN
1	D	409	GLN
1	A	407	SER
1	C	562	LYS
1	A	391	ASN
1	B	256	MET
1	B	364	MET
1	D	255	ASP
1	D	391	ASN
1	D	562	LYS
1	A	255	ASP
1	B	391	ASN
1	C	391	ASN

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	291/511 (57%)	278 (96%)	13 (4%)	34	14
1	B	291/511 (57%)	276 (95%)	15 (5%)	29	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	291/511 (57%)	276 (95%)	15 (5%)	29	10
1	D	291/511 (57%)	277 (95%)	14 (5%)	31	12
All	All	1164/2044 (57%)	1107 (95%)	57 (5%)	31	11

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	VAL
1	A	251	LEU
1	A	275	PHE
1	A	375	THR
1	A	392	ARG
1	A	407	SER
1	A	408	ASN
1	A	409	GLN
1	A	535	THR
1	A	543	MET
1	A	573	LEU
1	A	577	LEU
1	A	580	GLU
1	B	244	VAL
1	B	251	LEU
1	B	275	PHE
1	B	362	PHE
1	B	375	THR
1	B	388	GLN
1	B	405	ASP
1	B	407	SER
1	B	408	ASN
1	B	409	GLN
1	B	535	THR
1	B	543	MET
1	B	573	LEU
1	B	577	LEU
1	B	580	GLU
1	C	244	VAL
1	C	251	LEU
1	C	275	PHE
1	C	294	ARG
1	C	340	GLN
1	C	375	THR

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Mol	Chain	Res	Type
1	C	388	GLN
1	C	390	ASP
1	C	408	ASN
1	C	409	GLN
1	C	484	ARG
1	C	535	THR
1	C	573	LEU
1	C	577	LEU
1	C	580	GLU
1	D	244	VAL
1	D	251	LEU
1	D	275	PHE
1	D	356	GLN
1	D	375	THR
1	D	388	GLN
1	D	392	ARG
1	D	408	ASN
1	D	409	GLN
1	D	535	THR
1	D	543	MET
1	D	573	LEU
1	D	577	LEU
1	D	580	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	261	ASN
1	A	271	ASN
1	A	340	GLN
1	A	370	GLN
1	A	470	GLN
1	A	483	GLN
1	A	491	HIS
1	A	514	GLN
1	A	548	ASN
1	B	250	ASN
1	B	261	ASN
1	B	271	ASN
1	B	340	GLN
1	B	370	GLN

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Mol	Chain	Res	Type
1	B	470	GLN
1	B	483	GLN
1	B	491	HIS
1	C	250	ASN
1	C	261	ASN
1	C	271	ASN
1	C	368	GLN
1	C	470	GLN
1	C	483	GLN
1	C	491	HIS
1	D	250	ASN
1	D	261	ASN
1	D	271	ASN
1	D	340	GLN
1	D	368	GLN
1	D	470	GLN
1	D	483	GLN
1	D	486	ASN
1	D	491	HIS
1	D	514	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 carbohydrates 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	D	4
1	A	3
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	318:MET	C	319:ASP	N	1.19
1	B	296:MET	C	297:SER	N	1.17
1	D	498:LEU	C	499:MET	N	1.15
1	A	256:MET	C	257:GLY	N	1.13
1	A	498:LEU	C	499:MET	N	1.11
1	D	364:MET	C	365:PRO	N	1.05
1	B	498:LEU	C	499:MET	N	1.03
1	D	255:ASP	C	256:MET	N	1.03
1	C	256:MET	C	257:GLY	N	0.80
1	D	256:MET	C	257:GLY	N	0.80
1	B	256:MET	C	257:GLY	N	0.75
1	A	255:ASP	C	256:MET	N	0.61
1	C	255:ASP	C	256:MET	N	0.57
1	B	317:TYR	C	318:MET	N	0.36
1	B	255:ASP	C	256:MET	N	0.19

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	339/586 (57%)	-0.22	12 (3%) 48 44	17, 28, 59, 91	0
1	B	339/586 (57%)	-0.03	17 (5%) 32 29	21, 36, 73, 119	0
1	C	339/586 (57%)	-0.16	8 (2%) 62 59	18, 30, 65, 113	0
1	D	339/586 (57%)	-0.19	11 (3%) 51 47	19, 31, 65, 107	0
All	All	1356/2344 (57%)	-0.15	48 (3%) 48 44	17, 31, 67, 119	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	SER	9.4
1	C	386	TYR	7.9
1	B	364	MET	5.7
1	A	364	MET	5.3
1	A	243	SER	4.9
1	D	388	GLN	4.9
1	D	256	MET	4.7
1	C	388	GLN	4.7
1	D	243	SER	4.6
1	B	408	ASN	4.4
1	A	585	ALA	4.3
1	C	243	SER	4.2
1	B	406	ASP	4.2
1	C	390	ASP	4.1
1	B	366	ALA	4.1
1	B	410	LYS	4.1
1	C	256	MET	4.0
1	C	563	ILE	3.9
1	B	244	VAL	3.9
1	D	390	ASP	3.9
1	B	407	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	256	MET	3.6
1	B	361	ASP	3.5
1	D	244	VAL	3.2
1	D	563	ILE	3.1
1	D	570	LEU	3.1
1	D	574	LEU	2.9
1	B	405	ASP	2.8
1	B	245	GLN	2.7
1	A	361	ASP	2.7
1	D	386	TYR	2.7
1	A	244	VAL	2.6
1	A	406	ASP	2.6
1	B	585	ALA	2.5
1	B	362	PHE	2.4
1	A	256	MET	2.4
1	A	363	SER	2.3
1	A	407	SER	2.3
1	B	390	ASP	2.3
1	C	574	LEU	2.3
1	D	391	ASN	2.2
1	A	574	LEU	2.1
1	A	390	ASP	2.1
1	B	584	ILE	2.1
1	A	362	PHE	2.1
1	D	364	MET	2.1
1	C	543	MET	2.0
1	B	563	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.