



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:47 AM UTC

PDB ID : 5I5F / pdb_00005i5f
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

<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

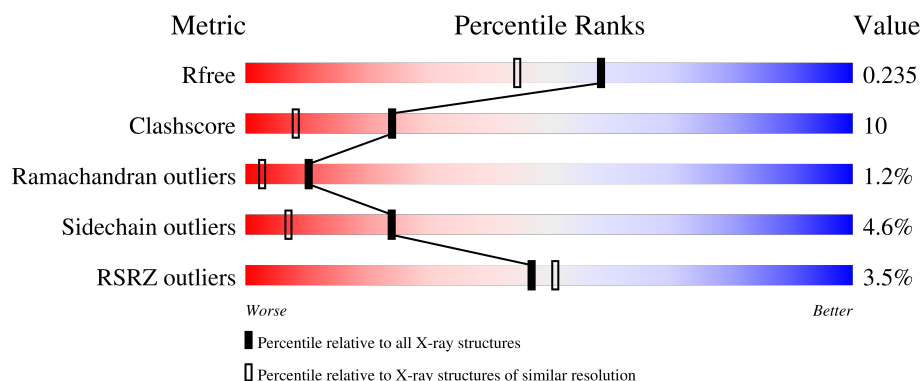
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	586	2% 45% 11% .. 42%
1	B	586	2% 46% 9% .. 42%
1	C	586	2% 45% 10% .. 42%
1	D	586	2% 47% 9% . 42%

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.

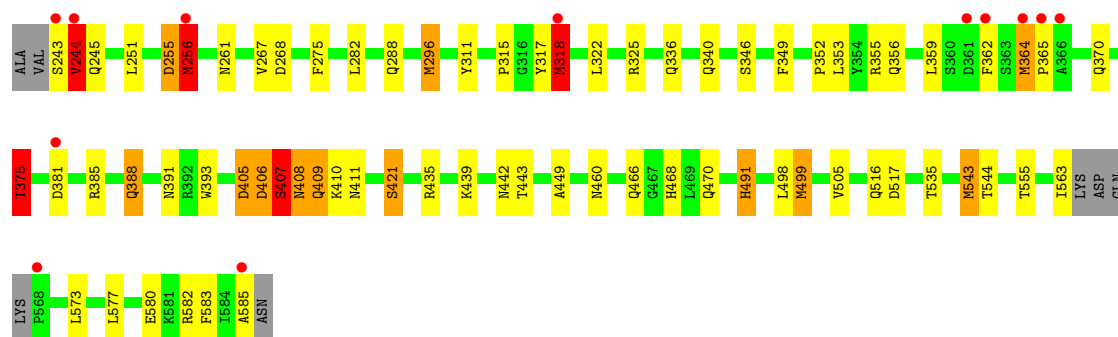
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inner membrane protein YejM.

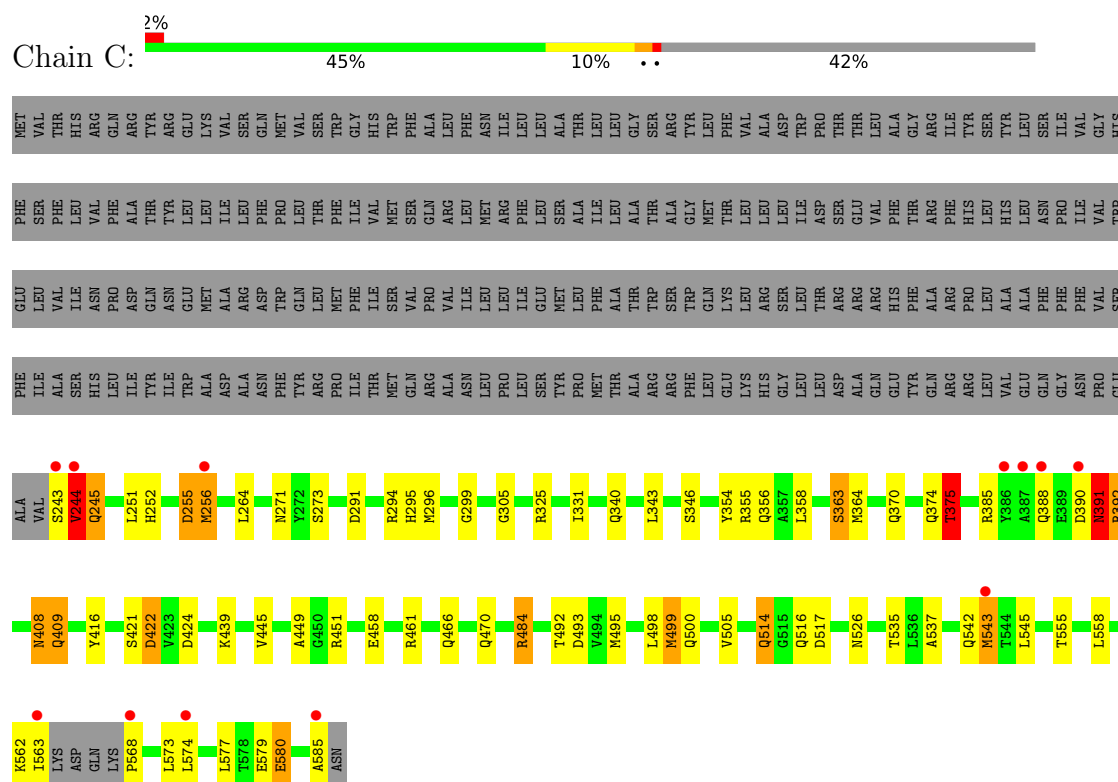
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			
1	B	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			
1	C	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			
1	D	339	Total	C	N	O	S	0	0	0
			2681	1690	468	515	8			

- Molecule 2 is water.

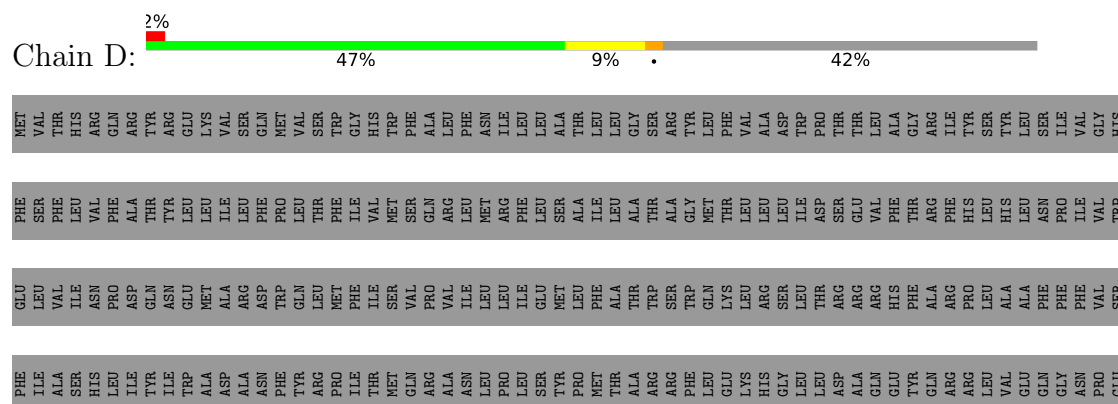
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	285	Total	O	0	0
			285	285		
2	B	187	Total	O	0	0
			187	187		
2	C	253	Total	O	0	0
			253	253		
2	D	235	Total	O	0	0
			235	235		

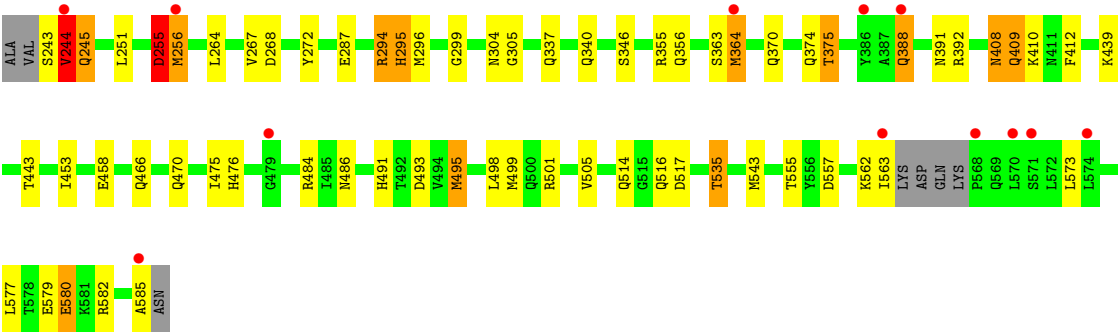


• Molecule 1: Inner membrane protein YejM



• 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 (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.911	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	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.*

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	1.78	18/2744 (0.7%)	1.30	21/3738 (0.6%)
1	B	2.65	16/2744 (0.6%)	1.87	19/3738 (0.5%)
1	C	1.88	29/2744 (1.1%)	1.44	28/3738 (0.7%)
1	D	1.57	17/2744 (0.6%)	1.63	18/3738 (0.5%)
All	All	2.01	80/10976 (0.7%)	1.57	86/14952 (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 (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	ASP	C-N	-81.74	0.19	1.33
1	B	317	TYR	C-N	-68.94	0.36	1.33
1	C	255	ASP	C-N	-57.01	0.57	1.33
1	A	255	ASP	C-N	-53.82	0.61	1.33
1	B	256	MET	C-N	-52.75	0.75	1.33
1	D	256	MET	C-N	-30.13	0.80	1.32
1	C	256	MET	C-N	-29.32	0.80	1.33
1	B	498	LEU	C-N	-23.71	1.03	1.33
1	D	364	MET	C-N	-23.00	1.05	1.33
1	D	255	ASP	C-N	-18.07	1.03	1.34
1	A	498	LEU	C-N	-17.79	1.11	1.33
1	D	498	LEU	C-N	-14.60	1.15	1.33
1	B	296	MET	C-N	-12.13	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	MET	C-N	-10.28	1.13	1.33
1	B	318	MET	C-N	-9.88	1.19	1.33
1	D	299	GLY	N-CA	9.53	1.55	1.45
1	B	543	MET	C-O	-9.40	1.14	1.24
1	A	296	MET	C-N	-9.09	1.21	1.33
1	D	363	SER	C-N	9.07	1.44	1.32
1	A	495	MET	C-O	-8.83	1.14	1.24
1	C	424	ASP	N-CA	8.63	1.56	1.46
1	C	493	ASP	N-CA	8.45	1.56	1.46
1	C	498	LEU	C-N	-8.44	1.23	1.33
1	B	544	THR	N-CA	8.11	1.56	1.46
1	D	495	MET	C-O	-8.02	1.14	1.24
1	C	363	SER	C-N	7.88	1.44	1.33
1	C	499	MET	C-N	-7.79	1.24	1.33
1	D	272	TYR	N-CA	7.53	1.55	1.46
1	A	499	MET	C-N	7.43	1.43	1.33
1	B	245	GLN	N-CA	7.25	1.55	1.46
1	C	495	MET	C-O	-7.24	1.15	1.24
1	D	493	ASP	N-CA	7.15	1.55	1.46
1	D	476	HIS	N-CA	7.14	1.54	1.46
1	A	421	SER	CB-OG	-6.85	1.28	1.42
1	C	542	GLN	C-N	6.84	1.42	1.33
1	A	494	VAL	CA-C	6.59	1.61	1.52
1	C	364	MET	C-N	-6.43	1.25	1.33
1	B	244	VAL	CA-C	6.40	1.60	1.52
1	A	540	THR	N-CA	6.39	1.50	1.46
1	B	245	GLN	CA-C	6.35	1.61	1.52
1	C	449	ALA	N-CA	6.31	1.53	1.45
1	D	453	ILE	N-CA	6.29	1.51	1.46
1	C	331	ILE	CA-CB	6.27	1.62	1.54
1	D	364	MET	CA-C	-6.12	1.45	1.52
1	D	305	GLY	N-CA	6.11	1.53	1.45
1	D	295	HIS	CA-C	6.10	1.60	1.52
1	C	299	GLY	N-CA	6.08	1.51	1.45
1	A	375	THR	CB-CG2	-6.00	1.32	1.52
1	A	543	MET	C-O	-5.97	1.17	1.24
1	C	543	MET	C-N	-5.93	1.25	1.33
1	C	445	VAL	N-CA	5.83	1.53	1.46
1	C	295	HIS	CA-CB	-5.71	1.45	1.53
1	C	537	ALA	N-CA	-5.67	1.39	1.46
1	D	304	ASN	CA-C	5.58	1.59	1.52
1	C	421	SER	CA-C	-5.50	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	TYR	C-O	-5.47	1.17	1.24
1	C	264	LEU	N-CA	-5.46	1.39	1.46
1	C	343	LEU	C-O	-5.43	1.17	1.24
1	B	421	SER	CB-OG	-5.42	1.31	1.42
1	D	264	LEU	N-CA	-5.41	1.39	1.46
1	C	451	ARG	N-CA	-5.38	1.39	1.45
1	A	385	ARG	CD-NE	-5.38	1.38	1.46
1	C	305	GLY	N-CA	5.36	1.52	1.45
1	A	317	TYR	C-N	5.27	1.40	1.33
1	B	375	THR	CB-CG2	-5.25	1.35	1.52
1	C	461	ARG	C-O	-5.22	1.17	1.24
1	B	468	HIS	N-CA	5.18	1.52	1.46
1	C	500	GLN	CA-C	-5.16	1.46	1.53
1	A	393	TRP	CA-C	-5.15	1.46	1.52
1	B	282	LEU	CA-C	5.14	1.59	1.52
1	C	492	THR	N-CA	-5.12	1.39	1.46
1	B	311	TYR	C-O	-5.11	1.17	1.24
1	A	540	THR	C-O	-5.11	1.19	1.24
1	C	358	LEU	N-CA	5.11	1.52	1.46
1	A	395	SER	CB-OG	-5.10	1.31	1.42
1	D	475	ILE	N-CA	-5.08	1.40	1.46
1	A	509	ALA	CA-CB	5.07	1.61	1.53
1	C	500	GLN	N-CA	5.06	1.52	1.46
1	C	492	THR	CA-C	5.03	1.59	1.52
1	C	271	ASN	CA-C	5.01	1.59	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	MET	O-C-N	-53.69	51.18	122.59
1	D	255	ASP	CA-C-N	-35.68	60.64	120.23
1	D	255	ASP	C-N-CA	-35.68	60.64	120.23
1	B	317	TYR	CA-C-N	28.00	172.11	121.70
1	B	317	TYR	C-N-CA	28.00	172.11	121.70
1	B	317	TYR	O-C-N	-27.97	77.65	122.41
1	B	255	ASP	CA-C-N	-26.53	70.87	121.54
1	B	255	ASP	C-N-CA	-26.53	70.87	121.54
1	C	256	MET	O-C-N	-26.47	90.58	122.34
1	B	256	MET	CA-C-N	23.36	158.59	120.51
1	B	256	MET	C-N-CA	23.36	158.59	120.51
1	D	256	MET	O-C-N	-20.28	98.72	122.05
1	D	364	MET	O-C-N	-20.10	104.23	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	MET	CA-C-N	19.82	157.74	122.66
1	D	256	MET	C-N-CA	19.82	157.74	122.66
1	C	256	MET	CA-C-N	17.41	151.33	121.39
1	C	256	MET	C-N-CA	17.41	151.33	121.39
1	B	296	MET	O-C-N	-13.57	107.15	123.30
1	D	364	MET	CA-C-N	13.22	133.12	120.03
1	D	364	MET	C-N-CA	13.22	133.12	120.03
1	C	498	LEU	CA-C-N	12.93	137.25	120.44
1	C	498	LEU	C-N-CA	12.93	137.25	120.44
1	B	498	LEU	CA-C-N	11.38	135.23	120.44
1	B	498	LEU	C-N-CA	11.38	135.23	120.44
1	A	498	LEU	CA-C-N	10.86	135.21	120.54
1	A	498	LEU	C-N-CA	10.86	135.21	120.54
1	C	255	ASP	O-C-N	10.51	136.57	122.59
1	A	296	MET	O-C-N	-10.25	111.10	123.30
1	A	256	MET	CA-C-N	10.20	139.59	121.32
1	A	256	MET	C-N-CA	10.20	139.59	121.32
1	D	498	LEU	CA-C-N	9.96	133.38	120.44
1	D	498	LEU	C-N-CA	9.96	133.38	120.44
1	D	255	ASP	O-C-N	9.94	135.81	122.59
1	C	543	MET	O-C-N	9.66	134.21	123.10
1	D	296	MET	O-C-N	-9.45	111.21	123.21
1	A	256	MET	O-C-N	-9.43	110.78	122.19
1	B	255	ASP	O-C-N	-9.13	110.45	122.59
1	C	296	MET	O-C-N	-8.49	112.19	123.23
1	C	244	VAL	CB-CA-C	7.85	117.97	111.06
1	D	244	VAL	CB-CA-C	7.76	117.89	111.06
1	A	405	ASP	N-CA-C	-7.46	103.77	113.17
1	B	245	GLN	N-CA-C	7.45	126.67	110.80
1	A	295	HIS	CA-C-N	-7.43	112.52	122.99
1	A	295	HIS	C-N-CA	-7.43	112.52	122.99
1	C	542	GLN	CA-C-N	7.42	134.04	121.87
1	C	542	GLN	C-N-CA	7.42	134.04	121.87
1	C	514	GLN	CB-CG-CD	7.30	125.01	112.60
1	B	244	VAL	N-CA-C	-7.25	97.04	107.77
1	C	542	GLN	O-C-N	-7.07	112.33	122.36
1	D	412	PHE	N-CA-C	-6.77	103.90	111.28
1	A	245	GLN	N-CA-C	6.53	120.05	107.44
1	C	392	ARG	CG-CD-NE	6.50	126.30	112.00
1	D	363	SER	O-C-N	-6.46	115.85	123.22
1	C	245	GLN	N-CA-C	6.35	119.69	107.44
1	C	416	TYR	N-CA-C	-6.19	104.53	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	TYR	N-CA-C	6.16	117.87	111.03
1	A	277	LYS	CB-CG-CD	6.12	125.37	111.30
1	D	294	ARG	CD-NE-CZ	6.10	132.94	124.40
1	C	439	LYS	CB-CA-C	-6.08	101.23	111.02
1	C	391	ASN	CA-C-N	5.95	132.41	121.70
1	C	391	ASN	C-N-CA	5.95	132.41	121.70
1	A	498	LEU	N-CA-C	5.84	117.32	111.07
1	C	422	ASP	N-CA-C	5.80	117.27	111.07
1	A	244	VAL	CB-CA-C	5.79	116.16	111.06
1	A	255	ASP	O-C-N	5.76	130.25	122.59
1	B	498	LEU	O-C-N	-5.76	116.01	122.12
1	A	543	MET	O-C-N	5.68	128.95	123.04
1	D	245	GLN	N-CA-C	5.67	118.39	107.44
1	C	375	THR	N-CA-CB	5.67	118.55	110.16
1	C	255	ASP	CA-C-N	-5.63	113.64	122.65
1	C	255	ASP	C-N-CA	-5.63	113.64	122.65
1	C	391	ASN	O-C-N	-5.63	115.11	122.59
1	D	295	HIS	O-C-N	5.53	129.51	123.27
1	A	385	ARG	CG-CD-NE	-5.41	100.10	112.00
1	B	318	MET	O-C-N	-5.37	114.41	123.00
1	A	274	ARG	N-CA-C	5.35	119.91	113.17
1	A	375	THR	N-CA-CB	5.29	117.99	110.16
1	B	375	THR	N-CA-CB	5.18	117.82	110.16
1	B	491	HIS	N-CA-C	5.16	117.64	111.71
1	C	295	HIS	CA-C-N	-5.16	115.20	122.94
1	C	295	HIS	C-N-CA	-5.16	115.20	122.94
1	A	421	SER	CB-CA-C	-5.14	102.58	110.81
1	A	317	TYR	CA-C-N	5.10	129.30	121.19
1	A	317	TYR	C-N-CA	5.10	129.30	121.19
1	B	499	MET	O-C-N	5.09	127.31	122.07
1	C	295	HIS	O-C-N	5.01	128.93	123.27

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
1	B	318	MET	Mainchain
1	B	407	SER	Peptide
1	C	391	ASN	Peptide
1	D	255	ASP	Mainchain

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Mol	Chain	Res	Type	Group
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	2581	76	1
1	B	2681	0	2579	52	0
1	C	2681	0	2582	49	0
1	D	2681	0	2581	37	0
2	A	285	0	0	23	1
2	B	187	0	0	17	0
2	C	253	0	0	21	0
2	D	235	0	0	11	0
All	All	11684	0	10323	210	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 10.

All (210) 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:C	1:C:256:MET:CA	1.76	1.55
1:A:255:ASP:C	1:A:256:MET:CA	1.86	1.49
1:C:255:ASP:CA	1:C:256:MET:N	1.72	1.48
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:A:543:MET:HE2	1:A:544:THR:N	1.61	1.11
1:C:526:ASN:HB2	2:C:617:HOH:O	1.52	1.08
1:C:543:MET:HE2	1:C:545:LEU:HB2	1.33	1.04
1:A:543:MET:CE	1:A:544:THR:C	2.35	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASP:O	1:C:256:MET:CA	2.13	0.90
1:A:543:MET:HE2	1:A:544:THR:CA	2.02	0.89
1:A:543:MET:HE2	1:A:543:MET:C	1.98	0.88
1:D:555:THR:HG22	1:D:563:ILE:HD12	1.56	0.87
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:HE1	1:A:544:THR:C	2.01	0.85
1:C:255:ASP:C	1:C:256:MET:HA	1.98	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: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:A:543:MET:HE1	1:A:545:LEU:N	1.99	0.78
1:C:422:ASP:HB2	2:C:735:HOH:O	1.84	0.78
1:C:543:MET:HE3	1:C:555:THR:OG1	1.83	0.77
1:A:255:ASP:CB	1:A:256:MET:N	2.47	0.76
1:A:407:SER:H	1:A:408:ASN:CG	1.95	0.75
1:A:388:GLN:HG2	2:A:703:HOH:O	1.87	0.74
1:A:378:GLN:CD	2:A:615:HOH:O	2.30	0.73
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: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:255:ASP:C	1:A:256:MET:N	0.61	0.71
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:359:LEU:HD13	1:A:364:MET:HE1	1.76	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:543:MET:HE2	1:A:544:THR:C	2.16	0.67
1:A:255:ASP:C	1:A:256:MET:HA	2.10	0.67
1:C:255:ASP:C	1:C:256:MET:N	0.57	0.66
1:B:499:MET:HE3	1:B:505:VAL:HG21	1.76	0.66
1:B:406:ASP:CG	1:B:407:SER:HA	2.22	0.65
1:A:340:GLN:HE22	1:A:388:GLN:H	1.46	0.64
1:A:499:MET:HE3	1:A:505:VAL:HG21	1.78	0.63
1:B:555:THR:CB	2:B:612:HOH:O	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:514:GLN:HB3	2:C:710:HOH:O	1.99	0.62
1:D:499:MET:HE3	1:D:505:VAL:HG21	1.80	0.62
1:A:535:THR:HG21	2:A:834:HOH:O	1.99	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: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:C:256:MET:HE3	2:C:770:HOH:O	2.03	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:B:364:MET:HB3	1:B:365:PRO:CD	2.34	0.58
1:D:579:GLU:CD	2:D:621:HOH:O	2.47	0.57
1:B:244:VAL:HB	1:B:585:ALA:HB3	1.87	0.57
1:B:325:ARG:HD3	1:B:356:GLN:O	2.04	0.57
1:B:256:MET:O	1:B:256:MET:HG2	2.04	0.57
1:A:381:ASP:OD1	1:A:385:ARG:HD3	2.04	0.57
1:C:499:MET:HE3	1:C:505:VAL:HG21	1.87	0.57
1:A:244:VAL:HB	1:A:585:ALA:HB3	1.87	0.56
1:A:460:ASN:CG	2:A:654:HOH:O	2.48	0.56
1:C:543:MET:CE	1:C:555:THR:OG1	2.51	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:B:340:GLN:HE22	1:B:388:GLN:H	1.54	0.55
1:D:256:MET:HG2	1:D:256:MET:O	2.07	0.55
1:A:407:SER:HB2	1:B:288:GLN:HA	1.89	0.55
1:D:408:ASN:N	1:D:408:ASN:OD1	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:C:385:ARG:HG3	2:C:740:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:HG2	1:A:256:MET:O	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
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: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:579:GLU:HG2	2:A:838:HOH:O	2.13	0.49
1:A:378:GLN:NE2	2:A:615:HOH:O	2.44	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:C:563:ILE:C	2:C:781:HOH:O	2.56	0.48
1:B:555:THR:HG23	1:B:563:ILE:HB	1.96	0.48
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:D:370:GLN:HE21	1:D:375:THR:HG22	1.79	0.47
1:A:514:GLN:OE1	2:A:603:HOH:O	2.20	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: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:C:516:GLN:O	1:C:517:ASP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASP:HB2	2:A:703:HOH:O	2.15	0.46
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: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:D:439:LYS:O	1:D:443:THR:OG1	2.33	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: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:C:543:MET:HE3	1:C:555:THR:HG1	1.79	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:D:579:GLU:CD	1:D:582:ARG:HH12	2.25	0.44
1:B:296:MET:HE3	2:B:772:HOH:O	2.18	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: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:516:GLN:O	1:A:517:ASP:C	2.61	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: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:A:543:MET:HE3	1:A:543:MET:HB2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:MET:HB3	2:B:775:HOH:O	2.18	0.42
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:D:516:GLN:O	1:D:517:ASP:C	2.62	0.42
1:B:346:SER:OG	1:B:375:THR:HG21	2.20	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:B:315:PRO:O	1:B:318:MET:CB	2.68	0.41
1:B:352:PRO:O	1:B:353:LEU:C	2.64	0.41
1:A:267:VAL:O	1:A:268:ASP:C	2.63	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:543:MET:CE	1:A:543:MET:C	2.84	0.41
1:A:543:MET:HE1	1:A:545:LEU:HB2	2.02	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:439:LYS:O	1:B:443:THR:OG1	2.35	0.40
1:B:516:GLN:O	1:B:517:ASP:C	2.64	0.40
1:D:267:VAL:O	1:D:268:ASP:C	2.60	0.40
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
1:B:267:VAL:O	1:B:268:ASP:C	2.64	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 [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	335/586 (57%)	316 (94%)	16 (5%)	3 (1%)	14	4
1	B	335/586 (57%)	311 (93%)	18 (5%)	6 (2%)	6	1
1	C	335/586 (57%)	319 (95%)	13 (4%)	3 (1%)	14	4
1	D	335/586 (57%)	321 (96%)	10 (3%)	4 (1%)	10	3
All	All	1340/2344 (57%)	1267 (95%)	57 (4%)	16 (1%)	10	3

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 [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	291/511 (57%)	277 (95%)	14 (5%)	23	6
1	B	291/511 (57%)	278 (96%)	13 (4%)	24	7
1	C	291/511 (57%)	277 (95%)	14 (5%)	23	6
1	D	291/511 (57%)	278 (96%)	13 (4%)	24	7
All	All	1164/2044 (57%)	1110 (95%)	54 (5%)	24	7

All (54) 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	281	GLU
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	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	573	LEU
1	B	577	LEU
1	B	580	GLU
1	C	244	VAL
1	C	251	LEU
1	C	294	ARG

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Mol	Chain	Res	Type
1	C	340	GLN
1	C	375	THR
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	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	250	ASN
1	A	261	ASN
1	A	271	ASN
1	A	304	ASN
1	A	340	GLN
1	A	370	GLN
1	A	378	GLN
1	A	470	GLN
1	A	483	GLN
1	A	491	HIS
1	A	514	GLN
1	A	542	GLN
1	A	552	HIS

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Mol	Chain	Res	Type
1	B	250	ASN
1	B	261	ASN
1	B	271	ASN
1	B	340	GLN
1	B	370	GLN
1	B	470	GLN
1	B	483	GLN
1	B	491	HIS
1	B	542	GLN
1	B	552	HIS
1	C	250	ASN
1	C	261	ASN
1	C	271	ASN
1	C	304	ASN
1	C	340	GLN
1	C	391	ASN
1	C	470	GLN
1	C	483	GLN
1	C	491	HIS
1	C	542	GLN
1	D	245	GLN
1	D	250	ASN
1	D	261	ASN
1	D	271	ASN
1	D	340	GLN
1	D	370	GLN
1	D	378	GLN
1	D	470	GLN
1	D	486	ASN
1	D	491	HIS
1	D	514	GLN
1	D	542	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 [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](#)

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%)	-0.03	12 (3%) 47 51	17, 28, 59, 91	0
1	B	339/586 (57%)	0.22	12 (3%) 47 51	21, 36, 73, 119	0
1	C	339/586 (57%)	0.03	12 (3%) 47 51	18, 30, 65, 113	0
1	D	339/586 (57%)	0.04	12 (3%) 47 51	19, 31, 65, 107	0
All	All	1356/2344 (57%)	0.07	48 (3%) 47 51	17, 31, 67, 119	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	MET	6.8
1	C	256	MET	6.7
1	B	256	MET	4.8
1	A	244	VAL	4.6
1	B	244	VAL	4.5
1	B	243	SER	4.3
1	B	364	MET	4.2
1	D	244	VAL	4.1
1	C	386	TYR	4.0
1	B	568	PRO	4.0
1	A	364	MET	3.9
1	D	574	LEU	3.9
1	C	568	PRO	3.4
1	A	243	SER	3.4
1	A	256	MET	3.3
1	B	365	PRO	3.2
1	A	361	ASP	3.2
1	A	407	SER	3.1
1	C	563	ILE	3.1
1	C	543	MET	3.1
1	B	366	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	318	MET	3.0
1	D	585	ALA	3.0
1	C	574	LEU	2.9
1	A	585	ALA	2.9
1	A	363	SER	2.8
1	B	585	ALA	2.8
1	D	563	ILE	2.8
1	D	364	MET	2.8
1	D	568	PRO	2.7
1	C	387	ALA	2.6
1	B	361	ASP	2.6
1	D	386	TYR	2.5
1	A	568	PRO	2.5
1	B	362	PHE	2.5
1	D	388	GLN	2.4
1	A	362	PHE	2.3
1	D	570	LEU	2.3
1	C	243	SER	2.2
1	C	390	ASP	2.2
1	C	244	VAL	2.2
1	C	585	ALA	2.2
1	D	571	SER	2.1
1	D	479	GLY	2.1
1	C	388	GLN	2.1
1	A	366	ALA	2.0
1	A	406	ASP	2.0
1	B	381	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.