



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:37 AM UTC

PDB ID : 5I5D / pdb_00005i5d
Title : Salmonella global domain 245
Authors : Dong, C.; Dong, H.
Deposited on : 2016-02-15
Resolution : 1.64 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
Mogul : 2022.3.0, CSD as543be (2022)
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

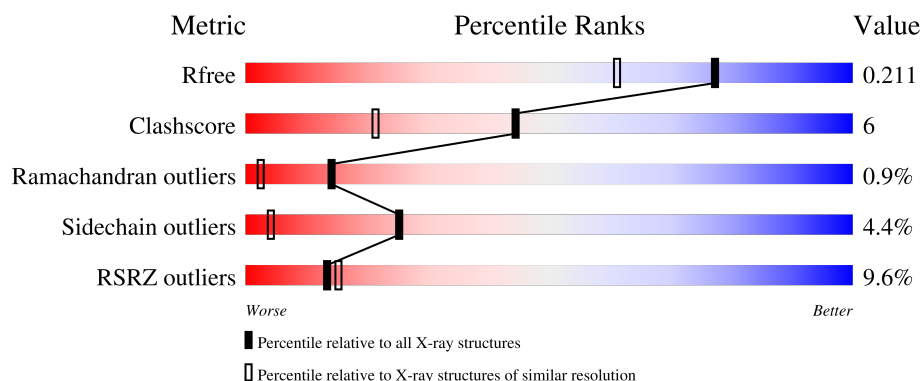
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	586	4% 50% 6% .. 42%
1	B	586	7% 51% 5% • 42%
1	C	586	7% 49% 7% .. 42%
1	D	586	4% 52% 5% • 42%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11987 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.

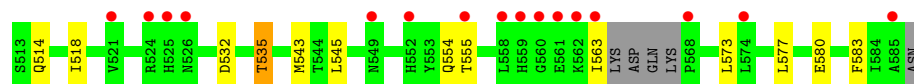
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	Se	0	0	0
			2681	1690	468	515	8			
1	B	340	Total	C	N	O	Se	0	0	0
			2686	1693	469	516	8			
1	C	338	Total	C	N	O	Se	0	0	0
			2675	1687	467	513	8			
1	D	342	Total	C	N	O	Se	0	0	0
			2702	1703	471	520	8			

- Molecule 2 is water.

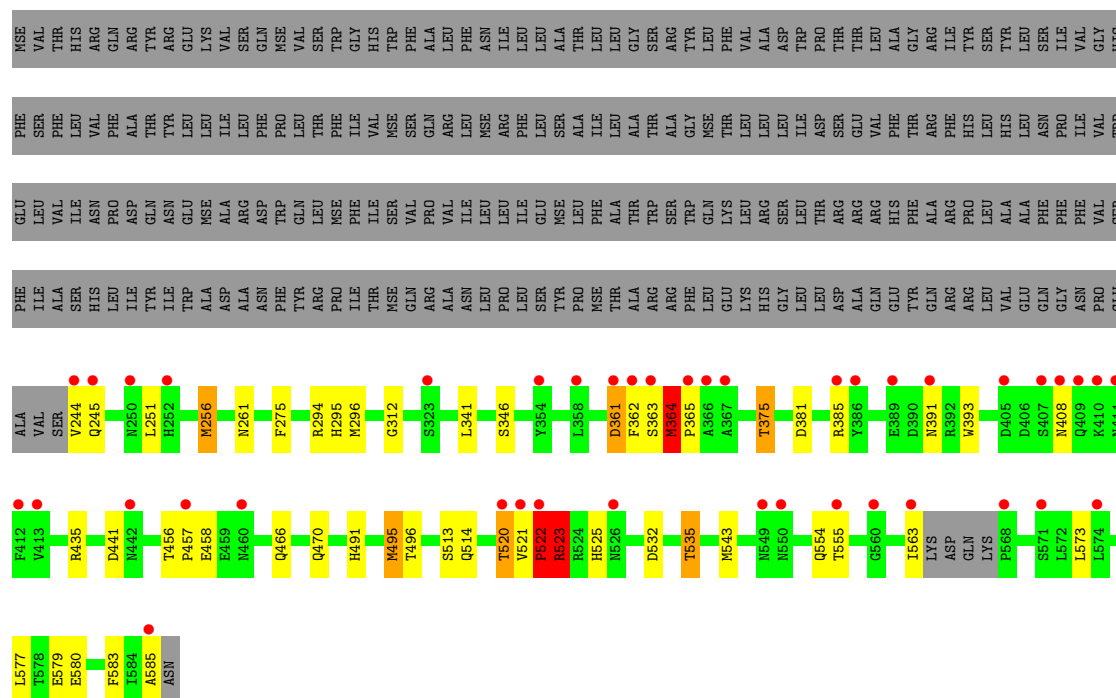
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	332	Total	O	0	0
			332	332		
2	B	316	Total	O	0	0
			316	316		
2	C	247	Total	O	0	0
			247	247		
2	D	348	Total	O	0	0
			348	348		

- Molecule 1: Inner membrane protein YejM

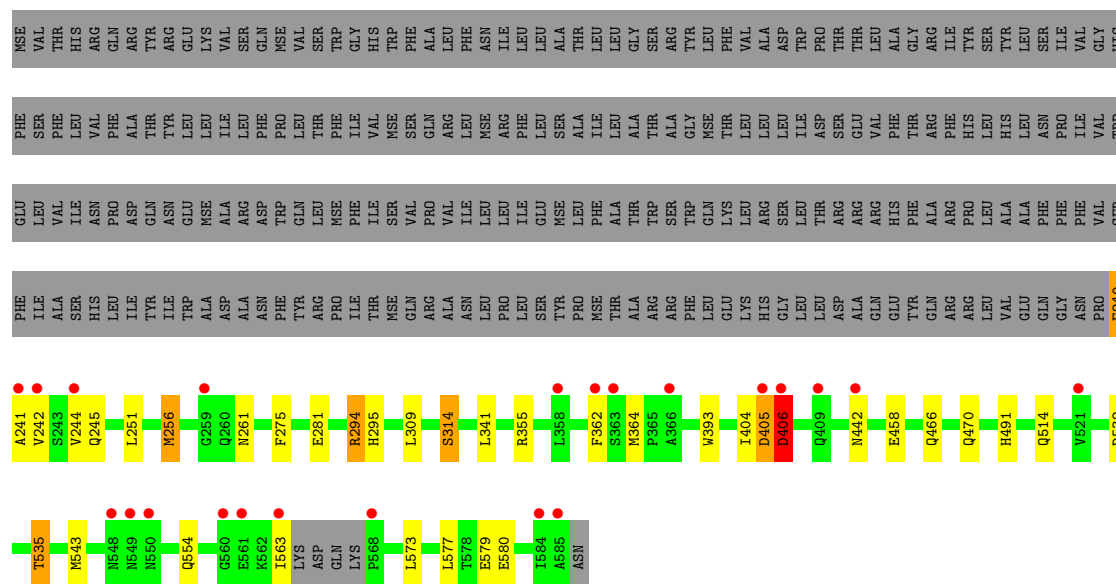




• Molecule 1: Inner membrane protein YejM



• 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	51.60Å 196.09Å 70.27Å 90.00° 95.79° 90.00°	Depositor
Resolution (Å)	98.04 – 1.64 98.04 – 1.64	Depositor EDS
% Data completeness (in resolution range)	85.8 (98.04-1.64) 85.8 (98.04-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.222 0.184 , 0.211	Depositor DCC
R_{free} test set	7305 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11987	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 71.57 % 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 2.5653e-06. 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	1.14	4/2736 (0.1%)	1.12	12/3714 (0.3%)
1	B	1.15	3/2741 (0.1%)	1.18	9/3721 (0.2%)
1	C	1.01	2/2730 (0.1%)	1.13	12/3706 (0.3%)
1	D	1.20	4/2757 (0.1%)	1.28	10/3743 (0.3%)
All	All	1.13	13/10964 (0.1%)	1.18	43/14884 (0.3%)

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	A	0	1
1	B	0	1
1	C	0	2
1	D	0	3
All	All	0	7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405	ASP	C-N	-16.18	1.11	1.33
1	D	404	ILE	C-N	-13.54	1.15	1.33
1	B	256	MSE	C-N	6.43	1.44	1.33
1	D	309	LEU	CB-CG	-6.28	1.40	1.53
1	A	243	SER	CA-CB	-6.26	1.41	1.53
1	B	244	VAL	N-CA	6.22	1.54	1.46
1	A	448	THR	C-O	5.66	1.30	1.23
1	A	244	VAL	CA-CB	5.29	1.60	1.54
1	B	244	VAL	CA-CB	5.27	1.61	1.54
1	D	314	SER	C-N	5.22	1.39	1.34
1	A	375	THR	CB-CG2	-5.18	1.35	1.52
1	C	361	ASP	CB-CG	5.11	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	THR	CA-C	5.05	1.59	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	ASP	O-C-N	-27.07	90.28	121.95
1	D	405	ASP	CA-C-N	16.23	152.54	121.54
1	D	405	ASP	C-N-CA	16.23	152.54	121.54
1	C	520	THR	CA-C-N	11.35	142.13	121.70
1	C	520	THR	C-N-CA	11.35	142.13	121.70
1	B	495	MSE	CG-SE-CE	10.46	121.93	98.92
1	B	514	GLN	CB-CG-CD	9.69	129.07	112.60
1	C	520	THR	O-C-N	-9.49	112.19	123.10
1	D	405	ASP	N-CA-C	-8.65	100.53	112.12
1	B	389	GLU	N-CA-C	-7.83	102.43	110.97
1	B	441	ASP	N-CA-C	-7.76	97.93	110.20
1	C	520	THR	CA-C-O	-7.48	112.46	121.28
1	A	244	VAL	N-CA-CB	7.20	118.50	110.51
1	D	406	ASP	N-CA-C	6.98	125.67	110.80
1	C	294	ARG	NE-CZ-NH2	6.84	125.35	119.20
1	B	442	ASN	N-CA-C	6.79	121.52	113.23
1	B	243	SER	CA-C-N	6.77	134.15	121.97
1	B	243	SER	C-N-CA	6.77	134.15	121.97
1	D	256	MSE	N-CA-CB	-6.75	99.49	110.42
1	A	325	ARG	CD-NE-CZ	6.52	133.53	124.40
1	C	256	MSE	CB-CA-C	-6.38	97.98	110.11
1	C	294	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	D	364	MSE	N-CA-C	-6.26	102.25	110.39
1	B	244	VAL	N-CA-C	6.21	122.25	109.34
1	D	256	MSE	CB-CA-C	-6.16	98.41	110.11
1	B	409	GLN	N-CA-C	6.05	123.69	110.80
1	A	562	LYS	N-CA-C	6.00	123.57	110.80
1	C	245	GLN	N-CA-C	5.91	123.39	110.80
1	C	522	PRO	CA-C-N	5.79	132.61	121.54
1	C	522	PRO	C-N-CA	5.79	132.61	121.54
1	C	523	ARG	N-CA-C	5.77	123.10	110.80
1	A	409	GLN	N-CA-C	5.74	123.03	110.80
1	A	543	MSE	CG-SE-CE	-5.62	86.55	98.92
1	A	471	VAL	CA-C-N	-5.59	114.02	119.78
1	A	471	VAL	C-N-CA	-5.59	114.02	119.78
1	C	543	MSE	CG-SE-CE	5.45	110.92	98.92
1	D	256	MSE	CG-SE-CE	-5.37	87.11	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	THR	CB-CA-C	5.18	119.40	110.79
1	D	294	ARG	CG-CD-NE	5.17	123.37	112.00
1	A	526	ASN	N-CA-CB	5.12	117.44	110.42
1	A	294	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	325	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	A	543	MSE	CB-CG-SE	-5.02	97.64	112.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	390	ASP	Peptide
1	B	255	ASP	Mainchain
1	C	522	PRO	Peptide
1	C	523	ARG	Peptide
1	D	240	GLU	Peptide
1	D	405	ASP	Mainchain,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	2681	0	2584	27	0
1	B	2686	0	2585	40	0
1	C	2675	0	2579	42	0
1	D	2702	0	2603	17	0
2	A	332	0	0	6	0
2	B	316	0	0	3	0
2	C	247	0	0	10	0
2	D	348	0	0	11	0
All	All	11987	0	10351	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (126) 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:B:255:ASP:C	1:B:256:MSE:CA	2.09	1.24
1:B:255:ASP:O	1:B:256:MSE:N	1.69	1.23
1:C:495:MSE:SE	2:C:814:HOH:O	2.10	1.17
1:B:255:ASP:CA	1:B:256:MSE:N	2.09	1.14
1:B:495:MSE:SE	2:B:851:HOH:O	2.15	1.12
1:C:495:MSE:HE1	1:C:513:SER:CB	1.85	1.07
1:C:296:MSE:SE	2:C:717:HOH:O	2.29	1.00
1:B:495:MSE:CE	1:B:496:THR:HA	1.96	0.96
1:B:495:MSE:HE2	1:B:496:THR:CA	1.98	0.94
1:D:442:ASN:HB3	2:D:734:HOH:O	1.68	0.92
1:D:244:VAL:HG11	2:D:910:HOH:O	1.68	0.90
1:B:255:ASP:C	1:B:256:MSE:N	0.80	0.90
1:B:495:MSE:HE2	1:B:496:THR:HA	1.51	0.89
1:A:294:ARG:NE	2:A:601:HOH:O	2.03	0.87
1:C:495:MSE:HE1	1:C:513:SER:HB2	1.60	0.83
1:C:495:MSE:HE1	1:C:513:SER:HB3	1.60	0.82
1:A:340:GLN:HE22	1:A:388:GLN:H	1.28	0.81
1:A:244:VAL:HG23	1:A:585:ALA:H	1.45	0.80
1:B:555:THR:HG23	1:B:563:ILE:HB	1.66	0.77
1:C:363:SER:HA	1:C:364:MSE:HB2	1.67	0.75
1:C:456:THR:HB	2:C:602:HOH:O	1.87	0.74
1:C:363:SER:HA	1:C:364:MSE:CB	2.17	0.73
1:B:495:MSE:HE1	1:B:512:TYR:HE1	1.51	0.73
1:C:466:GLN:HA	2:C:717:HOH:O	1.88	0.73
1:C:495:MSE:HE3	1:C:496:THR:N	2.04	0.73
1:D:281:GLU:HG2	2:D:618:HOH:O	1.88	0.72
1:B:495:MSE:HE1	1:B:512:TYR:CE1	2.24	0.72
1:C:495:MSE:CE	1:C:513:SER:HB2	2.19	0.72
1:B:495:MSE:HE2	1:B:496:THR:N	2.05	0.72
1:C:555:THR:HG23	1:C:563:ILE:HB	1.73	0.70
1:C:495:MSE:CE	1:C:513:SER:CB	2.68	0.70
1:A:484:ARG:HE	1:A:486:ASN:HD21	1.40	0.70
1:B:495:MSE:HE3	1:B:499:MSE:HG3	1.72	0.70
1:D:294:ARG:NE	2:D:602:HOH:O	2.22	0.67
1:D:244:VAL:HG21	2:D:910:HOH:O	1.95	0.66
1:C:244:VAL:HG12	1:C:585:ALA:H	1.62	0.65
1:B:495:MSE:HE3	1:B:499:MSE:CG	2.28	0.64
1:B:543:MSE:CE	1:B:545:LEU:HB2	2.27	0.63
1:A:555:THR:HG23	1:A:563:ILE:HB	1.80	0.63
1:B:495:MSE:HE3	1:B:496:THR:HA	1.80	0.62
1:C:364:MSE:H	1:C:365:PRO:CD	2.12	0.62
1:A:388:GLN:O	1:A:391:ASN:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:GLN:HE21	1:B:470:GLN:HE21	1.47	0.61
1:C:341:LEU:HD12	1:C:362:PHE:CZ	2.35	0.61
1:C:520:THR:O	1:C:523:ARG:NH1	2.30	0.61
1:C:381:ASP:OD1	1:C:385:ARG:NH1	2.33	0.60
1:D:466:GLN:HE21	1:D:470:GLN:HE21	1.50	0.59
1:C:364:MSE:H	1:C:365:PRO:HD3	1.68	0.59
1:B:543:MSE:HE3	1:B:545:LEU:HB2	1.84	0.58
1:A:244:VAL:HG22	1:A:584:ILE:HA	1.86	0.58
1:C:244:VAL:O	1:C:583:PHE:O	2.22	0.57
1:B:442:ASN:HA	1:B:478:PRO:HG2	1.86	0.57
1:A:466:GLN:HE21	1:A:470:GLN:HE21	1.51	0.56
1:A:466:GLN:HE21	1:A:470:GLN:NE2	2.04	0.56
1:C:466:GLN:HE21	1:C:470:GLN:HE21	1.53	0.56
1:D:458:GLU:O	2:D:601:HOH:O	2.18	0.56
1:A:408:ASN:OD1	1:A:408:ASN:N	2.37	0.55
1:B:422:ASP:HB2	2:D:621:HOH:O	2.06	0.55
1:C:457:PRO:N	2:C:602:HOH:O	2.40	0.55
1:B:543:MSE:HE1	1:B:545:LEU:HD12	1.89	0.55
1:D:281:GLU:CG	2:D:618:HOH:O	2.52	0.55
1:C:466:GLN:HE21	1:C:470:GLN:NE2	2.04	0.54
1:D:466:GLN:HE21	1:D:470:GLN:NE2	2.05	0.54
1:B:388:GLN:CD	1:B:388:GLN:H	2.14	0.54
1:C:346:SER:OG	1:C:375:THR:HG21	2.09	0.53
1:B:466:GLN:HE21	1:B:470:GLN:NE2	2.07	0.53
1:D:245:GLN:NE2	2:D:607:HOH:O	2.42	0.52
1:A:244:VAL:HG23	1:A:585:ALA:N	2.20	0.52
1:A:346:SER:OG	1:A:375:THR:HG21	2.09	0.52
1:B:388:GLN:HB2	1:B:391:ASN:H	1.75	0.51
1:A:254:ARG:NH2	2:A:604:HOH:O	2.40	0.51
1:D:261:ASN:HD22	1:D:393:TRP:H	1.56	0.51
1:B:495:MSE:CE	1:B:499:MSE:HG3	2.40	0.51
1:A:294:ARG:NH2	2:A:601:HOH:O	2.44	0.50
1:B:256:MSE:O	1:B:256:MSE:HG3	2.11	0.50
1:B:390:ASP:O	1:B:391:ASN:HB2	2.10	0.50
1:D:341:LEU:HD12	1:D:362:PHE:CZ	2.46	0.49
1:C:362:PHE:O	1:C:364:MSE:HG3	2.11	0.49
1:A:524:ARG:NH2	2:A:607:HOH:O	2.45	0.49
1:B:495:MSE:CE	1:B:496:THR:CA	2.69	0.49
1:A:408:ASN:O	1:A:410:LYS:N	2.46	0.49
1:B:255:ASP:CB	1:B:256:MSE:N	2.74	0.49
1:D:244:VAL:HG11	2:D:948:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ASP:O	1:B:256:MSE:CA	2.43	0.48
1:C:456:THR:CB	2:C:602:HOH:O	2.52	0.48
1:A:532:ASP:OD1	1:A:535:THR:HG23	2.14	0.48
1:A:294:ARG:CZ	2:A:601:HOH:O	2.55	0.48
1:B:532:ASP:OD1	1:B:535:THR:HG23	2.14	0.48
1:A:244:VAL:CG2	1:A:585:ALA:H	2.21	0.48
1:A:388:GLN:HB3	1:A:391:ASN:H	1.79	0.48
1:B:254:ARG:NH2	2:B:606:HOH:O	2.46	0.47
1:C:441:ASP:HA	2:C:736:HOH:O	2.13	0.47
1:A:370:GLN:HE21	1:A:375:THR:HG22	1.80	0.47
1:C:346:SER:OG	1:C:375:THR:CG2	2.62	0.47
1:D:355:ARG:HB2	2:D:661:HOH:O	2.13	0.47
1:B:244:VAL:O	1:B:583:PHE:O	2.32	0.47
1:B:408:ASN:O	1:B:410:LYS:N	2.48	0.47
1:D:314:SER:H	1:D:514:GLN:NE2	2.13	0.47
1:C:495:MSE:CE	1:C:513:SER:HB3	2.39	0.46
1:A:346:SER:OG	1:A:375:THR:CG2	2.63	0.46
1:C:495:MSE:HE3	1:C:496:THR:OG1	2.15	0.46
1:B:245:GLN:HG3	1:B:248:LEU:HD23	1.97	0.46
1:C:495:MSE:CE	1:C:496:THR:OG1	2.63	0.46
1:C:522:PRO:HA	1:C:523:ARG:HB2	1.97	0.46
1:C:435:ARG:HD3	2:C:737:HOH:O	2.16	0.45
1:C:523:ARG:O	1:C:525:HIS:N	2.49	0.45
1:A:261:ASN:HD22	1:A:393:TRP:H	1.63	0.45
1:C:532:ASP:OD1	1:C:535:THR:HG23	2.16	0.45
1:D:532:ASP:OD1	1:D:535:THR:HG23	2.16	0.45
1:B:555:THR:CG2	1:B:563:ILE:HB	2.41	0.45
1:A:540:THR:OG1	1:A:543:MSE:HG3	2.18	0.44
1:C:295:HIS:NE2	1:C:491:HIS:HD2	2.15	0.44
1:C:363:SER:CA	1:C:364:MSE:HB2	2.43	0.44
1:C:312:GLY:HA3	1:C:495:MSE:HE2	1.99	0.44
1:B:340:GLN:HG3	1:B:388:GLN:NE2	2.32	0.43
1:B:461:ARG:NH2	2:B:601:HOH:O	1.99	0.43
1:A:295:HIS:NE2	1:A:491:HIS:HD2	2.17	0.43
1:A:355:ARG:HB2	2:A:632:HOH:O	2.18	0.42
1:C:514:GLN:HG2	2:C:620:HOH:O	2.19	0.42
1:B:244:VAL:HB	1:B:245:GLN:H	1.64	0.42
1:B:442:ASN:HA	1:B:478:PRO:CG	2.49	0.42
1:D:295:HIS:NE2	1:D:491:HIS:HD2	2.18	0.41
1:A:516:GLN:O	1:A:517:ASP:C	2.64	0.41
1:C:261:ASN:HD22	1:C:393:TRP:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:GLU:HG3	2:C:620:HOH:O	2.20	0.40
1:C:555:THR:CG2	1:C:563:ILE:HB	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/586 (57%)	321 (96%)	11 (3%)	3 (1%)	14	2
1	B	336/586 (57%)	319 (95%)	14 (4%)	3 (1%)	14	2
1	C	334/586 (57%)	319 (96%)	12 (4%)	3 (1%)	14	2
1	D	338/586 (58%)	323 (96%)	12 (4%)	3 (1%)	14	2
All	All	1343/2344 (57%)	1282 (96%)	49 (4%)	12 (1%)	14	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	ASN
1	A	409	GLN
1	A	562	LYS
1	B	244	VAL
1	B	391	ASN
1	B	409	GLN
1	C	364	MSE
1	D	406	ASP
1	C	391	ASN
1	D	241	ALA
1	D	242	VAL
1	C	521	VAL

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	291/493 (59%)	278 (96%)	13 (4%)	24	4
1	B	291/493 (59%)	281 (97%)	10 (3%)	32	7
1	C	290/493 (59%)	275 (95%)	15 (5%)	21	3
1	D	293/493 (59%)	280 (96%)	13 (4%)	25	4
All	All	1165/1972 (59%)	1114 (96%)	51 (4%)	25	4

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	LEU
1	A	325	ARG
1	A	375	THR
1	A	388	GLN
1	A	391	ASN
1	A	408	ASN
1	A	518	ILE
1	A	535	THR
1	A	543	MSE
1	A	573	LEU
1	A	577	LEU
1	A	579	GLU
1	A	580	GLU
1	B	251	LEU
1	B	388	GLN
1	B	389	GLU
1	B	495	MSE
1	B	518	ILE
1	B	535	THR
1	B	554	GLN
1	B	573	LEU
1	B	577	LEU
1	B	580	GLU
1	C	251	LEU

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Mol	Chain	Res	Type
1	C	256	MSE
1	C	275	PHE
1	C	361	ASP
1	C	364	MSE
1	C	375	THR
1	C	408	ASN
1	C	458	GLU
1	C	495	MSE
1	C	523	ARG
1	C	535	THR
1	C	554	GLN
1	C	573	LEU
1	C	577	LEU
1	C	580	GLU
1	D	240	GLU
1	D	251	LEU
1	D	256	MSE
1	D	275	PHE
1	D	406	ASP
1	D	535	THR
1	D	543	MSE
1	D	554	GLN
1	D	563	ILE
1	D	573	LEU
1	D	577	LEU
1	D	579	GLU
1	D	580	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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	378	GLN
1	A	391	ASN
1	A	470	GLN
1	A	486	ASN
1	A	491	HIS
1	A	514	GLN

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Mol	Chain	Res	Type
1	B	250	ASN
1	B	252	HIS
1	B	261	ASN
1	B	271	ASN
1	B	388	GLN
1	B	470	GLN
1	B	483	GLN
1	B	491	HIS
1	C	250	ASN
1	C	261	ASN
1	C	340	GLN
1	C	388	GLN
1	C	470	GLN
1	C	491	HIS
1	C	514	GLN
1	C	525	HIS
1	C	554	GLN
1	D	252	HIS
1	D	261	ASN
1	D	271	ASN
1	D	370	GLN
1	D	378	GLN
1	D	411	ASN
1	D	442	ASN
1	D	470	GLN
1	D	491	HIS
1	D	514	GLN
1	D	548	ASN
1	D	554	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 [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	D	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	404:ILE	C	405:ASP	N	1.15
1	D	405:ASP	C	406:ASP	N	1.11
1	B	255:ASP	C	256:MSE	N	0.80

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	331/586 (56%)	0.31	24 (7%) 21 24	12, 21, 46, 71	0
1	B	332/586 (56%)	0.55	40 (12%) 9 10	11, 22, 51, 83	0
1	C	330/586 (56%)	0.79	41 (12%) 8 9	15, 27, 56, 84	0
1	D	334/586 (56%)	0.35	22 (6%) 24 28	12, 21, 45, 83	0
All	All	1327/2344 (56%)	0.50	127 (9%) 13 15	11, 23, 50, 84	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	VAL	8.8
1	D	563	ILE	8.1
1	D	242	VAL	6.8
1	C	244	VAL	6.6
1	B	568	PRO	5.4
1	D	568	PRO	5.4
1	C	366	ALA	5.1
1	B	386	TYR	5.1
1	A	243	SER	4.9
1	C	568	PRO	4.9
1	C	358	LEU	4.5
1	B	574	LEU	4.3
1	C	407	SER	4.3
1	A	244	VAL	4.3
1	A	568	PRO	4.2
1	C	574	LEU	4.1
1	A	479	GLY	4.1
1	C	386	TYR	4.1
1	B	563	ILE	4.0
1	A	386	TYR	4.0
1	B	388	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	241	ALA	3.9
1	B	242	VAL	3.8
1	B	387	ALA	3.8
1	B	391	ASN	3.8
1	B	407	SER	3.7
1	C	362	PHE	3.7
1	B	390	ASP	3.6
1	C	521	VAL	3.6
1	D	362	PHE	3.6
1	C	410	LYS	3.5
1	C	365	PRO	3.5
1	C	412	PHE	3.5
1	C	405	ASP	3.5
1	A	410	LYS	3.5
1	C	361	ASP	3.5
1	D	406	ASP	3.4
1	B	585	ALA	3.4
1	A	585	ALA	3.4
1	B	406	ASP	3.3
1	C	585	ALA	3.3
1	A	408	ASN	3.2
1	D	405	ASP	3.1
1	B	408	ASN	3.0
1	B	480	THR	2.9
1	C	522	PRO	2.9
1	C	457	PRO	2.9
1	A	391	ASN	2.9
1	B	521	VAL	2.8
1	D	561	GLU	2.8
1	A	480	THR	2.8
1	B	481	PRO	2.8
1	C	385	ARG	2.8
1	D	409	GLN	2.8
1	C	408	ASN	2.8
1	A	563	ILE	2.8
1	B	243	SER	2.8
1	C	389	GLU	2.7
1	D	244	VAL	2.7
1	B	558	LEU	2.7
1	A	407	SER	2.7
1	A	388	GLN	2.7
1	A	560	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	366	ALA	2.7
1	B	526	ASN	2.6
1	B	479	GLY	2.6
1	C	563	ILE	2.6
1	C	391	ASN	2.6
1	C	411	ASN	2.6
1	D	584	ILE	2.6
1	A	363	SER	2.6
1	C	442	ASN	2.6
1	B	561	GLU	2.6
1	B	560	GLY	2.5
1	D	560	GLY	2.5
1	A	482	ALA	2.5
1	A	584	ILE	2.5
1	C	549	ASN	2.4
1	C	413	VAL	2.4
1	C	550	ASN	2.4
1	C	560	GLY	2.4
1	A	390	ASP	2.4
1	B	389	GLU	2.4
1	B	385	ARG	2.4
1	A	577	LEU	2.4
1	B	287	GLU	2.4
1	D	521	VAL	2.4
1	A	552	HIS	2.4
1	C	409	GLN	2.3
1	C	460	ASN	2.3
1	D	549	ASN	2.3
1	B	555	THR	2.3
1	D	363	SER	2.3
1	C	363	SER	2.3
1	B	437	ALA	2.3
1	B	442	ASN	2.3
1	D	550	ASN	2.3
1	D	259	GLY	2.3
1	C	526	ASN	2.2
1	C	252	HIS	2.2
1	B	549	ASN	2.2
1	B	562	LYS	2.2
1	B	438	GLY	2.2
1	C	555	THR	2.2
1	C	323	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	387	ALA	2.2
1	D	358	LEU	2.2
1	C	245	GLN	2.1
1	A	574	LEU	2.1
1	C	520	THR	2.1
1	B	482	ALA	2.1
1	C	367	ALA	2.1
1	B	252	HIS	2.1
1	B	552	HIS	2.1
1	B	410	LYS	2.1
1	A	409	GLN	2.1
1	C	571	SER	2.1
1	C	354	TYR	2.1
1	B	525	HIS	2.1
1	D	548	ASN	2.1
1	A	570	LEU	2.1
1	C	250	ASN	2.0
1	D	442	ASN	2.0
1	B	524	ARG	2.0
1	B	286	ALA	2.0
1	D	585	ALA	2.0
1	B	559	HIS	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.