



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 AM UTC

PDB ID : 1TF5 / pdb_00001tf5
Title : Crystal structure of SecA in an open conformation from Bacillus Subtilis
Authors : Osborne, A.R.; Clemons Jr., W.M.; Rapoport, T.A.
Deposited on : 2004-05-26
Resolution : 2.18 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

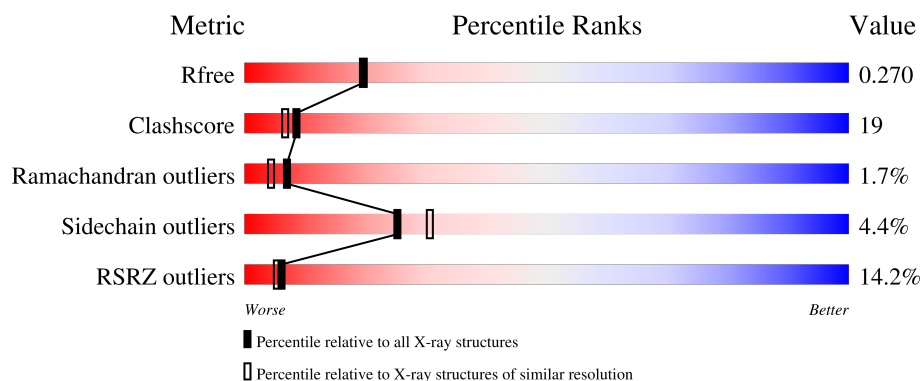
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	844	13% 60% 27% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6316 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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	775	Total	C	N	O	S	0	0	0
			6187	3872	1080	1201	34			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P28366
A	-1	PRO	-	cloning artifact	UNP P28366
A	0	HIS	-	cloning artifact	UNP P28366

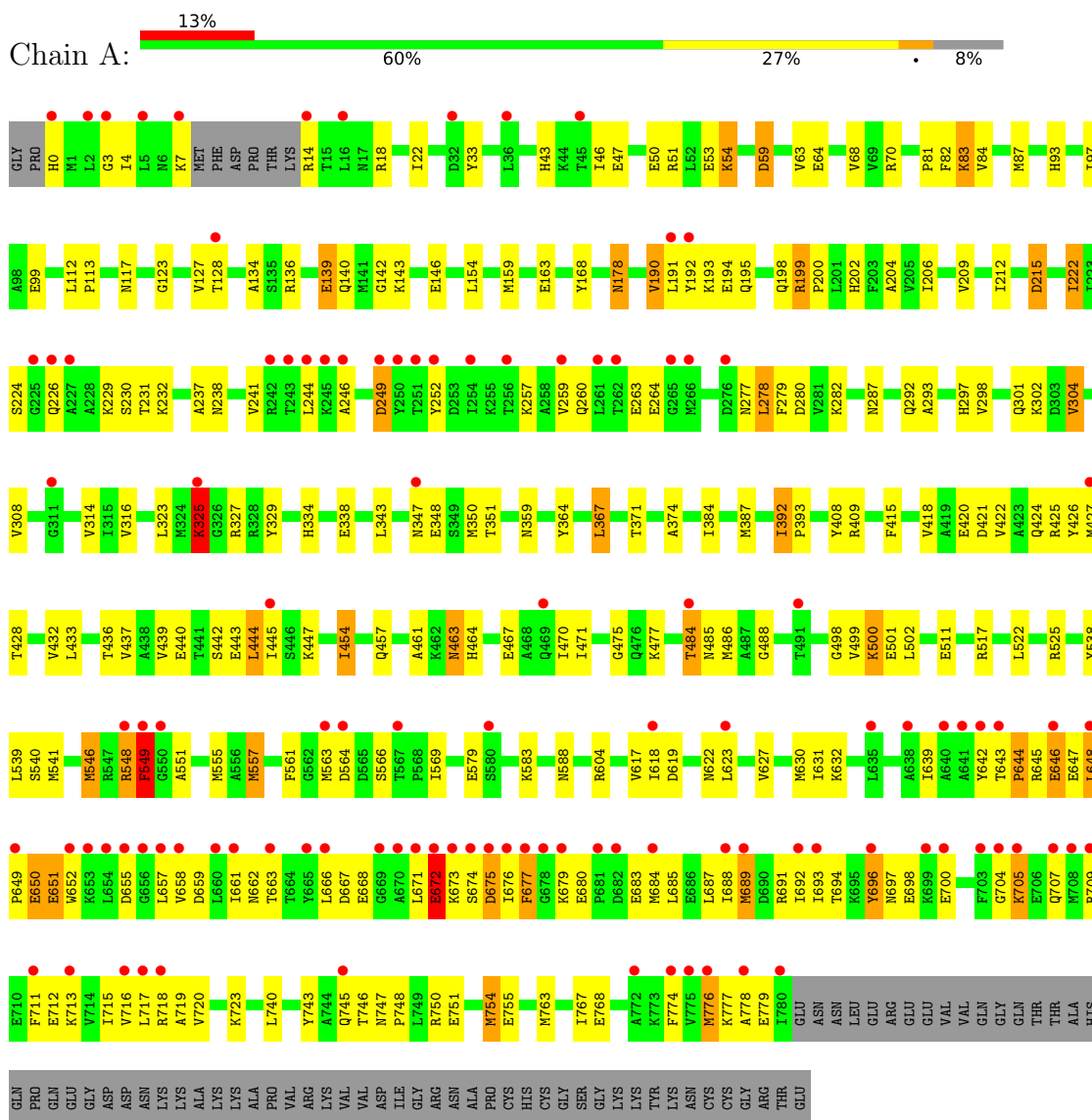
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	129	Total	O	0	0
			129	129		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Preprotein translocase secA subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.23Å 107.19Å 72.05Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	50.00 – 2.18 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.00-2.18) 90.5 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.273 0.239 , 0.270	Depositor DCC
R_{free} test set	3265 reflections (5.69%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6316	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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	0.42	0/6273	0.90	19/8434 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ALA	N-CA-C	7.46	119.05	111.07
1	A	454	ILE	N-CA-C	6.39	113.38	107.56
1	A	206	ILE	N-CA-C	6.13	116.94	107.99
1	A	212	ILE	N-CA-C	6.06	116.24	110.42
1	A	33	TYR	N-CA-C	-5.86	107.37	114.75
1	A	222	ILE	N-CA-C	5.81	116.85	108.48
1	A	325	LYS	N-CA-C	5.70	122.95	110.80
1	A	655	ASP	N-CA-C	5.67	117.64	108.41
1	A	484	THR	N-CA-C	-5.63	101.30	110.20
1	A	650	GLU	N-CA-C	5.61	120.08	113.23
1	A	464	HIS	N-CA-C	5.54	117.32	111.28
1	A	127	VAL	N-CA-C	5.43	116.12	108.36
1	A	209	VAL	N-CA-C	5.42	117.82	111.05
1	A	384	ILE	N-CA-C	5.40	116.06	110.82
1	A	199	ARG	N-CA-C	-5.40	103.83	110.31
1	A	392	ILE	CA-C-N	5.25	125.17	119.76
1	A	392	ILE	C-N-CA	5.25	125.17	119.76
1	A	329	TYR	N-CA-C	-5.18	103.69	110.53
1	A	215	ASP	N-CA-C	5.12	116.94	111.36

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	6187	0	6184	234	0
2	A	129	0	0	6	0
All	All	6316	0	6184	234	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 19.

All (234) 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:630:MET:HE2	1:A:768:GLU:HA	1.34	1.04
1:A:754:MET:C	1:A:754:MET:HE2	1.98	0.87
1:A:83:LYS:H	1:A:83:LYS:CD	1.84	0.86
1:A:658:VAL:HG11	1:A:672:GLU:HG2	1.58	0.86
1:A:83:LYS:H	1:A:83:LYS:HD3	1.39	0.85
1:A:630:MET:CE	1:A:768:GLU:HA	2.05	0.84
1:A:83:LYS:HD3	1:A:83:LYS:N	1.91	0.84
1:A:644:PRO:CB	1:A:647:GLU:HB2	2.11	0.81
1:A:671:LEU:HD11	1:A:691:ARG:HG3	1.62	0.81
1:A:644:PRO:HB2	1:A:647:GLU:HB2	1.64	0.80
1:A:693:ILE:HG22	1:A:697:ASN:HD21	1.48	0.79
1:A:159:MET:HE2	1:A:163:GLU:HG2	1.62	0.79
1:A:238:ASN:OD1	1:A:297:HIS:HE1	1.66	0.78
1:A:433:LEU:HD21	1:A:525:ARG:HD3	1.65	0.77
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.32	0.76
1:A:694:THR:HA	1:A:697:ASN:HD22	1.51	0.74
1:A:676:ILE:HG23	1:A:684:MET:HE2	1.68	0.74
1:A:159:MET:CE	1:A:163:GLU:HG2	2.17	0.73
1:A:622:ASN:HA	1:A:709:ARG:HD2	1.71	0.72
1:A:754:MET:HE2	1:A:755:GLU:N	2.04	0.72
1:A:436:THR:HG21	1:A:442:SER:OG	1.89	0.72
1:A:648:LEU:H	1:A:649:PRO:CD	2.05	0.69
1:A:747:ASN:HD22	1:A:748:PRO:CD	2.05	0.69
1:A:675:ASP:O	1:A:679:LYS:HG3	1.93	0.68
1:A:642:TYR:HD1	1:A:657:LEU:HB2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:MET:HA	1:A:486:MET:HE2	1.74	0.68
1:A:657:LEU:O	1:A:661:ILE:HG12	1.94	0.67
1:A:128:THR:CG2	1:A:134:ALA:HB2	2.25	0.67
1:A:415:PHE:CD2	1:A:445:ILE:HD11	2.31	0.65
1:A:457:GLN:NE2	1:A:470:ILE:HD12	2.11	0.65
1:A:549:PHE:HZ	1:A:588:ASN:ND2	1.95	0.65
1:A:627:VAL:HG21	1:A:712:GLU:HG2	1.78	0.65
1:A:658:VAL:CG1	1:A:672:GLU:HG2	2.26	0.65
1:A:51:ARG:HA	1:A:54:LYS:HG2	1.78	0.64
1:A:128:THR:HG21	1:A:134:ALA:HB2	1.79	0.64
1:A:557:MET:CE	1:A:561:PHE:HB2	2.27	0.64
1:A:222:ILE:HG23	1:A:351:THR:HG23	1.80	0.64
1:A:673:LYS:H	1:A:673:LYS:HD3	1.62	0.64
1:A:747:ASN:HD22	1:A:748:PRO:HD2	1.62	0.64
1:A:83:LYS:HG2	2:A:2014:HOH:O	1.98	0.63
1:A:0:HIS:O	1:A:4:ILE:HG13	1.99	0.63
1:A:675:ASP:HB3	1:A:687:LEU:HD13	1.81	0.63
1:A:557:MET:HE2	1:A:557:MET:O	1.99	0.63
1:A:648:LEU:H	1:A:649:PRO:HD2	1.64	0.62
1:A:277:ASN:ND2	1:A:279:PHE:H	1.98	0.62
1:A:715:ILE:HA	1:A:718:ARG:HD3	1.80	0.62
1:A:301:GLN:HB2	1:A:304:VAL:HG13	1.83	0.61
1:A:278:LEU:HD22	1:A:287:ASN:HB2	1.84	0.60
1:A:617:VAL:O	1:A:713:LYS:HE2	2.00	0.60
1:A:178:ASN:H	1:A:178:ASN:HD22	1.50	0.60
1:A:252:TYR:HD2	1:A:259:VAL:HG22	1.66	0.60
1:A:93:HIS:CD2	1:A:117:ASN:HD21	2.16	0.60
1:A:676:ILE:O	1:A:677:PHE:HB2	2.02	0.60
1:A:190:VAL:HG22	1:A:195:GLN:HB2	1.84	0.59
1:A:226:GLN:CD	1:A:226:GLN:H	2.10	0.59
1:A:252:TYR:CD2	1:A:259:VAL:HG22	2.37	0.59
1:A:644:PRO:HB3	1:A:647:GLU:HB2	1.82	0.59
1:A:557:MET:HE2	1:A:561:PHE:HB2	1.84	0.59
1:A:277:ASN:C	1:A:277:ASN:HD22	2.11	0.58
1:A:433:LEU:CD2	1:A:525:ARG:HD3	2.32	0.58
1:A:693:ILE:HG22	1:A:697:ASN:ND2	2.19	0.58
1:A:463:ASN:HD22	1:A:463:ASN:C	2.10	0.58
1:A:426:TYR:CD2	1:A:454:ILE:HD12	2.39	0.57
1:A:675:ASP:CB	1:A:687:LEU:HD13	2.35	0.57
1:A:617:VAL:HG13	1:A:623:LEU:HD21	1.87	0.57
1:A:648:LEU:HB2	1:A:649:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:O	1:A:241:VAL:HG23	2.05	0.56
1:A:260:GLN:HE21	1:A:740:LEU:HD22	1.69	0.56
1:A:84:VAL:HA	1:A:87:MET:HE3	1.87	0.56
1:A:308:VAL:HG13	1:A:343:LEU:HD11	1.88	0.56
1:A:754:MET:HE2	1:A:755:GLU:CA	2.36	0.56
1:A:549:PHE:HD1	1:A:549:PHE:H	1.53	0.55
1:A:231:THR:HG23	1:A:347:ASN:ND2	2.22	0.55
1:A:70:ARG:HG3	1:A:81:PRO:HD2	1.89	0.54
1:A:190:VAL:O	1:A:618:ILE:HD11	2.07	0.54
1:A:627:VAL:O	1:A:631:ILE:HG13	2.07	0.54
1:A:229:LYS:HD2	1:A:350:MET:HE3	1.90	0.54
1:A:754:MET:HE2	1:A:755:GLU:HA	1.89	0.54
1:A:671:LEU:O	1:A:672:GLU:HB2	2.06	0.54
1:A:477:LYS:HE2	1:A:502:LEU:HD11	1.89	0.53
1:A:99:GLU:HA	1:A:371:THR:O	2.08	0.53
1:A:685:LEU:C	1:A:685:LEU:HD13	2.34	0.53
1:A:538:TYR:O	1:A:539:LEU:HD23	2.08	0.53
1:A:642:TYR:CD1	1:A:657:LEU:HB2	2.43	0.53
1:A:662:ASN:HB3	1:A:668:GLU:HA	1.91	0.53
1:A:231:THR:CG2	1:A:347:ASN:HD22	2.22	0.52
1:A:359:ASN:OD1	1:A:604:ARG:HD3	2.08	0.52
1:A:673:LYS:HD3	1:A:673:LYS:N	2.25	0.52
1:A:178:ASN:H	1:A:178:ASN:ND2	2.05	0.52
1:A:549:PHE:CD1	1:A:549:PHE:N	2.78	0.52
1:A:763:MET:O	1:A:767:ILE:HG13	2.10	0.52
1:A:93:HIS:HD2	1:A:117:ASN:ND2	2.04	0.52
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.92	0.52
1:A:444:LEU:C	1:A:444:LEU:HD13	2.35	0.51
1:A:704:GLY:HA2	1:A:707:GLN:NE2	2.25	0.51
1:A:238:ASN:OD1	1:A:297:HIS:CE1	2.55	0.51
1:A:674:SER:O	1:A:676:ILE:HG13	2.10	0.51
1:A:14:ARG:HD3	1:A:14:ARG:N	2.25	0.51
1:A:231:THR:HG23	1:A:347:ASN:HD22	1.76	0.51
1:A:292:GLN:OE1	1:A:292:GLN:HA	2.10	0.51
1:A:659:ASP:O	1:A:663:THR:HG22	2.11	0.51
1:A:673:LYS:H	1:A:673:LYS:CD	2.23	0.51
1:A:463:ASN:O	1:A:467:GLU:HG3	2.11	0.51
1:A:677:PHE:C	1:A:679:LYS:H	2.19	0.51
1:A:191:LEU:HD23	1:A:192:TYR:CE1	2.45	0.50
1:A:715:ILE:HA	1:A:718:ARG:CD	2.41	0.50
1:A:280:ASP:OD2	1:A:282:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:HB3	1:A:549:PHE:HD1	1.77	0.50
1:A:743:TYR:O	1:A:746:THR:HB	2.12	0.50
1:A:128:THR:HG21	1:A:134:ALA:CA	2.41	0.50
1:A:191:LEU:HD12	1:A:717:LEU:HD12	1.92	0.50
1:A:715:ILE:O	1:A:718:ARG:HG2	2.12	0.50
1:A:260:GLN:HE21	1:A:740:LEU:CD2	2.25	0.50
1:A:648:LEU:N	1:A:649:PRO:CD	2.70	0.50
1:A:54:LYS:NZ	1:A:54:LYS:HB3	2.27	0.50
1:A:564:ASP:HB2	1:A:566:SER:OG	2.12	0.50
1:A:563:MET:SD	1:A:569:ILE:HG12	2.52	0.49
1:A:190:VAL:CG2	1:A:195:GLN:HB2	2.42	0.49
1:A:774:PHE:O	1:A:778:ALA:HB3	2.13	0.49
1:A:128:THR:HG21	1:A:134:ALA:N	2.28	0.49
1:A:630:MET:HE1	1:A:767:ILE:HG22	1.95	0.49
1:A:715:ILE:HD13	1:A:718:ARG:HD3	1.93	0.49
1:A:301:GLN:HB2	1:A:304:VAL:CG1	2.42	0.49
1:A:643:THR:N	1:A:644:PRO:HD3	2.28	0.49
1:A:541:MET:SD	1:A:563:MET:HE2	2.52	0.49
1:A:644:PRO:C	1:A:646:GLU:H	2.21	0.48
1:A:689:MET:HA	1:A:689:MET:HE2	1.96	0.48
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.42	0.48
1:A:461:ALA:HA	1:A:467:GLU:OE2	2.12	0.48
1:A:696:TYR:CD1	1:A:696:TYR:C	2.92	0.48
1:A:424:GLN:HA	1:A:424:GLN:NE2	2.29	0.48
1:A:193:LYS:HE2	1:A:619:ASP:OD1	2.14	0.48
1:A:711:PHE:O	1:A:715:ILE:HG12	2.13	0.48
1:A:549:PHE:HZ	1:A:588:ASN:HD21	1.61	0.48
1:A:334:HIS:O	1:A:338:GLU:HG3	2.13	0.47
1:A:18:ARG:O	1:A:22:ILE:HG12	2.14	0.47
1:A:705:LYS:HD3	1:A:705:LYS:N	2.29	0.47
1:A:277:ASN:HD22	1:A:278:LEU:N	2.12	0.47
1:A:776:MET:HE3	1:A:776:MET:HA	1.95	0.47
1:A:128:THR:HG21	1:A:134:ALA:CB	2.44	0.47
1:A:314:VAL:HG21	1:A:325:LYS:HE3	1.96	0.47
1:A:546:MET:HG3	1:A:555:MET:SD	2.54	0.47
1:A:651:GLU:HG3	1:A:652:TRP:N	2.30	0.47
1:A:549:PHE:CZ	1:A:588:ASN:ND2	2.80	0.47
1:A:63:VAL:HG23	2:A:2072:HOH:O	2.15	0.47
1:A:136:ARG:O	1:A:140:GLN:HG3	2.15	0.47
1:A:64:GLU:O	1:A:68:VAL:HG23	2.15	0.47
1:A:522:LEU:O	1:A:525:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:HB2	1:A:364:TYR:CE2	2.50	0.47
1:A:671:LEU:HD22	1:A:674:SER:HB2	1.96	0.46
1:A:224:SER:OG	2:A:2121:HOH:O	2.21	0.46
1:A:657:LEU:C	1:A:657:LEU:HD23	2.40	0.46
1:A:716:VAL:O	1:A:720:VAL:HG23	2.15	0.46
1:A:3:GLY:O	1:A:7:LYS:HG3	2.15	0.46
1:A:264:GLU:H	1:A:264:GLU:CD	2.23	0.46
1:A:551:ALA:O	1:A:555:MET:HG2	2.15	0.46
1:A:159:MET:HE3	1:A:163:GLU:HG2	1.98	0.46
1:A:230:SER:OG	1:A:232:LYS:HG2	2.15	0.46
1:A:650:GLU:O	1:A:651:GLU:HB3	2.15	0.46
1:A:463:ASN:C	1:A:463:ASN:ND2	2.70	0.45
1:A:277:ASN:HD21	1:A:279:PHE:HB2	1.81	0.45
1:A:316:VAL:HG22	1:A:323:LEU:CD2	2.46	0.45
1:A:425:ARG:HB2	1:A:432:VAL:HG21	1.99	0.45
1:A:302:LYS:NZ	2:A:2128:HOH:O	2.45	0.45
1:A:457:GLN:HG3	2:A:2104:HOH:O	2.15	0.45
1:A:676:ILE:HG23	1:A:684:MET:CE	2.43	0.45
1:A:671:LEU:HD22	1:A:674:SER:CB	2.47	0.45
1:A:751:GLU:OE1	1:A:755:GLU:OE2	2.35	0.45
1:A:51:ARG:HB3	2:A:2122:HOH:O	2.17	0.45
1:A:154:LEU:O	1:A:159:MET:HE1	2.17	0.45
1:A:241:VAL:HG21	1:A:293:ALA:HB3	1.98	0.45
1:A:471:ILE:HG13	1:A:488:GLY:HA3	1.98	0.45
1:A:97:ILE:HG13	1:A:387:MET:HE2	1.99	0.44
1:A:226:GLN:CD	1:A:226:GLN:N	2.75	0.44
1:A:475:GLY:O	1:A:499:VAL:HG21	2.16	0.44
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.83	0.44
1:A:409:ARG:HD3	1:A:563:MET:O	2.18	0.44
1:A:277:ASN:ND2	1:A:277:ASN:C	2.70	0.44
1:A:747:ASN:ND2	1:A:748:PRO:HD2	2.32	0.44
1:A:82:PHE:HD2	1:A:83:LYS:HZ1	1.66	0.44
1:A:142:GLY:O	1:A:146:GLU:HG3	2.18	0.44
1:A:437:VAL:HB	1:A:511:GLU:OE1	2.18	0.44
1:A:139:GLU:OE2	1:A:143:LYS:HE3	2.18	0.44
1:A:408:TYR:O	1:A:540:SER:HA	2.17	0.44
1:A:43:HIS:CD2	1:A:47:GLU:HG3	2.53	0.43
1:A:350:MET:HE2	1:A:350:MET:HA	2.00	0.43
1:A:70:ARG:CG	1:A:81:PRO:HD2	2.48	0.43
1:A:632:LYS:HD3	1:A:689:MET:HG3	2.00	0.43
1:A:639:ILE:O	1:A:643:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:CG	1:A:604:ARG:HD3	2.43	0.43
1:A:191:LEU:HD12	1:A:717:LEU:CD1	2.48	0.43
1:A:719:ALA:O	1:A:723:LYS:HG2	2.18	0.43
1:A:244:LEU:HB3	1:A:249:ASP:HB3	2.00	0.43
1:A:392:ILE:HA	1:A:393:PRO:HD3	1.88	0.43
1:A:651:GLU:HG3	1:A:652:TRP:H	1.84	0.43
1:A:680:GLU:HB2	1:A:683:GLU:HG3	2.01	0.42
1:A:747:ASN:HD22	1:A:748:PRO:N	2.17	0.42
1:A:50:GLU:O	1:A:53:GLU:HB3	2.19	0.42
1:A:747:ASN:HA	1:A:748:PRO:HD3	1.88	0.42
1:A:168:TYR:CZ	1:A:198:GLN:HG2	2.54	0.42
1:A:666:LEU:CD2	1:A:692:ILE:HD13	2.49	0.42
1:A:199:ARG:O	1:A:200:PRO:C	2.61	0.42
1:A:443:GLU:O	1:A:447:LYS:HG3	2.19	0.42
1:A:689:MET:HE2	1:A:692:ILE:HG13	2.01	0.42
1:A:754:MET:HE2	1:A:754:MET:O	2.17	0.42
1:A:371:THR:HG21	1:A:374:ALA:HB2	2.01	0.42
1:A:639:ILE:HA	1:A:657:LEU:CD1	2.49	0.42
1:A:424:GLN:HA	1:A:424:GLN:HE21	1.83	0.42
1:A:421:ASP:O	1:A:425:ARG:HG2	2.20	0.42
1:A:123:GLY:O	1:A:202:HIS:HD2	2.03	0.41
1:A:439:VAL:HG22	1:A:440:GLU:OE2	2.20	0.41
1:A:231:THR:CG2	1:A:347:ASN:ND2	2.83	0.41
1:A:418:VAL:O	1:A:422:VAL:HG23	2.20	0.41
1:A:688:ILE:O	1:A:692:ILE:HG12	2.20	0.41
1:A:46:ILE:O	1:A:50:GLU:HG3	2.20	0.41
1:A:327:ARG:HH11	1:A:327:ARG:HG3	1.86	0.41
1:A:364:TYR:HB2	1:A:367:LEU:HD13	2.02	0.41
1:A:500:LYS:H	1:A:500:LYS:CE	2.34	0.41
1:A:579:GLU:HG3	1:A:583:LYS:HE3	2.03	0.41
1:A:215:ASP:OD1	1:A:517:ARG:NH2	2.53	0.41
1:A:59:ASP:OD1	1:A:93:HIS:HE1	2.02	0.41
1:A:252:TYR:CD2	1:A:298:VAL:HG12	2.56	0.41
1:A:715:ILE:C	1:A:718:ARG:HG2	2.46	0.41
1:A:420:GLU:O	1:A:424:GLN:HG2	2.20	0.41
1:A:498:GLY:HA2	1:A:501:GLU:OE1	2.21	0.41
1:A:548:ARG:HB3	1:A:549:PHE:CD1	2.55	0.41
1:A:779:GLU:N	1:A:779:GLU:OE1	2.54	0.41
1:A:229:LYS:HG2	1:A:230:SER:N	2.36	0.41
1:A:424:GLN:O	1:A:428:THR:HG23	2.20	0.41
1:A:436:THR:HG22	1:A:484:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:O	1:A:259:VAL:HG23	2.20	0.40
1:A:178:ASN:ND2	1:A:178:ASN:N	2.68	0.40
1:A:563:MET:SD	1:A:569:ILE:CG1	3.10	0.40
1:A:667:ASP:HA	1:A:777:LYS:CE	2.51	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	771/844 (91%)	722 (94%)	36 (5%)	13 (2%)	7 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	PHE
1	A	672	GLU
1	A	485	ASN
1	A	645	ARG
1	A	651	GLU
1	A	675	ASP
1	A	677	PHE
1	A	700	GLU
1	A	249	ASP
1	A	698	GLU
1	A	548	ARG
1	A	644	PRO
1	A	648	LEU

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	665/723 (92%)	636 (96%)	29 (4%)	25	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	59	ASP
1	A	83	LYS
1	A	139	GLU
1	A	178	ASN
1	A	190	VAL
1	A	194	GLU
1	A	263	GLU
1	A	278	LEU
1	A	304	VAL
1	A	325	LYS
1	A	348	GLU
1	A	367	LEU
1	A	427	MET
1	A	444	LEU
1	A	463	ASN
1	A	500	LYS
1	A	546	MET
1	A	549	PHE
1	A	557	MET
1	A	646	GLU
1	A	672	GLU
1	A	689	MET
1	A	696	TYR
1	A	705	LYS
1	A	745	GLN
1	A	750	ARG
1	A	754	MET
1	A	776	MET

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	0	HIS
1	A	6	ASN
1	A	43	HIS
1	A	93	HIS
1	A	178	ASN
1	A	202	HIS
1	A	226	GLN
1	A	236	GLN
1	A	260	GLN
1	A	277	ASN
1	A	287	ASN
1	A	297	HIS
1	A	346	GLN
1	A	347	ASN
1	A	383	ASN
1	A	386	ASN
1	A	395	ASN
1	A	424	GLN
1	A	457	GLN
1	A	460	ASN
1	A	463	ASN
1	A	595	GLN
1	A	605	GLN
1	A	613	GLN
1	A	697	ASN
1	A	707	GLN
1	A	736	GLN
1	A	747	ASN

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](#)

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	775/844 (91%)	0.91	110 (14%) 6 5	27, 48, 116, 132	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	LEU	7.4
1	A	676	ILE	7.1
1	A	652	TRP	6.2
1	A	780	ILE	5.7
1	A	249	ASP	5.7
1	A	653	LYS	5.5
1	A	677	PHE	5.2
1	A	654	LEU	5.2
1	A	774	PHE	4.8
1	A	648	LEU	4.7
1	A	0	HIS	4.6
1	A	36	LEU	4.5
1	A	243	THR	4.3
1	A	655	ASP	4.2
1	A	703	PHE	4.1
1	A	642	TYR	4.0
1	A	673	LYS	4.0
1	A	772	ALA	3.9
1	A	696	TYR	3.9
1	A	666	LEU	3.9
1	A	665	TYR	3.8
1	A	623	LEU	3.6
1	A	681	PRO	3.6
1	A	745	GLN	3.6
1	A	192	TYR	3.6
1	A	649	PRO	3.5
1	A	3	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	692	ILE	3.3
1	A	656	GLY	3.3
1	A	244	LEU	3.2
1	A	658	VAL	3.2
1	A	32	ASP	3.1
1	A	670	ALA	3.1
1	A	661	ILE	3.1
1	A	246	ALA	3.1
1	A	16	LEU	3.0
1	A	191	LEU	3.0
1	A	716	VAL	3.0
1	A	674	SER	2.9
1	A	567	THR	2.9
1	A	245	LYS	2.8
1	A	689	MET	2.8
1	A	657	LEU	2.8
1	A	262	THR	2.8
1	A	660	LEU	2.8
1	A	491	THR	2.8
1	A	684	MET	2.7
1	A	128	THR	2.7
1	A	711	PHE	2.7
1	A	713	LYS	2.7
1	A	635	LEU	2.7
1	A	693	ILE	2.7
1	A	638	ALA	2.6
1	A	5	LEU	2.6
1	A	347	ASN	2.6
1	A	325	LYS	2.6
1	A	669	GLY	2.6
1	A	641	ALA	2.6
1	A	778	ALA	2.6
1	A	688	ILE	2.6
1	A	700	GLU	2.5
1	A	254	ILE	2.5
1	A	225	GLY	2.5
1	A	679	LYS	2.5
1	A	261	LEU	2.5
1	A	7	LYS	2.5
1	A	2	LEU	2.5
1	A	250	TYR	2.5
1	A	675	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	469	GLN	2.5
1	A	227	ALA	2.5
1	A	672	GLU	2.4
1	A	699	LYS	2.4
1	A	618	ILE	2.4
1	A	646	GLU	2.4
1	A	14	ARG	2.4
1	A	259	VAL	2.4
1	A	256	THR	2.4
1	A	640	ALA	2.3
1	A	226	GLN	2.3
1	A	707	GLN	2.3
1	A	252	TYR	2.3
1	A	242	ARG	2.3
1	A	548	ARG	2.3
1	A	563	MET	2.3
1	A	580	SER	2.3
1	A	45	THR	2.3
1	A	718	ARG	2.3
1	A	678	GLY	2.3
1	A	445	ILE	2.2
1	A	705	LYS	2.2
1	A	427	MET	2.2
1	A	682	ASP	2.2
1	A	708	MET	2.2
1	A	709	ARG	2.2
1	A	266	MET	2.2
1	A	775	VAL	2.2
1	A	484	THR	2.2
1	A	550	GLY	2.1
1	A	564	ASP	2.1
1	A	251	THR	2.1
1	A	643	THR	2.1
1	A	549	PHE	2.1
1	A	265	GLY	2.1
1	A	311	GLY	2.1
1	A	276	ASP	2.1
1	A	663	THR	2.1
1	A	704	GLY	2.1
1	A	776	MET	2.0
1	A	717	LEU	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.