



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:28 PM UTC

PDB ID : 5KYN / pdb_00005kyn
Title : Structure of Sec23 and TANGO1 complex
Authors : Ma, W.; Goldberg, J.
Deposited on : 2016-07-21
Resolution : 2.55 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

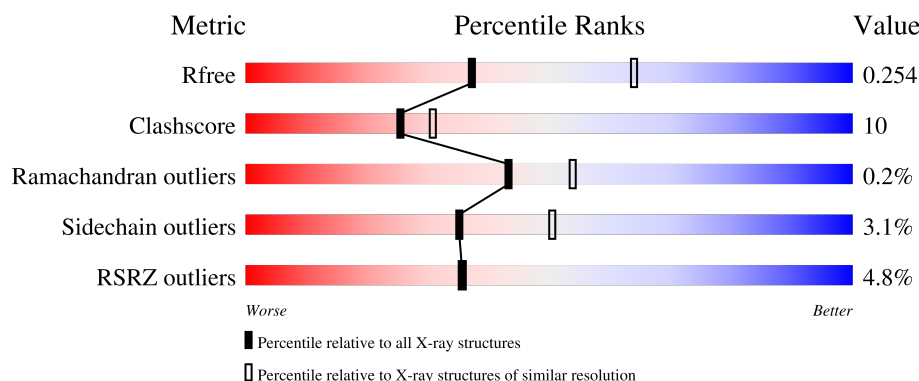
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	765	5% 77% 18% • 5%
1	B	765	5% 74% 18% • 6%
2	C	8	12% 25% 62%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11428 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5739	3661	988	1050	40			
1	B	719	Total	C	N	O	S	0	0	0
			5633	3596	961	1035	41			

- Molecule 2 is a protein called Melanoma inhibitory activity protein 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			21	15	3	3			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

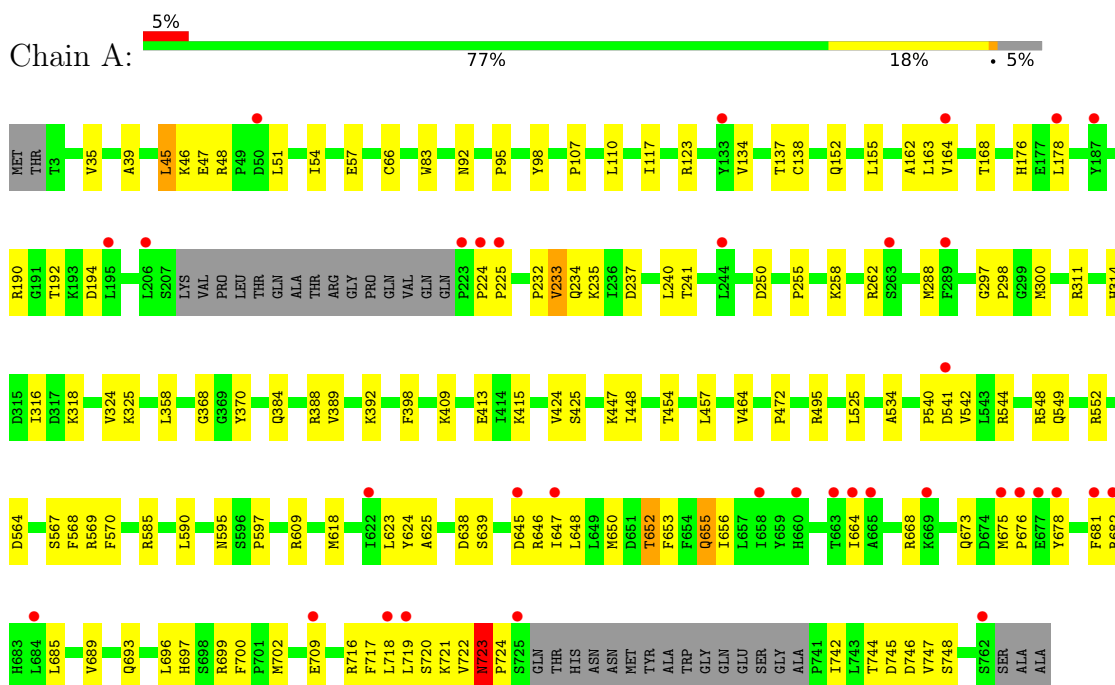
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	2	Total	O	0	0
			2	2		

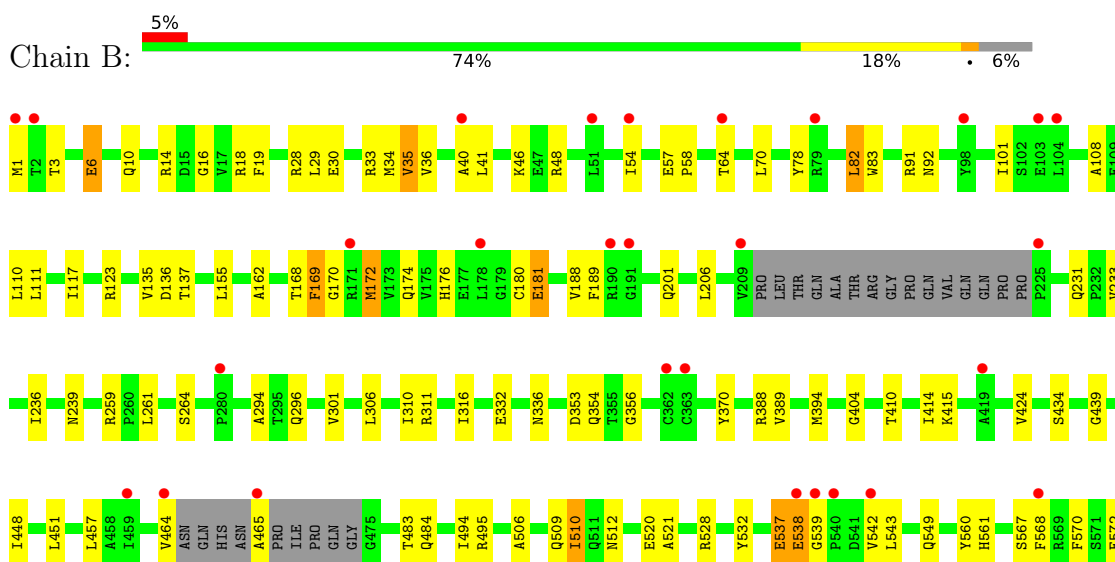
3 Residue-property plots

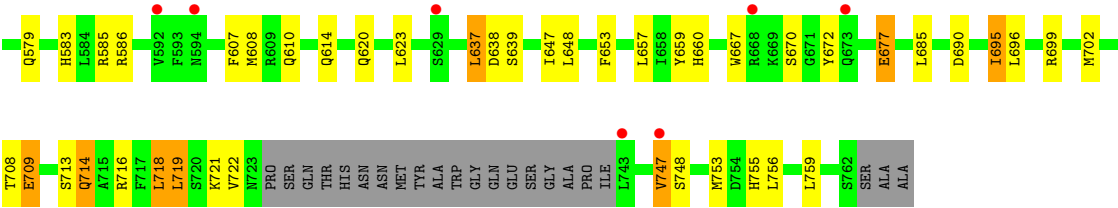
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Protein transport protein Sec23A



• Molecule 1: Protein transport protein Sec23A





● Molecule 2: Melanoma inhibitory activity protein 3

Chain C: 12% 25% 62%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.45Å 65.88Å 229.87Å 90.00° 97.39° 90.00°	Depositor
Resolution (Å)	47.94 – 2.55 47.94 – 2.55	Depositor EDS
% Data completeness (in resolution range)	87.8 (47.94-2.55) 83.5 (47.94-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.200 , 0.246 0.214 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11428	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.31	0/5879	0.47	9/7977 (0.1%)
1	B	0.25	2/5764 (0.0%)	0.44	7/7813 (0.1%)
2	C	0.21	0/23	0.35	0/32
All	All	0.28	2/11666 (0.0%)	0.45	16/15822 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	VAL	CA-C	-5.19	1.48	1.52
1	B	539	GLY	C-N	5.03	1.39	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	VAL	N-CA-C	10.94	120.92	110.42
1	A	742	ILE	N-CA-C	8.27	119.07	110.72
1	A	700	PHE	C-N-CD	7.07	136.15	120.60
1	A	233	VAL	CB-CA-C	-6.96	103.06	111.97
1	A	540	PRO	N-CA-CB	6.62	110.20	103.25
1	B	34	MET	N-CA-C	6.28	118.93	111.71
1	B	538	GLU	CB-CA-C	-6.16	100.88	111.23
1	B	537	GLU	N-CA-C	5.72	124.74	113.29
1	B	170	GLY	N-CA-C	-5.72	99.62	113.18
1	B	539	GLY	CA-C-N	-5.65	114.42	120.47
1	B	539	GLY	C-N-CA	-5.65	114.42	120.47
1	A	723	ASN	CA-C-N	-5.46	114.33	119.85
1	A	723	ASN	C-N-CA	-5.46	114.33	119.85
1	A	297	GLY	CA-C-N	-5.38	114.24	119.78
1	A	297	GLY	C-N-CA	-5.38	114.24	119.78
1	B	180	CYS	N-CA-C	5.05	117.33	111.02

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	5739	0	5647	107	0
1	B	5633	0	5552	109	0
2	C	21	0	23	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	0	5	0
4	B	2	0	0	0	0
All	All	11428	0	11222	217	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 10.

All (217) 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:675:MET:C	1:A:682:ARG:HH21	1.45	1.22
1:A:675:MET:O	1:A:682:ARG:NH2	1.75	1.19
1:B:135:VAL:C	1:B:169:PHE:HE1	1.56	1.14
1:A:744:THR:HG22	1:A:746:ASP:H	1.18	1.09
1:A:675:MET:C	1:A:682:ARG:NH2	2.09	1.09
1:B:135:VAL:C	1:B:169:PHE:CE1	2.39	1.01
1:B:136:ASP:HA	1:B:169:PHE:CE1	1.96	1.00
1:B:657:LEU:HD22	1:B:718:LEU:CD1	1.91	0.98
1:A:447:LYS:NZ	4:A:902:HOH:O	1.98	0.93
1:B:135:VAL:O	1:B:169:PHE:CD1	2.22	0.92
1:A:162:ALA:O	1:A:233:VAL:HG23	1.69	0.90
1:B:136:ASP:CA	1:B:169:PHE:CE1	2.53	0.90
1:B:136:ASP:N	1:B:169:PHE:HE1	1.69	0.90
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.54	0.86
1:B:135:VAL:O	1:B:169:PHE:CE1	2.28	0.86
1:B:136:ASP:N	1:B:169:PHE:CE1	2.46	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:SER:OG	4:A:901:HOH:O	1.94	0.84
1:A:653:PHE:HA	1:A:699:ARG:NH1	1.94	0.81
1:A:388:ARG:HH22	1:A:702:MET:CE	1.93	0.81
1:B:657:LEU:HD22	1:B:718:LEU:HD13	1.63	0.81
1:A:388:ARG:NH2	1:A:702:MET:CE	2.45	0.80
1:B:388:ARG:NH1	1:B:699:ARG:O	2.16	0.79
1:A:673:GLN:O	1:A:682:ARG:HG2	1.83	0.79
1:A:673:GLN:HB3	1:A:685:LEU:HD21	1.68	0.76
1:B:181:GLU:OE2	1:B:239:ASN:ND2	2.18	0.75
1:B:719:LEU:N	1:B:719:LEU:HD23	2.01	0.74
1:A:388:ARG:HH22	1:A:702:MET:HE2	1.51	0.74
1:B:135:VAL:O	1:B:169:PHE:HD1	1.72	0.72
1:B:721:LYS:HE2	1:B:721:LYS:HA	1.72	0.71
1:B:394:MET:SD	1:B:394:MET:N	2.64	0.71
1:B:332:GLU:O	1:B:336:ASN:ND2	2.24	0.71
1:B:1:MET:HG2	1:B:10:GLN:HE22	1.56	0.70
1:A:675:MET:O	1:A:682:ARG:CZ	2.39	0.70
1:B:657:LEU:CD2	1:B:718:LEU:HD13	2.22	0.70
1:B:311:ARG:NH1	1:B:354:GLN:OE1	2.24	0.69
1:A:668:ARG:NH1	1:A:709:GLU:OE2	2.25	0.69
1:B:415:LYS:HD2	1:B:464:VAL:HG21	1.75	0.69
1:A:720:SER:O	1:A:724:PRO:HB3	1.92	0.69
1:B:136:ASP:HB2	1:B:169:PHE:CZ	2.29	0.68
1:B:168:THR:HG1	1:B:176:HIS:HE2	1.42	0.68
1:B:560:TYR:HB3	1:B:568:PHE:HA	1.74	0.68
1:A:676:PRO:N	1:A:682:ARG:NH2	2.42	0.67
1:B:18:ARG:NH2	1:B:520:GLU:OE1	2.27	0.67
1:B:201:GLN:HG3	1:B:206:LEU:HB2	1.75	0.67
1:A:676:PRO:HA	1:A:682:ARG:NH2	2.10	0.67
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.76	0.66
1:A:623:LEU:HD11	1:A:648:LEU:HD13	1.78	0.66
1:A:746:ASP:OD1	1:A:748:SER:OG	2.14	0.66
1:B:660:HIS:HB2	1:B:709:GLU:HB3	1.77	0.66
1:A:676:PRO:HA	1:A:682:ARG:HH22	1.62	0.65
1:B:82:LEU:HD11	1:B:91:ARG:HB3	1.80	0.64
1:A:746:ASP:OD1	1:A:748:SER:N	2.15	0.64
1:B:659:TYR:CD2	1:B:718:LEU:HD22	2.32	0.64
1:B:506:ALA:O	1:B:510:ILE:HG12	1.99	0.63
1:B:714:GLN:HA	1:B:716:ARG:HH11	1.64	0.63
1:A:744:THR:HG22	1:A:746:ASP:N	2.03	0.62
1:B:653:PHE:CG	1:B:653:PHE:O	2.53	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.82	0.61
1:A:388:ARG:NH2	1:A:702:MET:HE3	2.16	0.61
1:A:638:ASP:C	1:A:722:VAL:HG11	2.25	0.61
1:A:152:GLN:NE2	1:A:241:THR:O	2.32	0.61
1:A:647:ILE:HG13	1:A:664:ILE:HD13	1.82	0.61
1:B:561:HIS:H	1:B:567:SER:HB2	1.65	0.60
1:A:676:PRO:CA	1:A:682:ARG:NH2	2.64	0.60
1:B:638:ASP:OD1	1:B:639:SER:N	2.34	0.60
1:A:46:LYS:O	1:A:495:ARG:NH2	2.34	0.60
1:A:645:ASP:O	1:A:664:ILE:HD11	2.02	0.60
1:B:657:LEU:CD2	1:B:718:LEU:CD1	2.76	0.59
1:A:66:CYS:O	1:A:409:LYS:NZ	2.25	0.59
1:A:673:GLN:O	1:A:682:ARG:CG	2.51	0.58
1:B:528:ARG:HA	1:B:608:MET:HE1	1.85	0.58
1:B:310:ILE:HD13	1:B:354:GLN:HB2	1.85	0.57
1:B:169:PHE:CD1	1:B:169:PHE:N	2.73	0.57
1:B:14:ARG:O	1:B:48:ARG:NH1	2.38	0.57
1:B:509:GLN:HB3	1:B:512:ASN:HB2	1.85	0.57
1:A:48:ARG:NH2	4:A:910:HOH:O	2.38	0.56
1:A:190:ARG:HB3	1:A:192:THR:HG22	1.86	0.56
1:B:174:GLN:HG2	1:B:188:VAL:HG22	1.87	0.56
1:A:676:PRO:CA	1:A:682:ARG:HH22	2.17	0.56
1:A:388:ARG:NH2	1:A:697:HIS:HA	2.21	0.56
1:A:35:VAL:HG11	1:A:552:ARG:HB2	1.88	0.56
1:B:647:ILE:HD11	1:B:685:LEU:HD23	1.88	0.56
1:B:670:SER:HB2	1:B:672:TYR:CE2	2.41	0.55
1:B:607:PHE:HD2	1:B:608:MET:HE2	1.72	0.55
1:A:138:CYS:O	1:A:262:ARG:NH1	2.34	0.55
1:B:136:ASP:HB2	1:B:169:PHE:HZ	1.72	0.55
1:A:719:LEU:O	1:A:722:VAL:O	2.25	0.54
1:A:262:ARG:NH2	4:A:912:HOH:O	2.40	0.54
1:A:541:ASP:OD2	1:A:544:ARG:NH2	2.40	0.54
1:B:78:TYR:HD1	1:B:101:ILE:HD12	1.72	0.54
1:B:83:TRP:NE1	1:B:92:ASN:HB2	2.23	0.54
1:A:163:LEU:CD2	1:A:232:PRO:HD3	2.38	0.54
1:B:667:TRP:CD2	2:C:2:PRO:HG2	2.43	0.53
1:A:678:TYR:O	1:A:682:ARG:HG3	2.08	0.53
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.90	0.53
1:A:137:THR:HG23	1:A:250:ASP:HB2	1.90	0.53
1:A:673:GLN:O	1:A:682:ARG:NE	2.41	0.53
1:B:537:GLU:OE1	1:B:537:GLU:HA	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:HA	1:B:111:LEU:HD12	1.90	0.53
1:A:650:MET:HE1	1:A:718:LEU:HA	1.90	0.53
1:A:448:ILE:HD11	1:A:457:LEU:HD11	1.92	0.52
1:B:136:ASP:CB	1:B:169:PHE:CZ	2.92	0.52
1:B:169:PHE:HD1	1:B:169:PHE:N	2.08	0.51
1:B:415:LYS:HB3	1:B:434:SER:HB3	1.92	0.51
1:A:647:ILE:HG13	1:A:664:ILE:CD1	2.40	0.51
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.46	0.51
1:A:652:THR:O	1:A:653:PHE:HB3	2.11	0.51
1:A:723:ASN:N	1:A:724:PRO:CD	2.73	0.50
1:B:610:GLN:HG2	1:B:614:GLN:HB2	1.92	0.50
1:B:264:SER:HB2	1:B:294:ALA:HB2	1.94	0.50
1:B:719:LEU:HD23	1:B:719:LEU:H	1.73	0.50
1:B:653:PHE:O	1:B:653:PHE:CD2	2.65	0.50
1:B:311:ARG:NH2	1:B:356:GLY:HA2	2.27	0.50
1:B:370:TYR:HE2	1:B:389:VAL:HG13	1.77	0.50
1:B:136:ASP:CA	1:B:169:PHE:CZ	2.95	0.49
1:B:718:LEU:HB3	1:B:719:LEU:HD23	1.94	0.49
1:B:259:ARG:HG3	1:B:306:LEU:HD21	1.94	0.49
1:B:753:MET:HA	1:B:756:LEU:HB3	1.93	0.49
1:B:30:GLU:CD	1:B:506:ALA:HB3	2.37	0.49
1:B:301:VAL:HG21	1:B:356:GLY:HA3	1.95	0.49
1:B:261:LEU:HD22	1:B:296:GLN:HG3	1.93	0.49
1:B:483:THR:HB	1:B:495:ARG:HB3	1.94	0.49
1:A:548:ARG:O	1:A:552:ARG:HG3	2.12	0.49
1:B:696:LEU:HG	1:B:702:MET:HE3	1.95	0.49
1:B:3:THR:HG23	1:B:6:GLU:H	1.77	0.48
1:B:583:HIS:HA	1:B:586:ARG:HG2	1.94	0.48
1:A:48:ARG:HG2	1:A:51:LEU:HD22	1.95	0.48
1:B:415:LYS:HD3	1:B:434:SER:HA	1.95	0.48
1:A:549:GLN:OE1	1:A:552:ARG:NH1	2.43	0.48
1:B:721:LYS:HE2	1:B:721:LYS:CA	2.41	0.48
1:B:231:GLN:HB3	1:B:236:ILE:HD13	1.95	0.48
1:B:448:ILE:HD11	1:B:457:LEU:HD11	1.96	0.47
1:B:677:GLU:CD	1:B:677:GLU:H	2.22	0.47
1:B:353:ASP:OD1	1:B:354:GLN:N	2.37	0.47
1:B:543:LEU:HD21	1:B:585:ARG:HB2	1.96	0.47
1:B:537:GLU:O	1:B:537:GLU:HG3	2.14	0.47
1:B:583:HIS:CE1	1:B:620:GLN:HE21	2.33	0.47
1:A:288:MET:HE3	1:A:288:MET:HB2	1.75	0.47
1:A:638:ASP:HA	1:A:722:VAL:HG13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:HH21	1:B:494:ILE:HD11	1.80	0.47
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.79	0.46
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.97	0.46
1:B:404:GLY:HA3	1:B:451:LEU:HD11	1.98	0.46
1:A:655:GLN:HG2	1:A:656:ILE:N	2.27	0.46
1:B:57:GLU:HG3	1:B:58:PRO:HD2	1.98	0.46
1:B:410:THR:HB	1:B:414:ILE:HB	1.97	0.46
1:B:54:ILE:HG13	1:B:117:ILE:HD11	1.97	0.46
1:B:708:THR:HB	1:B:714:GLN:HG3	1.97	0.46
1:A:618:MET:HE2	1:A:653:PHE:CE2	2.51	0.45
1:A:392:LYS:HE3	1:A:398:PHE:CE1	2.51	0.45
1:A:107:PRO:HD2	1:A:110:LEU:HD12	1.99	0.45
1:A:413:GLU:HG2	1:A:472:PRO:HG3	1.99	0.45
1:B:137:THR:OG1	1:B:169:PHE:O	2.29	0.45
1:A:717:PHE:CZ	1:A:721:LYS:HE2	2.51	0.45
1:A:693:GLN:HA	1:A:696:LEU:HD12	1.98	0.45
1:A:534:ALA:HB2	1:A:542:VAL:HG21	1.98	0.44
1:B:181:GLU:H	1:B:181:GLU:HG2	1.45	0.44
1:A:368:GLY:C	1:A:609:ARG:HH22	2.24	0.44
1:B:579:GLN:OE1	1:B:620:GLN:NE2	2.33	0.44
1:B:136:ASP:HA	1:B:169:PHE:CZ	2.48	0.44
1:A:234:GLN:HA	1:A:237:ASP:HB2	1.99	0.44
1:A:585:ARG:HA	1:A:590:LEU:HD12	2.00	0.44
1:A:57:GLU:OE2	1:A:123:ARG:NH2	2.36	0.43
1:A:568:PHE:C	1:A:569:ARG:HG3	2.43	0.43
1:A:716:ARG:H	1:A:716:ARG:HG2	1.60	0.43
1:A:233:VAL:O	1:A:237:ASP:HB2	2.18	0.43
1:A:564:ASP:O	1:A:567:SER:OG	2.27	0.43
1:B:484:GLN:HG2	1:B:494:ILE:HG12	2.01	0.43
1:A:370:TYR:CE2	1:A:389:VAL:HG13	2.54	0.43
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.99	0.43
1:B:29:LEU:O	1:B:33:ARG:HG3	2.19	0.43
1:A:664:ILE:HG23	1:A:681:PHE:HZ	1.84	0.43
1:A:388:ARG:NH1	1:A:699:ARG:O	2.52	0.43
1:B:172:MET:HG2	1:B:189:PHE:O	2.18	0.43
1:A:314:HIS:HB3	1:A:318:LYS:NZ	2.34	0.43
1:A:676:PRO:N	1:A:682:ARG:HH22	2.17	0.43
1:B:123:ARG:HH22	1:B:484:GLN:CD	2.27	0.43
1:B:747:VAL:HG12	1:B:748:SER:H	1.84	0.43
1:A:625:ALA:HB1	1:A:646:ARG:HD2	2.01	0.42
1:B:659:TYR:CG	1:B:718:LEU:HD22	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.54	0.42
1:A:746:ASP:OD1	1:A:747:VAL:N	2.53	0.42
1:A:311:ARG:NH1	1:A:597:PRO:HB2	2.34	0.42
1:A:388:ARG:HH21	1:A:697:HIS:HA	1.83	0.42
1:B:16:GLY:HA2	1:B:46:LYS:HD3	2.02	0.42
1:B:538:GLU:O	1:B:542:VAL:HG23	2.19	0.42
1:A:164:VAL:HG13	1:A:233:VAL:HG22	2.02	0.42
1:A:655:GLN:NE2	1:A:717:PHE:CE1	2.87	0.42
1:B:19:PHE:CE2	1:B:40:ALA:HB2	2.55	0.42
1:A:123:ARG:HA	1:A:123:ARG:HD3	1.85	0.42
1:B:162:ALA:O	1:B:233:VAL:HG23	2.20	0.42
1:A:702:MET:HE3	1:A:702:MET:HB2	1.90	0.42
1:B:623:LEU:HD11	1:B:648:LEU:HB3	2.02	0.42
1:A:595:ASN:OD1	4:A:903:HOH:O	2.22	0.42
1:A:325:LYS:HE3	1:A:325:LYS:HB2	1.88	0.41
1:A:639:SER:N	1:A:722:VAL:HG11	2.35	0.41
1:A:314:HIS:HB3	1:A:318:LYS:HZ2	1.85	0.41
1:B:719:LEU:N	1:B:719:LEU:CD2	2.72	0.41
1:A:224:PRO:HA	1:A:225:PRO:HD3	1.91	0.41
1:A:624:TYR:O	1:A:648:LEU:HA	2.21	0.41
1:B:18:ARG:HG2	1:B:521:ALA:HB2	2.02	0.41
1:B:439:GLY:HA2	1:B:532:TYR:CZ	2.56	0.41
1:A:311:ARG:HD3	1:A:324:VAL:HG22	2.02	0.41
1:B:28:ARG:HG3	1:B:465:ALA:N	2.36	0.41
1:B:70:LEU:HD11	1:B:110:LEU:HD21	2.01	0.41
1:A:45:LEU:HD22	1:A:495:ARG:HD3	2.02	0.41
1:A:168:THR:OG1	1:A:176:HIS:NE2	2.47	0.41
1:A:368:GLY:O	1:A:609:ARG:NH2	2.50	0.41
1:B:610:GLN:CG	1:B:614:GLN:HB2	2.51	0.41
1:A:178:LEU:HD22	1:A:240:LEU:HD11	2.01	0.41
1:B:713:SER:O	1:B:716:ARG:HD3	2.21	0.41
1:A:232:PRO:HB2	1:A:235:LYS:HB3	2.04	0.40
1:A:744:THR:HG22	1:A:745:ASP:N	2.37	0.40
1:B:695:ILE:H	1:B:695:ILE:HG13	1.63	0.40
1:B:755:HIS:O	1:B:759:LEU:HG	2.21	0.40
1:A:194:ASP:HB2	1:A:298:PRO:HG2	2.04	0.40
2:C:1:PRO:HA	2:C:2:PRO:HD2	1.95	0.40

There are no symmetry-related clashes.

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	724/765 (95%)	688 (95%)	35 (5%)	1 (0%)	48	60
1	B	710/765 (93%)	676 (95%)	32 (4%)	2 (0%)	36	44
2	C	1/8 (12%)	1 (100%)	0	0	100	100
All	All	1435/1538 (93%)	1365 (95%)	67 (5%)	3 (0%)	43	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	VAL
1	A	723	ASN
1	B	637	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	624/666 (94%)	611 (98%)	13 (2%)	47	63
1	B	613/666 (92%)	588 (96%)	25 (4%)	27	39
2	C	3/7 (43%)	3 (100%)	0	100	100
All	All	1240/1339 (93%)	1202 (97%)	38 (3%)	35	50

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	47	GLU
1	A	134	VAL
1	A	155	LEU
1	A	300	MET
1	A	316	ILE
1	A	384	GLN
1	A	424	VAL
1	A	454	THR
1	A	570	PHE
1	A	652	THR
1	A	655	GLN
1	A	689	VAL
1	B	6	GLU
1	B	35	VAL
1	B	41	LEU
1	B	64	THR
1	B	82	LEU
1	B	155	LEU
1	B	169	PHE
1	B	172	MET
1	B	181	GLU
1	B	316	ILE
1	B	424	VAL
1	B	510	ILE
1	B	549	GLN
1	B	570	PHE
1	B	572	GLU
1	B	637	LEU
1	B	677	GLU
1	B	690	ASP
1	B	695	ILE
1	B	709	GLU
1	B	714	GLN
1	B	718	LEU
1	B	719	LEU
1	B	722	VAL
1	B	747	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	296	GLN
1	A	336	ASN
1	A	395	HIS
1	A	610	GLN
1	A	614	GLN
1	A	620	GLN
1	A	655	GLN
1	B	10	GLN
1	B	105	ASN
1	B	201	GLN
1	B	296	GLN
1	B	336	ASN
1	B	445	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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	730/765 (95%)	0.38	35 (4%) 35 36	36, 81, 136, 176	0
1	B	719/765 (93%)	0.50	35 (4%) 35 35	70, 106, 152, 186	0
2	C	3/8 (37%)	1.25	0 100 100	149, 149, 158, 160	0
All	All	1452/1538 (94%)	0.44	70 (4%) 35 36	36, 95, 148, 186	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	ARG	7.2
1	A	677	GLU	5.4
1	A	225	PRO	5.4
1	A	709	GLU	5.1
1	A	664	ILE	4.7
1	B	465	ALA	4.2
1	A	178	LEU	4.0
1	A	224	PRO	3.7
1	A	678	TYR	3.7
1	A	718	LEU	3.6
1	A	676	PRO	3.6
1	A	223	PRO	3.6
1	B	104	LEU	3.4
1	A	675	MET	3.3
1	B	363	CYS	3.3
1	B	98	TYR	3.3
1	A	725	SER	3.2
1	A	669	LYS	3.2
1	B	743	LEU	3.2
1	A	681	PHE	3.0
1	B	673	GLN	3.0
1	A	195	LEU	2.9
1	B	79	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	684	LEU	2.9
1	B	2	THR	2.8
1	B	668	ARG	2.8
1	A	660	HIS	2.7
1	A	622	ILE	2.7
1	B	40	ALA	2.7
1	B	594	ASN	2.7
1	A	541	ASP	2.6
1	B	592	VAL	2.6
1	B	191	GLY	2.5
1	A	244	LEU	2.5
1	B	178	LEU	2.5
1	B	629	SER	2.5
1	A	719	LEU	2.4
1	B	54	ILE	2.4
1	A	663	THR	2.4
1	B	209	VAL	2.4
1	B	542	VAL	2.4
1	A	133	TYR	2.4
1	B	51	LEU	2.3
1	B	362	CYS	2.3
1	A	206	LEU	2.3
1	A	647	ILE	2.3
1	A	658	ILE	2.3
1	B	538	GLU	2.3
1	B	225	PRO	2.2
1	A	665	ALA	2.2
1	B	1	MET	2.2
1	B	539	GLY	2.2
1	A	289	PHE	2.2
1	B	190	ARG	2.2
1	B	540	PRO	2.2
1	B	419	ALA	2.2
1	A	645	ASP	2.2
1	B	568	PHE	2.2
1	A	187	TYR	2.1
1	A	762	SER	2.1
1	B	747	VAL	2.1
1	B	171	ARG	2.1
1	B	280	PRO	2.1
1	B	459	ILE	2.1
1	A	50	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	SER	2.1
1	A	164	VAL	2.0
1	B	64	THR	2.0
1	B	464	VAL	2.0
1	B	103	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	B	801	1/1	0.98	0.05	107,107,107,107	0
3	ZN	A	801	1/1	0.99	0.07	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.