



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:44 PM UTC

PDB ID : 5KYW / pdb_00005kyw
Title : crystal structure of Sec23 and TANGO1 peptide3 complex
Authors : Ma, W.; Goldberg, J.
Deposited on : 2016-07-22
Resolution : 3.20 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

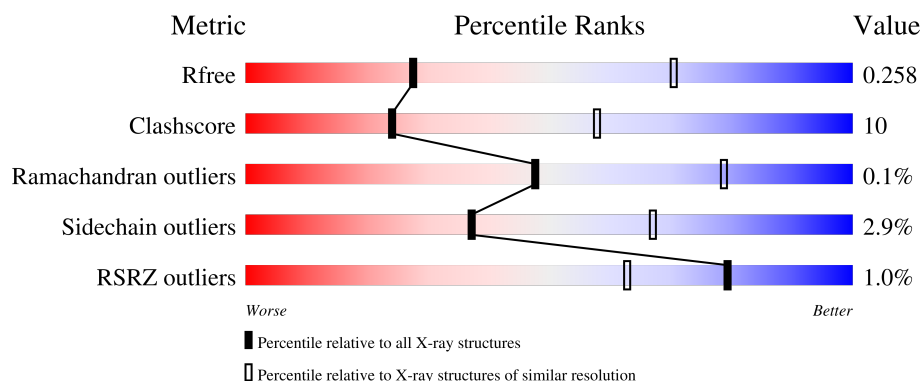
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	
2	B	770	
3	C	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11699 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	714	Total	C	N	O	S	0	0	0
			5668	3614	972	1042	40			

- Molecule 2 is a protein called Protein transport protein Sec24D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	766	Total	C	N	O	S	0	0	0
			6008	3823	1016	1115	54			

There are 3 discrepancies between the modelled and reference sequences:

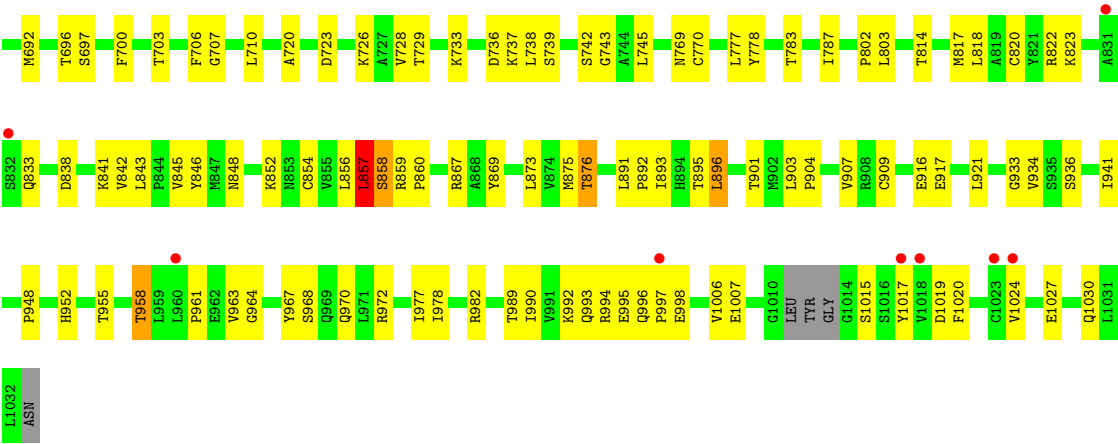
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP O94855
B	2	MET	-	expression tag	UNP O94855
B	3	GLY	-	expression tag	UNP O94855

- Molecule 3 is a protein called TANGO1 peptide3.

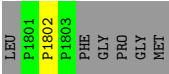
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			21	15	3	3			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



● Molecule 3: TANGO1 peptide3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.62Å 141.35Å 151.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.51 – 3.20 82.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (82.51-3.20) 88.7 (82.51-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.210 , 0.257 0.213 , 0.258	Depositor DCC
R_{free} test set	1829 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11699	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.24	0/5799	0.40	1/7850 (0.0%)
2	B	0.27	0/6136	0.49	8/8316 (0.1%)
3	C	0.22	0/23	0.36	0/32
All	All	0.25	0/11958	0.45	9/16198 (0.1%)

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
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	963	VAL	N-CA-C	13.52	124.41	110.62
2	B	469	MET	N-CA-C	6.77	119.50	111.71
2	B	858	SER	N-CA-C	6.38	120.03	110.14
2	B	407	GLY	N-CA-C	-6.28	106.86	113.58
1	A	744	THR	N-CA-C	5.65	116.73	108.14
2	B	857	LEU	N-CA-C	5.59	117.25	109.31
2	B	305	GLN	N-CA-C	5.50	119.02	111.54
2	B	459	VAL	N-CA-C	5.42	116.15	110.62
2	B	405	HIS	N-CA-C	-5.14	105.68	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	ASP	Peptide
2	B	901	THR	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	5668	0	5617	99	0
2	B	6008	0	5983	134	0
3	C	21	0	21	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	11699	0	11621	232	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 (232) 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:123:ARG:HG3	1:A:125:PRO:HD3	1.44	0.99
1:A:123:ARG:HG3	1:A:125:PRO:CD	1.96	0.95
2:B:286:THR:OG1	2:B:304:ASP:O	1.92	0.88
2:B:405:HIS:CD2	2:B:405:HIS:H	1.96	0.82
2:B:964:GLY:O	2:B:968:SER:HB3	1.80	0.82
1:A:638:ASP:OD1	1:A:639:SER:N	2.12	0.82
2:B:403:LEU:HD22	2:B:407:GLY:O	1.82	0.80
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.65	0.78
1:A:311:ARG:NH1	1:A:598:ASP:OD1	2.19	0.75
1:A:451:LEU:H	1:A:451:LEU:HD12	1.52	0.75
1:A:744:THR:OG1	1:A:747:VAL:HG21	1.88	0.74
2:B:637:LEU:HD21	2:B:643:VAL:HG11	1.69	0.73
2:B:469:MET:HE1	2:B:678:LEU:HG	1.69	0.72
1:A:745:ASP:O	1:A:747:VAL:HG22	1.89	0.71
2:B:317:THR:HG21	2:B:777:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:PHE:HB3	2:B:403:LEU:HD11	1.74	0.70
1:A:368:GLY:HA3	1:A:450:GLY:O	1.92	0.69
2:B:467:LYS:HB3	2:B:538:HIS:CE1	2.28	0.68
2:B:820:CYS:HA	2:B:823:LYS:HE2	1.77	0.66
2:B:288:THR:HB	2:B:291:GLN:HB2	1.78	0.65
2:B:462:ILE:O	2:B:466:LEU:HB2	1.97	0.65
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.78	0.64
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.80	0.64
1:A:123:ARG:C	1:A:125:PRO:HD3	2.23	0.64
2:B:697:SER:HB3	2:B:745:LEU:HB2	1.80	0.64
1:A:480:GLN:HG3	1:A:498:THR:HG22	1.79	0.63
2:B:407:GLY:O	2:B:408:ARG:C	2.40	0.63
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.33	0.62
2:B:948:PRO:HG2	2:B:952:HIS:ND1	2.14	0.62
1:A:451:LEU:HD12	1:A:451:LEU:N	2.15	0.61
1:A:745:ASP:CG	1:A:746:ASP:H	2.09	0.61
2:B:893:ILE:HD11	2:B:921:LEU:HB2	1.81	0.61
1:A:297:GLY:H	1:A:300:MET:HE3	1.65	0.61
2:B:641:GLN:HG2	2:B:642:TYR:H	1.66	0.61
2:B:1027:GLU:HA	2:B:1030:GLN:HB2	1.82	0.61
1:A:121:VAL:HG12	1:A:122:LEU:N	2.13	0.61
2:B:469:MET:HE1	2:B:678:LEU:CG	2.29	0.61
1:A:123:ARG:CG	1:A:125:PRO:HD3	2.27	0.61
1:A:636:LEU:HD23	1:A:638:ASP:CB	2.31	0.60
1:A:227:ASN:O	1:A:231:GLN:NE2	2.35	0.59
1:A:448:ILE:HD11	1:A:457:LEU:HD11	1.84	0.59
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.85	0.58
1:A:649:LEU:HD23	1:A:658:ILE:HG12	1.85	0.58
2:B:317:THR:HG22	2:B:319:CYS:H	1.67	0.58
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.85	0.58
1:A:63:ARG:O	1:A:67:ARG:HG2	2.02	0.58
2:B:578:LEU:HD12	2:B:633:VAL:HG22	1.86	0.58
2:B:518:VAL:HG21	2:B:560:PRO:HB3	1.85	0.58
1:A:636:LEU:HD23	1:A:638:ASP:HB2	1.84	0.58
2:B:367:CYS:HB2	2:B:389:CYS:SG	2.44	0.58
2:B:469:MET:CE	2:B:678:LEU:HG	2.34	0.58
1:A:504:ALA:HB1	1:A:509:GLN:HG3	1.86	0.58
2:B:961:PRO:O	2:B:972:ARG:NH1	2.38	0.57
1:A:369:GLY:O	1:A:609:ARG:NH2	2.37	0.57
2:B:606:ASP:HA	2:B:802:PRO:HG3	1.86	0.57
1:A:269:SER:HA	1:A:334:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:967:TYR:O	2:B:970:GLN:N	2.37	0.57
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.40	0.57
2:B:458:LEU:O	2:B:462:ILE:HG13	2.05	0.56
1:A:268:LEU:HD22	1:A:334:LEU:HD13	1.89	0.55
1:A:744:THR:OG1	1:A:747:VAL:CG2	2.53	0.55
2:B:707:GLY:HA2	2:B:875:MET:O	2.06	0.55
1:A:667:TRP:CE2	3:C:1802:PRO:HB2	2.42	0.55
2:B:454:ILE:HD13	2:B:459:VAL:HG21	1.89	0.54
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.88	0.54
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.88	0.54
1:A:147:LEU:HG	1:A:151:MET:HE2	1.90	0.54
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.89	0.54
1:A:28:ARG:HB2	1:A:464:VAL:HA	1.88	0.54
1:A:487:HIS:ND1	1:A:488:SER:O	2.41	0.54
2:B:736:ASP:OD1	2:B:737:LYS:N	2.37	0.54
2:B:814:THR:HA	2:B:817:MET:HE2	1.90	0.54
1:A:46:LYS:O	1:A:495:ARG:NH2	2.41	0.53
2:B:936:SER:HB3	2:B:941:ILE:HD11	1.90	0.53
2:B:405:HIS:CD2	2:B:405:HIS:N	2.73	0.53
2:B:470:LEU:HD12	2:B:530:TYR:CE1	2.43	0.53
1:A:3:THR:HG22	1:A:5:LEU:H	1.73	0.53
2:B:449:VAL:HG21	2:B:490:THR:HB	1.90	0.53
1:A:30:GLU:O	1:A:34:MET:HG3	2.09	0.53
2:B:996:GLN:C	2:B:998:GLU:H	2.17	0.53
2:B:803:LEU:HD13	2:B:856:LEU:HA	1.90	0.53
1:A:231:GLN:HB2	1:A:236:ILE:HG13	1.91	0.53
2:B:739:SER:OG	2:B:742:SER:OG	2.21	0.53
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.89	0.52
2:B:858:SER:C	2:B:860:PRO:HD2	2.34	0.52
1:A:121:VAL:CG1	1:A:122:LEU:N	2.73	0.52
2:B:466:LEU:HD22	2:B:470:LEU:HD21	1.91	0.52
2:B:743:GLY:HA2	2:B:770:CYS:HB2	1.92	0.51
2:B:449:VAL:HG12	2:B:454:ILE:HD11	1.92	0.51
2:B:632:SER:HA	2:B:655:THR:HB	1.91	0.51
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.41	0.51
2:B:461:LEU:O	2:B:465:GLU:HB2	2.11	0.51
2:B:891:LEU:HD12	2:B:978:ILE:HD11	1.92	0.50
1:A:51:LEU:HD21	1:A:117:ILE:HA	1.93	0.50
2:B:412:HIS:O	2:B:419:SER:HB3	2.12	0.50
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.92	0.50
1:A:178:LEU:HB3	1:A:236:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:958:THR:HG21	2:B:989:THR:HA	1.94	0.50
1:A:177:GLU:HG2	1:A:180:CYS:HB2	1.93	0.50
2:B:608:GLU:OE1	2:B:803:LEU:HG	2.10	0.50
1:A:743:LEU:O	1:A:755:HIS:ND1	2.45	0.50
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.94	0.50
1:A:655:GLN:HE22	1:A:717:PHE:HB3	1.77	0.50
2:B:845:VAL:HG22	2:B:1017:TYR:CZ	2.47	0.49
2:B:955:THR:HG21	2:B:997:PRO:HG3	1.93	0.49
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.93	0.49
2:B:818:LEU:HD12	2:B:1024:VAL:HG11	1.95	0.49
2:B:967:TYR:O	2:B:968:SER:C	2.54	0.49
2:B:276:ARG:HA	2:B:298:THR:HG23	1.95	0.49
2:B:684:LYS:O	2:B:686:ILE:HG13	2.13	0.49
1:A:312:SER:H	1:A:315:ASP:HB2	1.77	0.49
2:B:467:LYS:NZ	2:B:542:ASP:OD1	2.39	0.48
2:B:958:THR:HG23	2:B:990:ILE:HG13	1.94	0.48
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.95	0.48
2:B:321:PRO:HD3	2:B:777:LEU:HD13	1.96	0.48
1:A:143:ASP:OD1	1:A:376:SER:HB2	2.14	0.48
2:B:869:TYR:CE2	2:B:873:LEU:HD11	2.49	0.48
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.27	0.47
2:B:467:LYS:HB3	2:B:538:HIS:HE1	1.78	0.47
2:B:854:CYS:O	2:B:867:ARG:HD2	2.13	0.47
1:A:173:VAL:HG11	1:A:270:ILE:HD12	1.96	0.47
2:B:787:ILE:HG13	2:B:846:TYR:HB3	1.97	0.47
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.80	0.47
1:A:745:ASP:CG	1:A:746:ASP:N	2.72	0.47
2:B:481:THR:HG23	2:B:531:GLN:HG3	1.96	0.47
2:B:403:LEU:CD2	2:B:407:GLY:O	2.60	0.47
1:A:636:LEU:HD23	1:A:638:ASP:HB3	1.97	0.47
2:B:706:PHE:HB2	2:B:729:THR:HB	1.96	0.47
2:B:857:LEU:HD12	2:B:857:LEU:HA	1.55	0.47
2:B:609:LYS:O	2:B:613:GLN:HG3	2.15	0.47
2:B:560:PRO:HA	2:B:563:GLN:HB3	1.97	0.46
2:B:934:VAL:N	2:B:993:GLN:OE1	2.37	0.46
1:A:136:ASP:HB2	1:A:290:ILE:HA	1.97	0.46
1:A:35:VAL:HG11	1:A:549:GLN:O	2.15	0.46
1:A:624:TYR:HD2	1:A:649:LEU:HD12	1.81	0.46
1:A:231:GLN:CB	1:A:236:ILE:HG13	2.46	0.46
2:B:723:ASP:OD1	2:B:726:LYS:HG2	2.16	0.46
2:B:529:ASN:OD1	2:B:532:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1015:SER:HB2	2:B:1019:ASP:HB3	1.97	0.46
1:A:268:LEU:HD12	1:A:288:MET:SD	2.56	0.46
1:A:451:LEU:HD12	1:A:451:LEU:O	2.15	0.46
2:B:822:ARG:NH1	2:B:833:GLN:O	2.45	0.46
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.99	0.45
2:B:738:LEU:HB2	2:B:770:CYS:SG	2.56	0.45
2:B:626:CYS:HB3	2:B:631:CYS:O	2.16	0.45
1:A:568:PHE:HE2	1:A:570:PHE:CZ	2.34	0.45
1:A:744:THR:OG1	1:A:745:ASP:N	2.50	0.45
1:A:42:PHE:CZ	1:A:44:PRO:HA	2.51	0.45
2:B:903:LEU:HD13	2:B:977:ILE:HD11	1.99	0.45
1:A:401:GLY:O	1:A:451:LEU:HD12	2.17	0.45
2:B:487:GLY:HA3	2:B:527:LEU:HD23	1.99	0.45
2:B:909:CYS:O	2:B:1007:GLU:HB2	2.17	0.45
2:B:503:ASN:O	2:B:503:ASN:ND2	2.50	0.45
2:B:893:ILE:O	2:B:896:LEU:HB2	2.17	0.45
1:A:123:ARG:HD2	1:A:123:ARG:O	2.17	0.44
1:A:505:ASP:O	1:A:509:GLN:HG2	2.17	0.44
1:A:488:SER:O	1:A:489:SER:OG	2.29	0.44
2:B:896:LEU:HD21	2:B:904:PRO:HG3	1.98	0.44
1:A:637:LEU:HD12	1:A:722:VAL:HG22	1.98	0.44
2:B:624:LYS:HE2	2:B:624:LYS:HB3	1.82	0.44
1:A:41:LEU:CD1	1:A:525:LEU:HG	2.48	0.44
2:B:934:VAL:HG13	2:B:993:GLN:HB3	1.99	0.44
2:B:2:MET:HG2	2:B:1017:TYR:OH	2.18	0.44
2:B:403:LEU:HB3	2:B:407:GLY:O	2.18	0.44
2:B:520:VAL:HG12	2:B:522:LEU:H	1.83	0.44
2:B:859:ARG:N	2:B:860:PRO:HD2	2.33	0.44
2:B:401:GLN:HB2	2:B:409:ARG:CZ	2.47	0.43
1:A:139:MET:HE2	1:A:291:GLY:HA3	1.99	0.43
2:B:460:LYS:HA	2:B:545:PRO:HG3	1.99	0.43
2:B:838:ASP:OD1	2:B:841:LYS:HE3	2.18	0.43
2:B:852:LYS:NZ	2:B:1006:VAL:O	2.40	0.43
1:A:123:ARG:HG3	1:A:125:PRO:CG	2.47	0.43
2:B:994:ARG:HG2	2:B:995:GLU:HG3	2.00	0.43
2:B:680:ASN:O	2:B:684:LYS:HG3	2.19	0.43
2:B:848:ASN:HB2	2:B:1020:PHE:CD2	2.54	0.43
1:A:162:ALA:O	1:A:233:VAL:HG23	2.19	0.43
2:B:892:PRO:HB2	2:B:895:THR:HG22	2.01	0.43
1:A:18:ARG:NE	1:A:612:LEU:HD22	2.34	0.43
2:B:403:LEU:HB3	2:B:407:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.43	0.42
1:A:546:LEU:HD21	1:A:584:LEU:HD23	1.99	0.42
1:A:558:GLY:HA3	1:A:568:PHE:HE1	1.84	0.42
1:A:154:SER:HB3	1:A:386:PHE:HE2	1.84	0.42
1:A:700:PHE:HB3	1:A:701:PRO:HD3	2.00	0.42
2:B:562:ILE:HB	2:B:622:LEU:HD21	2.01	0.42
1:A:359:GLU:N	1:A:359:GLU:OE1	2.51	0.42
2:B:499:ASN:HB3	2:B:508:GLN:HB2	2.00	0.42
1:A:184:SER:N	2:B:506:GLN:OE1	2.53	0.42
1:A:531:ILE:HB	1:A:608:MET:HE3	2.01	0.42
2:B:543:GLN:HB3	2:B:547:MET:HE3	2.01	0.42
2:B:916:GLU:HG2	2:B:993:GLN:HE22	1.84	0.42
2:B:696:THR:OG1	2:B:700:PHE:O	2.28	0.42
1:A:41:LEU:HD12	1:A:525:LEU:HG	2.02	0.42
2:B:284:TYR:CE2	2:B:286:THR:HG22	2.55	0.42
2:B:467:LYS:HD3	2:B:538:HIS:ND1	2.35	0.42
1:A:570:PHE:CE2	1:A:578:PRO:HG2	2.55	0.42
2:B:996:GLN:O	2:B:998:GLU:N	2.47	0.42
2:B:296:VAL:HG12	2:B:314:ARG:CZ	2.49	0.42
2:B:500:VAL:O	2:B:528:VAL:HG21	2.20	0.42
1:A:35:VAL:HG21	1:A:553:LEU:N	2.35	0.41
1:A:121:VAL:CG1	1:A:122:LEU:H	2.33	0.41
1:A:753:MET:O	1:A:757:LYS:N	2.50	0.41
2:B:391:CYS:SG	2:B:392:VAL:N	2.93	0.41
2:B:570:LYS:HE2	2:B:629:HIS:CE1	2.55	0.41
2:B:703:THR:HG21	2:B:733:LYS:HB2	2.01	0.41
2:B:982:ARG:HD3	2:B:982:ARG:HA	1.76	0.41
2:B:458:LEU:HD12	2:B:458:LEU:HA	1.78	0.41
2:B:654:LEU:HD13	2:B:710:LEU:HD13	2.02	0.41
2:B:726:LYS:HD3	2:B:876:THR:OG1	2.19	0.41
1:A:154:SER:HB3	1:A:386:PHE:CE2	2.56	0.41
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.21	0.41
2:B:620:ASP:OD1	2:B:650:LEU:HD21	2.20	0.41
1:A:78:TYR:CD1	1:A:103:GLU:HG2	2.55	0.41
1:A:350:CYS:HB2	1:A:377:PHE:CE1	2.55	0.41
1:A:14:ARG:HA	1:A:48:ARG:NH1	2.36	0.41
2:B:446:MET:HE3	2:B:580:ILE:HG12	2.03	0.41
2:B:499:ASN:HB2	2:B:522:LEU:HD11	2.02	0.41
1:A:679:GLU:O	1:A:683:HIS:ND1	2.48	0.41
2:B:453:ASN:O	2:B:459:VAL:HG23	2.21	0.41
2:B:692:MET:HE1	2:B:728:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:933:GLY:HA2	2:B:993:GLN:HB2	2.03	0.41
2:B:996:GLN:C	2:B:998:GLU:N	2.78	0.41
1:A:14:ARG:NH1	1:A:15:ASP:OD2	2.54	0.41
2:B:332:ILE:HD11	2:B:778:TYR:CE1	2.55	0.41
2:B:461:LEU:HD22	2:B:667:MET:SD	2.61	0.41
1:A:556:LYS:HG2	1:A:557:PHE:CE2	2.57	0.40
2:B:858:SER:HB3	2:B:860:PRO:HD2	2.03	0.40
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.03	0.40
1:A:511:GLN:OE1	1:A:511:GLN:N	2.34	0.40
2:B:466:LEU:HA	2:B:466:LEU:HD23	1.82	0.40
2:B:655:THR:O	2:B:720:ALA:HB3	2.21	0.40
2:B:783:THR:HG23	2:B:843:LEU:HD12	2.04	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	702/765 (92%)	665 (95%)	36 (5%)	1 (0%)	48	79
2	B	762/770 (99%)	714 (94%)	48 (6%)	0	100	100
3	C	1/9 (11%)	1 (100%)	0	0	100	100
All	All	1465/1544 (95%)	1380 (94%)	84 (6%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO

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%)	606 (97%)	18 (3%)	37	67
2	B	674/682 (99%)	654 (97%)	20 (3%)	36	66
3	C	3/7 (43%)	3 (100%)	0	100	100
All	All	1301/1355 (96%)	1263 (97%)	38 (3%)	37	67

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

Mol	Chain	Res	Type
1	A	17	VAL
1	A	45	LEU
1	A	101	ILE
1	A	103	GLU
1	A	105	ASN
1	A	106	GLN
1	A	109	GLU
1	A	122	LEU
1	A	437	GLU
1	A	451	LEU
1	A	508	THR
1	A	509	GLN
1	A	636	LEU
1	A	637	LEU
1	A	646	ARG
1	A	695	ILE
1	A	696	LEU
1	A	722	VAL
2	B	269	ILE
2	B	296	VAL
2	B	325	ASP
2	B	334	LEU
2	B	405	HIS
2	B	449	VAL
2	B	486	VAL
2	B	506	GLN

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Mol	Chain	Res	Type
2	B	518	VAL
2	B	523	LEU
2	B	533	SER
2	B	536	VAL
2	B	566	MET
2	B	842	VAL
2	B	857	LEU
2	B	876	THR
2	B	896	LEU
2	B	907	VAL
2	B	917	GLU
2	B	958	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	201	GLN
1	A	281	ASN
1	A	296	GLN
1	A	397	GLN
1	A	491	GLN
1	A	519	GLN
1	A	549	GLN
1	A	555	GLN
1	A	591	GLN
1	A	610	GLN
1	A	620	GLN
1	A	655	GLN
2	B	305	GLN
2	B	405	HIS
2	B	496	HIS
2	B	543	GLN
2	B	813	GLN
2	B	824	ASN
2	B	848	ASN
2	B	965	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	714/765 (93%)	-0.16	6 (0%) 82 67	54, 93, 153, 220	0
2	B	766/770 (99%)	-0.09	9 (1%) 76 58	55, 96, 183, 304	0
3	C	3/9 (33%)	0.51	0 100 100	176, 176, 177, 209	0
All	All	1483/1544 (96%)	-0.12	15 (1%) 79 63	54, 95, 168, 304	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1017	TYR	4.0
2	B	960	LEU	3.3
2	B	1018	VAL	3.2
1	A	540	PRO	2.9
1	A	209	VAL	2.9
2	B	832	SER	2.9
1	A	570	PHE	2.7
2	B	1023	CYS	2.6
2	B	3	GLY	2.4
1	A	464	VAL	2.4
2	B	1024	VAL	2.3
1	A	742	ILE	2.2
1	A	741	PRO	2.1
2	B	997	PRO	2.1
2	B	831	ALA	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($\text{\AA}^2$)	Q<0.9
4	ZN	B	1101	1/1	0.88	0.15	75,75,75,75	0
4	ZN	A	801	1/1	0.98	0.14	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.