Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 07:28 am BST

PDB ID	:	5KYW
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
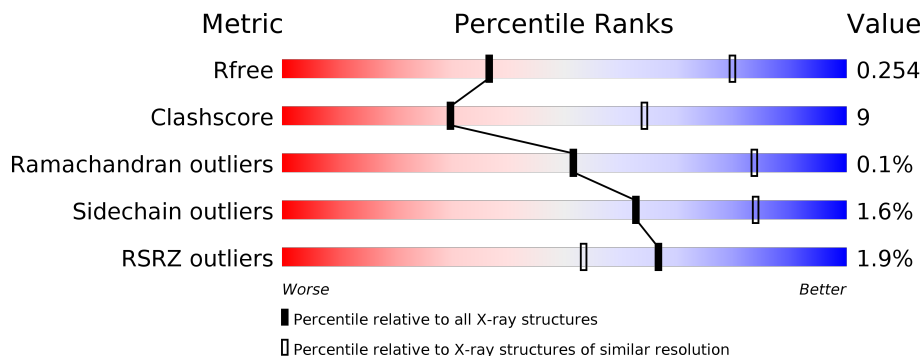with specific help available everywhere you see the (i) symbol.

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	Percentile Ranks	Value
Rfree		0.254
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		1.6%
RSRZ outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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 <=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	76% 17% • 7%
2	B	770	3% 74% 24% ••
3	C	9	22% 11% 67%

2 Entry composition (i)

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 (three-letter code: ZN) (formula: Zn).

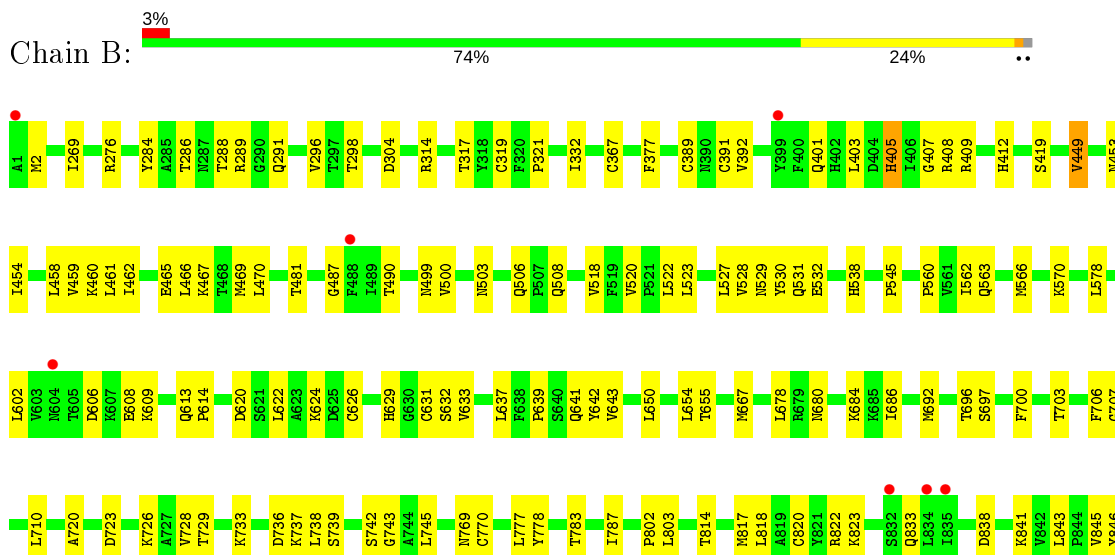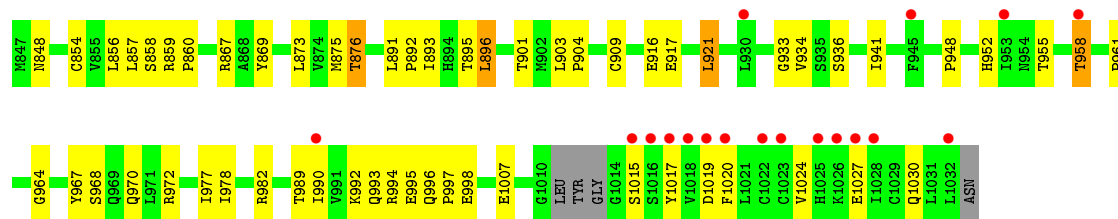| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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
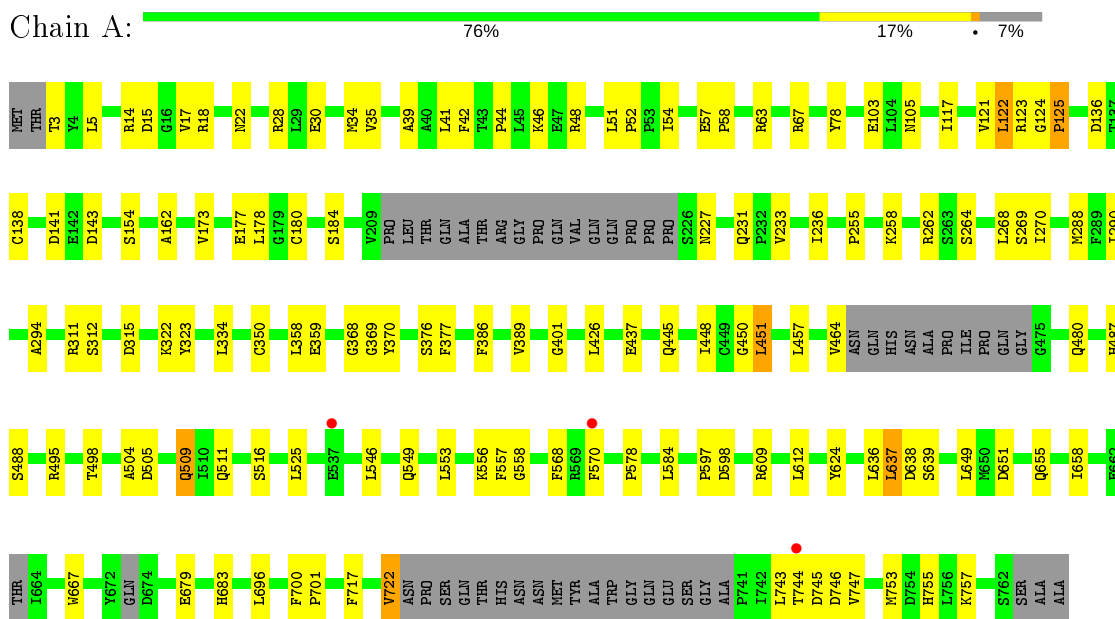
- Molecule 2: Protein transport protein Sec24D

M847 N848 C854 V855 L856 L857 S858 R859 P860 R867 A868 Y869 L873 V874 M875 T876 L891 P892 I893 H894 T895 L896 T901 M902 L903 P904 C909 E916 E917 L921 L930 G933 V934 S935 S936 I941 F945 P948 H952 I953 N954 T955 T958 P961

G964 Y967 S968 Q969 Q970 L971 R972 I977 I978 R982 T989 I990 V991 K992 Q993 R994 E995 Q996 P997 E998 E1007 G1010 LEU TYR GLY G1014 S1015 S1016 Y1017 V1018 D1019 F1020 L1021 C1022 C1023 V1024 H1025 K1026 E1027 I1028 C1029 Q1030 L1031 L1032 ASN

• **Molecule 3: TANGO1 peptide3**

Chain C:

22%   11%   67%

LEU P1801 P1802 P1803 PHE GLY PRO GLY MET
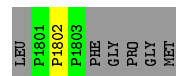
4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [1]	1.59 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.210 , 0.257 0.211 , 0.254	Depositor DCC
R_{free} test set	1829 reflections (5.00%)	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)	0.29 , 47.5	EDS
L-test for twinning [2]	$<|L|> = 0.45$, $<L^2> = 0.28$	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.29	0/5799	0.46	1/7850 (0.0%)
2	B	0.30	0/6136	0.48	0/8316
3	C	0.27	0/23	0.39	0/32
All	All	0.29	0/11958	0.47	1/16198 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	GLY	C-N-CD	5.00	138.91	128.40

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 (i)

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	92	0
2	B	6008	0	5983	128	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	219	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 9.

All (219) 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:H	2:B:405:HIS:CD2	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:HD12	1:A:451:LEU:H	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:893:ILE:HD11	2:B:921:LEU:HB2	1.81	0.61
2:B:1027:GLU:HA	2:B:1030:GLN:HB2	1.82	0.61
2:B:641:GLN:HG2	2:B:642:TYR:H	1.66	0.61
1:A:121:VAL:HG12	1:A:122:LEU:N	2.13	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:123:ARG:C	1:A:125:PRO:HD3	2.23	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
2:B:407:GLY:O	2:B:408:ARG:C	2.40	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
2:B:469:MET:HE2	2:B:678:LEU:HG	1.84	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
2:B:967:TYR:O	2:B:970:GLN:N	2.37	0.57
1:A:745:ASP:CG	1:A:746:ASP:H	2.09	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
2:B:814:THR:HA	2:B:817:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:N	2:B:405:HIS:CD2	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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:958:THR:HG23	2:B:990:ILE:HG13	1.94	0.48
2:B:996:GLN:C	2:B:998:GLU:H	2.17	0.48
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.95	0.48
2:B:858:SER:C	2:B:860:PRO:HD2	2.34	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
2:B:481:THR:HG23	2:B:531:GLN:HG3	1.96	0.47
2:B:692:MET:HE1	2:B:728:VAL:HG11	1.96	0.47
2:B:403:LEU:CD2	2:B:407:GLY:O	2.60	0.47
2:B:706:PHE:HB2	2:B:729:THR:HB	1.96	0.47
1:A:636:LEU:HD23	1:A:638:ASP:HB3	1.97	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
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:909:CYS:O	2:B:1007:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:GLY:HA3	2:B:527:LEU:HD23	1.99	0.45
2:B:503:ASN:ND2	2:B:503:ASN:O	2.50	0.45
2:B:893:ILE:O	2:B:896:LEU:HB2	2.17	0.45
1:A:123:ARG:O	1:A:123:ARG:HD2	2.17	0.44
1:A:505:ASP:O	1:A:509:GLN:HG2	2.17	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
2:B:967:TYR:O	2:B:968:SER:C	2.54	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
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
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:848:ASN:HB2	2:B:1020:PHE:CD2	2.54	0.43
2:B:680:ASN:O	2:B:684:LYS:HG3	2.19	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
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:745:ASP:CG	1:A:746:ASP:N	2.72	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
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:391:CYS:SG	2:B:392:VAL:N	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:VAL:CG1	1:A:122:LEU:H	2.33	0.41
1:A:35:VAL:HG21	1:A:553:LEU:N	2.35	0.41
1:A:753:MET:O	1:A:757:LYS:N	2.50	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:620:ASP:OD1	2:B:650:LEU:HD21	2.20	0.41
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.21	0.41
1:A:350:CYS:HB2	1:A:377:PHE:CE1	2.55	0.41
1:A:78:TYR:CD1	1:A:103:GLU:HG2	2.55	0.41
1:A:14:ARG:HA	1:A:48:ARG:NH1	2.36	0.41
2:B:499:ASN:HB2	2:B:522:LEU:HD11	2.02	0.41
2:B:453:ASN:O	2:B:459:VAL:HG23	2.21	0.41
2:B:933:GLY:HA2	2:B:993:GLN:HB2	2.03	0.41
1:A:679:GLU:O	1:A:683:HIS:ND1	2.48	0.41
1:A:14:ARG:NH1	1:A:15:ASP:OD2	2.54	0.41
2:B:461:LEU:HD22	2:B:667:MET:SD	2.61	0.41
2:B:332:ILE:HD11	2:B:778:TYR:CE1	2.55	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:511:GLN:N	1:A:511:GLN:OE1	2.34	0.40
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.03	0.40
2:B:466:LEU:HD23	2:B:466:LEU:HA	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 (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	702/765 (92%)	665 (95%)	36 (5%)	1 (0%)	51	83
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%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	624/666 (94%)	614 (98%)	10 (2%)	62	84
2	B	674/682 (99%)	663 (98%)	11 (2%)	62	84
3	C	3/7 (43%)	3 (100%)	0	100	100
All	All	1301/1355 (96%)	1280 (98%)	21 (2%)	62	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	141	ASP
1	A	437	GLU
1	A	451	LEU
1	A	509	GLN
1	A	637	LEU
1	A	696	LEU
1	A	722	VAL
2	B	269	ILE
2	B	405	HIS
2	B	449	VAL
2	B	523	LEU
2	B	566	MET
2	B	602	LEU
2	B	876	THR
2	B	896	LEU
2	B	917	GLU
2	B	921	LEU
2	B	958	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
2	B	305	GLN
2	B	405	HIS
2	B	496	HIS
2	B	965	ASN

5.3.3 RNA (i)

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 carbohydrates 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%)	0.05	3 (0%)	92	89	54, 93, 153, 220	0
2	B	766/770 (99%)	0.14	25 (3%)	46	30	55, 96, 183, 304	0
3	C	3/9 (33%)	1.00	0	100	100	176, 176, 177, 209	0
All	All	1483/1544 (96%)	0.09	28 (1%)	66	53	54, 95, 168, 304	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	832	SER	7.1
2	B	1017	TYR	6.5
2	B	1027	GLU	5.8
2	B	1016	SER	4.9
2	B	604	ASN	4.7
2	B	1018	VAL	3.7
2	B	1028	ILE	3.7
2	B	1023	CYS	3.4
2	B	1032	LEU	3.3
2	B	1	ALA	3.2
2	B	1026	LYS	3.2
2	B	1019	ASP	2.8
2	B	1022	CYS	2.7
1	A	537	GLU	2.7
2	B	399	TYR	2.6
2	B	834	LEU	2.6
1	A	570	PHE	2.4
2	B	1015	SER	2.3
2	B	953	ILE	2.3
2	B	1020	PHE	2.3
2	B	1025	HIS	2.3
2	B	958	THR	2.3
2	B	835	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	744	THR	2.2
2	B	945	PHE	2.1
2	B	990	ILE	2.1
2	B	930	LEU	2.1
2	B	488	PHE	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 carbohydrates 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
4	ZN	B	1101	1/1	0.49	0.12	75,75,75,75	0
4	ZN	A	801	1/1	0.95	0.04	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.