



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2016 – 04:33 PM EDT

PDB ID : 5KYN
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

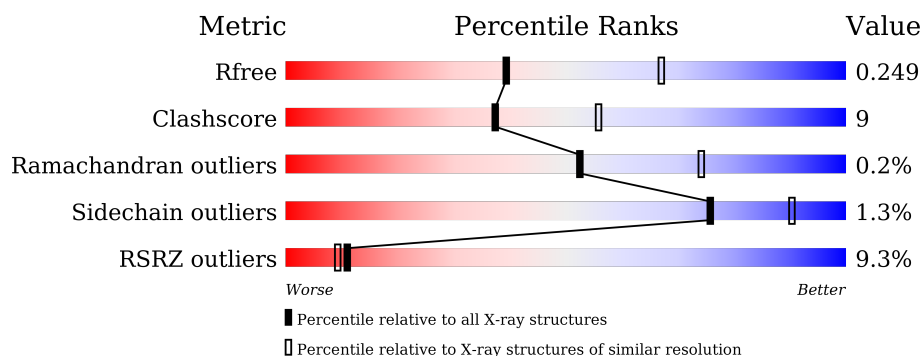
1 Overall quality at a glance

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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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. 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	<div> <div>7%</div> <div>79% 16% 5%</div> </div>
1	B	765	<div> <div>11%</div> <div>75% 18% 6%</div> </div>
2	C	8	<div> <div>13% 25% 63%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	801	-	-	-	X

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.

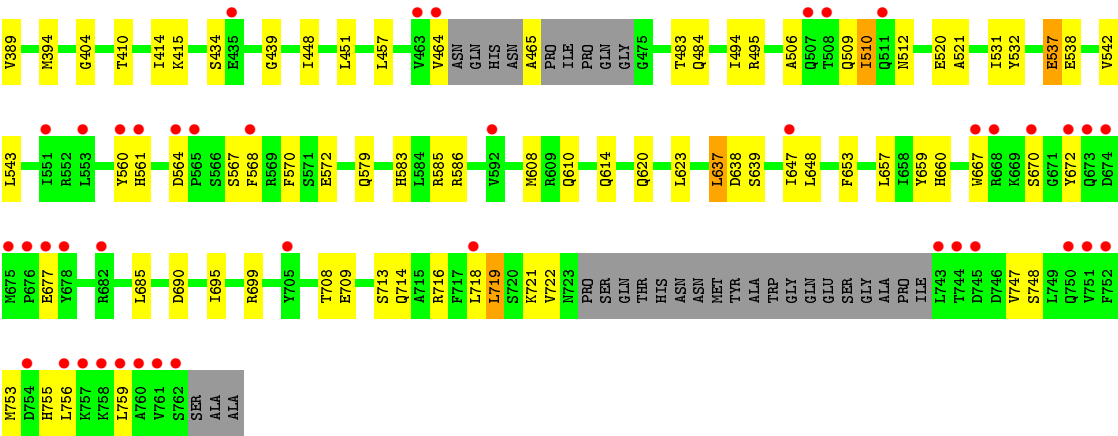
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			21	15	3	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



● Molecule 2: Melanoma inhibitory activity protein 3



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	2.93 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.200 , 0.246 0.206 , 0.249	Depositor DCC
R_{free} test set	1876 reflections (3.46%)	DCC
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.6	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	0.94	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 4.10% 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 [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	0.33	0/5879	0.47	1/7977 (0.0%)
1	B	0.28	0/5764	0.48	2/7813 (0.0%)
2	C	0.27	0/23	0.41	0/32
All	All	0.31	0/11666	0.48	3/15822 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	PRO	N-CA-CB	5.75	110.20	103.30
1	B	170	GLY	N-CA-C	-5.39	99.62	113.10
1	B	537	GLU	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

There are no planarity outliers.

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	5739	0	5647	103	0
1	B	5633	0	5552	107	0
2	C	21	0	23	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	0	5	0
4	B	2	0	0	0	0
All	All	11428	0	11222	211	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 (211) 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:O	1:A:682:ARG:NH2	1.75	1.19
1:A:675:MET:C	1:A:682:ARG:HH21	1.45	1.17
1:A:744:THR:HG22	1:A:746:ASP:H	1.18	1.09
1:B:135:VAL:C	1:B:169:PHE:HE1	1.56	1.09
1:A:675:MET:C	1:A:682:ARG:NH2	2.09	1.05
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:B:135:VAL:C	1:B:169:PHE:CE1	2.39	0.96
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:A:388:ARG:HH22	1:A:702:MET:HE2	1.41	0.85
1:B:136:ASP:N	1:B:169:PHE:CE1	2.46	0.84
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:HD23	1:B:719:LEU:N	2.01	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:N	1:B:394:MET:SD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:168:THR:HG1	1:B:176:HIS:HE2	1.44	0.64
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:O	1:B:653:PHE:CG	2.53	0.61
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.82	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:673:GLN:O	1:A:682:ARG:CG	2.51	0.58
1:B:310:ILE:HD13	1:B:354:GLN:HB2	1.85	0.57
1:B:169:PHE:N	1:B:169:PHE:CD1	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:190:ARG:HB3	1:A:192:THR:HG22	1.86	0.56
1:A:48:ARG:NH2	4:A:910:HOH:O	2.38	0.56
1:B:174:GLN:HG2	1:B:188:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ASP:C	1:A:722:VAL:HG11	2.25	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:A:746:ASP:OD1	1:A:748:SER:OG	2.14	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:137:THR:HG23	1:A:250:ASP:HB2	1.90	0.53
1:A:39:ALA:HB3	1:A:525:LEU:HD13	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
1:B:108:ALA:HA	1:B:111:LEU:HD12	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:B:531:ILE:HB	1:B:608:MET:HE3	1.93	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:A:655:GLN:HG2	1:A:656:ILE:N	2.27	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:MET:HA	1:B:756:LEU:HB3	1.93	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:564:ASP:O	1:B:567:SER:OG	2.22	0.48
1:B:583:HIS:HA	1:B:586:ARG:HG2	1.94	0.48
1:B:3:THR:HG23	1:B:6:GLU:H	1.77	0.48
1:A:48:ARG:HG2	1:A:51:LEU:HD22	1.95	0.48
1:A:66:CYS:O	1:A:409:LYS:NZ	2.25	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:A:388:ARG:NH2	1:A:702:MET:HE3	2.28	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: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:638:ASP:HA	1:A:722:VAL:HG13	1.97	0.47
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:B:410:THR:HB	1:B:414:ILE:HB	1.97	0.46
1:B:57:GLU:HG3	1:B:58:PRO:HD2	1.98	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: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:268:LEU:HD13	1:A:288:MET:HE3	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:610:GLN:HG3	1:A:618:MET:HE1	1.98	0.44
1:A:534:ALA:HB2	1:A:542:VAL:HG21	1.98	0.44
1:B:30:GLU:CD	1:B:506:ALA:HB3	2.37	0.44
1:B:181:GLU:HG2	1:B:181:GLU:H	1.45	0.44
1:B:579:GLN:OE1	1:B:620:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:716:ARG:HG2	1:A:716:ARG:H	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:B:677:GLU:H	1:B:677:GLU:CD	2.22	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:314:HIS:HB3	1:A:318:LYS:HZ1	1.84	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:747:VAL:HG12	1:B:748:SER:H	1.84	0.43
1:A:447:LYS:NZ	4:A:902:HOH:O	1.98	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
1:A:746:ASP:OD1	1:A:747:VAL:N	2.53	0.42
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.54	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: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:HB2	1:A:325:LYS:HE3	1.88	0.41
1:A:639:SER:N	1:A:722:VAL:HG11	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:LEU:HD11	1:B:110:LEU:HD21	2.01	0.41
1:B:28:ARG:HG3	1:B:465:ALA:N	2.36	0.41
1:A:168:THR:OG1	1:A:176:HIS:NE2	2.47	0.41
1:A:45:LEU:HD22	1:A:495:ARG:HD3	2.02	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:HG13	1:B:695:ILE:H	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 [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	724/765 (95%)	688 (95%)	35 (5%)	1 (0%)	56	78
1	B	710/765 (93%)	676 (95%)	32 (4%)	2 (0%)	46	68
2	C	1/8 (12%)	1 (100%)	0	0	100	100
All	All	1435/1538 (93%)	1365 (95%)	67 (5%)	3 (0%)	52	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	VAL

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Mol	Chain	Res	Type
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%)	619 (99%)	5 (1%)	86	95
1	B	613/666 (92%)	602 (98%)	11 (2%)	66	86
2	C	3/7 (43%)	3 (100%)	0	100	100
All	All	1240/1339 (93%)	1224 (99%)	16 (1%)	76	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	155	LEU
1	A	319	ASP
1	A	570	PHE
1	A	655	GLN
1	B	41	LEU
1	B	82	LEU
1	B	169	PHE
1	B	181	GLU
1	B	510	ILE
1	B	570	PHE
1	B	572	GLU
1	B	637	LEU
1	B	690	ASP
1	B	719	LEU
1	B	722	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	B	336	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

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%)	0.47	50 (6%) 20 18	36, 81, 136, 176	0
1	B	719/765 (93%)	0.67	85 (11%) 6 5	70, 106, 152, 186	0
2	C	3/8 (37%)	-0.28	0 100 100	149, 149, 158, 160	0
All	All	1452/1538 (94%)	0.57	135 (9%) 11 9	36, 95, 148, 186	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	LEU	8.7
1	B	761	VAL	5.9
1	A	681	PHE	5.7
1	B	673	GLN	5.0
1	B	257	GLY	4.7
1	A	664	ILE	4.6
1	B	110	LEU	4.5
1	B	568	PHE	4.5
1	A	677	GLU	4.5
1	B	307	LYS	4.4
1	A	682	ARG	4.4
1	B	672	TYR	4.3
1	A	717	PHE	4.3
1	B	674	ASP	4.2
1	B	104	LEU	4.2
1	B	667	TRP	4.1
1	A	718	LEU	4.0
1	A	719	LEU	4.0
1	B	125	PRO	4.0
1	A	679	GLU	3.9
1	B	551	ILE	3.9
1	A	683	HIS	3.9
1	B	310	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	191	GLY	3.8
1	B	1	MET	3.8
1	A	658	ILE	3.7
1	B	759	LEU	3.7
1	B	318	LYS	3.6
1	B	324	VAL	3.6
1	B	744	THR	3.6
1	B	256	GLN	3.6
1	B	228	ARG	3.5
1	A	668	ARG	3.5
1	B	30	GLU	3.5
1	A	225	PRO	3.4
1	B	306	LEU	3.3
1	A	626	TYR	3.3
1	B	675	MET	3.3
1	B	314	HIS	3.3
1	B	464	VAL	3.3
1	B	677	GLU	3.3
1	B	682	ARG	3.2
1	A	195	LEU	3.2
1	B	754	ASP	3.2
1	B	123	ARG	3.2
1	B	676	PRO	3.2
1	B	670	SER	3.1
1	B	752	PHE	3.1
1	A	636	LEU	3.1
1	B	508	THR	3.1
1	A	674	ASP	3.0
1	B	751	VAL	3.0
1	B	678	TYR	3.0
1	B	705	TYR	3.0
1	A	684	LEU	3.0
1	B	756	LEU	3.0
1	B	561	HIS	2.9
1	B	762	SER	2.9
1	A	631	PRO	2.9
1	A	244	LEU	2.9
1	B	565	PRO	2.9
1	B	89	TYR	2.9
1	A	680	ASN	2.9
1	B	208	LYS	2.9
1	B	101	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	705	TYR	2.8
1	A	224	PRO	2.8
1	B	592	VAL	2.8
1	B	668	ARG	2.8
1	B	463	VAL	2.7
1	A	665	ALA	2.7
1	B	209	VAL	2.7
1	B	745	ASP	2.7
1	A	660	HIS	2.7
1	B	309	PRO	2.7
1	A	303	GLY	2.7
1	B	302	VAL	2.7
1	B	435	GLU	2.7
1	B	111	LEU	2.7
1	B	305	GLU	2.7
1	A	164	VAL	2.7
1	A	456	THR	2.7
1	B	308	THR	2.7
1	A	721	LYS	2.7
1	B	718	LEU	2.7
1	B	303	GLY	2.7
1	B	758	LYS	2.6
1	B	564	ASP	2.6
1	A	141	ASP	2.6
1	B	29	LEU	2.6
1	B	507	GLN	2.6
1	A	709	GLU	2.5
1	B	750	GLN	2.5
1	B	107	PRO	2.5
1	B	51	LEU	2.5
1	A	675	MET	2.5
1	A	179	GLY	2.5
1	A	181	GLU	2.5
1	A	541	ASP	2.4
1	B	33	ARG	2.4
1	A	178	LEU	2.4
1	B	50	ASP	2.3
1	B	560	TYR	2.3
1	A	451	LEU	2.3
1	A	383	LYS	2.3
1	B	238	MET	2.3
1	B	757	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	511	GLN	2.3
1	A	184	SER	2.3
1	B	319	ASP	2.3
1	B	97	SER	2.2
1	A	323	TYR	2.2
1	A	104	LEU	2.2
1	B	198	LYS	2.2
1	B	180	CYS	2.2
1	B	553	LEU	2.2
1	A	612	LEU	2.2
1	B	139	MET	2.1
1	A	696	LEU	2.1
1	B	54	ILE	2.1
1	B	647	ILE	2.1
1	A	453	PRO	2.1
1	B	102	SER	2.1
1	A	454	THR	2.1
1	B	98	TYR	2.1
1	A	452	SER	2.1
1	B	760	ALA	2.1
1	B	119	TYR	2.1
1	A	132	LEU	2.1
1	A	457	LEU	2.1
1	A	152	GLN	2.1
1	A	165	GLY	2.1
1	B	207	SER	2.0
1	A	569	ARG	2.0
1	B	121	VAL	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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	801	1/1	0.99	0.20	3.54	63,63,63,63	0
3	ZN	B	801	1/1	0.97	0.13	0.42	107,107,107,107	0

6.5 Other polymers

There are no such residues in this entry.