



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:28 am BST

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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

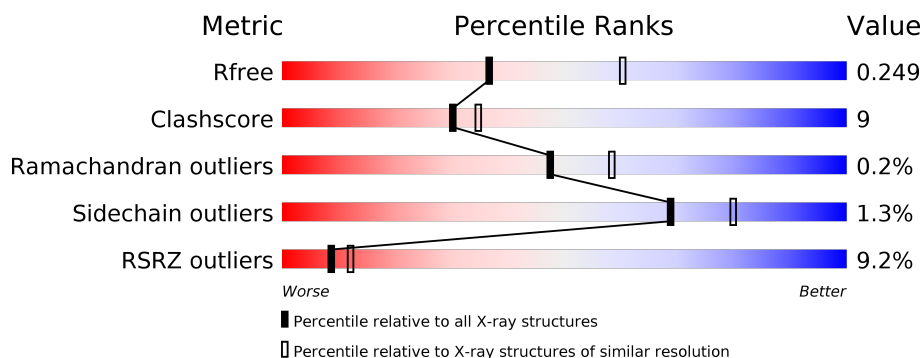
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
1	B	765	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>6%</div> </div> </div>
2	C	8	<div> <div>13%</div> <div>25%</div> <div>63%</div> </div>

## 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		

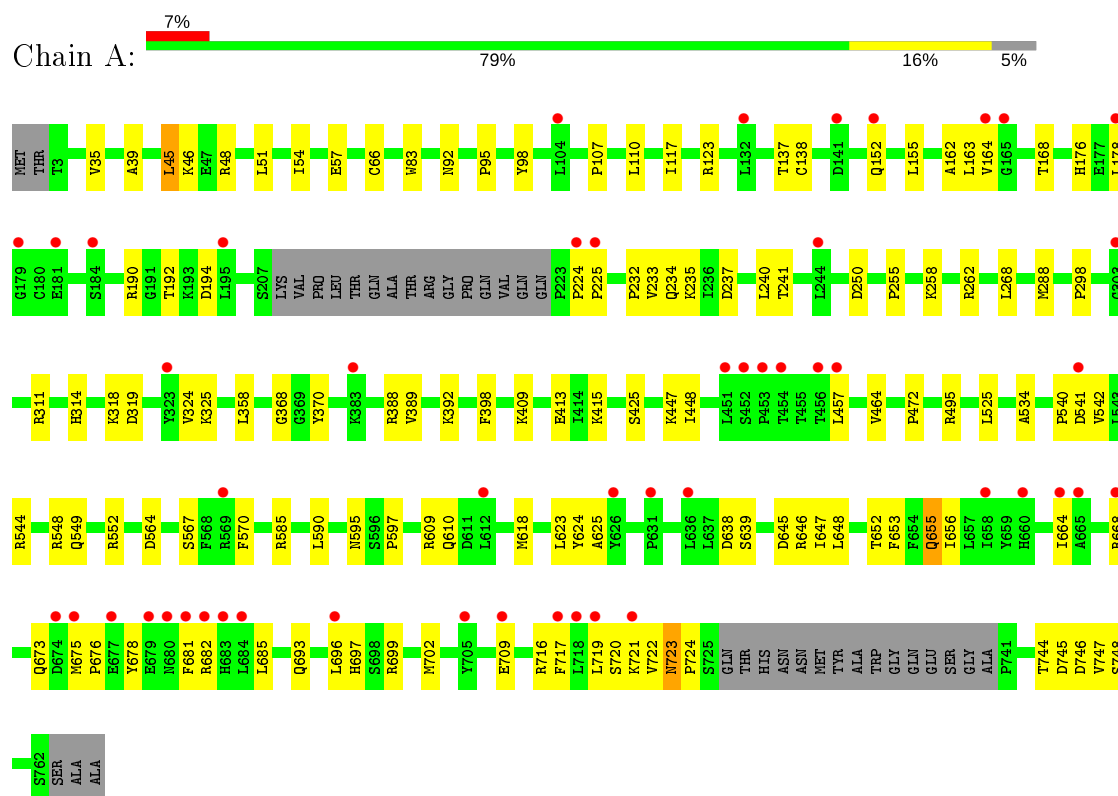
- Molecule 4 is water.

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

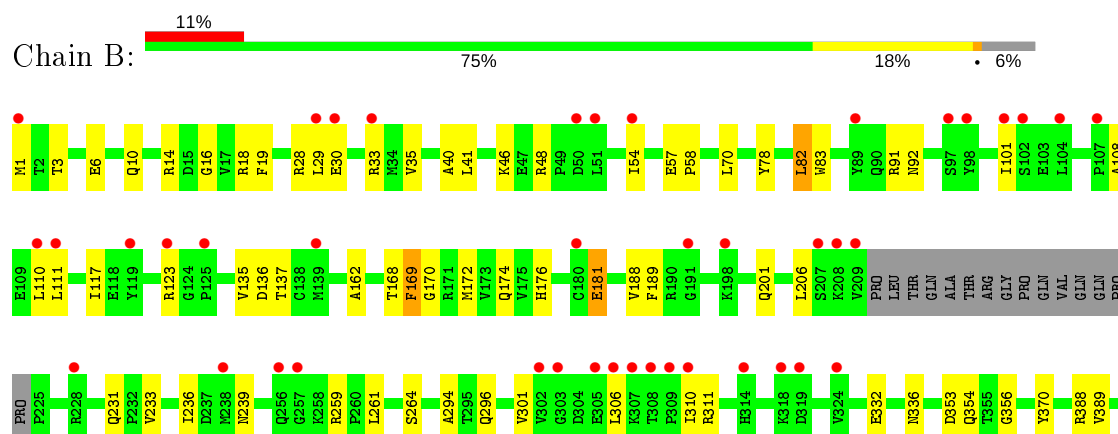
### 3 Residue-property plots [i](#)

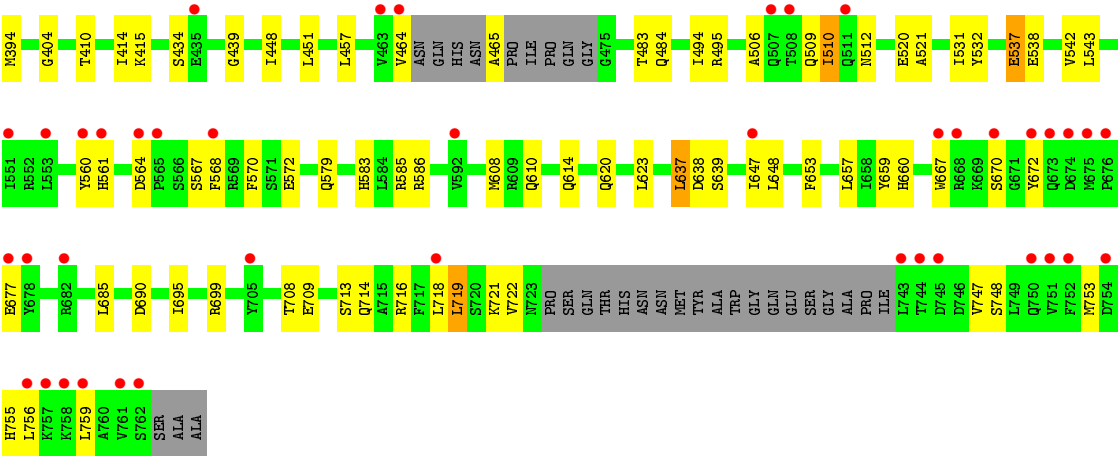
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 1: Protein transport protein Sec23A





● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.200 , 0.246 0.208 , 0.249	Depositor DCC
$R_{free}$ test set	2000 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: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: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:388:ARG:HH21	1:A:697:HIS:HA	1.83	0.42
1:A:311:ARG:NH1	1:A:597:PRO:HB2	2.34	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: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: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%)	51	65
1	B	710/765 (93%)	676 (95%)	32 (4%)	2 (0%)	41	50
2	C	1/8 (12%)	1 (100%)	0	0	100	100
All	All	1435/1538 (93%)	1365 (95%)	67 (5%)	3 (0%)	47	58

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%)	81	88
1	B	613/666 (92%)	602 (98%)	11 (2%)	59	73
2	C	3/7 (43%)	3 (100%)	0	100	100
All	All	1240/1339 (93%)	1224 (99%)	16 (1%)	69	80

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	730/765 (95%)	0.47	50 (6%) 17 22	36, 81, 136, 176	0
1	B	719/765 (93%)	0.67	83 (11%) 4 7	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	133 (9%) 9 12	36, 95, 148, 186	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	LEU	8.7
1	B	761	VAL	5.8
1	A	681	PHE	5.6
1	B	673	GLN	5.0
1	B	257	GLY	4.7
1	A	664	ILE	4.6
1	A	677	GLU	4.5
1	B	568	PHE	4.5
1	B	110	LEU	4.5
1	B	307	LYS	4.4
1	A	682	ARG	4.3
1	B	672	TYR	4.3
1	A	717	PHE	4.3
1	B	674	ASP	4.2
1	B	667	TRP	4.1
1	B	104	LEU	4.1
1	A	718	LEU	4.0
1	B	125	PRO	4.0
1	A	719	LEU	4.0
1	A	679	GLU	3.9
1	A	683	HIS	3.9
1	B	551	ILE	3.9
1	B	310	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.8
1	A	658	ILE	3.7
1	B	744	THR	3.7
1	B	759	LEU	3.7
1	B	191	GLY	3.7
1	B	324	VAL	3.6
1	B	256	GLN	3.6
1	B	318	LYS	3.6
1	B	228	ARG	3.6
1	A	668	ARG	3.5
1	B	30	GLU	3.5
1	A	225	PRO	3.4
1	B	306	LEU	3.4
1	A	626	TYR	3.3
1	B	677	GLU	3.3
1	B	675	MET	3.3
1	B	464	VAL	3.3
1	B	314	HIS	3.3
1	A	195	LEU	3.3
1	B	123	ARG	3.2
1	B	682	ARG	3.2
1	B	676	PRO	3.2
1	B	754	ASP	3.2
1	B	752	PHE	3.1
1	A	636	LEU	3.1
1	B	670	SER	3.1
1	B	751	VAL	3.1
1	B	508	THR	3.1
1	B	705	TYR	3.0
1	B	678	TYR	3.0
1	B	561	HIS	2.9
1	A	684	LEU	2.9
1	B	89	TYR	2.9
1	B	565	PRO	2.9
1	B	756	LEU	2.9
1	A	674	ASP	2.9
1	B	762	SER	2.9
1	A	224	PRO	2.9
1	A	631	PRO	2.9
1	B	208	LYS	2.9
1	A	244	LEU	2.8
1	A	680	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	101	ILE	2.8
1	A	705	TYR	2.8
1	A	303	GLY	2.8
1	B	668	ARG	2.8
1	B	463	VAL	2.8
1	A	660	HIS	2.8
1	B	592	VAL	2.7
1	A	721	LYS	2.7
1	B	111	LEU	2.7
1	B	309	PRO	2.7
1	B	209	VAL	2.7
1	B	302	VAL	2.7
1	B	305	GLU	2.7
1	B	745	ASP	2.7
1	B	303	GLY	2.7
1	B	435	GLU	2.7
1	A	456	THR	2.7
1	A	665	ALA	2.7
1	A	164	VAL	2.7
1	B	308	THR	2.7
1	B	564	ASP	2.6
1	B	758	LYS	2.6
1	B	718	LEU	2.6
1	A	141	ASP	2.6
1	A	675	MET	2.6
1	A	179	GLY	2.6
1	B	29	LEU	2.5
1	B	507	GLN	2.5
1	B	750	GLN	2.5
1	A	709	GLU	2.5
1	B	51	LEU	2.5
1	A	181	GLU	2.5
1	B	107	PRO	2.4
1	A	178	LEU	2.4
1	A	541	ASP	2.4
1	B	33	ARG	2.4
1	B	50	ASP	2.4
1	B	757	LYS	2.3
1	B	560	TYR	2.3
1	B	238	MET	2.3
1	A	451	LEU	2.3
1	A	383	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	184	SER	2.3
1	B	511	GLN	2.3
1	B	319	ASP	2.3
1	A	323	TYR	2.2
1	B	97	SER	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	B	139	MET	2.1
1	A	612	LEU	2.1
1	A	696	LEU	2.1
1	B	54	ILE	2.1
1	A	453	PRO	2.1
1	A	454	THR	2.1
1	B	647	ILE	2.1
1	A	452	SER	2.1
1	B	102	SER	2.1
1	A	152	GLN	2.1
1	B	98	TYR	2.1
1	A	132	LEU	2.1
1	A	457	LEU	2.0
1	A	165	GLY	2.0
1	B	119	TYR	2.0
1	A	569	ARG	2.0
1	B	207	SER	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, 95<sup>th</sup> 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
3	ZN	B	801	1/1	0.97	0.13	107,107,107,107	0
3	ZN	A	801	1/1	0.99	0.20	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.