



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:33 am BST

PDB ID : 5VNJ
Title : Crystal structure of Sec23a/Sec24a/Sec22 complexed with a C-terminal FF sorting motif (ERGIC-53)
Authors : Ma, W.; Goldberg, J.
Deposited on : 2017-04-30
Resolution : 2.81 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 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

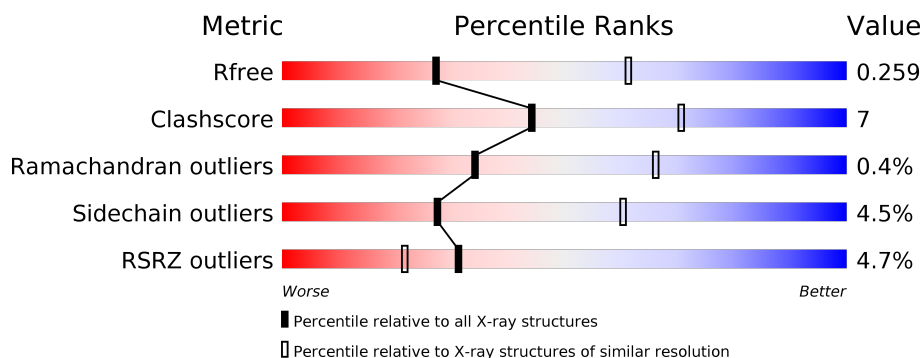
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	764	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	748	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
3	C	157	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
4	D	5	<div> <div>40%</div> <div> <div>20%</div> <div>20%</div> <div>60%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12497 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	697	Total	C	N	O	S	0	0	0
			5524	3521	951	1013	39			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5770	3685	980	1071	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1056	ALA	ARG	conflict	UNP O95486

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1103	708	182	205	8			

- Molecule 4 is a protein called C-terminal FF Ergic-53.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			23	18	2	3			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0

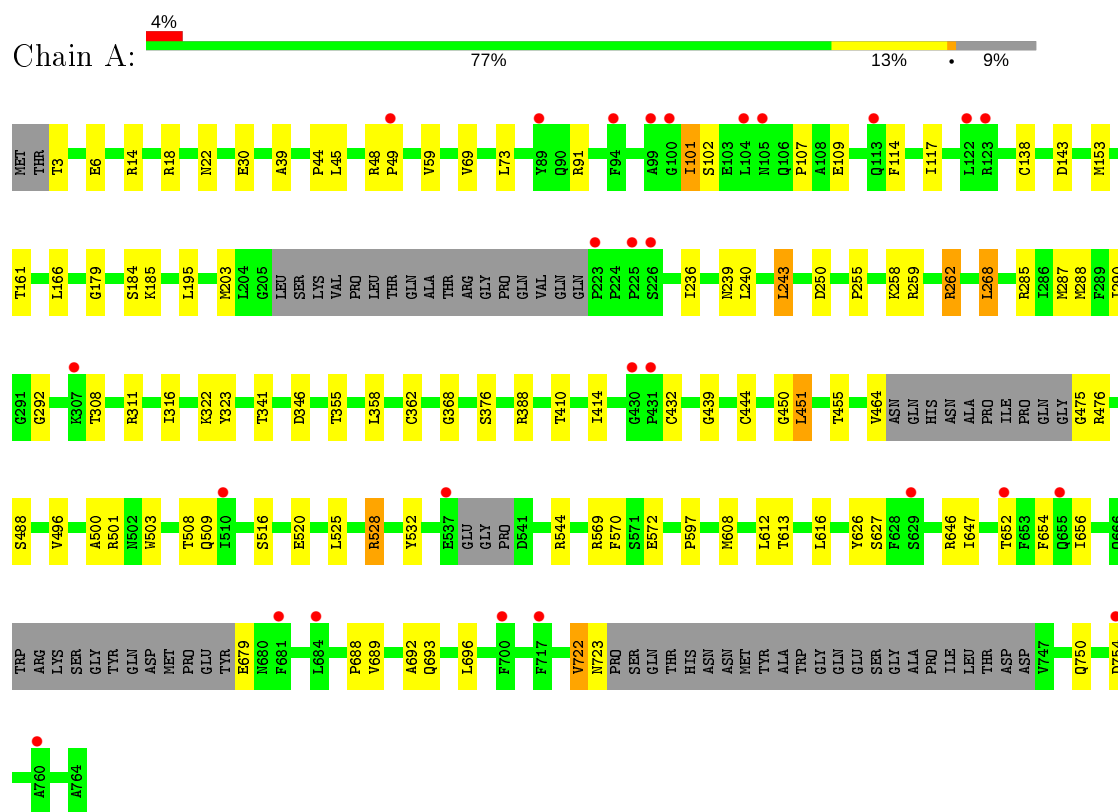
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	40	Total 40	O 40	0	0
6	B	34	Total 34	O 34	0	0
6	C	1	Total 1	O 1	0	0

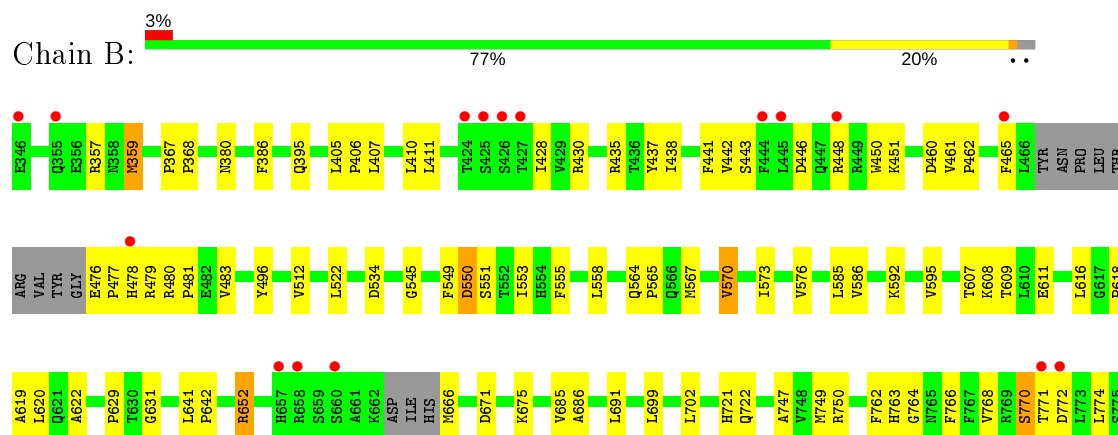
3 Residue-property plots [i](#)

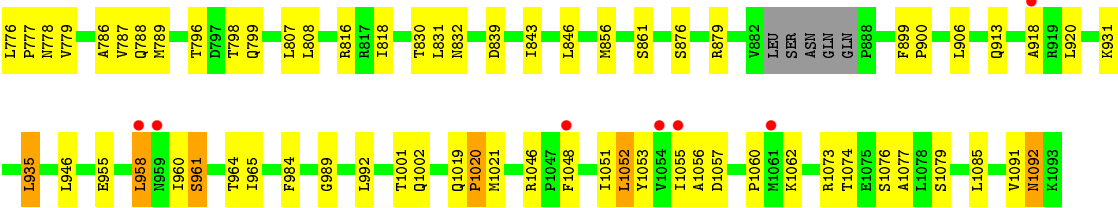
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

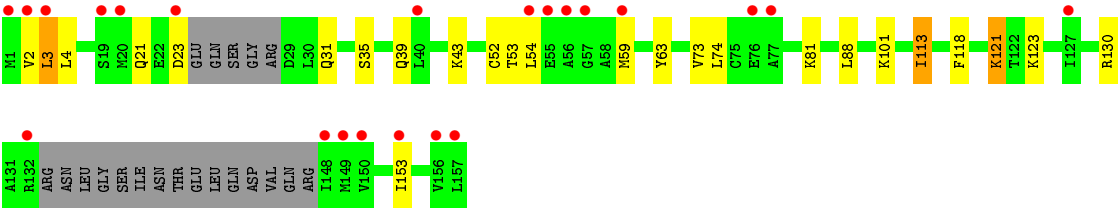


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: C-terminal FF Ergic-53



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.96Å 96.98Å 129.55Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	48.83 – 2.81 48.83 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.83-2.81) 99.3 (48.83-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.221 , 0.261 0.221 , 0.259	Depositor DCC
R_{free} test set	1999 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12497	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	0.29	0/5651	0.45	0/7651
2	B	0.29	0/5894	0.47	0/8012
3	C	0.24	0/1122	0.42	0/1510
4	D	0.41	0/24	0.31	0/29
All	All	0.29	0/12691	0.45	0/17202

There are no bond length outliers.

There are no bond angle outliers.

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	5524	0	5487	55	0
2	B	5770	0	5820	96	0
3	C	1103	0	1109	15	0
4	D	23	0	20	8	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	40	0	0	5	0
6	B	34	0	0	4	0
6	C	1	0	0	0	0
All	All	12497	0	12436	163	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 7.

All (163) 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)
2:B:750:ARG:HD3	2:B:772:ASP:O	1.76	0.84
2:B:770:SER:O	2:B:771:THR:C	2.17	0.83
2:B:550:ASP:OD1	2:B:551:SER:N	2.13	0.81
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.63	0.80
2:B:480:ARG:HG3	2:B:481:PRO:HD2	1.67	0.77
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.70	0.74
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.18	0.74
2:B:1074:THR:HG23	2:B:1076:SER:H	1.53	0.71
2:B:960:ILE:HD13	2:B:960:ILE:N	2.06	0.70
2:B:788:GLN:NE2	6:B:1202:HOH:O	2.22	0.69
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.74	0.68
1:A:362:CYS:SG	6:A:937:HOH:O	2.51	0.68
2:B:460:ASP:O	2:B:462:PRO:HD3	1.94	0.67
2:B:357:ARG:NH2	6:B:1203:HOH:O	2.27	0.67
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.76	0.67
2:B:609:THR:HG22	2:B:611:GLU:H	1.60	0.67
2:B:652:ARG:NH2	6:B:1204:HOH:O	2.28	0.66
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.78	0.65
1:A:3:THR:HG22	1:A:6:GLU:H	1.61	0.65
2:B:965:ILE:O	2:B:965:ILE:HG22	1.96	0.64
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.80	0.63
2:B:879:ARG:NH1	2:B:1092:ASN:OD1	2.33	0.61
1:A:250:ASP:O	3:C:130:ARG:NH2	2.28	0.61
1:A:528:ARG:NH1	6:A:901:HOH:O	1.96	0.60
2:B:480:ARG:HG3	2:B:481:PRO:CD	2.31	0.60
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.83	0.60
1:A:341:THR:OG1	6:A:902:HOH:O	2.17	0.60
2:B:430:ARG:HH22	4:D:2:PHE:HB3	1.68	0.59
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.84	0.59
2:B:478:HIS:CD2	2:B:478:HIS:H	2.21	0.59
2:B:808:LEU:HD22	4:D:1:PHE:H1	1.68	0.59
1:A:679:GLU:N	6:A:907:HOH:O	2.34	0.59
1:A:59:VAL:O	1:A:59:VAL:HG12	2.03	0.58
2:B:808:LEU:HB2	4:D:2:PHE:CZ	2.39	0.58
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.86	0.58
2:B:1055:ILE:O	2:B:1057:ASP:N	2.36	0.57
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.87	0.56
1:A:410:THR:HB	1:A:414:ILE:HB	1.87	0.56
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.71	0.56
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.86	0.55
1:A:259:ARG:NH2	1:A:308:THR:O	2.36	0.55
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.88	0.55
2:B:960:ILE:O	2:B:961:SER:C	2.45	0.55
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.73	0.54
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.88	0.54
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.89	0.54
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.90	0.54
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.90	0.53
1:A:143:ASP:OD1	1:A:376:SER:OG	2.24	0.53
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.74	0.52
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.92	0.52
3:C:54:LEU:HD13	3:C:153:ILE:HG13	1.90	0.52
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.25	0.52
1:A:69:VAL:HG11	1:A:496:VAL:HG21	1.92	0.52
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.92	0.52
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.92	0.52
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.92	0.52
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.91	0.51
2:B:512:VAL:HG22	2:B:549:PHE:O	2.11	0.51
2:B:407:LEU:HG	2:B:789:MET:HG3	1.92	0.51
2:B:955:GLU:OE1	2:B:955:GLU:N	2.43	0.51
1:A:572:GLU:O	6:A:903:HOH:O	2.19	0.51
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.76	0.51
1:A:722:VAL:HG22	1:A:723:ASN:H	1.76	0.51
1:A:750:GLN:OE1	1:A:750:GLN:N	2.41	0.51
2:B:430:ARG:HH22	4:D:2:PHE:HA	1.77	0.50
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.94	0.50
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.94	0.50
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.94	0.49
2:B:437:TYR:HH	4:D:2:PHE:HD1	1.59	0.49
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.94	0.49
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.94	0.49
2:B:839:ASP:OD1	6:B:1201:HOH:O	2.19	0.49
1:A:195:LEU:HD13	1:A:203:MET:CE	2.43	0.49
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.94	0.49
1:A:475:GLY:HA2	1:A:503:TRP:HB2	1.94	0.48
2:B:913:GLN:HE21	2:B:918:ALA:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:ALA:HB3	2:B:776:LEU:HB2	1.95	0.48
2:B:992:LEU:HB2	2:B:1052:LEU:HB2	1.95	0.48
2:B:476:GLU:N	2:B:477:PRO:CD	2.77	0.48
2:B:666:MET:HB3	2:B:856:MET:CE	2.43	0.48
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.96	0.48
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.49	0.48
1:A:14:ARG:O	1:A:48:ARG:NH1	2.47	0.47
1:A:285:ARG:NE	1:A:346:ASP:OD2	2.47	0.47
1:A:287:MET:HA	1:A:346:ASP:HB2	1.97	0.47
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.97	0.47
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.97	0.46
2:B:406:PRO:HB2	2:B:846:LEU:HD23	1.98	0.46
2:B:446:ASP:C	2:B:448:ARG:H	2.19	0.46
1:A:290:ILE:HG23	1:A:292:GLY:H	1.80	0.46
2:B:430:ARG:HD3	2:B:435:ARG:HH21	1.81	0.46
2:B:749:MET:HB2	2:B:807:LEU:HD13	1.98	0.46
2:B:856:MET:H	2:B:856:MET:HG2	1.60	0.46
2:B:430:ARG:NH2	4:D:2:PHE:HB3	2.29	0.45
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.98	0.45
2:B:1053:TYR:HD2	2:B:1055:ILE:HB	1.82	0.45
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.98	0.45
1:A:114:PHE:HB3	1:A:117:ILE:HD12	1.97	0.45
2:B:450:TRP:HD1	2:B:461:VAL:HG22	1.81	0.45
2:B:438:ILE:HD12	2:B:442:VAL:HG11	1.98	0.45
1:A:184:SER:OG	1:A:184:SER:O	2.24	0.45
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.99	0.45
2:B:558:LEU:HD13	2:B:595:VAL:HG12	1.98	0.45
3:C:39:GLN:O	3:C:43:LYS:HG2	2.16	0.45
2:B:428:ILE:HG21	2:B:437:TYR:HE1	1.81	0.44
2:B:989:GLY:O	2:B:1046:ARG:NH1	2.50	0.44
2:B:666:MET:HB3	2:B:856:MET:HE2	1.98	0.44
2:B:395:GLN:HE21	2:B:796:THR:HA	1.82	0.44
3:C:3:LEU:HD11	3:C:21:GLN:HB2	2.00	0.44
3:C:52:CYS:SG	3:C:53:THR:N	2.90	0.44
2:B:691:LEU:HD22	2:B:699:LEU:HD13	1.99	0.44
3:C:3:LEU:HB3	3:C:123:LYS:HD3	1.98	0.44
2:B:1019:GLN:O	2:B:1055:ILE:HG23	2.18	0.44
2:B:545:GLY:HA3	2:B:585:LEU:HD23	2.00	0.43
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.57	0.43
3:C:35:SER:O	3:C:39:GLN:HG2	2.19	0.43
2:B:750:ARG:NE	4:D:2:PHE:OXT	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD23	1:A:243:LEU:HD13	2.01	0.43
2:B:958:LEU:HD12	2:B:964:THR:HG23	2.00	0.43
2:B:777:PRO:O	2:B:778:ASN:ND2	2.52	0.43
2:B:405:LEU:HD22	2:B:843:ILE:HD13	1.99	0.43
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.84	0.42
3:C:73:VAL:HB	3:C:88:LEU:HD21	2.00	0.42
1:A:528:ARG:HA	1:A:608:MET:HE1	2.00	0.42
3:C:118:PHE:HA	3:C:121:LYS:HG2	2.00	0.42
1:A:73:LEU:HD11	1:A:500:ALA:HB2	2.00	0.42
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.35	0.42
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.54	0.42
2:B:359:MET:N	2:B:359:MET:SD	2.90	0.42
2:B:808:LEU:HD22	4:D:1:PHE:N	2.34	0.42
2:B:958:LEU:H	2:B:958:LEU:HD22	1.85	0.42
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.54	0.42
3:C:113:ILE:HD13	3:C:113:ILE:H	1.83	0.42
2:B:553:ILE:HG12	2:B:619:ALA:HA	2.01	0.42
1:A:656:ILE:HD12	1:A:696:LEU:HD13	2.01	0.42
2:B:496:TYR:CD2	2:B:818:ILE:HD11	2.54	0.42
1:A:500:ALA:O	1:A:501:ARG:NH1	2.48	0.41
1:A:652:THR:HG22	1:A:654:PHE:H	1.85	0.41
2:B:721:HIS:CD2	2:B:722:GLN:HG3	2.55	0.41
1:A:44:PRO:HD2	1:A:455:THR:O	2.21	0.41
2:B:830:THR:HG22	2:B:832:ASN:H	1.84	0.41
2:B:564:GLN:HE21	2:B:564:GLN:HB3	1.65	0.41
2:B:671:ASP:OD2	2:B:675:LYS:HE3	2.20	0.41
2:B:616:LEU:O	2:B:620:LEU:HG	2.20	0.41
2:B:768:VAL:HG22	2:B:774:LEU:CD2	2.50	0.41
1:A:101:ILE:HD13	1:A:102:SER:H	1.86	0.41
1:A:268:LEU:HG	1:A:288:MET:SD	2.61	0.41
2:B:410:LEU:HD22	2:B:935:LEU:HG	2.01	0.41
2:B:764:GLY:HA2	2:B:931:LYS:O	2.20	0.41
1:A:358:LEU:HD22	1:A:597:PRO:HB3	2.03	0.41
2:B:876:SER:HA	2:B:1091:VAL:HG13	2.02	0.41
2:B:550:ASP:CG	2:B:551:SER:H	2.20	0.41
2:B:946:LEU:HD11	2:B:984:PHE:HB3	2.02	0.41
1:A:107:PRO:HB2	1:A:109:GLU:OE2	2.21	0.40
1:A:368:GLY:HA3	1:A:450:GLY:O	2.21	0.40
2:B:395:GLN:NE2	2:B:796:THR:HA	2.36	0.40
3:C:54:LEU:HB3	3:C:153:ILE:HB	2.03	0.40
1:A:689:VAL:O	1:A:693:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ALA:O	1:A:696:LEU:HB2	2.21	0.40
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.96	0.40
2:B:762:PHE:HB3	2:B:766:PHE:CZ	2.57	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	685/764 (90%)	650 (95%)	32 (5%)	3 (0%)	34	66
2	B	723/748 (97%)	676 (94%)	44 (6%)	3 (0%)	34	66
3	C	131/157 (83%)	120 (92%)	11 (8%)	0	100	100
All	All	1539/1669 (92%)	1446 (94%)	87 (6%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1056	ALA
1	A	476	ARG
2	B	550	ASP
1	A	509	GLN
2	B	1020	PRO
1	A	722	VAL

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	609/666 (91%)	585 (96%)	24 (4%)	32	66
2	B	660/678 (97%)	629 (95%)	31 (5%)	26	59
3	C	120/138 (87%)	113 (94%)	7 (6%)	20	50
4	D	2/5 (40%)	1 (50%)	1 (50%)	0	0
All	All	1391/1487 (94%)	1328 (96%)	63 (4%)	27	60

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	91	ARG
1	A	101	ILE
1	A	153	MET
1	A	161	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	262	ARG
1	A	268	LEU
1	A	311	ARG
1	A	316	ILE
1	A	355	THR
1	A	388	ARG
1	A	451	LEU
1	A	464	VAL
1	A	488	SER
1	A	508	THR
1	A	528	ARG
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE
1	A	613	THR
1	A	754	ASP
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	465	PHE
2	B	479	ARG
2	B	483	VAL
2	B	522	LEU

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Mol	Chain	Res	Type
2	B	570	VAL
2	B	607	THR
2	B	608	LYS
2	B	641	LEU
2	B	652	ARG
2	B	770	SER
2	B	787	VAL
2	B	798	THR
2	B	799	GLN
2	B	816	ARG
2	B	831	LEU
2	B	861	SER
2	B	906	LEU
2	B	920	LEU
2	B	935	LEU
2	B	958	LEU
2	B	961	SER
2	B	1001	THR
2	B	1002	GLN
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1085	LEU
2	B	1092	ASN
3	C	2	VAL
3	C	3	LEU
3	C	31	GLN
3	C	81	LYS
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
4	D	2	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
2	B	478	HIS
2	B	913	GLN

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	697/764 (91%)	0.26	27 (3%) 39 29	35, 71, 119, 177	0
2	B	731/748 (97%)	0.14	23 (3%) 49 39	33, 58, 114, 184	0
3	C	137/157 (87%)	0.99	22 (16%) 1 1	54, 91, 145, 155	0
4	D	2/5 (40%)	3.02	2 (100%) 0 0	129, 129, 129, 148	0
All	All	1567/1674 (93%)	0.27	74 (4%) 31 22	33, 66, 122, 184	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	8.8
3	C	1	MET	8.5
3	C	57	GLY	7.9
2	B	424	THR	7.7
3	C	148	ILE	5.4
2	B	959	ASN	5.1
2	B	346	GLU	4.8
2	B	772	ASP	4.6
3	C	149	MET	4.6
3	C	157	LEU	4.6
1	A	225	PRO	3.8
3	C	20	MET	3.5
3	C	127	ILE	3.4
2	B	444	PHE	3.3
4	D	2	PHE	3.2
1	A	123	ARG	3.2
3	C	153	ILE	3.1
1	A	700	PHE	3.1
2	B	426	SER	3.1
3	C	156	VAL	3.0
1	A	510	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	77	ALA	3.0
1	A	113	GLN	3.0
1	A	754	ASP	2.9
3	C	55	GLU	2.8
4	D	1	PHE	2.8
2	B	427	THR	2.8
1	A	99	ALA	2.7
1	A	223	PRO	2.7
1	A	629	SER	2.7
3	C	3	LEU	2.7
1	A	430	GLY	2.7
3	C	56	ALA	2.7
2	B	771	THR	2.7
1	A	537	GLU	2.7
3	C	54	LEU	2.7
2	B	448	ARG	2.6
1	A	681	PHE	2.6
2	B	660	SER	2.6
2	B	658	ARG	2.5
1	A	94	PHE	2.5
1	A	49	PRO	2.5
1	A	89	TYR	2.5
2	B	425	SER	2.5
3	C	2	VAL	2.5
3	C	132	ARG	2.5
2	B	478	HIS	2.4
3	C	40	LEU	2.4
1	A	122	LEU	2.3
1	A	100	GLY	2.3
3	C	150	VAL	2.3
2	B	1048	PHE	2.3
2	B	445	LEU	2.3
2	B	1054	VAL	2.3
1	A	684	LEU	2.3
1	A	655	GLN	2.3
3	C	19	SER	2.2
3	C	23	ASP	2.2
1	A	760	ALA	2.2
2	B	465	PHE	2.2
3	C	59	MET	2.2
1	A	105	ASN	2.2
1	A	431	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	918	ALA	2.1
2	B	1061	MET	2.1
1	A	226	SER	2.1
1	A	307	LYS	2.1
1	A	104	LEU	2.1
1	A	717	PHE	2.1
2	B	958	LEU	2.1
2	B	355	GLN	2.1
2	B	657	HIS	2.0
1	A	652	THR	2.0
3	C	76	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
5	ZN	B	1101	1/1	0.85	0.36	174,174,174,174	0
5	ZN	A	801	1/1	0.99	0.08	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.