Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:26 PM EDT

PDB ID	:	5VNE
Title	:	Crystal structure of Sec23a/Sec24a/Sec22 complexed with Emp24 sorting motif
Authors	:	Ma, W.; Goldberg, J.
Deposited on	:	2017-04-30
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

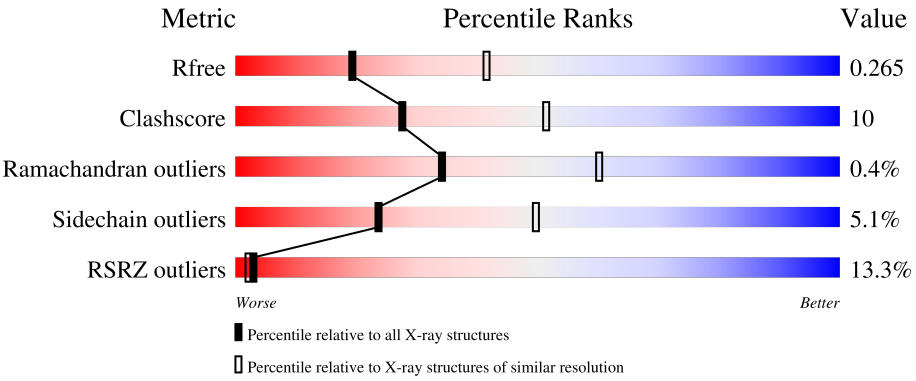
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	10% 74% 17% · 7%
2	B	748	10% 75% 21% · ·
3	C	157	36% 53% 29% · 14%
4	D	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12570 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	708	Total	C	N	O	S	0	0	0
			5624	3582	968	1034	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5747	3664	980	1069	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	135	Total	C	N	O	S	0	0	0
			1077	693	173	203	8			

- Molecule 4 is a protein called EMP24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			22	14	3	5			

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

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

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

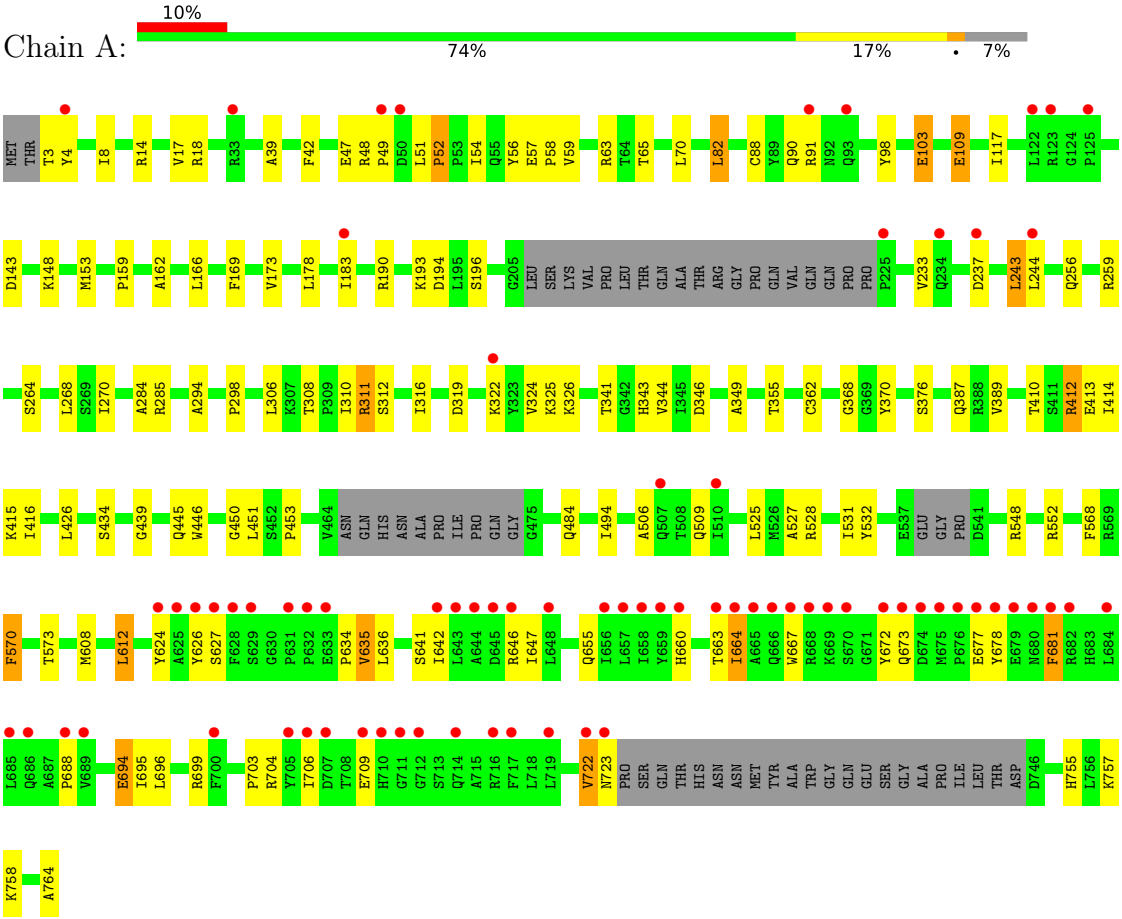
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	57	Total O 57 57	0	0
6	B	38	Total O 38 38	0	0
6	C	3	Total O 3 3	0	0

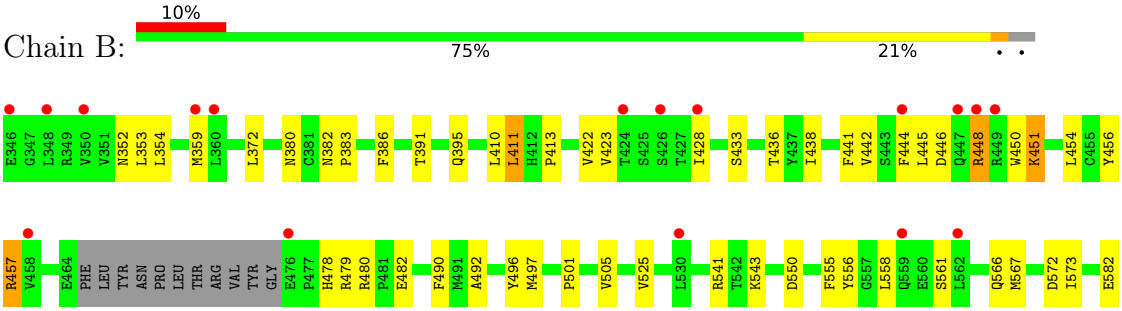
3 Residue-property plots (i)

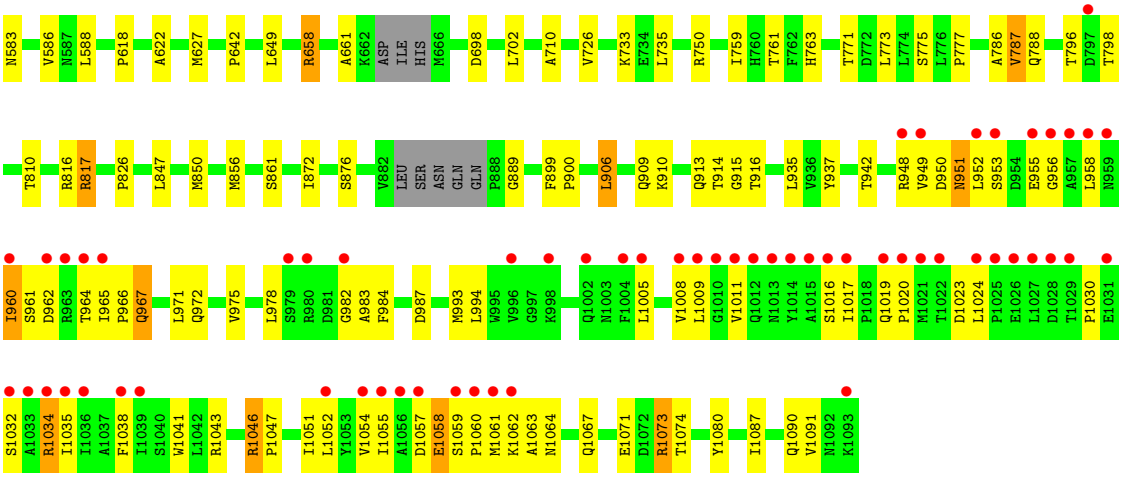
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

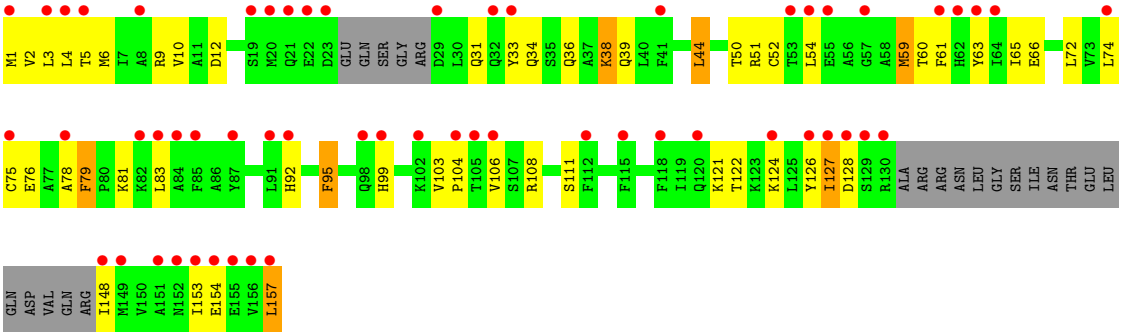


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: EMP24

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.76Å 96.50Å 126.57Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	49.80 – 2.70 49.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.80-2.70) 99.8 (49.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.224 , 0.266 0.225 , 0.265	Depositor DCC
R_{free} test set	2013 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12570	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/5755	0.44	0/7791
2	B	0.28	0/5869	0.47	0/7977
3	C	0.25	0/1096	0.44	0/1478
4	D	0.17	0/21	0.37	0/26
All	All	0.28	0/12741	0.46	0/17272

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

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	5624	0	5565	80	0
2	B	5747	0	5792	124	0
3	C	1077	0	1069	48	0
4	D	22	0	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	57	0	0	2	0
6	B	38	0	0	2	0
6	C	3	0	0	2	0
All	All	12570	0	12450	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (248) 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:965:ILE:HG22	2:B:965:ILE:O	1.76	0.82
3:C:4:LEU:HD23	3:C:74:LEU:HD23	1.59	0.81
2:B:950:ASP:OD1	2:B:951:ASN:OD1	2.00	0.79
2:B:960:ILE:HG22	2:B:960:ILE:O	1.81	0.79
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.48	0.77
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.66	0.77
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.69	0.74
2:B:987:ASP:CG	2:B:1046:ARG:HH22	1.89	0.74
1:A:285:ARG:NH1	1:A:346:ASP:OD2	2.21	0.74
2:B:949:VAL:HA	2:B:952:LEU:HD11	1.68	0.74
2:B:1063:ALA:O	6:B:1201:HOH:O	2.04	0.74
3:C:75:CYS:HB2	3:C:79:PHE:CD2	2.22	0.73
3:C:59:MET:HA	3:C:76:GLU:HA	1.68	0.73
2:B:987:ASP:OD1	2:B:1046:ARG:NH2	2.22	0.73
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.71	0.72
2:B:950:ASP:OD2	2:B:982:GLY:HA3	1.89	0.72
3:C:33:TYR:HD2	3:C:74:LEU:HD21	1.54	0.71
2:B:501:PRO:O	2:B:541:ARG:NH2	2.24	0.70
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.73	0.70
2:B:952:LEU:HD12	2:B:952:LEU:H	1.58	0.69
2:B:1034:ARG:O	2:B:1034:ARG:NH1	2.26	0.69
1:A:672:TYR:HB3	1:A:681:PHE:HE2	1.58	0.68
2:B:987:ASP:OD2	2:B:1046:ARG:NH2	2.21	0.68
2:B:987:ASP:CG	2:B:1046:ARG:NH2	2.47	0.67
2:B:948:ARG:HG3	2:B:971:LEU:HD11	1.77	0.67
3:C:3:LEU:HG	3:C:127:ILE:HD11	1.77	0.67
1:A:237:ASP:OD1	6:A:901:HOH:O	2.13	0.66
2:B:1064:ASN:O	2:B:1067:GLN:HG2	1.95	0.66
1:A:548:ARG:NH2	1:A:764:ALA:O	2.28	0.66
2:B:952:LEU:HD12	2:B:952:LEU:N	2.11	0.66
2:B:952:LEU:H	2:B:952:LEU:CD1	2.09	0.65
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.79	0.65
2:B:956:GLY:HA2	2:B:967:GLN:HB2	1.78	0.65
3:C:103:VAL:HG23	3:C:104:PRO:HD3	1.79	0.65
3:C:6:MET:SD	3:C:38:LYS:NZ	2.69	0.65
1:A:722:VAL:O	1:A:723:ASN:HB2	1.97	0.64
2:B:733:LYS:HG3	2:B:1051:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:THR:OG1	2:B:915:GLY:N	2.30	0.64
2:B:952:LEU:HB2	2:B:1034:ARG:HE	1.61	0.63
3:C:74:LEU:HD12	3:C:75:CYS:H	1.64	0.63
2:B:948:ARG:HG2	2:B:984:PHE:CE1	2.34	0.63
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.52	0.63
3:C:50:THR:O	3:C:51:ARG:NH1	2.33	0.61
2:B:1023:ASP:OD1	2:B:1024:LEU:N	2.34	0.61
1:A:410:THR:HB	1:A:414:ILE:HB	1.81	0.61
2:B:411:LEU:HD12	2:B:413:PRO:HG3	1.82	0.61
2:B:382:ASN:HD22	2:B:383:PRO:HD2	1.66	0.61
1:A:755:HIS:HA	1:A:758:LYS:HE3	1.83	0.60
2:B:1054:VAL:HG12	2:B:1054:VAL:O	2.01	0.60
2:B:478:HIS:CD2	2:B:479:ARG:HH11	2.20	0.59
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.84	0.59
1:A:169:PHE:HB2	1:A:173:VAL:HG12	1.85	0.59
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.83	0.59
2:B:352:ASN:HD21	2:B:889:GLY:HA3	1.68	0.59
1:A:678:TYR:HB3	1:A:681:PHE:HB2	1.85	0.59
2:B:442:VAL:HG21	2:B:450:TRP:HE3	1.68	0.58
2:B:497:MET:HB3	2:B:816:ARG:HD3	1.84	0.58
2:B:978:LEU:HA	2:B:984:PHE:HE2	1.68	0.58
1:A:14:ARG:NH2	6:A:907:HOH:O	2.36	0.58
3:C:66:GLU:OE1	3:C:92:HIS:NE2	2.36	0.58
2:B:1062:LYS:O	2:B:1062:LYS:HG3	2.03	0.57
2:B:1073:ARG:NH1	6:B:1205:HOH:O	2.37	0.57
3:C:76:GLU:HB2	3:C:79:PHE:CE1	2.40	0.57
3:C:61:PHE:HD2	3:C:72:LEU:HD11	1.70	0.57
3:C:39:GLN:HB3	3:C:157:LEU:HD11	1.87	0.56
3:C:95:PHE:HE1	3:C:99:HIS:HB2	1.70	0.56
3:C:126:TYR:O	3:C:128:ASP:N	2.38	0.56
2:B:949:VAL:CA	2:B:952:LEU:HD11	2.34	0.56
2:B:410:LEU:HD12	2:B:935:LEU:HD22	1.87	0.56
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.71	0.56
3:C:3:LEU:CG	3:C:127:ILE:HD11	2.36	0.56
2:B:1064:ASN:HB2	2:B:1067:GLN:NE2	2.21	0.56
3:C:31:GLN:OE1	3:C:31:GLN:N	2.37	0.56
2:B:847:LEU:HD23	2:B:850:MET:HE3	1.86	0.56
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.88	0.55
2:B:436:THR:HG21	2:B:454:LEU:HD13	1.88	0.55
2:B:953:SER:HB2	2:B:955:GLU:OE1	2.06	0.55
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.89	0.54
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.42	0.54
2:B:451:LYS:HZ3	2:B:457:ARG:N	2.06	0.54
1:A:193:LYS:NZ	2:B:572:ASP:OD2	2.30	0.54
1:A:626:TYR:N	1:A:647:ILE:O	2.40	0.54
2:B:1059:SER:O	2:B:1059:SER:OG	2.25	0.54
1:A:183:ILE:HG13	2:B:567:MET:HB2	1.89	0.53
2:B:994:LEU:HB3	2:B:1054:VAL:HG13	1.90	0.53
1:A:528:ARG:HA	1:A:608:MET:HE1	1.90	0.53
2:B:960:ILE:O	2:B:961:SER:OG	2.24	0.53
2:B:966:PRO:HD2	2:B:1038:PHE:HB2	1.89	0.53
2:B:1058:GLU:HA	2:B:1058:GLU:OE1	2.07	0.53
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.90	0.53
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.24	0.52
1:A:696:LEU:HD12	1:A:703:PRO:HD2	1.90	0.52
1:A:641:SER:OG	1:A:646:ARG:NH2	2.43	0.52
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.92	0.52
2:B:960:ILE:O	2:B:960:ILE:CG2	2.54	0.52
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.92	0.52
1:A:527:ALA:O	1:A:531:ILE:HG12	2.11	0.51
1:A:143:ASP:OD1	1:A:376:SER:OG	2.27	0.51
1:A:98:TYR:OH	1:A:109:GLU:OE2	2.13	0.51
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.93	0.51
2:B:750:ARG:NH2	2:B:773:LEU:HD13	2.26	0.51
2:B:950:ASP:HB3	2:B:983:ALA:H	1.75	0.50
3:C:79:PHE:N	3:C:79:PHE:CD1	2.78	0.50
3:C:126:TYR:C	3:C:128:ASP:N	2.64	0.50
3:C:126:TYR:C	3:C:128:ASP:H	2.14	0.50
1:A:47:GLU:HG3	1:A:453:PRO:HB3	1.93	0.50
3:C:1:MET:HG2	3:C:79:PHE:CE1	2.47	0.50
1:A:412:ARG:H	1:A:412:ARG:HD3	1.77	0.50
2:B:661:ALA:HB3	2:B:861:SER:HB3	1.94	0.49
2:B:1019:GLN:O	2:B:1055:ILE:CB	2.60	0.49
1:A:663:THR:HG23	1:A:664:ILE:HD13	1.94	0.49
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.93	0.49
2:B:913:GLN:HG3	2:B:916:THR:HG21	1.93	0.49
3:C:75:CYS:HB2	3:C:79:PHE:CE2	2.46	0.49
3:C:121:LYS:N	6:C:202:HOH:O	2.30	0.49
1:A:506:ALA:HA	1:A:509:GLN:HG3	1.94	0.49
2:B:480:ARG:NH1	2:B:482:GLU:OE2	2.46	0.49
1:A:284:ALA:HB3	1:A:343:HIS:ND1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.77	0.49
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.94	0.49
2:B:876:SER:HA	2:B:1091:VAL:HG13	1.95	0.49
2:B:975:VAL:HG23	2:B:978:LEU:HD12	1.95	0.49
2:B:1034:ARG:NH2	2:B:1035:ILE:HA	2.28	0.49
1:A:655:GLN:HB2	1:A:706:ILE:HD11	1.95	0.48
3:C:60:THR:N	3:C:75:CYS:O	2.46	0.48
2:B:952:LEU:CB	2:B:1034:ARG:HE	2.26	0.48
2:B:965:ILE:HD13	2:B:1041:TRP:CD1	2.48	0.48
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.94	0.48
2:B:972:GLN:HB3	2:B:1071:GLU:OE1	2.13	0.48
1:A:4:TYR:O	1:A:8:ILE:HG12	2.14	0.48
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.95	0.48
1:A:48:ARG:HA	1:A:49:PRO:HD3	1.68	0.48
3:C:154:GLU:O	6:C:201:HOH:O	2.20	0.48
2:B:451:LYS:HE2	2:B:456:TYR:HA	1.93	0.48
1:A:194:ASP:HB2	1:A:298:PRO:HG2	1.96	0.48
2:B:994:LEU:HB3	2:B:1054:VAL:HG22	1.95	0.48
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.28	0.48
1:A:256:GLN:N	3:C:1:MET:SD	2.87	0.48
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.96	0.48
3:C:9:ARG:NH2	3:C:106:VAL:O	2.46	0.48
2:B:1043:ARG:NH2	2:B:1052:LEU:HD22	2.29	0.47
1:A:173:VAL:HG21	1:A:270:ILE:HD12	1.94	0.47
2:B:422:VAL:HG11	2:B:817:ARG:HH12	1.80	0.47
2:B:442:VAL:HG21	2:B:450:TRP:CE3	2.49	0.47
2:B:948:ARG:HG2	2:B:984:PHE:CZ	2.49	0.47
2:B:994:LEU:HD11	2:B:1035:ILE:HD11	1.96	0.47
2:B:1005:LEU:HA	2:B:1009:LEU:HD12	1.96	0.47
2:B:993:MET:HE3	2:B:1064:ASN:OD1	2.15	0.47
3:C:54:LEU:HB3	3:C:61:PHE:HB2	1.97	0.47
2:B:950:ASP:OD2	2:B:982:GLY:CA	2.62	0.47
2:B:993:MET:CE	2:B:1064:ASN:OD1	2.63	0.47
1:A:103:GLU:H	1:A:103:GLU:HG3	1.52	0.46
1:A:368:GLY:HA3	1:A:450:GLY:O	2.15	0.46
2:B:353:LEU:HD22	2:B:359:MET:HE2	1.96	0.46
1:A:310:ILE:HD12	1:A:310:ILE:H	1.79	0.46
1:A:660:HIS:HB3	1:A:664:ILE:HG22	1.97	0.46
2:B:505:VAL:HG22	2:B:543:LYS:HB2	1.97	0.46
1:A:694:GLU:HG2	1:A:695:ILE:HG13	1.97	0.46
3:C:33:TYR:CD2	3:C:74:LEU:HD21	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:GLN:OE1	3:C:153:ILE:HG12	2.16	0.46
2:B:446:ASP:C	2:B:448:ARG:H	2.20	0.45
2:B:448:ARG:HD2	2:B:448:ARG:O	2.17	0.45
3:C:51:ARG:NH1	3:C:65:ILE:H	2.13	0.45
3:C:153:ILE:HD11	3:C:157:LEU:HD23	1.98	0.45
2:B:1030:PRO:O	2:B:1034:ARG:HB2	2.17	0.45
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.97	0.45
2:B:810:THR:OG1	2:B:816:ARG:NH1	2.50	0.45
3:C:95:PHE:CE1	3:C:99:HIS:HB2	2.52	0.45
1:A:178:LEU:HD21	1:A:243:LEU:HD12	1.99	0.45
1:A:312:SER:O	1:A:316:ILE:HG12	2.16	0.45
2:B:372:LEU:HG	2:B:826:PRO:HG3	1.98	0.45
2:B:658:ARG:HH11	2:B:658:ARG:HB3	1.81	0.45
1:A:82:LEU:HD21	1:A:91:ARG:HB3	1.99	0.45
2:B:1005:LEU:O	2:B:1009:LEU:HB2	2.16	0.45
1:A:341:THR:HB	1:A:343:HIS:HD2	1.82	0.45
1:A:699:ARG:HD2	1:A:703:PRO:HG3	1.98	0.45
1:A:412:ARG:NE	1:A:413:GLU:OE1	2.50	0.45
1:A:159:PRO:HG2	1:A:162:ALA:HB2	1.99	0.44
2:B:952:LEU:N	2:B:952:LEU:CD1	2.73	0.44
3:C:10:VAL:HG13	3:C:44:LEU:HB3	1.99	0.44
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.97	0.44
3:C:81:LYS:HE3	3:C:148:ILE:HG21	1.99	0.44
2:B:444:PHE:CE1	2:B:450:TRP:HB3	2.52	0.44
2:B:451:LYS:HD2	2:B:451:LYS:HA	1.50	0.44
2:B:1032:SER:HA	2:B:1035:ILE:HG22	2.00	0.44
2:B:438:ILE:HG23	2:B:482:GLU:HB3	1.99	0.44
3:C:1:MET:HG2	3:C:79:PHE:CZ	2.52	0.44
1:A:59:VAL:HB	1:A:70:LEU:HB2	1.99	0.44
1:A:635:VAL:HG12	1:A:636:LEU:H	1.83	0.44
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.99	0.44
1:A:568:PHE:HB3	1:A:757:LYS:HG2	2.00	0.44
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.82	0.44
2:B:958:LEU:HG	2:B:964:THR:HA	2.00	0.44
1:A:548:ARG:HE	1:A:552:ARG:HE	1.65	0.43
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.86	0.43
3:C:79:PHE:N	3:C:79:PHE:HD1	2.16	0.43
1:A:319:ASP:O	1:A:322:LYS:NZ	2.34	0.43
1:A:59:VAL:HB	1:A:70:LEU:CB	2.48	0.43
1:A:63:ARG:HE	1:A:90:GLN:HB2	1.84	0.43
2:B:978:LEU:HA	2:B:984:PHE:CE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:ARG:HD2	3:C:12:ASP:OD1	2.19	0.43
3:C:34:GLN:HB2	3:C:38:LYS:HZ1	1.83	0.43
1:A:17:VAL:HG23	1:A:42:PHE:HD1	1.84	0.43
2:B:761:THR:HB	2:B:788:GLN:HB2	1.99	0.43
1:A:285:ARG:HA	1:A:344:VAL:HG12	2.00	0.43
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.53	0.43
2:B:395:GLN:NE2	2:B:796:THR:HA	2.34	0.43
2:B:582:GLU:OE2	2:B:583:ASN:ND2	2.52	0.43
2:B:952:LEU:HB2	2:B:1034:ARG:NE	2.32	0.43
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.19	0.43
1:A:148:LYS:HE3	1:A:244:LEU:O	2.19	0.42
2:B:948:ARG:HA	2:B:984:PHE:CD1	2.54	0.42
1:A:570:PHE:HD1	1:A:570:PHE:HA	1.73	0.42
2:B:391:THR:O	2:B:826:PRO:HD2	2.18	0.42
2:B:961:SER:OG	2:B:962:ASP:N	2.52	0.42
2:B:428:ILE:HD11	2:B:490:PHE:CD2	2.54	0.42
2:B:1011:VAL:HG21	2:B:1017:ILE:HD13	2.01	0.42
2:B:1034:ARG:HH12	2:B:1038:PHE:H	1.67	0.42
1:A:233:VAL:HG22	1:A:237:ASP:HB3	2.01	0.42
1:A:259:ARG:HG2	1:A:306:LEU:HD12	2.02	0.42
2:B:899:PHE:HB3	2:B:900:PRO:HD3	2.00	0.42
2:B:937:TYR:OH	2:B:1047:PRO:HD2	2.19	0.42
1:A:57:GLU:HA	1:A:58:PRO:HD3	1.88	0.42
2:B:556:TYR:HA	2:B:566:GLN:O	2.20	0.42
2:B:642:PRO:HG3	2:B:702:LEU:HD21	2.02	0.42
1:A:311:ARG:HG3	1:A:316:ILE:HD11	2.02	0.42
1:A:415:LYS:HB3	1:A:434:SER:HB2	2.03	0.41
2:B:956:GLY:HA3	2:B:966:PRO:HA	2.02	0.41
2:B:1057:ASP:HB2	2:B:1058:GLU:H	1.67	0.41
1:A:51:LEU:HA	1:A:52:PRO:HD3	1.91	0.41
2:B:582:GLU:HG3	3:C:124:LYS:NZ	2.35	0.41
1:A:166:LEU:HD23	1:A:243:LEU:HD13	2.03	0.41
2:B:909:GLN:HG2	2:B:910:LYS:N	2.35	0.41
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.56	0.41
2:B:847:LEU:HA	2:B:850:MET:HE2	2.03	0.41
3:C:39:GLN:HB3	3:C:157:LEU:CD1	2.50	0.41
3:C:10:VAL:HG21	3:C:65:ILE:HG23	2.03	0.41
1:A:63:ARG:NE	1:A:88:CYS:SG	2.89	0.41
1:A:153:MET:SD	1:A:387:GLN:HB3	2.61	0.40
3:C:83:LEU:HB3	3:C:126:TYR:CE2	2.56	0.40
3:C:157:LEU:HD13	3:C:157:LEU:HA	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ILE:HG21	1:A:446:TRP:HH2	1.85	0.40
1:A:624:TYR:CE1	1:A:634:PRO:HB3	2.56	0.40
2:B:1051:ILE:H	2:B:1051:ILE:HG12	1.75	0.40
3:C:83:LEU:HB3	3:C:126:TYR:HE2	1.86	0.40
2:B:492:ALA:HB1	2:B:496:TYR:HB2	2.04	0.40
2:B:1071:GLU:HG2	2:B:1080:TYR:HB2	2.03	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	698/764 (91%)	669 (96%)	27 (4%)	2 (0%)	41 66
2	B	721/748 (96%)	675 (94%)	44 (6%)	2 (0%)	41 66
3	C	129/157 (82%)	116 (90%)	11 (8%)	2 (2%)	9 24
4	D	1/3 (33%)	1 (100%)	0	0	100 100
All	All	1549/1672 (93%)	1461 (94%)	82 (5%)	6 (0%)	34 60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	960	ILE
2	B	951	ASN
3	C	127	ILE
1	A	52	PRO
3	C	78	ALA
1	A	642	ILE

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	618/666 (93%)	589 (95%)	29 (5%)	26 54
2	B	657/678 (97%)	626 (95%)	31 (5%)	26 54
3	C	117/138 (85%)	106 (91%)	11 (9%)	8 20
4	D	3/3 (100%)	3 (100%)	0	100 100
All	All	1395/1485 (94%)	1324 (95%)	71 (5%)	24 50

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	65	THR
1	A	82	LEU
1	A	103	GLU
1	A	109	GLU
1	A	190	ARG
1	A	196	SER
1	A	243	LEU
1	A	268	LEU
1	A	308	THR
1	A	311	ARG
1	A	324	VAL
1	A	325	LYS
1	A	326	LYS
1	A	362	CYS
1	A	412	ARG
1	A	451	LEU
1	A	570	PHE
1	A	573	THR
1	A	612	LEU
1	A	635	VAL
1	A	664	ILE
1	A	667	TRP
1	A	673	GLN

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Mol	Chain	Res	Type
1	A	677	GLU
1	A	681	PHE
1	A	694	GLU
1	A	704	ARG
1	A	722	VAL
2	B	354	LEU
2	B	386	PHE
2	B	411	LEU
2	B	423	VAL
2	B	433	SER
2	B	445	LEU
2	B	448	ARG
2	B	451	LYS
2	B	457	ARG
2	B	550	ASP
2	B	561	SER
2	B	588	LEU
2	B	627	MET
2	B	658	ARG
2	B	726	VAL
2	B	771	THR
2	B	775	SER
2	B	787	VAL
2	B	798	THR
2	B	817	ARG
2	B	856	MET
2	B	906	LEU
2	B	967	GLN
2	B	1008	VAL
2	B	1016	SER
2	B	1034	ARG
2	B	1046	ARG
2	B	1058	GLU
2	B	1061	MET
2	B	1073	ARG
2	B	1074	THR
3	C	2	VAL
3	C	5	THR
3	C	38	LYS
3	C	44	LEU
3	C	59	MET
3	C	79	PHE

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Mol	Chain	Res	Type
3	C	95	PHE
3	C	108	ARG
3	C	111	SER
3	C	122	THR
3	C	157	LEU

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

Mol	Chain	Res	Type
2	B	382	ASN
2	B	478	HIS
2	B	532	ASN
2	B	583	ASN
2	B	736	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 monosaccharides 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^{th} 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	708/764 (92%)	0.56	75 (10%) 6 4	33, 62, 182, 273	0
2	B	729/748 (97%)	0.53	78 (10%) 6 4	33, 65, 185, 277	0
3	C	135/157 (85%)	1.84	57 (42%) 0 0	75, 142, 213, 269	0
4	D	3/3 (100%)	0.34	0 100 100	82, 82, 87, 89	0
All	All	1575/1672 (94%)	0.65	210 (13%) 3 2	33, 68, 191, 277	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	684	LEU	14.5
2	B	958	LEU	10.8
1	A	685	LEU	10.8
1	A	677	GLU	10.5
1	A	717	PHE	10.3
2	B	1061	MET	10.3
2	B	1035	ILE	9.7
1	A	678	TYR	9.5
2	B	1009	LEU	9.5
1	A	675	MET	8.7
2	B	1024	LEU	8.4
3	C	128	ASP	8.3
1	A	628	PHE	8.3
1	A	659	TYR	8.0
3	C	57	GLY	7.9
1	A	688	PRO	7.4
2	B	1028	ASP	6.8
2	B	1036	ILE	6.8
1	A	49	PRO	6.6
2	B	962	ASP	6.6
1	A	50	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	6.5
1	A	709	GLU	6.4
1	A	711	GLY	6.4
3	C	23	ASP	6.3
2	B	1010	GLY	6.3
1	A	122	LEU	6.2
2	B	476	GLU	6.2
2	B	1022	THR	6.0
3	C	154	GLU	6.0
2	B	426	SER	6.0
1	A	644	ALA	5.9
3	C	55	GLU	5.8
2	B	1027	LEU	5.7
1	A	123	ARG	5.7
1	A	663	THR	5.7
2	B	949	VAL	5.6
1	A	669	LYS	5.6
1	A	643	LEU	5.6
1	A	666	GLN	5.5
3	C	83	LEU	5.5
2	B	346	GLU	5.4
3	C	99	HIS	5.4
2	B	1026	GLU	5.3
1	A	658	ILE	5.3
1	A	665	ALA	5.3
1	A	667	TRP	5.2
1	A	676	PRO	5.2
2	B	963	ARG	5.2
3	C	61	PHE	5.1
3	C	1	MET	5.1
1	A	627	SER	5.0
3	C	20	MET	5.0
2	B	1029	THR	5.0
2	B	980	ARG	4.9
2	B	1005	LEU	4.9
2	B	1014	TYR	4.9
1	A	680	ASN	4.8
1	A	689	VAL	4.8
2	B	1056	ALA	4.7
2	B	1016	SER	4.7
2	B	1015	ALA	4.7
2	B	1032	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	648	LEU	4.6
2	B	956	GLY	4.6
1	A	642	ILE	4.6
1	A	707	ASP	4.6
1	A	681	PHE	4.5
1	A	225	PRO	4.5
1	A	714	GLN	4.4
3	C	91	LEU	4.4
3	C	63	TYR	4.3
3	C	74	LEU	4.3
3	C	126	TYR	4.3
1	A	93	GLN	4.2
2	B	964	THR	4.2
2	B	1039	ILE	4.2
3	C	29	ASP	4.1
1	A	706	ILE	4.1
1	A	673	GLN	4.1
3	C	152	ASN	4.0
1	A	510	ILE	4.0
1	A	664	ILE	4.0
2	B	1012	GLN	3.9
2	B	1019	GLN	3.9
1	A	670	SER	3.8
1	A	723	ASN	3.8
1	A	716	ARG	3.8
1	A	682	ARG	3.7
2	B	965	ILE	3.7
1	A	629	SER	3.7
3	C	54	LEU	3.7
1	A	672	TYR	3.7
2	B	959	ASN	3.7
3	C	153	ILE	3.7
1	A	668	ARG	3.7
2	B	1002	GLN	3.7
1	A	244	LEU	3.6
1	A	674	ASP	3.6
2	B	1033	ALA	3.5
2	B	1025	PRO	3.5
3	C	148	ILE	3.5
3	C	78	ALA	3.5
3	C	155	GLU	3.4
1	A	507	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	447	GLN	3.4
3	C	62	HIS	3.4
3	C	127	ILE	3.4
2	B	1011	VAL	3.4
3	C	115	PHE	3.3
1	A	710	HIS	3.3
1	A	657	LEU	3.3
1	A	625	ALA	3.3
1	A	646	ARG	3.3
2	B	957	ALA	3.2
2	B	359	MET	3.2
1	A	626	TYR	3.1
3	C	130	ARG	3.1
2	B	1093	LYS	3.1
3	C	8	ALA	3.1
1	A	624	TYR	3.1
1	A	705	TYR	3.1
1	A	234	GLN	3.0
2	B	1004	PHE	3.0
2	B	1013	ASN	3.0
2	B	1054	VAL	3.0
2	B	953	SER	2.9
2	B	1057	ASP	2.9
2	B	444	PHE	2.9
3	C	106	VAL	2.9
1	A	660	HIS	2.9
2	B	1059	SER	2.9
1	A	679	GLU	2.9
2	B	428	ILE	2.8
1	A	632	PRO	2.8
2	B	1031	GLU	2.8
2	B	559	GLN	2.8
3	C	32	GLN	2.8
1	A	700	PHE	2.8
3	C	118	PHE	2.8
3	C	104	PRO	2.8
2	B	1062	LYS	2.7
3	C	64	ILE	2.7
3	C	157	LEU	2.7
1	A	91	ARG	2.7
2	B	1060	PRO	2.6
2	B	952	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	3	LEU	2.6
2	B	955	GLU	2.6
3	C	92	HIS	2.6
1	A	686	GLN	2.6
3	C	33	TYR	2.6
2	B	562	LEU	2.6
2	B	424	THR	2.6
3	C	75	CYS	2.6
2	B	948	ARG	2.6
3	C	4	LEU	2.6
3	C	98	GLN	2.5
2	B	979	SER	2.5
3	C	22	GLU	2.5
2	B	1017	ILE	2.5
2	B	996	VAL	2.5
2	B	998	LYS	2.4
1	A	183	ILE	2.4
1	A	712	GLY	2.4
3	C	156	VAL	2.4
2	B	530	LEU	2.4
3	C	19	SER	2.4
1	A	645	ASP	2.4
2	B	797	ASP	2.4
3	C	112	PHE	2.4
1	A	722	VAL	2.4
2	B	1052	LEU	2.3
1	A	631	PRO	2.3
2	B	1021	MET	2.3
2	B	348	LEU	2.3
2	B	360	LEU	2.3
1	A	656	ILE	2.3
2	B	458	VAL	2.3
3	C	53	THR	2.3
1	A	125	PRO	2.3
2	B	1020	PRO	2.3
1	A	633	GLU	2.3
2	B	960	ILE	2.2
3	C	124	LYS	2.2
3	C	41	PHE	2.2
3	C	85	PHE	2.2
3	C	129	SER	2.2
3	C	151	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1008	VAL	2.2
1	A	237	ASP	2.2
2	B	982	GLY	2.2
3	C	105	THR	2.2
3	C	82	LYS	2.1
2	B	1038	PHE	2.1
3	C	120	GLN	2.1
1	A	33	ARG	2.1
3	C	5	THR	2.1
2	B	449	ARG	2.1
1	A	322	LYS	2.1
3	C	149	MET	2.1
2	B	350	VAL	2.1
3	C	21	GLN	2.1
3	C	84	ALA	2.0
1	A	719	LEU	2.0
2	B	1034	ARG	2.0
3	C	87	TYR	2.0
2	B	448	ARG	2.0
1	A	4	TYR	2.0
3	C	102	LYS	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 monosaccharides 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^{th} 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
5	ZN	A	801	1/1	0.96	0.14	91,91,91,91	0
5	ZN	B	1101	1/1	0.97	0.15	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.