



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 PM UTC

PDB ID : 5VNE / pdb_00005vne
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

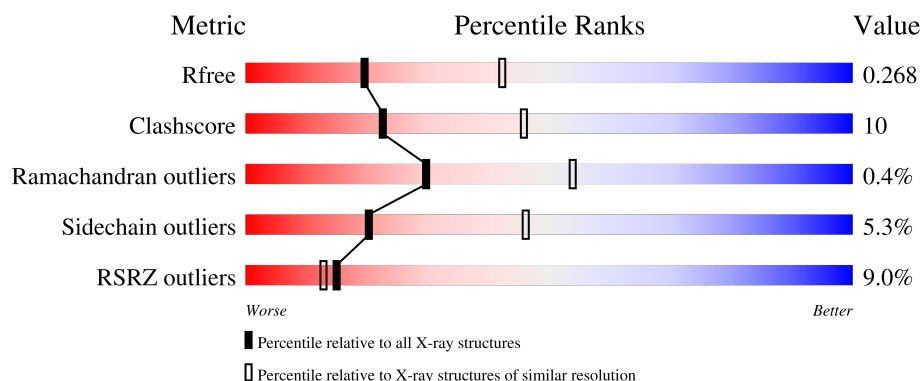
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

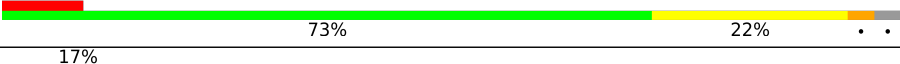
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	
2	B	748	
3	C	157	
4	D	3	

2 Entry composition

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 (CCD ID: 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 1	Zn 1	0	0

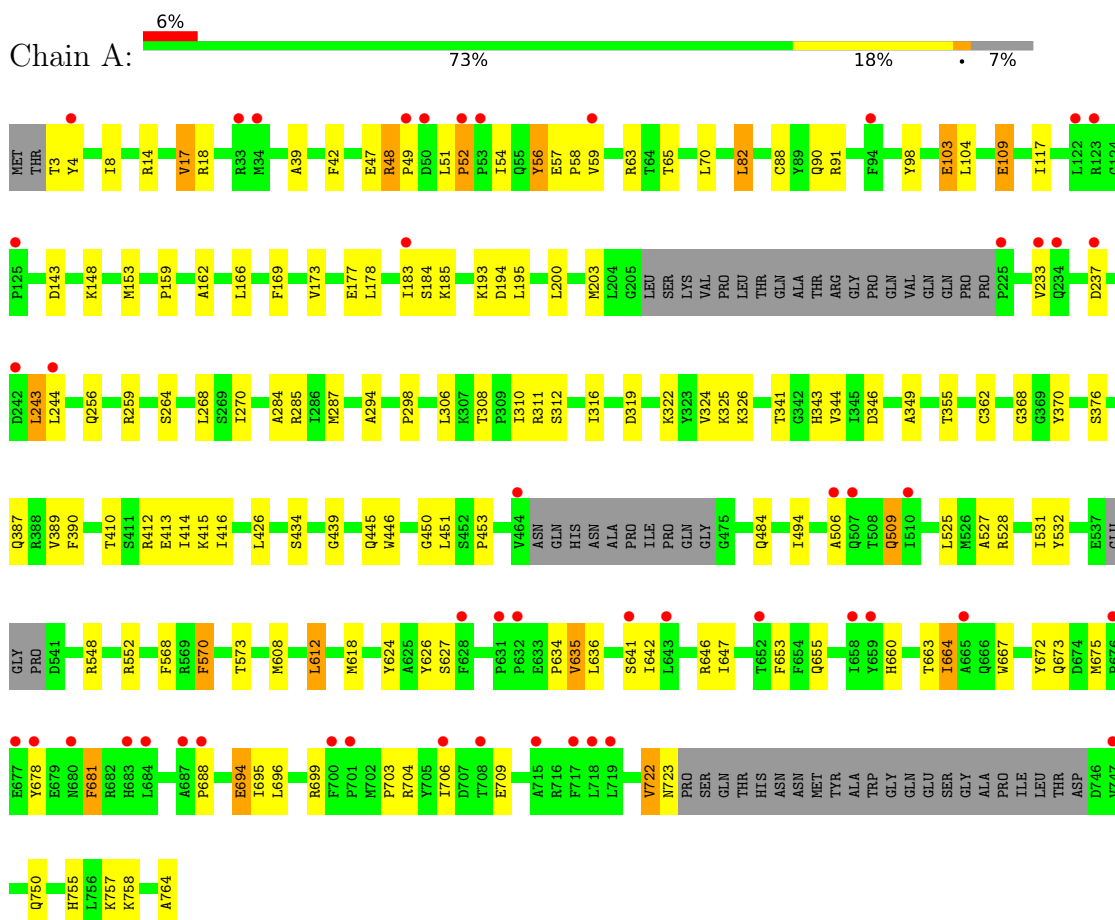
- Molecule 6 is water.

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

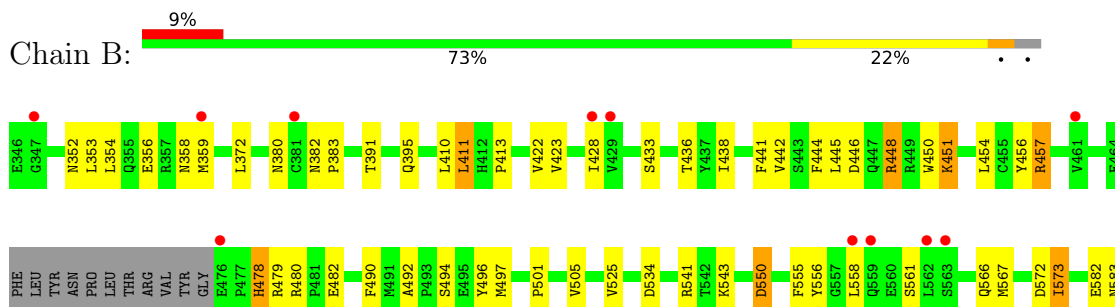
3 Residue-property plots

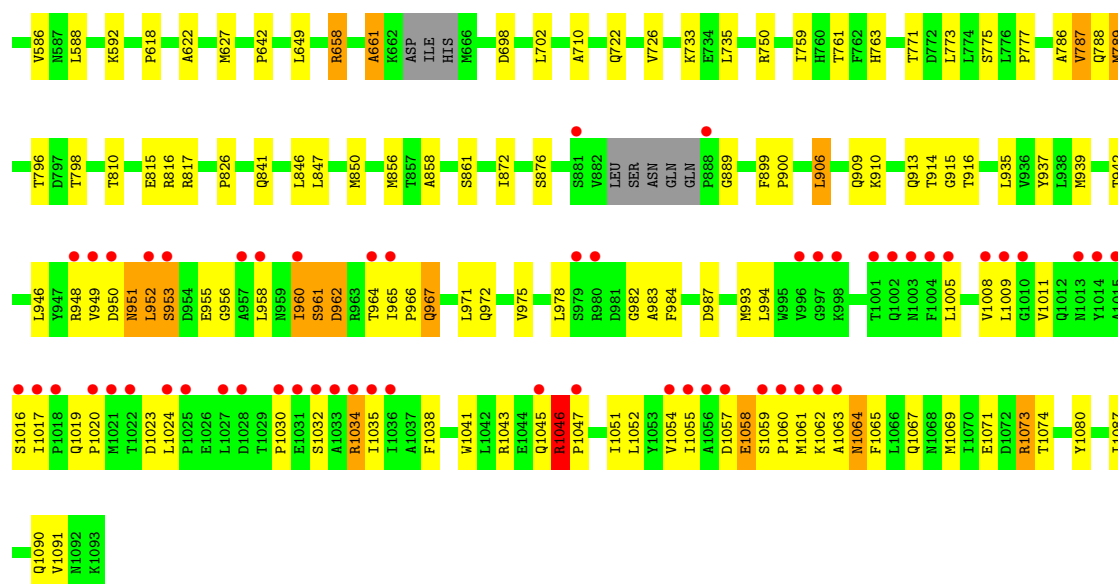
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

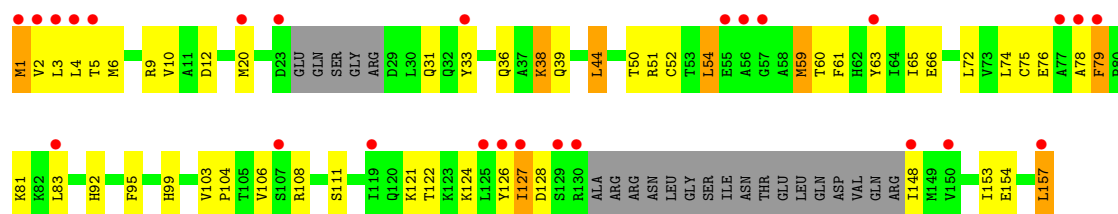


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: EMP24



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.224 , 0.266 0.227 , 0.268	Depositor DCC
R_{free} test set	2013 reflections (3.84%)	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)	0.31 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

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	0.18	1/5755 (0.0%)	0.37	3/7791 (0.0%)
2	B	0.22	0/5869	0.47	12/7977 (0.2%)
3	C	0.11	0/1096	0.35	0/1478
4	D	0.06	0/21	0.23	0/26
All	All	0.19	1/12741 (0.0%)	0.42	15/17272 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	TYR	C-O	-5.27	1.17	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	ASP	N-CA-C	9.48	124.12	108.48
2	B	961	SER	CB-CA-C	-7.67	107.73	116.63
2	B	858	ALA	N-CA-C	7.62	122.70	111.34
1	A	48	ARG	CA-C-N	7.43	127.30	119.05
1	A	48	ARG	C-N-CA	7.43	127.30	119.05
2	B	962	ASP	N-CA-C	7.12	121.74	110.70
2	B	1046	ARG	N-CA-C	7.00	119.57	108.23
2	B	952	LEU	N-CA-C	6.55	119.47	110.24
2	B	1045	GLN	N-CA-C	-6.39	104.64	112.88
2	B	1064	ASN	N-CA-C	-6.25	105.29	113.17
2	B	1065	PHE	N-CA-C	-5.93	104.89	111.36
2	B	953	SER	N-CA-C	5.63	118.86	110.14
2	B	661	ALA	N-CA-C	-5.09	99.95	110.80
2	B	550	ASP	CB-CA-C	-5.08	105.33	114.52
1	A	184	SER	N-CA-C	5.01	117.28	111.02

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	86	0
2	B	5747	0	5792	129	0
3	C	1077	0	1069	50	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	261	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 (261) 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:987:ASP:CG	2:B:1046:ARG:HH22	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:987:ASP:CG	2:B:1046:ARG:NH2	2.47	0.72
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: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
2:B:993:MET:HE3	2:B:1064:ASN:OD1	1.97	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:846:LEU:HG	2:B:850:MET:HE2	1.77	0.64
2:B:733:LYS:HG3	2:B:1051:ILE:HD11	1.80	0.64
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
1:A:528:ARG:HA	1:A:608:MET:HE1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.86	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:451:LYS:HZ3	2:B:457:ARG:N	2.03	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
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.32	0.56
2:B:847:LEU:HA	2:B:850:MET:HE3	1.87	0.56
3:C:126:TYR:C	3:C:128:ASP:N	2.64	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
1:A:98:TYR:OH	1:A:109:GLU:OE2	2.13	0.56
3:C:31:GLN:OE1	3:C:31:GLN:N	2.37	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
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
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
3:C:4:LEU:HD11	3:C:20:MET:HE2	1.90	0.54
3:C:126:TYR:C	3:C:128:ASP:H	2.14	0.54
2:B:841:GLN:HG2	2:B:939:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:966:PRO:HD2	2:B:1038:PHE:HB2	1.89	0.53
2:B:1058:GLU:OE1	2:B:1058:GLU:HA	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
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
2:B:446:ASP:C	2:B:448:ARG:H	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
3:C:36:GLN:OE1	3:C:153:ILE:HG12	2.16	0.46
2:B:353:LEU:HD22	2:B:359:MET:HE2	1.98	0.46
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
3:C:1:MET:HE2	3:C:79:PHE:CE1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:618:MET:HE2	1:A:653:PHE:CD1	2.52	0.44
3:C:81:LYS:HE3	3:C:148:ILE:HG21	1.99	0.44
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.43	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:993:MET:CE	2:B:1064:ASN:OD1	2.63	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
1:A:750:GLN:H	1:A:750:GLN:CD	2.25	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
3:C:9:ARG:HD2	3:C:12:ASP:OD1	2.19	0.43
1:A:17:VAL:HG23	1:A:42:PHE:HD1	1.84	0.43
2:B:356:GLU:C	2:B:358:ASN:H	2.26	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
2:B:946:LEU:HD22	2:B:1069:MET:HE1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:287:MET:HE1	1:A:390:PHE:HZ	1.83	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:494:SER:HA	2:B:497:MET:HE3	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:200:LEU:HA	1:A:203:MET:HE2	2.01	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
3:C:39:GLN:HB3	3:C:157:LEU:CD1	2.50	0.41
3:C:59:MET:HE2	3:C:76:GLU:HG2	2.03	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
2:B:789:MET:HB3	2:B:789:MET:HE3	1.84	0.40
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	60
2	B	721/748 (96%)	675 (94%)	44 (6%)	2 (0%)	36	60
3	C	129/157 (82%)	116 (90%)	11 (8%)	2 (2%)	7	20
4	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1549/1672 (93%)	1461 (94%)	82 (5%)	6 (0%)	30	54

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%)	590 (96%)	28 (4%)	24	52
2	B	657/678 (97%)	623 (95%)	34 (5%)	21	47
3	C	117/138 (85%)	105 (90%)	12 (10%)	7	18
4	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1395/1485 (94%)	1321 (95%)	74 (5%)	20	46

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	17	VAL
1	A	65	THR
1	A	82	LEU
1	A	103	GLU
1	A	104	LEU
1	A	109	GLU
1	A	243	LEU
1	A	268	LEU
1	A	308	THR
1	A	324	VAL
1	A	325	LYS
1	A	326	LYS
1	A	362	CYS
1	A	451	LEU
1	A	509	GLN
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
1	A	675	MET
1	A	681	PHE
1	A	694	GLU
1	A	704	ARG
1	A	722	VAL
2	B	354	LEU
2	B	411	LEU
2	B	423	VAL

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Mol	Chain	Res	Type
2	B	433	SER
2	B	445	LEU
2	B	448	ARG
2	B	451	LYS
2	B	457	ARG
2	B	478	HIS
2	B	550	ASP
2	B	561	SER
2	B	573	ILE
2	B	588	LEU
2	B	627	MET
2	B	658	ARG
2	B	722	GLN
2	B	726	VAL
2	B	771	THR
2	B	775	SER
2	B	787	VAL
2	B	789	MET
2	B	798	THR
2	B	815	GLU
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	1	MET
3	C	2	VAL
3	C	5	THR
3	C	38	LYS
3	C	44	LEU
3	C	54	LEU
3	C	59	MET
3	C	79	PHE
3	C	108	ARG
3	C	111	SER
3	C	122	THR

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Mol	Chain	Res	Type
3	C	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	387	GLN
1	A	502	ASN
1	A	555	GLN
1	A	594	ASN
1	A	614	GLN
2	B	352	ASN
2	B	382	ASN
2	B	515	ASN
2	B	532	ASN
2	B	583	ASN
2	B	683	GLN
2	B	727	GLN
2	B	736	GLN
2	B	780	ASN
2	B	832	ASN
2	B	959	ASN
2	B	1068	ASN
2	B	1090	GLN
3	C	32	GLN
3	C	67	GLN
3	C	152	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 oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	708/764 (92%)	0.42	49 (6%)	23 20	33, 62, 182, 273	0
2	B	729/748 (97%)	0.41	67 (9%)	14 12	33, 65, 185, 277	0
3	C	135/157 (85%)	1.20	26 (19%)	3 3	75, 142, 213, 269	0
4	D	3/3 (100%)	0.26	0	100 100	82, 82, 87, 89	0
All	All	1575/1672 (94%)	0.48	142 (9%)	15 13	33, 68, 191, 277	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1056	ALA	6.3
2	B	1035	ILE	5.7
2	B	562	LEU	5.7
2	B	1024	LEU	5.4
2	B	1054	VAL	5.0
2	B	957	ALA	5.0
1	A	122	LEU	4.9
2	B	1036	ILE	4.6
2	B	1030	PRO	4.4
2	B	428	ILE	4.3
3	C	127	ILE	4.2
1	A	700	PHE	4.2
2	B	949	VAL	4.2
1	A	225	PRO	4.0
2	B	965	ILE	4.0
2	B	1005	LEU	3.8
1	A	183	ILE	3.8
2	B	1017	ILE	3.8
1	A	510	ILE	3.7
2	B	1025	PRO	3.7
1	A	684	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	2	VAL	3.6
2	B	1062	LYS	3.6
1	A	52	PRO	3.5
1	A	717	PHE	3.5
2	B	1009	LEU	3.5
2	B	888	PRO	3.5
1	A	659	TYR	3.4
2	B	347	GLY	3.4
2	B	958	LEU	3.4
2	B	1047	PRO	3.3
2	B	1032	SER	3.3
1	A	701	PRO	3.3
1	A	718	LEU	3.3
2	B	1063	ALA	3.3
1	A	680	ASN	3.3
1	A	244	LEU	3.3
1	A	677	GLU	3.2
2	B	1018	PRO	3.2
2	B	881	SER	3.2
1	A	706	ILE	3.2
1	A	678	TYR	3.2
2	B	1014	TYR	3.2
2	B	1057	ASP	3.1
2	B	1016	SER	3.1
2	B	953	SER	3.0
3	C	126	TYR	3.0
2	B	1034	ARG	3.0
1	A	628	PHE	3.0
1	A	234	GLN	3.0
2	B	559	GLN	2.9
1	A	59	VAL	2.9
2	B	1027	LEU	2.9
1	A	632	PRO	2.9
3	C	148	ILE	2.9
3	C	20	MET	2.9
1	A	4	TYR	2.9
1	A	34	MET	2.8
3	C	4	LEU	2.8
3	C	129	SER	2.8
1	A	631	PRO	2.7
1	A	658	ILE	2.7
1	A	506	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	429	VAL	2.7
2	B	1055	ILE	2.7
1	A	643	LEU	2.7
2	B	1033	ALA	2.7
2	B	1015	ALA	2.6
2	B	960	ILE	2.6
2	B	1003	ASN	2.6
3	C	77	ALA	2.6
2	B	359	MET	2.6
1	A	687	ALA	2.6
1	A	688	PRO	2.6
2	B	1004	PHE	2.6
3	C	3	LEU	2.6
1	A	665	ALA	2.6
1	A	747	VAL	2.6
2	B	1060	PRO	2.5
2	B	1010	GLY	2.5
2	B	1061	MET	2.5
2	B	1022	THR	2.5
2	B	948	ARG	2.5
1	A	715	ALA	2.5
2	B	1001	THR	2.5
1	A	676	PRO	2.5
2	B	1020	PRO	2.4
3	C	1	MET	2.4
1	A	507	GLN	2.4
3	C	83	LEU	2.4
2	B	381	CYS	2.4
1	A	683	HIS	2.3
2	B	964	THR	2.3
3	C	5	THR	2.3
1	A	33	ARG	2.3
1	A	233	VAL	2.3
3	C	79	PHE	2.3
2	B	979	SER	2.3
3	C	78	ALA	2.3
1	A	708	THR	2.3
2	B	1028	ASP	2.3
2	B	461	VAL	2.3
2	B	996	VAL	2.3
3	C	56	ALA	2.2
3	C	119	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1013	ASN	2.2
3	C	23	ASP	2.2
3	C	150	VAL	2.2
1	A	652	THR	2.2
1	A	53	PRO	2.2
1	A	50	ASP	2.2
2	B	997	GLY	2.2
3	C	125	LEU	2.2
2	B	1021	MET	2.2
1	A	125	PRO	2.1
3	C	33	TYR	2.1
1	A	719	LEU	2.1
2	B	558	LEU	2.1
2	B	952	LEU	2.1
1	A	237	ASP	2.1
1	A	242	ASP	2.1
2	B	1045	GLN	2.1
2	B	1008	VAL	2.1
1	A	94	PHE	2.1
3	C	130	ARG	2.1
1	A	49	PRO	2.1
1	A	464	VAL	2.1
2	B	950	ASP	2.1
2	B	563	SER	2.1
3	C	107	SER	2.1
1	A	123	ARG	2.1
2	B	980	ARG	2.1
3	C	157	LEU	2.1
3	C	63	TYR	2.1
2	B	476	GLU	2.0
1	A	641	SER	2.0
2	B	1059	SER	2.0
2	B	998	LYS	2.0
3	C	57	GLY	2.0
2	B	1031	GLU	2.0
3	C	55	GLU	2.0
2	B	1002	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	ZN	A	801	1/1	0.98	0.06	91,91,91,91	0
5	ZN	B	1101	1/1	0.99	0.05	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.