Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 09:11 PM EST

PDB ID	:	3MZK
Title	:	Sec13/Sec16 complex, S.cerevisiae
Authors	:	Whittle, J.R.; Schwartz, T.U.
Deposited on	:	2010-05-12
Resolution	:	2.69 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:

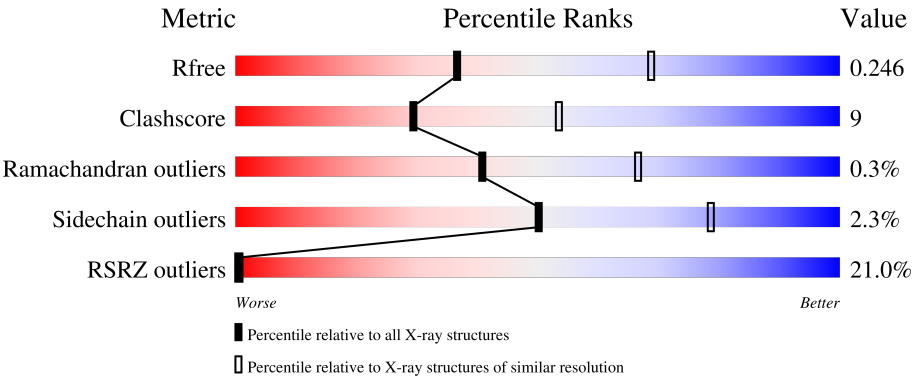
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.69 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	297	80% 19%
1	D	297	74% 77% 23%
2	B	441	74% 13% 13%
2	C	441	13% 65% 21% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10662 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 SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2329	1481	400	444	4			
1	D	297	Total	C	N	O	S	0	0	0
			2322	1477	398	443	4			

- Molecule 2 is a protein called Protein transport protein SEC16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2932	1904	472	544	12			
2	C	381	Total	C	N	O	S	0	0	0
			2904	1890	467	536	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	980	GLY	-	expression tag	UNP P48415
B	981	PRO	-	expression tag	UNP P48415
B	982	GLY	-	expression tag	UNP P48415
B	983	SER	-	expression tag	UNP P48415
C	980	GLY	-	expression tag	UNP P48415
C	981	PRO	-	expression tag	UNP P48415
C	982	GLY	-	expression tag	UNP P48415
C	983	SER	-	expression tag	UNP P48415

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	48	Total	O	0	0
			48	48		

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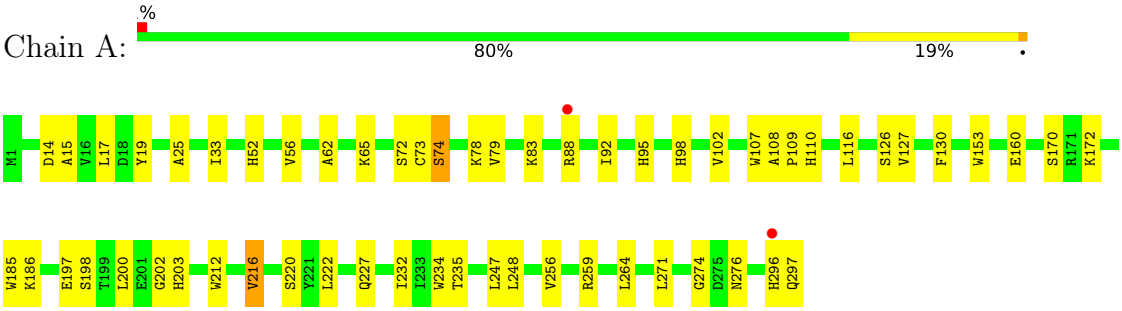
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	10	Total O 10 10	0	0
3	D	1	Total O 1 1	0	0

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.

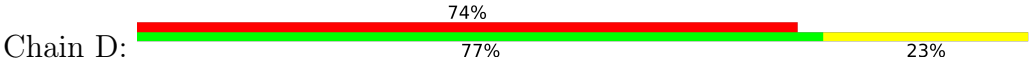
• Molecule 1: Protein transport protein SEC13

Chain A:



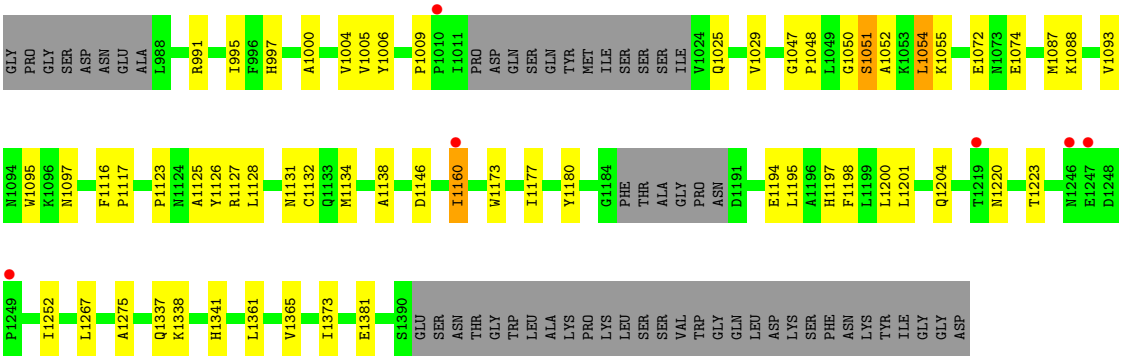
• Molecule 1: Protein transport protein SEC13

Chain D:



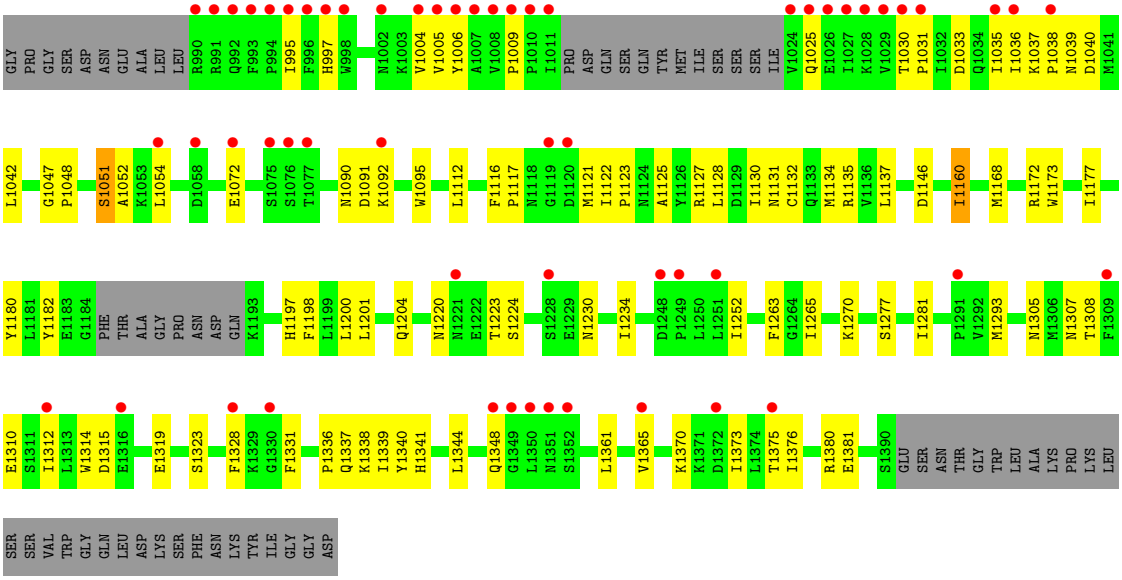
• Molecule 2: Protein transport protein SEC16

Chain B:



• Molecule 2: Protein transport protein SEC16

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.73Å 139.01Å 205.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.71 – 2.69 30.71 – 2.69	Depositor EDS
% Data completeness (in resolution range)	92.3 (30.71-2.69) 98.1 (30.71-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.198 , 0.243 0.200 , 0.246	Depositor DCC
R_{free} test set	2292 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 79.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10662	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

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	0.34	0/2392	0.53	0/3263
1	D	0.31	0/2385	0.51	0/3255
2	B	0.29	0/2999	0.42	0/4094
2	C	0.24	0/2971	0.41	0/4057
All	All	0.30	0/10747	0.47	0/14669

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	2329	0	2254	41	0
1	D	2322	0	2239	65	0
2	B	2932	0	2818	49	0
2	C	2904	0	2791	87	0
3	A	116	0	0	3	0
3	B	48	0	0	5	0
3	C	10	0	0	0	0
3	D	1	0	0	0	0
All	All	10662	0	10102	195	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 (195) 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:1128:LEU:HD22	2:B:1160:ILE:HD12	1.46	0.97
1:D:227:GLN:HA	1:D:256:VAL:HG23	1.49	0.95
2:C:1128:LEU:HD22	2:C:1160:ILE:HD12	1.47	0.94
1:A:227:GLN:HA	1:A:256:VAL:HG23	1.47	0.93
2:C:1381:GLU:HB3	1:D:216:VAL:HG22	1.55	0.89
2:C:1310:GLU:HB2	1:D:285:LEU:HD21	1.56	0.86
2:C:1033:ASP:HA	2:C:1036:ILE:O	1.76	0.85
2:C:1337:GLN:HA	1:D:217:LEU:HD21	1.62	0.81
1:D:83:LYS:HB2	1:D:92:ILE:HD13	1.64	0.79
2:C:1039:ASN:HD21	2:C:1042:LEU:HG	1.47	0.78
1:A:83:LYS:HB2	1:A:92:ILE:HD13	1.65	0.78
1:A:52:HIS:CD2	1:A:74:SER:HB3	2.19	0.77
2:C:1035:ILE:HG22	2:C:1036:ILE:HG13	1.67	0.77
2:B:1127:ARG:HB2	2:C:1125:ALA:HB2	1.65	0.77
2:C:1339:ILE:CG2	1:D:216:VAL:HG11	2.15	0.77
2:B:1125:ALA:HB2	2:C:1127:ARG:HB2	1.67	0.76
2:C:1380:ARG:CZ	1:D:156:ALA:O	2.36	0.74
1:D:52:HIS:CD2	1:D:74:SER:HB3	2.23	0.73
1:D:92:ILE:HD12	1:D:130:PHE:CZ	2.24	0.73
1:A:92:ILE:HD12	1:A:130:PHE:CZ	2.23	0.72
2:C:1339:ILE:HB	1:D:216:VAL:HG11	1.70	0.72
2:B:1128:LEU:HD22	2:B:1160:ILE:CD1	2.19	0.71
2:C:1128:LEU:HD22	2:C:1160:ILE:CD1	2.20	0.71
1:D:232:ILE:HD13	1:D:247:LEU:HD23	1.75	0.69
2:B:1132:CYS:SG	2:C:1116:PHE:HZ	2.16	0.69
2:B:1132:CYS:HG	2:C:1116:PHE:HZ	1.42	0.67
1:D:170:SER:HB2	1:D:186:LYS:HE3	1.77	0.66
1:A:232:ILE:HD13	1:A:247:LEU:HD23	1.79	0.65
2:C:1339:ILE:CB	1:D:216:VAL:HG11	2.27	0.65
2:B:1116:PHE:CD1	2:C:1135:ARG:HD2	2.32	0.64
2:C:1373:ILE:HD11	1:D:160:GLU:HB2	1.80	0.63
1:D:33:ILE:HD11	1:D:56:VAL:HG11	1.81	0.62
1:A:79:VAL:HB	1:A:95:HIS:HB3	1.82	0.62
1:D:212:TRP:CD2	1:D:222:LEU:HD21	2.34	0.62
1:D:98:HIS:HE1	1:D:126:SER:OG	1.82	0.62
1:A:33:ILE:CD1	1:A:56:VAL:HG11	2.30	0.62
1:A:212:TRP:CD2	1:A:222:LEU:HD21	2.34	0.62
2:C:1323:SER:HA	2:C:1328:PHE:CD2	2.36	0.61
1:D:79:VAL:HB	1:D:95:HIS:HB3	1.83	0.61
1:A:98:HIS:HE1	1:A:126:SER:OG	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1123:PRO:HB2	2:C:1123:PRO:HB2	1.83	0.60
1:D:33:ILE:CD1	1:D:56:VAL:HG11	2.32	0.60
2:C:1314:TRP:CH2	1:D:285:LEU:HD11	2.36	0.59
1:A:78:LYS:HD2	3:A:358:HOH:O	2.01	0.59
2:C:1319:GLU:HA	2:C:1331:PHE:HE2	1.68	0.58
2:B:1116:PHE:CD1	2:B:1117:PRO:HD2	2.39	0.58
2:C:1337:GLN:HA	1:D:217:LEU:CD2	2.34	0.57
1:A:170:SER:HB2	1:A:186:LYS:HE3	1.86	0.57
2:C:1339:ILE:HB	1:D:216:VAL:CG1	2.35	0.57
2:B:1054:LEU:HD22	2:B:1055:LYS:N	2.20	0.56
2:C:1052:ALA:C	2:C:1054:LEU:H	2.08	0.56
1:A:259:ARG:HD3	3:A:376:HOH:O	2.04	0.56
2:B:1267:LEU:HD13	2:B:1275:ALA:HB1	1.88	0.56
2:C:1381:GLU:HB3	1:D:216:VAL:CG2	2.31	0.55
2:B:1200:LEU:O	2:B:1204:GLN:HG2	2.06	0.55
2:C:1030:THR:OG1	2:C:1031:PRO:HD2	2.07	0.55
2:C:1370:LYS:HA	2:C:1375:THR:HG21	1.89	0.55
1:A:33:ILE:HD11	1:A:56:VAL:HG11	1.90	0.54
1:A:108:ALA:HB2	1:A:153:TRP:CE2	2.43	0.54
2:C:1005:VAL:CG2	1:D:17:LEU:HG	2.37	0.54
2:C:1336:PRO:HG2	1:D:218:LEU:HG	1.90	0.54
2:C:1339:ILE:HG22	1:D:216:VAL:HG11	1.87	0.54
2:C:1344:LEU:HD21	1:D:267:ASN:ND2	2.22	0.54
2:B:1088:LYS:HE2	3:B:226:HOH:O	2.07	0.54
1:D:108:ALA:HB2	1:D:153:TRP:CE2	2.44	0.53
2:B:1052:ALA:C	2:B:1054:LEU:H	2.11	0.53
2:C:1200:LEU:O	2:C:1204:GLN:HG2	2.07	0.53
2:C:1308:THR:HG21	1:D:284:ASN:C	2.29	0.53
2:B:1050:GLY:HA2	3:B:264:HOH:O	2.10	0.52
2:C:1090:ASN:O	2:C:1091:ASP:HB2	2.09	0.52
2:C:1197:HIS:HE2	2:C:1223:THR:HG22	1.74	0.52
2:C:1323:SER:HA	2:C:1328:PHE:HD2	1.74	0.52
1:A:17:LEU:HG	2:B:1005:VAL:CG2	2.38	0.52
2:B:1009:PRO:HA	2:B:1025:GLN:HE22	1.74	0.52
2:C:1305:ASN:ND2	1:D:283:GLU:HB3	2.25	0.52
1:A:172:LYS:HA	1:A:185:TRP:O	2.10	0.52
2:C:997:HIS:HE1	1:D:14:ASP:OD1	1.93	0.52
1:D:83:LYS:HB2	1:D:92:ILE:CD1	2.39	0.52
2:C:1265:ILE:HD11	2:C:1293:MET:HB3	1.91	0.51
2:C:1009:PRO:HA	2:C:1025:GLN:HE22	1.76	0.51
2:B:1138:ALA:HB3	2:C:1112:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1194:GLU:HA	2:B:1197:HIS:HD1	1.76	0.50
2:C:1039:ASN:O	2:C:1039:ASN:OD1	2.30	0.50
2:C:1095:TRP:CH2	2:C:1252:ILE:HG12	2.48	0.49
1:D:52:HIS:CD2	1:D:74:SER:CB	2.94	0.49
2:C:1307:ASN:CB	1:D:283:GLU:OE1	2.60	0.49
2:C:1376:ILE:HG21	1:D:158:ILE:HG13	1.93	0.49
1:D:172:LYS:HA	1:D:185:TRP:O	2.12	0.49
2:C:1224:SER:HB2	2:C:1270:LYS:NZ	2.27	0.48
1:A:19:TYR:HA	3:B:102:HOH:O	2.12	0.48
1:A:220:SER:O	1:A:235:THR:HA	2.13	0.48
1:A:52:HIS:CD2	1:A:74:SER:CB	2.93	0.48
2:C:1224:SER:CB	2:C:1270:LYS:HZ1	2.26	0.48
2:B:1160:ILE:HG12	2:C:1180:TYR:OH	2.14	0.48
2:C:1376:ILE:CG2	1:D:158:ILE:HG13	2.43	0.48
2:C:1380:ARG:NH1	1:D:156:ALA:O	2.47	0.48
1:A:116:LEU:O	1:A:127:VAL:HA	2.13	0.48
1:A:108:ALA:HB1	1:A:109:PRO:HD2	1.97	0.47
2:C:1182:TYR:HE2	2:C:1200:LEU:HD22	1.79	0.47
1:A:65:LYS:HE2	1:A:110:HIS:ND1	2.29	0.47
2:B:991:ARG:NE	3:B:291:HOH:O	2.47	0.47
2:C:1048:PRO:O	2:C:1051:SER:HB3	2.14	0.47
1:A:92:ILE:HD12	1:A:130:PHE:CE2	2.49	0.47
2:B:1126:TYR:HE1	2:C:1121:MET:O	1.98	0.47
2:C:1220:ASN:CG	2:C:1223:THR:HG23	2.35	0.47
1:D:220:SER:O	1:D:235:THR:HA	2.15	0.47
1:D:81:ILE:HB	1:D:93:ALA:HB3	1.97	0.46
1:D:108:ALA:HB2	1:D:153:TRP:CZ2	2.50	0.46
1:A:88:ARG:HG2	3:A:396:HOH:O	2.16	0.46
1:A:227:GLN:HG2	1:A:256:VAL:HG21	1.97	0.46
2:B:1048:PRO:O	2:B:1051:SER:HB3	2.15	0.46
2:B:1220:ASN:CG	2:B:1223:THR:HG23	2.36	0.46
1:D:116:LEU:O	1:D:127:VAL:HA	2.15	0.46
2:B:1195:LEU:HD23	2:C:1137:LEU:HD23	1.97	0.46
2:B:1127:ARG:CB	2:C:1125:ALA:HB2	2.41	0.45
2:B:1132:CYS:SG	2:C:1116:PHE:CZ	2.97	0.45
2:C:1038:PRO:HB3	2:C:1348:GLN:NE2	2.31	0.45
2:C:1338:LYS:O	2:C:1341:HIS:HB3	2.16	0.45
2:C:1314:TRP:HH2	1:D:285:LEU:HD11	1.81	0.45
1:A:108:ALA:HB2	1:A:153:TRP:CZ2	2.51	0.45
2:B:1128:LEU:HG	2:B:1132:CYS:CB	2.47	0.45
2:B:1338:LYS:O	2:B:1341:HIS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1361:LEU:O	2:C:1365:VAL:HG23	2.17	0.45
2:C:995:ILE:O	2:C:1006:TYR:HA	2.16	0.45
2:B:1087:MET:HE2	2:B:1093:VAL:HG23	1.99	0.45
2:B:1131:ASN:HA	2:B:1134:MET:HE2	1.97	0.45
1:D:62:ALA:HB2	1:D:107:TRP:CE2	2.51	0.45
2:B:1095:TRP:CH2	2:B:1252:ILE:HG12	2.52	0.45
2:C:1319:GLU:HA	2:C:1331:PHE:CE2	2.51	0.45
2:C:1128:LEU:HG	2:C:1132:CYS:CB	2.46	0.45
1:A:108:ALA:HA	1:A:153:TRP:CD1	2.52	0.44
1:D:108:ALA:HA	1:D:153:TRP:CD1	2.52	0.44
2:C:1131:ASN:HA	2:C:1134:MET:HE2	1.99	0.44
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.98	0.44
2:B:1051:SER:O	2:B:1054:LEU:HB2	2.18	0.44
2:B:1125:ALA:HB2	2:C:1127:ARG:CB	2.43	0.44
1:D:92:ILE:HD12	1:D:130:PHE:CE2	2.51	0.44
1:A:203:HIS:CE1	1:A:232:ILE:HG12	2.53	0.44
1:D:65:LYS:HE3	1:D:110:HIS:HB2	1.99	0.44
1:D:274:GLY:C	1:D:276:ASN:H	2.20	0.44
1:D:227:GLN:HG2	1:D:256:VAL:HG21	1.99	0.44
1:D:108:ALA:HB1	1:D:109:PRO:HD2	2.00	0.44
1:A:200:LEU:HB3	1:A:234:TRP:CZ3	2.52	0.44
2:B:995:ILE:O	2:B:1006:TYR:HA	2.18	0.43
2:C:1168:MET:CE	2:C:1172:ARG:HD2	2.48	0.43
2:B:1005:VAL:HG22	2:B:1029:VAL:HG22	2.00	0.43
1:D:200:LEU:HB3	1:D:234:TRP:CZ3	2.52	0.43
2:C:1312:ILE:HD11	2:C:1340:TYR:CE2	2.53	0.43
2:C:1090:ASN:HB3	2:C:1092:LYS:HD3	2.00	0.43
2:C:1277:SER:O	2:C:1281:ILE:HG13	2.18	0.43
2:C:1116:PHE:HA	2:C:1117:PRO:HD3	1.90	0.43
2:C:1130:ILE:HD12	2:C:1130:ILE:HA	1.92	0.43
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.53	0.43
2:B:1361:LEU:O	2:B:1365:VAL:HG23	2.19	0.43
1:D:213:SER:HA	1:D:214:PRO:HD3	1.87	0.43
1:A:274:GLY:C	1:A:276:ASN:H	2.23	0.43
2:C:1009:PRO:CA	2:C:1025:GLN:HE22	2.31	0.43
2:B:1009:PRO:CA	2:B:1025:GLN:HE22	2.31	0.42
2:B:1087:MET:HE1	2:B:1097:ASN:HB2	2.01	0.42
1:D:154:ALA:HB2	1:D:212:TRP:CE3	2.54	0.42
2:C:1230:ASN:O	2:C:1234:ILE:HG13	2.20	0.42
2:C:1380:ARG:NH2	1:D:157:THR:HG22	2.35	0.42
1:D:15:ALA:HA	1:D:25:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:HIS:CE1	1:D:232:ILE:HG12	2.54	0.42
2:C:1308:THR:HG21	1:D:285:LEU:HA	2.02	0.42
1:D:296:HIS:O	1:D:297:GLN:C	2.57	0.42
1:A:15:ALA:HA	1:A:25:ALA:O	2.19	0.42
1:A:14:ASP:OD1	2:B:997:HIS:HE1	2.02	0.42
2:B:1173:TRP:NE1	2:B:1177:ILE:HD11	2.35	0.42
2:C:1305:ASN:ND2	1:D:283:GLU:CB	2.83	0.41
1:D:212:TRP:HA	1:D:222:LEU:HD23	2.01	0.41
1:D:229:ARG:HD2	1:D:253:PHE:O	2.20	0.41
2:C:1052:ALA:C	2:C:1054:LEU:N	2.72	0.41
1:D:282:LYS:HG2	1:D:292:ALA:HB2	2.02	0.41
1:A:52:HIS:HE1	1:A:72:SER:OG	2.02	0.41
1:A:160:GLU:N	2:B:1373:ILE:HD11	2.35	0.41
2:C:1037:LYS:HA	2:C:1038:PRO:HD3	1.78	0.41
2:C:1315:ASP:CB	2:C:1337:GLN:HE22	2.34	0.41
1:A:264:LEU:HD11	2:B:1000:ALA:HA	2.03	0.41
2:B:1180:TYR:OH	2:C:1160:ILE:HG12	2.21	0.41
1:A:216:VAL:HG22	2:B:1381:GLU:HB3	2.03	0.41
1:A:296:HIS:O	1:A:297:GLN:C	2.58	0.41
2:B:1337:GLN:NE2	3:B:34:HOH:O	2.53	0.41
2:C:1168:MET:HE2	2:C:1172:ARG:HD2	2.03	0.41
2:C:1197:HIS:NE2	2:C:1223:THR:HG22	2.35	0.41
2:C:1319:GLU:HG3	2:C:1331:PHE:CD2	2.55	0.41
2:C:1336:PRO:HB3	1:D:217:LEU:HA	2.02	0.41
1:A:73:CYS:HB2	1:A:102:VAL:HG12	2.02	0.41
2:B:1197:HIS:NE2	2:B:1223:THR:HG22	2.36	0.41
1:D:52:HIS:HE1	1:D:72:SER:OG	2.04	0.41
1:D:29:SER:HA	1:D:55:PRO:HB3	2.02	0.40
2:B:1173:TRP:O	2:B:1177:ILE:HG13	2.21	0.40
1:A:248:LEU:HD22	1:A:271:LEU:HD11	2.04	0.40
2:B:1087:MET:HE2	2:B:1087:MET:HB3	1.97	0.40
2:C:1173:TRP:NE1	2:C:1177:ILE:HD11	2.36	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	295/297 (99%)	278 (94%)	16 (5%)	1 (0%)	41	66
1	D	295/297 (99%)	284 (96%)	10 (3%)	1 (0%)	41	66
2	B	379/441 (86%)	360 (95%)	18 (5%)	1 (0%)	41	66
2	C	375/441 (85%)	347 (92%)	27 (7%)	1 (0%)	41	66
All	All	1344/1476 (91%)	1269 (94%)	71 (5%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1047	GLY
2	C	1047	GLY
1	D	202	GLY
1	A	202	GLY

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	250/252 (99%)	246 (98%)	4 (2%)	62	85
1	D	248/252 (98%)	246 (99%)	2 (1%)	81	93
2	B	306/395 (78%)	297 (97%)	9 (3%)	42	71
2	C	302/395 (76%)	292 (97%)	10 (3%)	38	67
All	All	1106/1294 (86%)	1081 (98%)	25 (2%)	50	78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	197	GLU

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Mol	Chain	Res	Type
1	A	198	SER
1	A	216	VAL
2	B	1004	VAL
2	B	1051	SER
2	B	1054	LEU
2	B	1072	GLU
2	B	1074	GLU
2	B	1146	ASP
2	B	1160	ILE
2	B	1198	PHE
2	B	1201	LEU
2	C	1004	VAL
2	C	1040	ASP
2	C	1051	SER
2	C	1072	GLU
2	C	1122	ILE
2	C	1146	ASP
2	C	1160	ILE
2	C	1198	PHE
2	C	1201	LEU
2	C	1263	PHE
1	D	197	GLU
1	D	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	98	HIS
2	B	997	HIS
2	B	1341	HIS
2	C	997	HIS
2	C	1039	ASN
2	C	1305	ASN
2	C	1337	GLN
2	C	1341	HIS
2	C	1348	GLN
1	D	52	HIS
1	D	98	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	297/297 (100%)	-0.40	2 (0%) 87 89	20, 39, 90, 133	0
1	D	297/297 (100%)	4.22	220 (74%) 0 0	122, 243, 326, 392	0
2	B	385/441 (87%)	-0.23	6 (1%) 72 74	33, 72, 123, 174	0
2	C	381/441 (86%)	0.63	57 (14%) 2 1	49, 99, 228, 287	0
All	All	1360/1476 (92%)	0.94	285 (20%) 1 0	20, 84, 276, 392	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	THR	19.6
1	D	67	GLY	15.4
1	D	189	SER	15.1
1	D	272	SER	14.0
1	D	253	PHE	13.4
1	D	114	PRO	13.2
1	D	197	GLU	12.9
1	D	87	GLY	12.8
1	D	56	VAL	12.3
1	D	181	LEU	12.2
2	C	1010	PRO	11.4
1	D	120	SER	11.4
1	D	167	THR	11.4
1	D	3	VAL	11.0
1	D	259	ARG	10.8
1	D	49	LEU	10.8
1	D	187	TYR	10.5
1	D	258	TRP	10.2
1	D	65	LYS	10.2
2	C	1009	PRO	10.1
1	D	9	ASN	9.9

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Mol	Chain	Res	Type	RSRZ
1	D	6	ASN	9.7
1	D	225	VAL	9.6
1	D	7	ALA	9.5
2	C	1006	TYR	9.5
2	C	1011	ILE	9.3
2	C	1026	GLU	9.1
2	C	1008	VAL	8.8
1	D	36	PHE	8.7
1	D	203	HIS	8.7
1	D	297	GLN	8.6
1	D	240	GLN	8.6
1	D	277	LYS	8.6
1	D	23	ARG	8.5
1	D	151	ALA	8.4
1	D	55	PRO	8.3
1	D	13	HIS	8.3
2	C	1027	ILE	8.2
1	D	193	THR	8.0
1	D	296	HIS	8.0
1	D	139	ILE	8.0
2	C	991	ARG	7.8
1	D	58	ARG	7.8
1	D	251	GLU	7.7
1	D	104	SER	7.7
1	D	194	TYR	7.6
1	D	271	LEU	7.6
1	D	252	LYS	7.5
1	D	14	ASP	7.4
1	D	82	TRP	7.4
1	D	239	GLU	7.3
2	C	996	PHE	7.3
1	D	255	ASP	7.2
1	D	209	ASP	7.2
1	D	261	SER	7.1
1	D	44	LYS	7.1
1	D	11	LEU	7.1
1	D	173	PHE	7.0
1	D	153	TRP	6.9
2	C	1007	ALA	6.8
1	D	106	GLN	6.7
1	D	250	GLU	6.6
1	D	128	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	192	GLN	6.6
1	D	45	LEU	6.5
1	D	10	GLU	6.5
1	D	95	HIS	6.5
1	D	89	TRP	6.4
1	D	1	MET	6.4
2	C	995	ILE	6.4
1	D	5	ALA	6.4
1	D	8	HIS	6.4
1	D	29	SER	6.3
1	D	160	GLU	6.3
1	D	260	ALA	6.3
2	C	1025	GLN	6.3
1	D	234	TRP	6.2
1	D	281	TRP	6.1
1	D	211	ALA	6.0
1	D	25	ALA	5.9
2	C	1002	ASN	5.9
1	D	269	LEU	5.9
2	C	997	HIS	5.9
1	D	37	GLU	5.8
1	D	207	VAL	5.8
1	D	143	ALA	5.8
1	D	64	PRO	5.7
1	D	208	ARG	5.7
1	D	257	LEU	5.6
1	D	57	TRP	5.6
1	D	24	LEU	5.6
2	C	993	PHE	5.6
1	D	107	TRP	5.6
2	C	1028	LYS	5.6
1	D	256	VAL	5.6
1	D	119	ALA	5.5
1	D	176	GLY	5.5
2	C	1035	ILE	5.4
1	D	117	LEU	5.3
1	D	21	GLY	5.3
1	D	190	ASP	5.3
1	D	12	ILE	5.3
1	D	126	SER	5.3
1	D	26	THR	5.2
1	D	130	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	158	ILE	5.2
1	D	88	ARG	5.2
1	D	20	TYR	5.2
2	C	1004	VAL	5.1
1	D	206	TRP	5.1
1	D	185	TRP	5.1
2	C	1030	THR	5.0
1	D	212	TRP	5.0
1	D	70	LEU	5.0
1	D	244	LYS	5.0
1	D	152	SER	4.9
1	D	4	ILE	4.9
2	C	992	GLN	4.8
1	D	148	VAL	4.8
1	D	247	LEU	4.8
1	D	50	THR	4.8
1	D	16	VAL	4.7
1	D	17	LEU	4.7
1	D	295	VAL	4.7
1	D	15	ALA	4.7
1	D	105	VAL	4.6
2	C	990	ARG	4.6
2	C	1024	VAL	4.6
1	D	133	ASN	4.6
1	D	183	LYS	4.6
1	D	32	THR	4.5
1	D	113	GLY	4.5
1	D	243	TRP	4.5
1	D	75	TYR	4.5
1	D	73	CYS	4.5
1	D	60	ASP	4.4
1	D	142	ASP	4.4
1	D	171	ARG	4.3
1	D	226	SER	4.3
1	D	248	LEU	4.3
1	D	144	HIS	4.3
1	D	186	LYS	4.3
1	D	230	THR	4.3
2	C	994	PRO	4.3
1	D	51	GLY	4.2
1	D	141	ILE	4.2
1	D	33	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	149	ASN	4.1
2	C	1221	ASN	4.1
1	D	41	GLU	4.0
1	D	118	VAL	4.0
1	D	27	CYS	4.0
1	D	195	VAL	4.0
1	D	270	ALA	3.9
1	D	59	VAL	3.9
1	D	71	ALA	3.8
1	D	140	ILE	3.8
1	D	224	SER	3.8
1	D	169	GLU	3.8
1	D	262	TRP	3.8
1	D	78	LYS	3.7
1	D	205	ASP	3.7
1	D	287	GLY	3.7
1	D	174	VAL	3.7
1	D	63	HIS	3.7
1	D	254	PRO	3.6
1	D	290	GLU	3.6
2	C	998	TRP	3.6
1	D	48	THR	3.6
2	B	1246	ASN	3.6
2	C	1092	LYS	3.6
2	C	1251	LEU	3.5
1	D	157	THR	3.5
1	D	61	TRP	3.5
1	D	86	ASN	3.5
1	D	42	THR	3.5
2	C	1077	THR	3.5
1	D	98	HIS	3.5
1	D	175	THR	3.5
1	D	131	LYS	3.5
1	D	69	ILE	3.5
1	D	47	ASP	3.5
1	D	99	SER	3.4
1	D	145	ALA	3.4
1	D	108	ALA	3.4
2	C	1349	GLY	3.4
1	D	227	GLN	3.4
1	D	210	VAL	3.4
1	D	127	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	1219	THR	3.3
1	D	38	VAL	3.3
2	C	1029	VAL	3.3
1	D	217	LEU	3.3
1	D	84	GLU	3.3
1	D	115	LEU	3.3
1	D	179	ASP	3.2
1	D	34	LYS	3.2
1	D	43	HIS	3.2
1	D	172	LYS	3.2
2	C	1075	SER	3.2
2	C	1351	ASN	3.1
1	D	28	SER	3.1
1	D	232	ILE	3.1
1	D	268	VAL	3.1
1	D	159	GLU	3.0
1	D	221	TYR	3.0
2	C	1072	GLU	3.0
1	D	102	VAL	3.0
1	D	180	ASN	3.0
1	D	92	ILE	3.0
1	D	111	GLU	3.0
1	D	184	ILE	3.0
1	D	116	LEU	3.0
1	D	19	TYR	2.9
1	D	154	ALA	2.9
1	D	90	SER	2.9
2	C	1076	SER	2.9
2	C	1054	LEU	2.9
1	D	74	SER	2.9
2	C	1036	ILE	2.8
1	A	88	ARG	2.8
1	D	292	ALA	2.8
1	D	134	GLY	2.7
1	D	100	ALA	2.7
1	D	245	LYS	2.7
1	D	278	VAL	2.7
1	D	62	ALA	2.7
1	D	223	ALA	2.7
1	D	150	SER	2.7
1	D	246	THR	2.7
1	D	238	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	1372	ASP	2.6
1	D	81	ILE	2.6
2	C	1312	ILE	2.6
2	B	1247	GLU	2.6
1	D	52	HIS	2.6
1	D	242	PRO	2.6
2	C	1005	VAL	2.5
1	D	218	LEU	2.5
1	D	229	ARG	2.5
1	D	155	PRO	2.5
1	D	137	SER	2.4
1	D	204	SER	2.4
2	C	1365	VAL	2.4
1	D	216	VAL	2.4
2	C	1375	THR	2.4
2	C	1248	ASP	2.4
1	D	103	ASN	2.4
2	C	1038	PRO	2.3
1	D	166	GLY	2.3
1	D	188	ASN	2.3
1	D	201	GLU	2.3
2	B	1010	PRO	2.3
2	C	1352	SER	2.3
1	D	72	SER	2.3
1	D	80	LEU	2.3
1	D	222	LEU	2.3
1	D	124	LYS	2.3
2	C	1058	ASP	2.3
2	C	1291	PRO	2.3
2	C	1348	GLN	2.3
1	D	97	VAL	2.3
1	D	54	GLY	2.2
1	D	215	THR	2.2
2	C	1309	PHE	2.2
2	C	1228	SER	2.2
2	C	1031	PRO	2.2
2	C	1350	LEU	2.2
2	C	1119	GLY	2.2
2	C	1249	PRO	2.2
1	D	249	LYS	2.2
2	C	1330	GLY	2.2
1	D	168	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	1316	GLU	2.1
2	B	1249	PRO	2.1
1	D	289	TRP	2.1
1	D	122	ASP	2.1
1	D	263	SER	2.1
2	C	1120	ASP	2.1
2	B	1160	ILE	2.0
1	D	132	GLU	2.0
1	D	273	GLY	2.0
2	C	1328	PHE	2.0
1	D	200	LEU	2.0
1	A	296	HIS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.