



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 3MZK / pdb_00003mzk
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	:	4-5-2 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

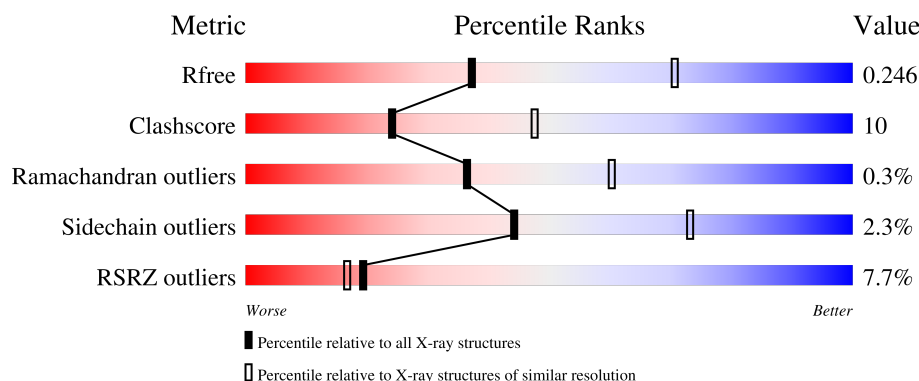
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	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	297	
1	D	297	
2	B	441	
2	C	441	

2 Entry composition

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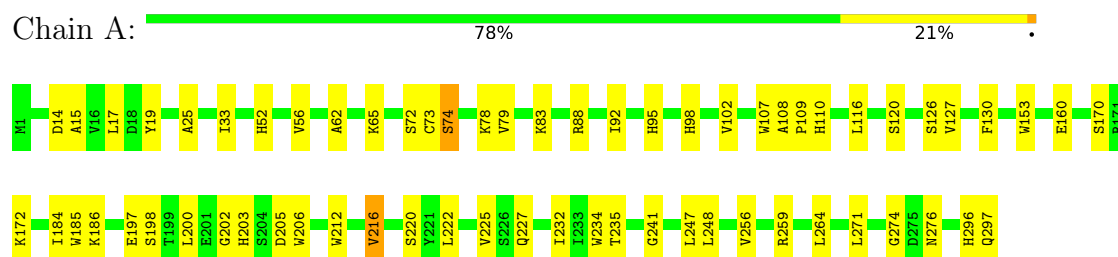
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	10	Total	O	0	0
			10	10		
3	D	1	Total	O	0	0
			1	1		

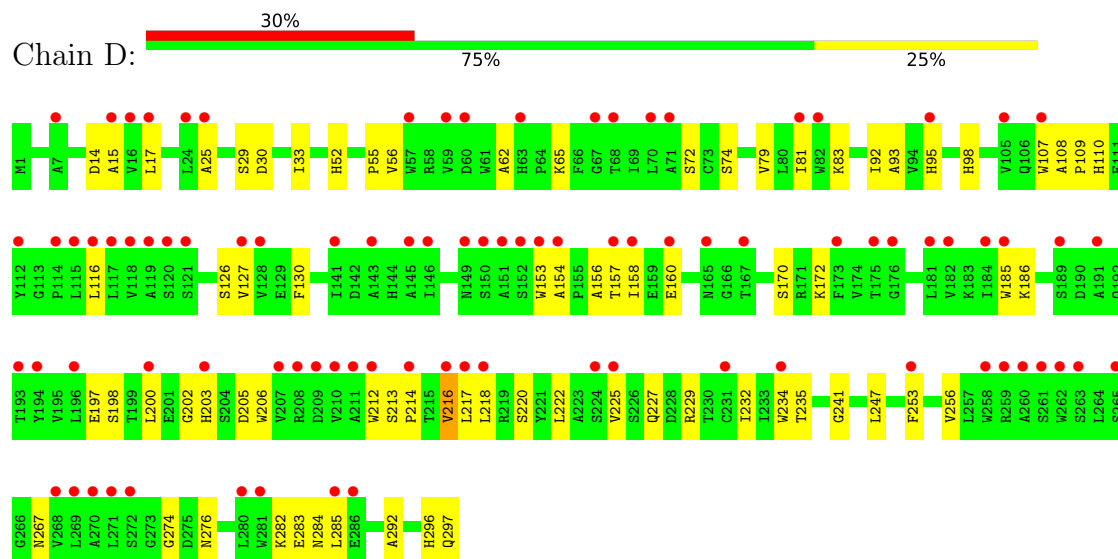
3 Residue-property plots

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.

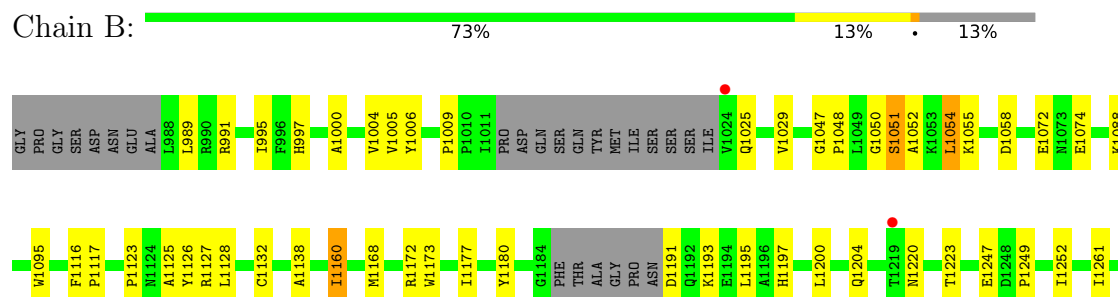
• Molecule 1: Protein transport protein SEC13

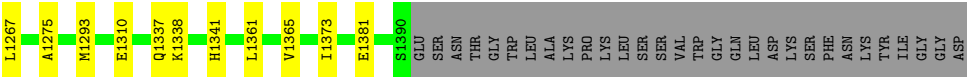


• Molecule 1: Protein transport protein SEC13

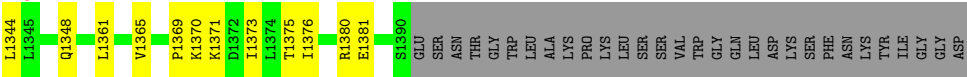
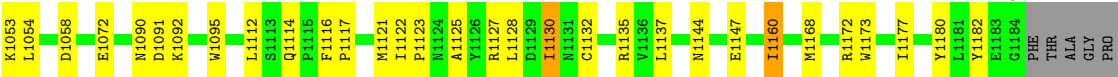
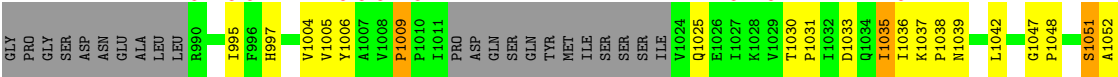


• Molecule 2: Protein transport protein SEC16





● Molecule 2: Protein transport protein SEC16



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.198 , 0.243 0.201 , 0.246	Depositor DCC
R_{free} test set	2292 reflections (4.97%)	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 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

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	0.41	0/2392	0.79	3/3263 (0.1%)
1	D	0.40	0/2385	0.77	2/3255 (0.1%)
2	B	0.38	0/2999	0.74	1/4094 (0.0%)
2	C	0.33	0/2971	0.75	5/4057 (0.1%)
All	All	0.38	0/10747	0.76	11/14669 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1009	PRO	CA-C-N	6.97	126.96	119.78
2	C	1009	PRO	C-N-CA	6.97	126.96	119.78
1	D	241	GLY	CA-C-N	6.67	126.61	120.21
1	D	241	GLY	C-N-CA	6.67	126.61	120.21
1	A	241	GLY	CA-C-N	6.44	126.39	120.21
1	A	241	GLY	C-N-CA	6.44	126.39	120.21
2	B	989	LEU	N-CA-C	-6.39	105.23	113.16
2	C	1114	GLN	CA-C-N	5.46	125.39	119.76
2	C	1114	GLN	C-N-CA	5.46	125.39	119.76
2	C	1053	LYS	N-CA-C	-5.43	105.87	113.37
1	A	120	SER	N-CA-C	5.09	117.12	109.23

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	42	0
1	D	2322	0	2239	68	0
2	B	2932	0	2818	51	0
2	C	2904	0	2791	92	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	205	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 (205) 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
1:D:170:SER:HB2	1:D:186:LYS:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1132:CYS:HG	2:C:1116:PHE:HZ	1.43	0.65
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
2:C:1052:ALA:C	2:C:1054:LEU:H	2.08	0.60
1:A:98:HIS:HE1	1:A:126:SER:OG	1.85	0.60
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:1308:THR:HG21	1:D:284:ASN:C	2.29	0.57
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:1052:ALA:C	2:B:1054:LEU:H	2.11	0.57
2:B:1054:LEU:HD22	2:B:1055:LYS:N	2.20	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
2:C:1168:MET:HE2	2:C:1172:ARG:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ALA:HB2	1:D:153:TRP:CE2	2.44	0.53
2:C:1200:LEU:O	2:C:1204:GLN:HG2	2.07	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
2:C:1306:MET:HE2	2:C:1337:GLN:HB2	1.92	0.52
1:D:83:LYS:HB2	1:D:92:ILE:CD1	2.39	0.52
2:C:1220:ASN:CG	2:C:1223:THR:HG23	2.35	0.51
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:1220:ASN:CG	2:B:1223:THR:HG23	2.36	0.50
2:B:1138:ALA:HB3	2:C:1112:LEU:HD21	1.93	0.50
2:B:1197:HIS:HE2	2:B:1223:THR:HG22	1.75	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
1:D:274:GLY:C	1:D:276:ASN:H	2.20	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
1:A:274:GLY:C	1:A:276:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1052:ALA:C	2:C:1054:LEU:N	2.72	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:B:1168:MET:HE2	2:B:1172:ARG:HD2	1.95	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
1:D:296:HIS:O	1:D:297:GLN:C	2.57	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
1:A:296:HIS:O	1:A:297:GLN:C	2.58	0.45
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
2:B:1052:ALA:C	2:B:1054:LEU:N	2.75	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
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
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
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
2:B:1191:ASP:C	2:B:1193:LYS:H	2.25	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
2:B:1261:ILE:CG2	2:B:1293:MET:HE2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HB3	1:A:234:TRP:CZ3	2.52	0.44
2:B:1247:GLU:C	2:B:1249:PRO:HD3	2.43	0.44
2:B:995:ILE:O	2:B:1006:TYR:HA	2.18	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:1168:MET:CE	2:C:1172:ARG:HD2	2.48	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:1336:PRO:C	1:D:217:LEU:HD23	2.43	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:205:ASP:O	1:D:206:TRP:C	2.62	0.43
2:C:1310:GLU:CD	2:C:1310:GLU:H	2.26	0.43
1:D:213:SER:HA	1:D:214:PRO:HD3	1.87	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
1:D:154:ALA:HB2	1:D:212:TRP:CE3	2.54	0.42
1:A:205:ASP:O	1:A:206:TRP:C	2.61	0.42
2:B:1310:GLU:H	2:B:1310:GLU:CD	2.28	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
1:D:30:ASP:OD1	1:D:30:ASP:C	2.61	0.42
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: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
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
2:C:1369:PRO:C	2:C:1371:LYS:H	2.28	0.41
1:A:160:GLU:N	2:B:1373:ILE:HD11	2.35	0.41
2:C:1090:ASN:C	2:C:1092:LYS:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1337:GLN:NE2	3:B:34:HOH:O	2.53	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:C:1144:ASN:CG	2:C:1147:GLU:HB2	2.46	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%)	36	60
1	D	295/297 (99%)	284 (96%)	10 (3%)	1 (0%)	36	60
2	B	379/441 (86%)	360 (95%)	18 (5%)	1 (0%)	36	60
2	C	375/441 (85%)	347 (92%)	27 (7%)	1 (0%)	36	60
All	All	1344/1476 (91%)	1269 (94%)	71 (5%)	4 (0%)	36	60

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 ⓘ

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%)	244 (98%)	6 (2%)	43	72
1	D	248/252 (98%)	244 (98%)	4 (2%)	55	80
2	B	306/395 (78%)	299 (98%)	7 (2%)	44	73
2	C	302/395 (76%)	294 (97%)	8 (3%)	40	70
All	All	1106/1294 (86%)	1081 (98%)	25 (2%)	44	73

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

Mol	Chain	Res	Type
1	A	74	SER
1	A	184	ILE
1	A	197	GLU
1	A	198	SER
1	A	216	VAL
1	A	225	VAL
2	B	1004	VAL
2	B	1051	SER
2	B	1054	LEU
2	B	1058	ASP
2	B	1072	GLU
2	B	1074	GLU
2	B	1160	ILE
2	C	1004	VAL
2	C	1035	ILE
2	C	1051	SER
2	C	1058	ASP
2	C	1072	GLU

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Mol	Chain	Res	Type
2	C	1122	ILE
2	C	1130	ILE
2	C	1160	ILE
1	D	197	GLU
1	D	198	SER
1	D	216	VAL
1	D	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	52	HIS
1	A	98	HIS
2	B	1337	GLN
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	1346	GLN
2	C	1348	GLN
1	D	6	ASN
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 oligosaccharides 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, 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	297/297 (100%)	-0.74	0 100 100	20, 39, 90, 133	0
1	D	297/297 (100%)	1.65	90 (30%) 1 1	122, 243, 326, 392	0
2	B	385/441 (87%)	-0.19	2 (0%) 87 86	33, 72, 123, 174	0
2	C	381/441 (86%)	0.22	13 (3%) 48 44	49, 99, 228, 287	0
All	All	1360/1476 (92%)	0.21	105 (7%) 19 17	20, 84, 276, 392	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	VAL	6.0
1	D	153	TRP	5.7
1	D	216	VAL	5.7
1	D	173	PHE	5.4
1	D	258	TRP	5.0
1	D	194	TYR	4.7
2	C	996	PHE	4.7
1	D	189	SER	4.3
2	C	1006	TYR	4.3
1	D	262	TRP	4.3
2	C	990	ARG	4.2
1	D	260	ALA	4.1
1	D	24	LEU	4.1
1	D	212	TRP	4.1
1	D	217	LEU	4.0
1	D	208	ARG	4.0
1	D	218	LEU	3.9
2	C	1027	ILE	3.8
1	D	269	LEU	3.8
1	D	70	LEU	3.7
1	D	261	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	211	ALA	3.6
1	D	118	VAL	3.6
1	D	128	VAL	3.4
2	C	995	ILE	3.3
1	D	15	ALA	3.3
1	D	225	VAL	3.3
1	D	146	ILE	3.3
1	D	271	LEU	3.3
1	D	167	THR	3.2
1	D	141	ILE	3.2
1	D	165	ASN	3.1
1	D	95	HIS	3.0
1	D	151	ALA	3.0
1	D	191	ALA	3.0
1	D	185	TRP	3.0
1	D	68	THR	2.9
2	C	1007	ALA	2.9
1	D	270	ALA	2.9
1	D	114	PRO	2.9
1	D	285	LEU	2.9
1	D	259	ARG	2.8
1	D	107	TRP	2.8
1	D	121	SER	2.8
1	D	120	SER	2.8
1	D	234	TRP	2.7
1	D	119	ALA	2.7
1	D	145	ALA	2.7
1	D	154	ALA	2.7
2	C	1010	PRO	2.7
1	D	214	PRO	2.7
1	D	116	LEU	2.7
1	D	117	LEU	2.7
1	D	17	LEU	2.6
1	D	182	VAL	2.6
1	D	253	PHE	2.6
1	D	272	SER	2.6
1	D	127	VAL	2.6
2	B	1024	VAL	2.6
1	D	158	ILE	2.6
2	C	1029	VAL	2.5
1	D	281	TRP	2.5
1	D	105	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	25	ALA	2.5
1	D	115	LEU	2.4
1	D	224	SER	2.4
2	C	1036	ILE	2.4
1	D	63	HIS	2.4
1	D	82	TRP	2.4
1	D	209	ASP	2.4
1	D	176	GLY	2.4
1	D	67	GLY	2.4
1	D	181	LEU	2.3
1	D	196	LEU	2.3
1	D	81	ILE	2.3
1	D	16	VAL	2.3
2	C	1008	VAL	2.3
1	D	150	SER	2.3
1	D	112	TYR	2.3
1	D	193	THR	2.3
2	C	1345	LEU	2.3
1	D	203	HIS	2.3
1	D	157	THR	2.3
1	D	175	THR	2.3
1	D	149	ASN	2.3
2	C	1184	GLY	2.3
1	D	200	LEU	2.2
1	D	152	SER	2.2
1	D	265	SER	2.2
1	D	59	VAL	2.2
1	D	71	ALA	2.2
1	D	143	ALA	2.2
1	D	231	CYS	2.2
1	D	60	ASP	2.2
1	D	263	SER	2.2
1	D	7	ALA	2.2
1	D	286	GLU	2.2
1	D	184	ILE	2.2
1	D	57	TRP	2.1
1	D	160	GLU	2.1
2	B	1219	THR	2.1
1	D	280	LEU	2.0
2	C	1332	SER	2.0
1	D	207	VAL	2.0
1	D	268	VAL	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 oligosaccharides 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.