



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:44 am GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

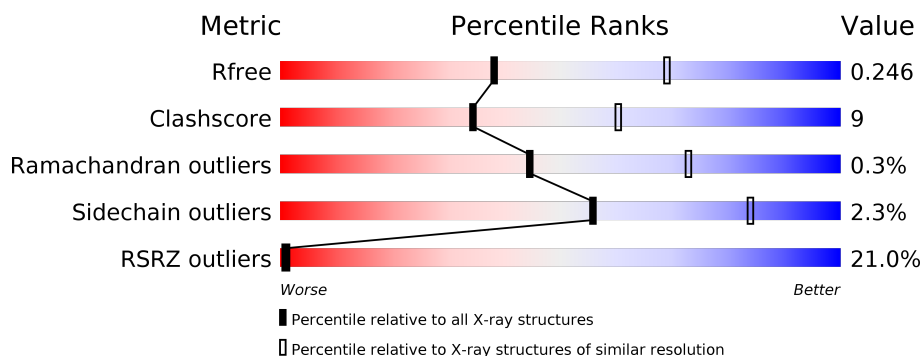
1 Overall quality at a glance

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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div>80% 19% .</div> </div>
1	D	297	<div> <div>74%</div> <div>77% 23%</div> </div>
2	B	441	<div> <div></div> <div>74% 13% . 13%</div> </div>
2	C	441	<div> <div>13%</div> <div>65% 21% 14%</div> </div>

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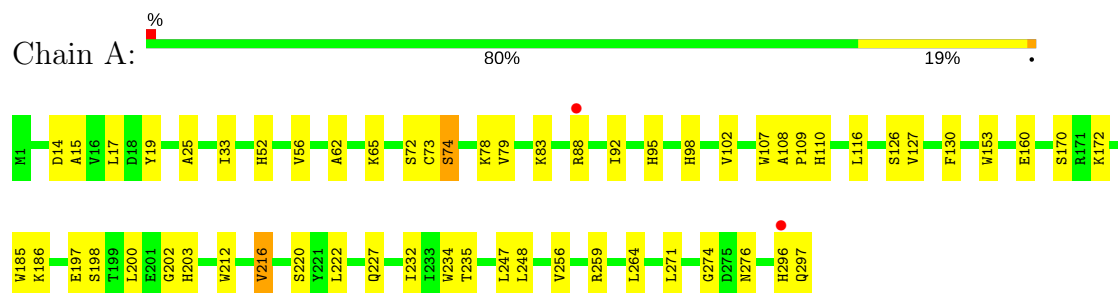
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	10	Total	O	0	0
			10	10		
3	D	1	Total	O	0	0
			1	1		

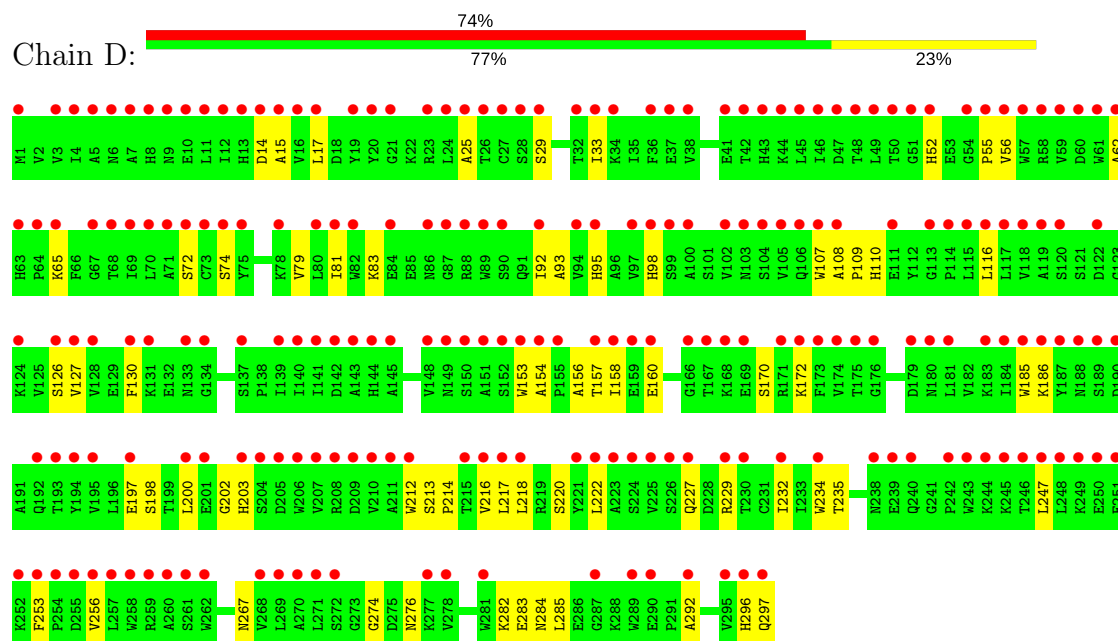
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

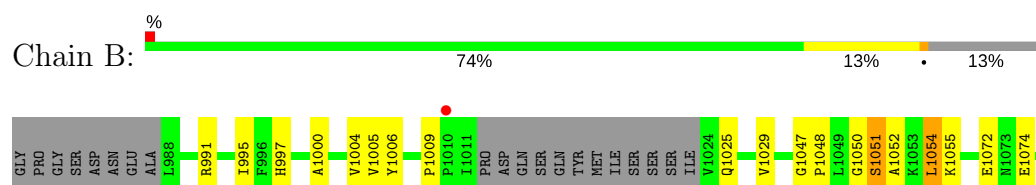
• Molecule 1: Protein transport protein SEC13

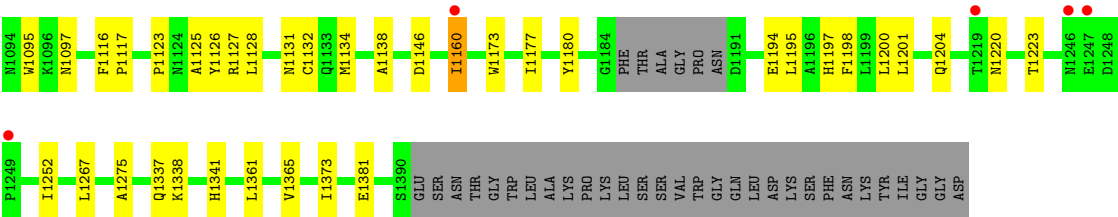


• Molecule 1: Protein transport protein SEC13

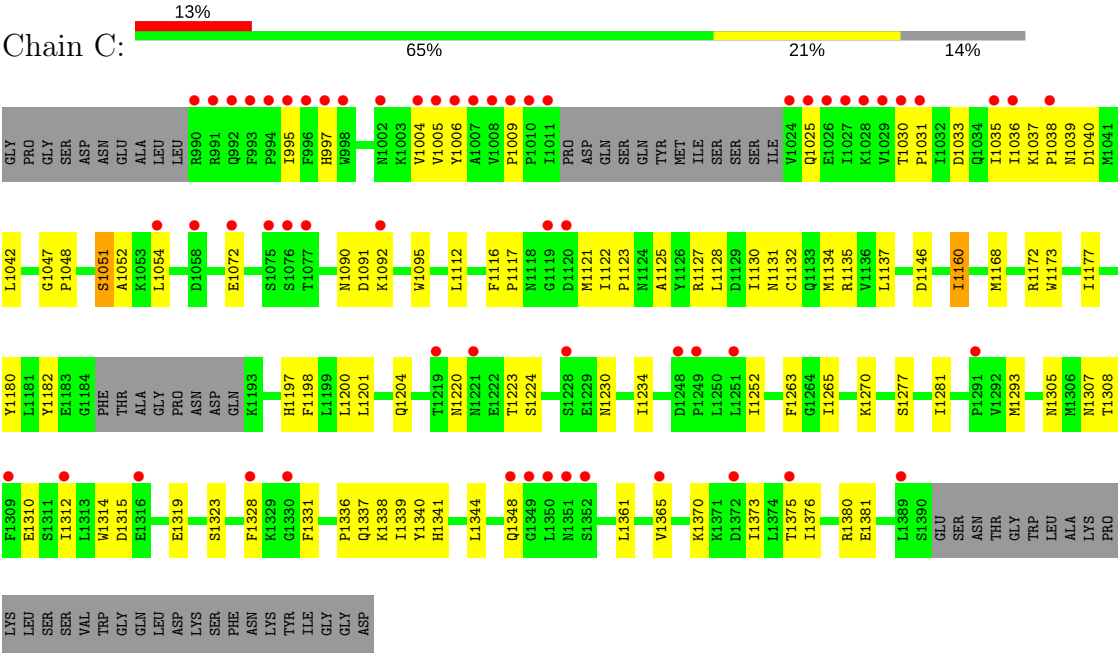


• Molecule 2: Protein transport protein SEC16





● 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 0.198 , 0.246	Depositor DCC
R_{free} test set	2289 reflections (5.06%)	DCC
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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:212:TRP:CD2	1:A:222:LEU:HD21	2.34	0.62
1:A:33:ILE:CD1	1:A:56:VAL:HG11	2.30	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:108:ALA:HB2	1:A:153:TRP:CE2	2.43	0.54
1:A:33:ILE:HD11	1:A:56:VAL:HG11	1.90	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:1344:LEU:HD21	1:D:267:ASN:ND2	2.22	0.54
2:C:1339:ILE:HG22	1:D:216:VAL:HG11	1.87	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:1194:GLU:HA	2:B:1197:HIS:HD1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1138:ALA:HB3	2:C:1112:LEU:HD21	1.93	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:1376:ILE:HG21	1:D:158:ILE:HG13	1.93	0.49
2:C:1307:ASN:CB	1:D:283:GLU:OE1	2.60	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:1132:CYS:SG	2:C:1116:PHE:CZ	2.97	0.45
2:B:1127:ARG:CB	2:C:1125:ALA:HB2	2.41	0.45
2:C:1338:LYS:O	2:C:1341:HIS:HB3	2.16	0.45
2:C:1038:PRO:HB3	2:C:1348:GLN:NE2	2.31	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:HA	2:C:1130:ILE:HD12	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
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:296:HIS:O	1:A:297:GLN:C	2.58	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:HB3	2:B:1087:MET:HE2	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	44	73
1	D	295/297 (99%)	284 (96%)	10 (3%)	1 (0%)	44	73
2	B	379/441 (86%)	360 (95%)	18 (5%)	1 (0%)	44	73
2	C	375/441 (85%)	347 (92%)	27 (7%)	1 (0%)	44	73
All	All	1344/1476 (91%)	1269 (94%)	71 (5%)	4 (0%)	44	73

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%)	246 (98%)	4 (2%)	68	89
1	D	248/252 (98%)	246 (99%)	2 (1%)	85	95
2	B	306/395 (78%)	297 (97%)	9 (3%)	48	77
2	C	302/395 (76%)	292 (97%)	10 (3%)	43	73
All	All	1106/1294 (86%)	1081 (98%)	25 (2%)	56	84

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

Some 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/297 (100%)	-0.41	2 (0%) 87 88	20, 39, 90, 133	0
1	D	297/297 (100%)	4.21	219 (73%) 0 0	122, 243, 326, 392	0
2	B	385/441 (87%)	-0.23	6 (1%) 72 73	33, 72, 123, 174	0
2	C	381/441 (86%)	0.63	59 (15%) 2 2	49, 99, 228, 287	0
All	All	1360/1476 (92%)	0.94	286 (21%) 1 1	20, 84, 276, 392	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	THR	19.2
1	D	67	GLY	14.8
1	D	189	SER	14.6
1	D	272	SER	13.6
1	D	114	PRO	13.3
1	D	253	PHE	13.1
1	D	197	GLU	12.6
1	D	56	VAL	12.4
1	D	87	GLY	12.4
1	D	181	LEU	12.3
1	D	167	THR	11.5
1	D	3	VAL	11.5
1	D	120	SER	11.4
2	C	1010	PRO	11.3
1	D	259	ARG	10.9
1	D	49	LEU	10.6
1	D	65	LYS	10.6
1	D	187	TYR	10.5
2	C	1009	PRO	10.2
1	D	9	ASN	10.1
1	D	258	TRP	10.1

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Mol	Chain	Res	Type	RSRZ
1	D	225	VAL	9.7
1	D	6	ASN	9.7
1	D	7	ALA	9.6
2	C	1006	TYR	9.4
2	C	1011	ILE	9.0
1	D	55	PRO	8.9
2	C	1026	GLU	8.8
2	C	1008	VAL	8.7
1	D	297	GLN	8.7
1	D	203	HIS	8.7
1	D	240	GLN	8.5
1	D	277	LYS	8.5
1	D	23	ARG	8.4
1	D	151	ALA	8.4
1	D	13	HIS	8.3
1	D	296	HIS	8.3
1	D	36	PHE	8.2
2	C	991	ARG	8.2
1	D	193	THR	8.1
2	C	1027	ILE	8.1
1	D	139	ILE	8.0
1	D	251	GLU	7.8
1	D	194	TYR	7.8
1	D	252	LYS	7.8
1	D	58	ARG	7.7
1	D	104	SER	7.7
1	D	14	ASP	7.6
1	D	261	SER	7.5
1	D	82	TRP	7.4
1	D	209	ASP	7.4
1	D	239	GLU	7.4
1	D	255	ASP	7.3
1	D	11	LEU	7.3
2	C	996	PHE	7.3
1	D	271	LEU	7.2
1	D	173	PHE	7.0
1	D	250	GLU	6.9
1	D	44	LYS	6.9
1	D	153	TRP	6.8
2	C	1007	ALA	6.8
1	D	192	GLN	6.7
1	D	10	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	89	TRP	6.7
1	D	45	LEU	6.6
1	D	95	HIS	6.6
1	D	8	HIS	6.6
1	D	128	VAL	6.5
1	D	106	GLN	6.4
1	D	1	MET	6.4
1	D	160	GLU	6.3
1	D	5	ALA	6.2
1	D	234	TRP	6.2
2	C	1025	GLN	6.2
1	D	25	ALA	6.1
2	C	995	ILE	6.1
1	D	281	TRP	6.1
1	D	211	ALA	6.0
1	D	143	ALA	5.9
2	C	1002	ASN	5.9
1	D	269	LEU	5.9
1	D	29	SER	5.9
1	D	260	ALA	5.8
1	D	37	GLU	5.8
1	D	57	TRP	5.8
1	D	24	LEU	5.7
1	D	64	PRO	5.7
1	D	107	TRP	5.7
1	D	208	ARG	5.7
1	D	207	VAL	5.6
2	C	993	PHE	5.6
1	D	257	LEU	5.6
2	C	997	HIS	5.5
2	C	1028	LYS	5.5
1	D	119	ALA	5.4
1	D	148	VAL	5.4
1	D	117	LEU	5.3
1	D	244	LYS	5.3
1	D	190	ASP	5.2
1	D	176	GLY	5.2
1	D	158	ILE	5.2
2	C	1004	VAL	5.2
1	D	12	ILE	5.2
2	C	1035	ILE	5.1
1	D	20	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	185	TRP	5.1
1	D	126	SER	5.1
1	D	130	PHE	5.1
1	D	21	GLY	5.1
1	D	256	VAL	5.1
1	D	105	VAL	5.0
1	D	206	TRP	5.0
2	C	992	GLN	5.0
2	C	1030	THR	4.9
1	D	88	ARG	4.9
1	D	212	TRP	4.9
1	D	70	LEU	4.9
1	D	4	ILE	4.9
1	D	50	THR	4.9
1	D	26	THR	4.8
2	C	1024	VAL	4.7
1	D	16	VAL	4.7
1	D	295	VAL	4.7
1	D	133	ASN	4.7
2	C	990	ARG	4.7
1	D	247	LEU	4.6
1	D	152	SER	4.6
1	D	32	THR	4.6
1	D	243	TRP	4.6
1	D	15	ALA	4.6
1	D	17	LEU	4.5
1	D	183	LYS	4.4
1	D	226	SER	4.4
1	D	33	ILE	4.4
1	D	75	TYR	4.4
2	C	994	PRO	4.4
1	D	142	ASP	4.4
1	D	60	ASP	4.4
1	D	248	LEU	4.3
1	D	73	CYS	4.3
1	D	171	ARG	4.3
1	D	144	HIS	4.3
1	D	186	LYS	4.3
1	D	113	GLY	4.3
1	D	141	ILE	4.3
2	C	1221	ASN	4.1
1	D	230	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	41	GLU	4.0
1	D	51	GLY	4.0
1	D	27	CYS	4.0
1	D	118	VAL	4.0
1	D	149	ASN	4.0
1	D	195	VAL	4.0
1	D	169	GLU	3.9
1	D	59	VAL	3.8
1	D	270	ALA	3.8
1	D	254	PRO	3.8
1	D	140	ILE	3.8
1	D	71	ALA	3.8
1	D	262	TRP	3.7
1	D	224	SER	3.7
1	D	98	HIS	3.7
1	D	174	VAL	3.7
1	D	78	LYS	3.7
1	D	290	GLU	3.7
1	D	287	GLY	3.7
1	D	205	ASP	3.6
1	D	227	GLN	3.6
2	C	1092	LYS	3.6
2	C	998	TRP	3.6
1	D	48	THR	3.6
1	D	157	THR	3.6
1	D	86	ASN	3.6
1	D	63	HIS	3.6
1	D	38	VAL	3.6
1	D	69	ILE	3.6
2	B	1246	ASN	3.6
2	C	1077	THR	3.5
1	D	61	TRP	3.5
1	D	210	VAL	3.5
1	D	145	ALA	3.5
1	D	43	HIS	3.4
1	D	108	ALA	3.4
2	C	1251	LEU	3.4
1	D	131	LYS	3.4
1	D	115	LEU	3.4
1	D	127	VAL	3.4
1	D	175	THR	3.4
1	D	99	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	217	LEU	3.3
1	D	42	THR	3.3
2	C	1349	GLY	3.3
2	B	1219	THR	3.3
1	D	172	LYS	3.2
2	C	1029	VAL	3.2
1	D	84	GLU	3.2
1	D	34	LYS	3.2
1	D	47	ASP	3.1
2	C	1075	SER	3.1
1	D	92	ILE	3.1
1	D	232	ILE	3.1
1	D	111	GLU	3.0
2	C	1351	ASN	3.0
2	C	1072	GLU	3.0
1	D	179	ASP	3.0
1	D	28	SER	3.0
1	D	221	TYR	3.0
1	D	102	VAL	3.0
1	D	19	TYR	3.0
2	C	1076	SER	3.0
1	D	159	GLU	3.0
1	D	268	VAL	3.0
1	D	154	ALA	2.9
1	D	278	VAL	2.9
1	D	184	ILE	2.9
1	D	116	LEU	2.9
1	D	90	SER	2.8
1	D	245	LYS	2.8
1	D	292	ALA	2.8
1	A	88	ARG	2.8
2	C	1054	LEU	2.8
1	D	180	ASN	2.8
1	D	74	SER	2.7
2	C	1036	ILE	2.7
1	D	62	ALA	2.7
1	D	223	ALA	2.7
1	D	238	ASN	2.7
1	D	242	PRO	2.6
1	D	134	GLY	2.6
2	C	1005	VAL	2.6
2	C	1372	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	1312	ILE	2.6
1	D	216	VAL	2.6
1	D	246	THR	2.6
1	D	100	ALA	2.6
1	D	229	ARG	2.6
1	D	150	SER	2.6
1	D	201	GLU	2.5
2	B	1247	GLU	2.5
1	D	81	ILE	2.5
2	C	1365	VAL	2.5
1	D	103	ASN	2.5
2	C	1031	PRO	2.5
1	D	218	LEU	2.5
1	D	137	SER	2.4
1	D	52	HIS	2.4
1	D	155	PRO	2.4
2	B	1010	PRO	2.4
1	D	72	SER	2.4
2	C	1248	ASP	2.4
1	D	188	ASN	2.3
1	D	204	SER	2.3
1	D	215	THR	2.3
2	C	1348	GLN	2.3
2	C	1291	PRO	2.3
2	C	1352	SER	2.3
1	D	166	GLY	2.3
1	D	222	LEU	2.3
2	C	1375	THR	2.3
1	D	249	LYS	2.2
2	C	1058	ASP	2.2
1	D	97	VAL	2.2
2	C	1119	GLY	2.2
2	C	1350	LEU	2.2
1	D	94	VAL	2.2
2	C	1038	PRO	2.2
2	C	1309	PHE	2.2
1	D	124	LYS	2.2
1	D	289	TRP	2.2
2	C	1120	ASP	2.1
1	D	122	ASP	2.1
2	B	1249	PRO	2.1
2	C	1330	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	LYS	2.1
2	C	1316	GLU	2.1
2	C	1219	THR	2.1
1	D	54	GLY	2.1
1	D	80	LEU	2.1
2	C	1389	LEU	2.1
2	C	1249	PRO	2.1
2	C	1228	SER	2.1
1	A	296	HIS	2.0
1	D	46	ILE	2.0
2	C	1328	PHE	2.0
1	D	200	LEU	2.0
2	B	1160	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.