Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 11:58 AM JST

PDB ID	:	5X6B
Title	:	Crystal structure of SepCysE-SepCysS in complex with tRNACys from Methanocaldococcus jannaschii
Authors	:	Chen, M.; Kato, K.; Yao, M.
Deposited on	:	2017-02-21
Resolution	:	2.60 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:

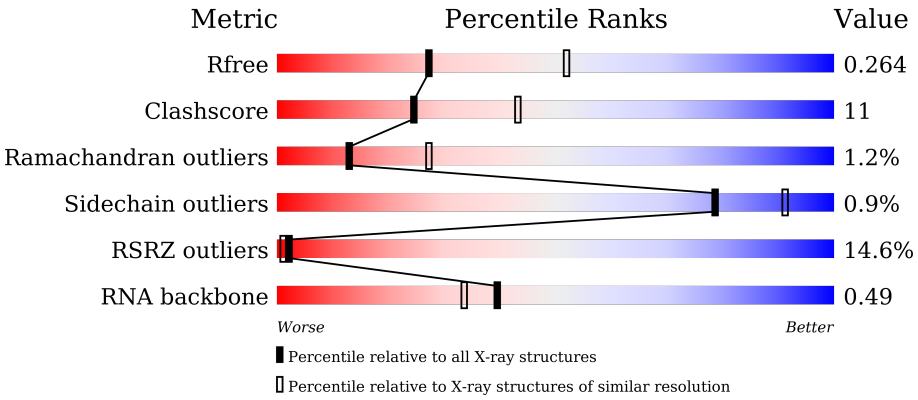
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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.



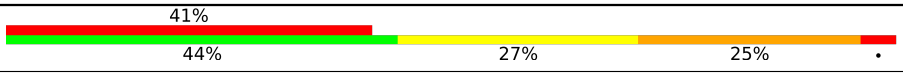
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	I	417	6% 71% 16% 12%
1	J	417	8% 72% 18% • 10%
2	E	216	27% • 69%
2	F	216	30% 50% 28% • • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	75	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9621 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 O-phospho-L-seryl-tRNA:Cys-tRNA synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	I	367	Total	C	N	O	P	S	0	0	0
			2944	1892	490	547	1	14			
1	J	377	Total	C	N	O	P	S	0	0	0
			3016	1936	500	564	1	15			

- Molecule 2 is a protein called Uncharacterized protein MJ1481.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	68	Total	C	N	O	S	0	0	0
			562	368	89	103	2			
2	F	177	Total	C	N	O	S	0	0	0
			1455	941	236	273	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	MET	-	initiating methionine	UNP Q58876
E	-1	ASN	-	expression tag	UNP Q58876
E	0	HIS	-	expression tag	UNP Q58876
F	-2	MET	-	initiating methionine	UNP Q58876
F	-1	ASN	-	expression tag	UNP Q58876
F	0	HIS	-	expression tag	UNP Q58876

- Molecule 3 is a RNA chain called tRNACys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	75	Total	C	N	O	P	0	0	0
			1599	712	286	526	75			

- Molecule 4 is water.

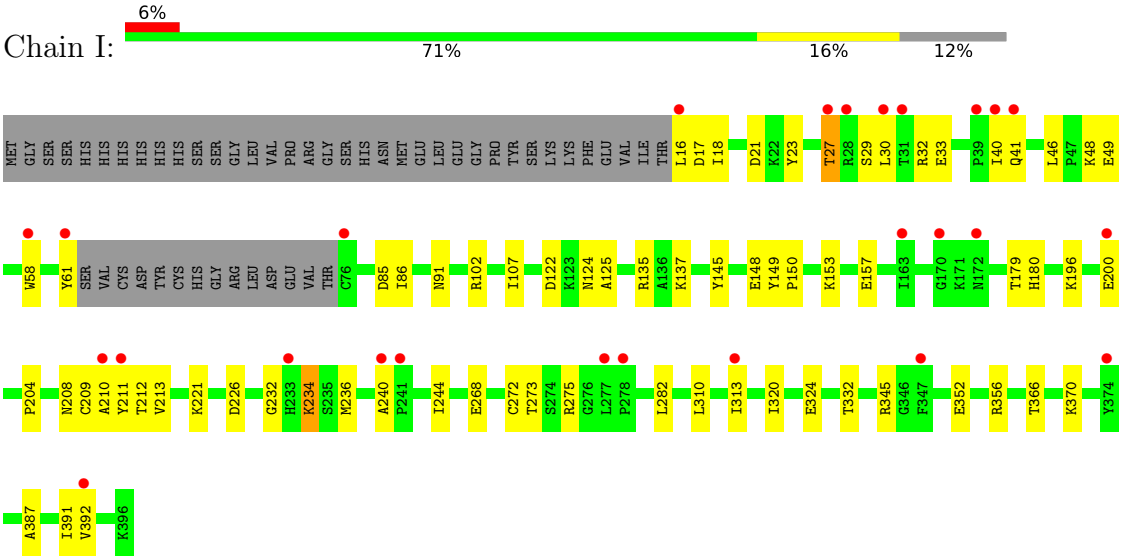
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	20	Total O 20 20	0	0
4	J	17	Total O 17 17	0	0
4	E	5	Total O 5 5	0	0
4	F	2	Total O 2 2	0	0
4	P	1	Total O 1 1	0	0

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.

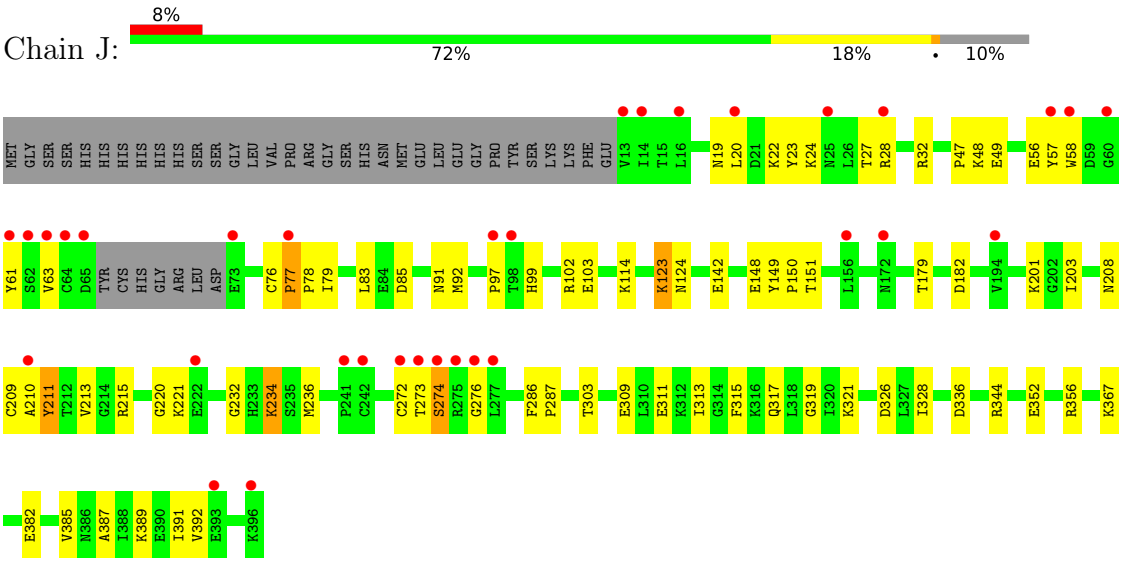
• Molecule 1: O-phospho-L-seryl-tRNA:Cys-tRNA synthase

Chain I:



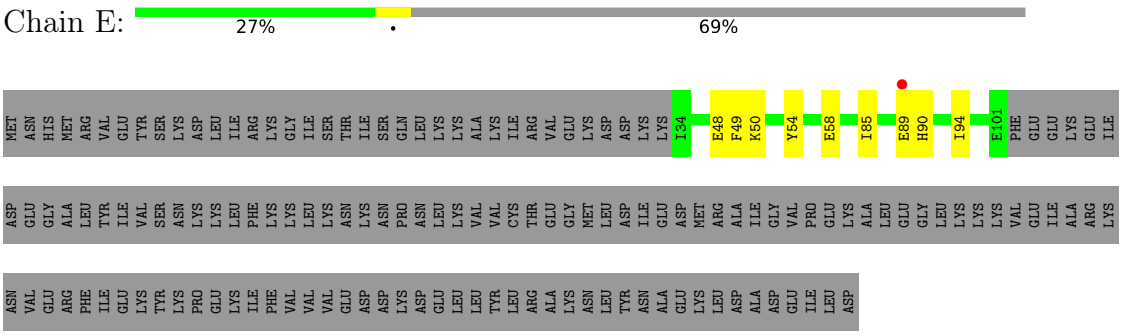
• Molecule 1: O-phospho-L-seryl-tRNA:Cys-tRNA synthase

Chain J:



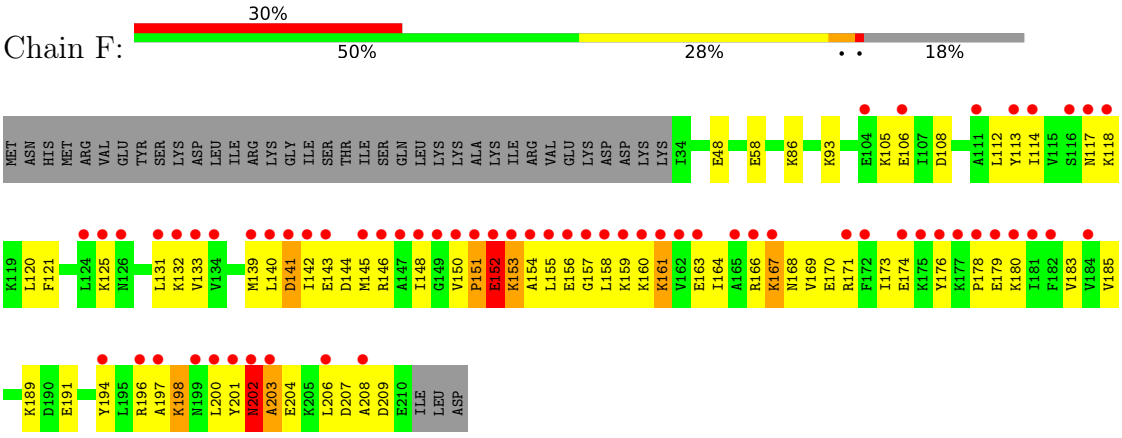
• Molecule 2: Uncharacterized protein MJ1481

Chain E:



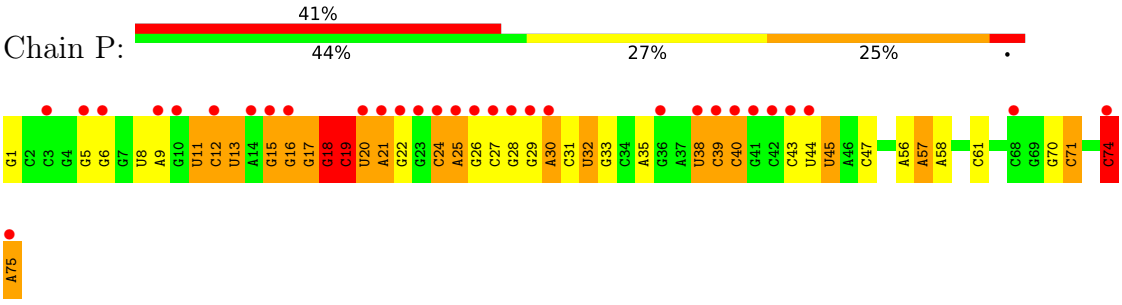
• Molecule 2: Uncharacterized protein MJ1481

Chain F:



• Molecule 3: tRNACys

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.25Å 107.25Å 551.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.22 – 2.60 48.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.22-2.60) 99.7 (48.22-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.225 , 0.261 0.228 , 0.264	Depositor DCC
R_{free} test set	2927 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	I	0.27	0/2976	0.47	0/4000
1	J	0.27	0/3048	0.48	0/4100
2	E	0.27	0/573	0.37	0/765
2	F	0.50	1/1477 (0.1%)	0.83	3/1973 (0.2%)
3	P	0.37	1/1785 (0.1%)	0.89	8/2779 (0.3%)
All	All	0.33	2/9859 (0.0%)	0.63	11/13617 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	F	0	4
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	G	OP3-P	-10.65	1.48	1.61
2	F	152	GLU	CB-CG	5.21	1.62	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	161	LYS	CD-CE-NZ	11.08	137.19	111.70
3	P	38	U	OP1-P-O3'	-10.89	81.23	105.20
3	P	38	U	OP2-P-O3'	-9.63	84.02	105.20
3	P	19	C	N3-C4-C5	7.89	125.06	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	39	C	OP1-P-OP2	7.22	130.43	119.60
3	P	74	C	C6-N1-C1'	-7.11	112.27	120.80
2	F	167	LYS	CA-CB-CG	6.61	127.95	113.40
3	P	74	C	C2-N1-C1'	6.59	126.05	118.80
2	F	152	GLU	OE1-CD-OE2	-6.18	115.89	123.30
3	P	74	C	N1-C2-O2	5.87	122.42	118.90
3	P	18	G	O4'-C1'-N9	5.34	112.47	108.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	141	ASP	Peptide
2	F	153	LYS	Peptide
2	F	176	TYR	Peptide
2	F	198	LYS	Peptide
1	J	274	SER	Peptide

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	I	2944	0	2987	47	0
1	J	3016	0	3060	52	0
2	E	562	0	571	7	0
2	F	1455	0	1505	94	0
3	P	1599	0	813	34	0
4	E	5	0	0	0	0
4	F	2	0	0	0	0
4	I	20	0	0	4	0
4	J	17	0	0	3	0
4	P	1	0	0	0	0
All	All	9621	0	8936	200	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 11.

All (200) 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)
1:J:28:ARG:HB2	2:E:50:LYS:HE3	1.43	0.99
2:F:198:LYS:HA	2:F:201:TYR:H	1.31	0.96
2:F:153:LYS:HE3	2:F:156:GLU:HB2	1.47	0.93
1:J:210:ALA:O	4:J:401:HOH:O	1.85	0.92
2:F:168:ASN:HA	2:F:171:ARG:HG3	1.51	0.92
2:F:118:LYS:HA	2:F:121:PHE:HB3	1.55	0.86
2:F:113:TYR:HB2	2:F:133:VAL:HG12	1.58	0.85
2:F:164:ILE:HA	2:F:167:LYS:HG2	1.57	0.84
3:P:13:U:H3	3:P:21:A:H61	1.26	0.83
2:F:194:TYR:CE1	2:F:204:GLU:HB2	2.12	0.83
1:I:352:GLU:HB3	1:I:391:ILE:HD12	1.62	0.82
1:J:352:GLU:HB3	1:J:391:ILE:HD12	1.60	0.80
2:F:161:LYS:HE2	3:P:18:G:O2'	1.83	0.79
2:F:163:GLU:O	2:F:167:LYS:N	2.17	0.77
2:F:118:LYS:NZ	3:P:57:A:H3'	1.99	0.77
1:J:382:GLU:OE2	4:J:402:HOH:O	2.02	0.76
2:F:118:LYS:NZ	3:P:58:A:OP2	2.21	0.73
1:I:179:THR:HA	1:I:208:ASN:HB3	1.72	0.72
2:F:161:LYS:NZ	3:P:19:C:O4'	2.23	0.71
2:F:161:LYS:HE3	3:P:18:G:O3'	1.90	0.70
2:E:48:GLU:OE2	2:E:90:HIS:ND1	2.20	0.70
2:F:152:GLU:O	2:F:155:LEU:HB2	1.90	0.70
2:F:206:LEU:O	2:F:208:ALA:N	2.23	0.69
1:I:49:GLU:HG2	1:J:24:LYS:HE3	1.75	0.69
1:I:46:LEU:HD22	1:J:58:TRP:HB3	1.75	0.68
1:I:240:ALA:HB3	1:J:276:GLY:HA3	1.75	0.68
1:I:209:CYS:HB3	1:I:213:VAL:HG23	1.77	0.67
1:I:125:ALA:HA	1:I:179:THR:HG21	1.76	0.66
1:J:27:THR:O	2:E:54:TYR:OH	2.12	0.65
2:F:141:ASP:HA	2:F:166:ARG:HH22	1.61	0.65
2:F:151:PRO:HA	2:F:152:GLU:OE1	1.96	0.65
2:F:160:LYS:O	2:F:164:ILE:N	2.26	0.65
2:F:198:LYS:HA	2:F:201:TYR:N	2.09	0.65
2:F:152:GLU:HG3	2:F:155:LEU:HD22	1.81	0.63
2:F:108:ASP:O	2:F:113:TYR:OH	2.12	0.62
1:J:336:ASP:OD2	1:J:367:LYS:HG2	2.00	0.61
1:I:27:THR:HA	1:J:56:GLU:HG3	1.82	0.61
1:I:210:ALA:O	4:I:401:HOH:O	2.16	0.60
1:J:232:GLY:HA2	1:J:236:MET:HB2	1.83	0.60
1:I:107:ILE:HG23	1:I:268:GLU:HG2	1.84	0.59
2:F:141:ASP:O	2:F:144:ASP:HB2	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:17:G:H21	3:P:57:A:H5'	1.68	0.59
2:F:118:LYS:HZ3	3:P:57:A:H3'	1.65	0.59
2:F:151:PRO:HB3	2:F:152:GLU:HB2	1.85	0.59
2:F:118:LYS:CA	2:F:121:PHE:HB3	2.31	0.59
1:I:272:CYS:HA	1:I:273:THR:HB	1.84	0.58
1:I:29:SER:HB2	1:J:57:TYR:CZ	2.39	0.58
2:F:114:ILE:HB	2:F:183:VAL:HG22	1.85	0.58
2:F:170:GLU:N	2:F:170:GLU:OE1	2.37	0.57
1:I:234:LLP:OP1	1:J:61:TYR:OH	2.20	0.57
1:J:77:PRO:O	1:J:79:ILE:N	2.38	0.57
2:F:198:LYS:HZ3	2:F:203:ALA:N	2.03	0.57
3:P:13:U:H3	3:P:21:A:N6	1.99	0.57
1:J:209:CYS:HB3	1:J:213:VAL:HG23	1.88	0.56
1:J:123:LYS:HG3	1:J:142:GLU:HB3	1.86	0.56
2:F:139:MET:HG2	2:F:148:ILE:HD11	1.86	0.56
2:F:143:GLU:HB3	2:F:146:ARG:HH21	1.72	0.55
2:F:198:LYS:HD2	2:F:202:ASN:C	2.26	0.55
1:I:387:ALA:O	1:I:391:ILE:HG12	2.06	0.55
1:I:180:HIS:ND1	1:I:212:THR:HG21	2.21	0.55
1:I:196:LYS:O	1:I:200:GLU:HG2	2.06	0.55
2:F:118:LYS:HA	2:F:121:PHE:CB	2.34	0.55
2:F:170:GLU:O	2:F:174:GLU:N	2.36	0.55
1:I:370:LYS:HD3	3:P:74:C:N4	2.22	0.55
1:I:21:ASP:OD2	3:P:61:C:O2'	2.25	0.55
2:F:169:VAL:O	2:F:173:ILE:HG22	2.08	0.54
2:F:194:TYR:CZ	2:F:204:GLU:HB2	2.43	0.54
2:F:146:ARG:HD3	2:F:152:GLU:OE2	2.07	0.54
2:F:191:GLU:O	2:F:194:TYR:HB3	2.07	0.54
2:F:161:LYS:HZ2	3:P:19:C:C5'	2.20	0.54
2:F:197:ALA:C	2:F:198:LYS:HG3	2.27	0.53
1:I:40:ILE:HG13	1:I:41:GLN:HG3	1.90	0.53
1:I:32:ARG:NH2	1:J:58:TRP:HE1	2.07	0.53
1:J:387:ALA:O	1:J:391:ILE:HG12	2.07	0.53
2:F:194:TYR:CE1	2:F:198:LYS:NZ	2.75	0.53
2:F:141:ASP:C	2:F:144:ASP:HB2	2.29	0.53
1:I:157:GLU:H	1:I:157:GLU:CD	2.13	0.53
1:J:61:TYR:HB3	1:J:63:VAL:HG22	1.91	0.52
1:J:215:ARG:NH2	1:J:326:ASP:OD1	2.42	0.52
2:F:141:ASP:HB3	2:F:144:ASP:CG	2.29	0.52
1:J:102:ARG:NH1	1:J:234:LLP:OP2	2.42	0.52
1:J:309:GLU:HG2	1:J:385:VAL:HG11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:198:LYS:HD2	2:F:202:ASN:O	2.10	0.52
2:F:142:ILE:HA	2:F:145:MET:HB3	1.91	0.52
2:F:170:GLU:HA	2:F:173:ILE:CG2	2.40	0.52
2:F:167:LYS:O	2:F:170:GLU:HB2	2.10	0.52
2:F:161:LYS:HA	2:F:164:ILE:HB	1.92	0.51
2:F:141:ASP:HA	2:F:166:ARG:NH2	2.24	0.51
2:F:118:LYS:HZ3	3:P:58:A:P	2.32	0.51
1:I:61:TYR:HE2	1:I:275:ARG:HB3	1.77	0.50
2:F:144:ASP:OD2	2:F:196:ARG:HG3	2.11	0.50
1:I:86:ILE:HG21	1:I:244:ILE:HG21	1.93	0.50
3:P:27:C:H2'	3:P:28:G:C8	2.47	0.49
1:I:324:GLU:OE1	4:I:403:HOH:O	2.20	0.49
1:J:179:THR:OG1	4:J:403:HOH:O	2.20	0.49
2:F:161:LYS:NZ	3:P:19:C:N1	2.58	0.49
2:F:198:LYS:HG2	2:F:201:TYR:C	2.33	0.49
2:F:140:LEU:HG	2:F:166:ARG:HH21	1.77	0.48
1:I:102:ARG:NH2	1:J:272:CYS:HA	2.28	0.48
2:F:198:LYS:NZ	2:F:203:ALA:N	2.61	0.48
1:J:344:ARG:NH2	1:J:352:GLU:OE2	2.37	0.48
2:F:142:ILE:O	2:F:145:MET:HB3	2.14	0.48
2:E:49:PHE:HA	2:E:94:ILE:HD11	1.96	0.48
1:I:232:GLY:HA2	1:I:236:MET:HB2	1.95	0.48
1:J:99:HIS:HB2	1:J:103:GLU:HG3	1.94	0.48
2:F:105:LYS:HB3	2:F:106:GLU:H	1.51	0.48
2:F:113:TYR:HE2	2:F:131:LEU:HD11	1.78	0.48
2:E:50:LYS:HE2	2:E:54:TYR:CE2	2.49	0.47
2:F:161:LYS:HE2	3:P:18:G:HO2'	1.78	0.47
2:F:170:GLU:HA	2:F:173:ILE:HG22	1.96	0.47
2:E:85:ILE:O	2:E:89:GLU:HG3	2.13	0.47
2:F:161:LYS:HE3	3:P:19:C:P	2.55	0.47
3:P:5:G:H2'	3:P:6:G:O4'	2.14	0.47
1:J:210:ALA:O	1:J:211:TYR:HB2	2.14	0.47
2:F:198:LYS:HB3	2:F:202:ASN:N	2.29	0.47
1:I:153:LYS:HG3	1:I:320:ILE:HD11	1.96	0.47
2:F:163:GLU:HB3	2:F:167:LYS:HZ2	1.80	0.46
1:J:83:LEU:HD11	1:J:97:PRO:HD3	1.96	0.46
1:J:352:GLU:O	1:J:356:ARG:HG3	2.15	0.46
1:I:310:LEU:O	1:I:313:ILE:HG12	2.15	0.46
1:I:234:LLP:HG2	1:J:61:TYR:HE2	1.80	0.46
2:F:125:LYS:NZ	3:P:45:U:O5'	2.49	0.45
2:F:143:GLU:HA	2:F:146:ARG:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:197:ALA:O	2:F:200:LEU:HB2	2.17	0.45
2:F:143:GLU:HB3	2:F:146:ARG:NH2	2.31	0.45
2:F:151:PRO:HA	2:F:152:GLU:CB	2.47	0.45
2:F:151:PRO:CA	2:F:152:GLU:HB2	2.45	0.45
2:F:161:LYS:CE	3:P:18:G:O2'	2.60	0.45
1:J:76:CYS:HA	1:J:77:PRO:C	2.37	0.45
3:P:32:U:H2'	3:P:33:G:C8	2.52	0.45
1:I:16:LEU:O	1:I:18:ILE:N	2.50	0.45
3:P:24:C:O2'	3:P:25:A:H5'	2.17	0.44
1:J:149:TYR:HA	1:J:150:PRO:HA	1.81	0.44
3:P:29:G:H2'	3:P:30:A:C8	2.52	0.44
3:P:30:A:H61	3:P:38:U:H3	1.65	0.44
1:I:85:ASP:OD2	1:J:23:TYR:OH	2.27	0.44
1:J:47:PRO:HB2	1:J:49:GLU:OE1	2.17	0.44
1:J:124:ASN:HB3	1:J:182:ASP:HB3	1.98	0.44
2:F:121:PHE:CE1	2:F:133:VAL:HG23	2.52	0.44
1:J:311:GLU:HG2	1:J:315:PHE:O	2.18	0.44
2:F:151:PRO:CB	2:F:152:GLU:HB2	2.46	0.44
2:F:159:LYS:HE3	2:F:159:LYS:HB2	1.80	0.44
1:J:201:LYS:O	1:J:203:ILE:HG13	2.18	0.44
3:P:15:G:O2'	3:P:16:G:OP1	2.30	0.44
3:P:74:C:H1'	3:P:75:A:H5'	1.99	0.44
2:F:154:ALA:O	2:F:158:LEU:HD13	2.18	0.43
2:F:152:GLU:HA	2:F:155:LEU:HD13	2.00	0.43
1:I:145:TYR:CD2	1:I:148:GLU:HG2	2.53	0.43
1:I:91:ASN:O	1:I:221:LYS:HG3	2.18	0.43
1:J:313:ILE:HD12	1:J:392:VAL:HG21	1.99	0.43
3:P:30:A:N6	3:P:38:U:H3	2.16	0.43
1:J:91:ASN:O	1:J:221:LYS:HG3	2.19	0.43
1:J:317:GLN:HB3	1:J:321:LYS:HE2	2.01	0.43
1:J:114:LYS:HD3	1:J:114:LYS:HA	1.78	0.43
1:J:303:THR:HG23	1:J:328:ILE:HD11	2.00	0.43
1:I:149:TYR:HA	1:I:150:PRO:HA	1.72	0.42
1:J:48:LYS:HD2	2:F:58:GLU:HG2	2.00	0.42
2:F:155:LEU:O	2:F:158:LEU:HB2	2.19	0.42
2:F:198:LYS:HZ3	2:F:203:ALA:C	2.22	0.42
3:P:20:U:O2'	3:P:21:A:OP1	2.29	0.42
1:J:309:GLU:OE2	1:J:389:LYS:NZ	2.49	0.42
1:I:313:ILE:HD12	1:I:392:VAL:HG21	2.01	0.42
1:J:151:THR:O	1:J:319:GLY:HA2	2.19	0.42
2:F:117:ASN:OD1	3:P:56:A:H5"	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:19:ASN:HB3	1:J:22:LYS:NZ	2.35	0.42
3:P:39:C:H2'	3:P:40:C:O4'	2.19	0.42
1:I:48:LYS:HD2	2:E:58:GLU:HG2	2.02	0.42
1:I:345:ARG:NH2	3:P:71:C:H5"	2.34	0.42
2:F:118:LYS:HZ2	2:F:118:LYS:HG3	1.68	0.42
2:F:179:GLU:O	2:F:180:LYS:HD2	2.19	0.42
1:I:352:GLU:O	1:I:356:ARG:HG3	2.20	0.42
2:F:105:LYS:HG3	2:F:209:ASP:HA	2.02	0.42
1:I:23:TYR:OH	1:J:85:ASP:OD2	2.30	0.42
1:J:92:MET:SD	1:J:220:GLY:HA3	2.60	0.42
2:F:48:GLU:OE2	2:F:93:LYS:HD2	2.20	0.42
3:P:11:U:HO2'	3:P:12:C:P	2.43	0.42
2:F:142:ILE:HG12	2:F:155:LEU:HD23	2.02	0.41
2:F:191:GLU:HA	2:F:194:TYR:HB3	2.02	0.41
1:I:30:LEU:HD22	1:I:33:GLU:OE2	2.19	0.41
1:I:332:THR:OG1	1:I:366:THR:O	2.31	0.41
2:F:112:LEU:HD13	2:F:132:LYS:NZ	2.35	0.41
1:J:179:THR:HA	1:J:208:ASN:HB3	2.03	0.41
2:F:173:ILE:HG13	2:F:178:PRO:HD2	2.02	0.41
3:P:21:A:H2'	3:P:22:G:O4'	2.20	0.41
1:I:204:PRO:HA	1:I:226:ASP:OD2	2.21	0.41
2:F:141:ASP:HB3	2:F:144:ASP:OD2	2.21	0.41
2:F:155:LEU:C	2:F:157:GLY:H	2.24	0.41
1:I:122:ASP:OD2	1:I:124:ASN:HB2	2.21	0.41
1:J:19:ASN:OD1	1:J:20:LEU:N	2.54	0.41
1:J:286:PHE:HB3	1:J:287:PRO:HD3	2.03	0.41
2:F:118:LYS:CE	3:P:57:A:H3'	2.51	0.41
1:I:282:LEU:O	4:I:404:HOH:O	2.21	0.41
2:F:117:ASN:HD22	2:F:120:LEU:HD13	1.86	0.40
2:F:160:LYS:O	2:F:164:ILE:HG13	2.20	0.40
1:I:58:TRP:HE1	1:J:32:ARG:NH1	2.19	0.40
1:I:135:ARG:C	1:I:137:LYS:H	2.24	0.40
2:F:185:VAL:HG11	2:F:191:GLU:HG3	2.02	0.40
2:F:198:LYS:HB3	2:F:202:ASN:H	1.86	0.40
1:I:324:GLU:O	4:I:403:HOH:O	2.22	0.40
2:F:143:GLU:OE1	2:F:143:GLU:N	2.53	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	I	362/417 (87%)	347 (96%)	13 (4%)	2 (1%)	25 47
1	J	372/417 (89%)	356 (96%)	11 (3%)	5 (1%)	12 24
2	E	66/216 (31%)	65 (98%)	1 (2%)	0	100 100
2	F	175/216 (81%)	157 (90%)	13 (7%)	5 (3%)	4 7
All	All	975/1266 (77%)	925 (95%)	38 (4%)	12 (1%)	13 27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	17	ASP
1	J	77	PRO
2	F	202	ASN
2	F	203	ALA
2	F	207	ASP
1	I	27	THR
1	J	273	THR
1	J	274	SER
2	F	152	GLU
2	F	150	VAL
1	J	148	GLU
1	J	78	PRO

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	I	314/359 (88%)	313 (100%)	1 (0%)	92 98
1	J	324/359 (90%)	322 (99%)	2 (1%)	86 95
2	E	60/195 (31%)	60 (100%)	0	100 100
2	F	158/195 (81%)	153 (97%)	5 (3%)	39 65
All	All	856/1108 (77%)	848 (99%)	8 (1%)	78 91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	211	TYR
1	J	123	LYS
1	J	211	TYR
2	F	86	LYS
2	F	151	PRO
2	F	152	GLU
2	F	189	LYS
2	F	202	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	74/75 (98%)	28 (37%)	4 (5%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	8	U
3	P	9	A
3	P	11	U
3	P	12	C
3	P	13	U
3	P	16	G
3	P	17	G
3	P	18	G
3	P	19	C
3	P	20	U
3	P	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	24	C
3	P	25	A
3	P	26	G
3	P	30	A
3	P	31	C
3	P	32	U
3	P	35	A
3	P	40	C
3	P	43	C
3	P	44	U
3	P	45	U
3	P	47	C
3	P	57	A
3	P	70	G
3	P	71	C
3	P	74	C
3	P	75	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	P	15	G
3	P	16	G
3	P	20	U
3	P	31	C

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	I	234	1	23,24,25	2.61	6 (26%)	25,32,34	1.34	3 (12%)
1	LLP	J	234	1	23,24,25	2.66	8 (34%)	25,32,34	1.45	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	I	234	1	-	8/16/17/19	0/1/1/1
1	LLP	J	234	1	-	6/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	234	LLP	C4-C4'	8.05	1.61	1.46
1	J	234	LLP	C4-C4'	7.87	1.61	1.46
1	J	234	LLP	C4'-NZ	4.84	1.43	1.27
1	I	234	LLP	C4'-NZ	4.81	1.43	1.27
1	J	234	LLP	C4-C5	-4.64	1.36	1.42
1	I	234	LLP	C4-C5	-4.20	1.36	1.42
1	J	234	LLP	C2'-C2	3.57	1.56	1.50
1	I	234	LLP	C2'-C2	3.51	1.56	1.50
1	I	234	LLP	C6-N1	3.02	1.40	1.34
1	J	234	LLP	C6-N1	2.94	1.40	1.34
1	J	234	LLP	C3-C2	2.27	1.43	1.40
1	J	234	LLP	C4-C3	-2.08	1.37	1.40
1	I	234	LLP	C3-C2	2.02	1.42	1.40
1	J	234	LLP	CB-CA	-2.00	1.50	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	234	LLP	CE-NZ-C4'	-3.42	108.41	118.90
1	J	234	LLP	C4-C4'-NZ	-3.38	108.77	124.31
1	J	234	LLP	CE-NZ-C4'	-3.21	109.04	118.90
1	I	234	LLP	C4-C4'-NZ	-3.04	110.36	124.31
1	J	234	LLP	C5-C6-N1	-2.64	119.42	123.82
1	J	234	LLP	C3-C4-C5	2.53	120.20	118.26
1	I	234	LLP	C5-C6-N1	-2.42	119.79	123.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	234	LLP	C4-C4'-NZ-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	I	234	LLP	C5'-OP4-P-OP1
1	I	234	LLP	C5'-OP4-P-OP2
1	I	234	LLP	N-CA-CB-CG
1	I	234	LLP	C-CA-CB-CG
1	J	234	LLP	C4-C4'-NZ-CE
1	I	234	LLP	CG-CD-CE-NZ
1	J	234	LLP	CG-CD-CE-NZ
1	J	234	LLP	CA-CB-CG-CD
1	J	234	LLP	CD-CE-NZ-C4'
1	I	234	LLP	CD-CE-NZ-C4'
1	J	234	LLP	CE-CD-CG-CB
1	I	234	LLP	C3-C4-C4'-NZ
1	J	234	LLP	C4-C5-C5'-OP4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	234	LLP	2	0
1	J	234	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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	I	366/417 (87%)	0.76	26 (7%) 16 11	39, 65, 93, 124	0
1	J	376/417 (90%)	0.72	33 (8%) 10 7	40, 66, 101, 126	0
2	E	68/216 (31%)	0.32	1 (1%) 73 70	42, 53, 65, 85	0
2	F	177/216 (81%)	1.87	64 (36%) 0 0	46, 107, 143, 172	0
3	P	75/75 (100%)	2.00	31 (41%) 0 0	94, 127, 184, 189	0
All	All	1062/1341 (79%)	0.99	155 (14%) 2 1	39, 67, 135, 189	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	153	LYS	12.2
3	P	43	C	11.5
3	P	25	A	9.9
3	P	42	C	9.7
2	F	139	MET	9.6
2	F	150	VAL	8.2
3	P	41	G	8.1
2	F	151	PRO	7.6
2	F	203	ALA	7.6
2	F	172	PHE	7.5
3	P	26	G	6.6
3	P	22	G	6.6
1	I	76	CYS	6.5
2	F	165	ALA	6.4
2	F	157	GLY	6.0
3	P	16	G	6.0
1	J	63	VAL	6.0
2	F	175	LYS	5.8
2	F	156	GLU	5.8
2	F	158	LEU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	162	VAL	5.7
2	F	154	ALA	5.5
2	F	148	ILE	5.5
3	P	40	C	5.5
3	P	75	A	5.4
2	F	181	ILE	5.4
2	F	171	ARG	5.4
3	P	44	U	5.3
3	P	23	G	5.3
2	F	155	LEU	5.2
2	F	182	PHE	5.0
2	F	146	ARG	4.9
2	F	166	ARG	4.8
1	I	27	THR	4.8
1	J	77	PRO	4.8
2	F	178	PRO	4.8
2	F	140	LEU	4.7
1	J	273	THR	4.6
3	P	10	G	4.6
2	F	163	GLU	4.5
3	P	27	C	4.5
2	F	143	GLU	4.5
2	F	131	LEU	4.3
2	F	200	LEU	4.3
3	P	9	A	4.2
2	F	177	LYS	4.2
2	F	202	ASN	4.2
2	F	152	GLU	4.2
2	F	132	LYS	4.2
3	P	24	C	4.0
1	J	65	ASP	3.9
1	J	62	SER	3.9
1	J	16	LEU	3.6
2	F	199	ASN	3.6
3	P	29	G	3.6
2	F	201	TYR	3.5
2	F	174	GLU	3.5
2	F	197	ALA	3.5
2	F	167	LYS	3.4
1	I	200	GLU	3.4
1	J	73	GLU	3.4
3	P	15	G	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	274	SER	3.4
2	F	125	LYS	3.3
2	F	176	TYR	3.3
3	P	20	U	3.3
1	J	28	ARG	3.3
1	J	61	TYR	3.1
2	F	118	LYS	3.1
1	I	240	ALA	3.0
2	F	106	GLU	3.0
1	J	13	VAL	3.0
1	J	14	ILE	3.0
1	J	58	TRP	3.0
1	I	58	TRP	2.9
1	J	172	ASN	2.8
2	F	114	ILE	2.8
2	F	208	ALA	2.8
2	F	134	VAL	2.8
1	I	39	PRO	2.8
1	I	241	PRO	2.8
3	P	3	C	2.8
2	F	194	TYR	2.8
2	F	126	ASN	2.8
3	P	74	C	2.8
1	J	60	GLY	2.7
1	I	16	LEU	2.7
1	I	30	LEU	2.7
2	F	142	ILE	2.7
2	F	117	ASN	2.7
1	J	242	CYS	2.7
2	F	141	ASP	2.7
1	J	393	GLU	2.7
2	F	161	LYS	2.6
1	J	276	GLY	2.6
2	F	159	LYS	2.6
3	P	39	C	2.6
1	I	61	TYR	2.6
3	P	5	G	2.6
3	P	36	G	2.6
2	F	111	ALA	2.6
1	I	41	GLN	2.6
2	F	124	LEU	2.6
2	F	196	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	P	68	C	2.6
1	I	347	PHE	2.6
1	I	28	ARG	2.6
2	F	145	MET	2.5
1	J	156	LEU	2.5
1	J	194	VAL	2.5
1	J	20	LEU	2.5
1	I	170	GLY	2.5
1	J	275	ARG	2.5
1	I	392	VAL	2.5
1	J	210	ALA	2.5
1	J	57	TYR	2.4
2	F	160	LYS	2.4
3	P	14	A	2.4
1	I	40	ILE	2.4
1	J	272	CYS	2.4
2	F	147	ALA	2.3
3	P	21	A	2.3
1	I	31	THR	2.3
1	I	210	ALA	2.3
2	E	89	GLU	2.3
1	I	374	TYR	2.3
1	J	222	GLU	2.3
1	J	241	PRO	2.2
1	J	25	ASN	2.2
2	F	206	LEU	2.2
2	F	179	GLU	2.2
2	F	113	TYR	2.2
2	F	116	SER	2.2
2	F	133	VAL	2.2
1	J	97	PRO	2.2
1	I	211	TYR	2.2
1	I	233	HIS	2.2
2	F	180	LYS	2.2
1	I	172	ASN	2.2
1	J	277	LEU	2.1
2	F	184	VAL	2.1
3	P	12	C	2.1
2	F	104	GLU	2.1
3	P	38	U	2.1
3	P	28	G	2.1
1	I	278	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	163	ILE	2.1
1	I	313	ILE	2.1
1	J	98	THR	2.1
3	P	6	G	2.0
2	F	149	GLY	2.0
3	P	30	A	2.0
1	J	64	CYS	2.0
1	J	396	LYS	2.0
1	I	277	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	I	234	24/25	0.97	0.28	38,65,76,77	0
1	LLP	J	234	24/25	0.97	0.22	44,61,72,73	0

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.