Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 07:31 am BST

PDB ID	:	5L75
Title	:	A protein structure
Authors	:	Dong, C.; Dong, H.; Zhang, Z.; Paterson, N.; Tang, X.
Deposited on	:	2016-06-01
Resolution	:	3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

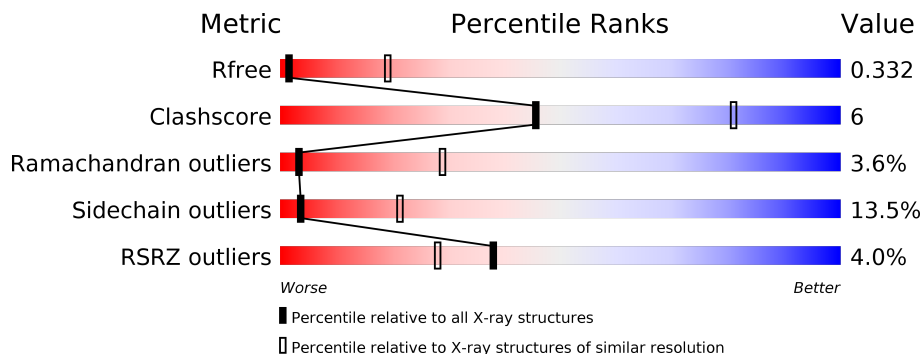|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.332
Clashscore		6
Ramachandran outliers		3.6%
Sidechain outliers		13.5%
RSRZ outliers		4.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	241	2% / 68% 24% 5% ·
1	B	241	% / 76% 21% ··
2	F	365	5% / 57% 25% 5% 12%
3	G	360	6% / 74% 18% · 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8824 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 Lipopolysaccharide ABC transporter, ATP-binding protein LptB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total 1833	C 1149	N 335	O 345	S 4	0	0	0
1	B	237	Total 1850	C 1159	N 337	O 349	S 5	0	0	0

- Molecule 2 is a protein called FIG000988: Predicted permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	323	Total 2503	C 1636	N 418	O 433	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	107	VAL	LEU	conflict	UNP W1B830
F	204	TYR	VAL	conflict	UNP W1B830

- Molecule 3 is a protein called FIG000906: Predicted Permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	340	Total 2636	C 1720	N 433	O 465	S 18	0	0	0

- Molecule 4 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Pt 1	0	0
4	A	1	Total 1	Pt 1	0	0

3 Residue-property plots (i)

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: Lipopolysaccharide ABC transporter, ATP-binding protein LptB
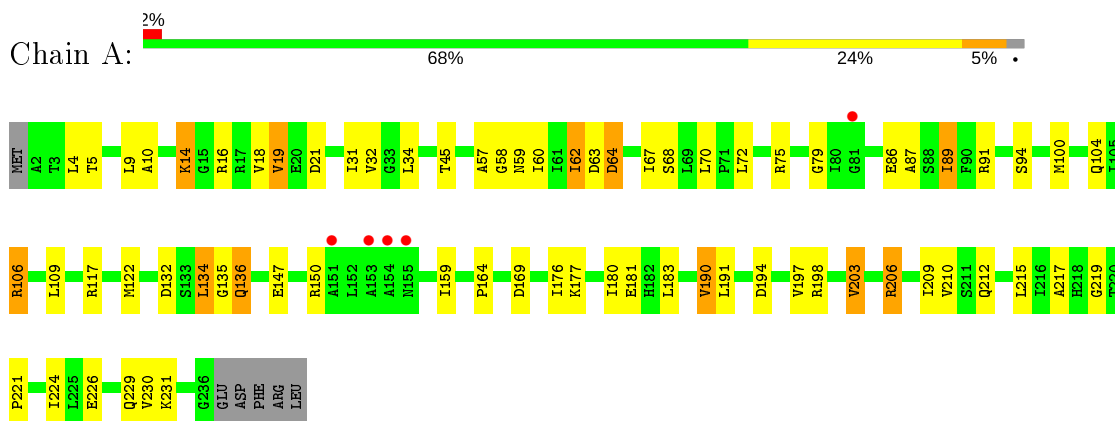
- Molecule 1: Lipopolysaccharide ABC transporter, ATP-binding protein LptB
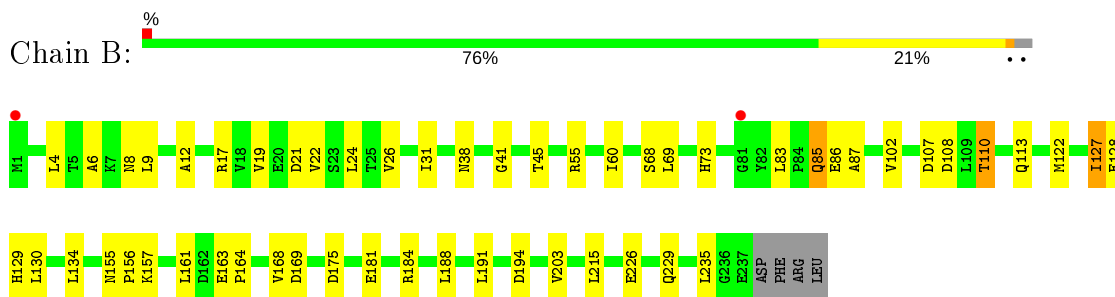
- Molecule 2: FIG000988: Predicted permease

I278 M282 V283 V284 P285 V288 V289 N290 Q293 G294 R295 V296 L297 L300 L307 F310 L311 L312 Q313 K317 G320 G321 K322 G323 K324 M325 D326 P327 A328 I329 W330 M331 W332 A333 I334 N335 Y338 L344 L345 W348 ASP THR VAL PRO MET ARG ARG PHE ARG

ALA ARG PHE ASN LYS GLY ALA ALA
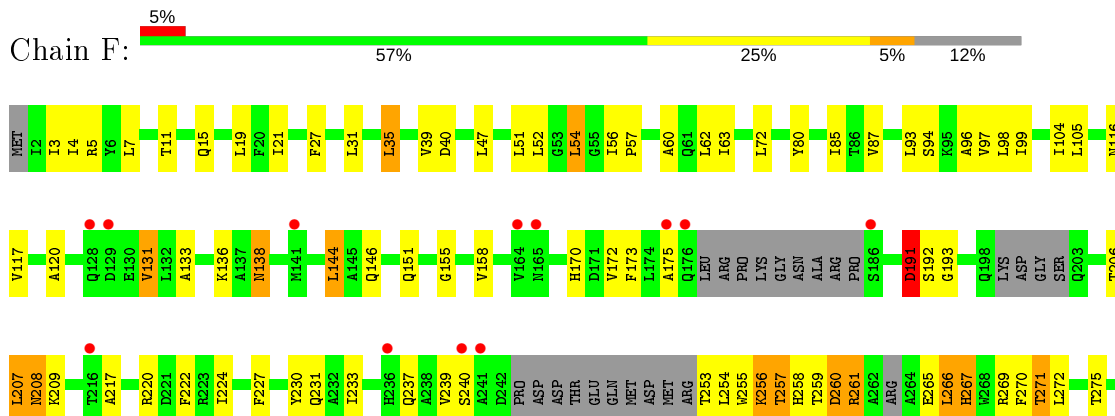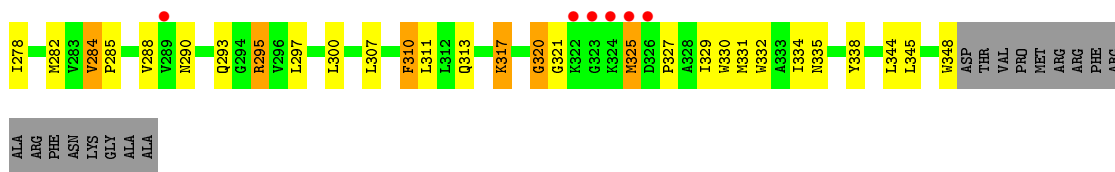
- **Molecule 3: FIG000906: Predicted Permease**

Chain G:

6%

74%   18%   •   6%

MET GLN ALA PHE GLY V6 L7 D8 R9 I15 F24 I29 I32 I33 K40 G45 L50 Y55 V60 P61 K62 D63 I64 F68 L73 L80 R86 L89 T98 Q101 L104 L116 T117 I120 G121 Q139 M140 Y141 L145

T148 Q149 Q150 G151 L152 W153 K167 G168 N169 V175 S176 F180 R184 R190 D198 S199 E200 N201 LYS VAL W204 V209 D210 E211 T215 D216 Q219 S223 Q224 M225 V226 SER GLY THR TRP LYS THR N233 L234 L239 L244 A248 L249 V258 K259

Y260 LEU LYS SER GLY GLN ASP P268 Y271 Q272 L273 N274 M275 W276 S277 F280 L290 L293 I296 F297 G298 P299 L300 R301 S302 G306 V307 R308 V309 V310 I313 F326 G327 P328 L329 P337 L343 M357 R358 K359 A360

4   Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.26Å 210.52Å 258.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.70 29.96 – 3.70	Depositor EDS
% Data completeness (in resolution range)	65.3 (29.96-3.70) 65.3 (29.96-3.70)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.65 (at 3.75Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.284 , 0.322 0.305 , 0.332	Depositor DCC
R_{free} test set	1041 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	124.0	Xtriage
Anisotropy	1.734	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 72.9	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8824	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.42	0/1858	0.64	0/2512
1	B	0.42	0/1875	0.64	0/2534
2	F	0.45	0/2550	0.67	0/3459
3	G	0.46	0/2691	0.70	0/3639
All	All	0.44	0/8974	0.67	0/12144

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	1833	0	1871	26	0
1	B	1850	0	1889	18	0
2	F	2503	0	2595	48	3
3	G	2636	0	2715	28	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
All	All	8824	0	9070	115	3

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 6.

All (115) 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:F:257:THR:HG23	2:F:258:HIS:H	1.31	0.96
2:F:253:THR:HG22	2:F:256:LYS:NZ	1.89	0.87
1:A:89:ILE:HA	1:A:150:ARG:HH21	1.42	0.83
2:F:275:THR:HA	2:F:278:ILE:HG22	1.61	0.83
2:F:253:THR:HG22	2:F:256:LYS:HZ1	1.49	0.77
1:A:60:ILE:H	1:A:68:SER:HB3	1.52	0.74
3:G:273:LEU:HA	3:G:337:PRO:HB3	1.69	0.74
3:G:209:VAL:HB	3:G:225:MET:HG3	1.71	0.72
1:B:22:VAL:HG23	1:B:215:LEU:HB2	1.76	0.67
2:F:257:THR:HG23	2:F:258:HIS:N	2.05	0.67
2:F:260:ASP:O	2:F:261:ARG:HB2	1.97	0.65
2:F:116:ASN:HA	2:F:120:ALA:HB3	1.77	0.64
2:F:117:VAL:HG13	2:F:269:ARG:HG3	1.82	0.62
3:G:64:ILE:HD11	3:G:120:ILE:HG13	1.82	0.62
1:B:60:ILE:H	1:B:68:SER:HB3	1.65	0.61
1:B:164:PRO:HD2	1:B:194:ASP:HB2	1.84	0.60
1:A:164:PRO:HD2	1:A:194:ASP:HB2	1.84	0.59
1:A:31:ILE:HB	1:A:190:VAL:HG22	1.84	0.59
1:A:206:ARG:HE	1:A:219:GLY:HA2	1.68	0.59
1:B:19:VAL:HG11	1:B:45:THR:HB	1.83	0.59
2:F:285:PRO:HG2	2:F:345:LEU:HG	1.86	0.58
2:F:257:THR:CG2	2:F:258:HIS:H	2.12	0.57
2:F:60:ALA:HA	2:F:63:ILE:HG12	1.86	0.57
3:G:60:VAL:HG13	3:G:61:PRO:HD3	1.87	0.57
2:F:56:ILE:HG13	2:F:57:PRO:HD3	1.85	0.57
1:A:177:LYS:HE3	1:A:203:VAL:HG13	1.87	0.57
1:B:122:MET:HB3	1:B:128:GLU:HG3	1.87	0.56
3:G:64:ILE:HD12	3:G:117:THR:HA	1.88	0.56
2:F:151:GLN:HE22	2:F:155:GLY:H	1.55	0.55
2:F:256:LYS:O	2:F:257:THR:C	2.45	0.55
3:G:64:ILE:HG23	3:G:117:THR:HG22	1.87	0.55
1:A:34:LEU:HD21	1:A:45:THR:HB	1.89	0.54
3:G:293:LEU:HA	3:G:296:ILE:HG22	1.89	0.54
1:A:10:ALA:HB3	1:A:57:ALA:HB3	1.88	0.54
2:F:334:ILE:O	2:F:338:TYR:HB2	2.09	0.53
2:F:253:THR:HG22	2:F:256:LYS:HZ2	1.71	0.53
1:B:157:LYS:HG3	1:B:188:LEU:HD23	1.91	0.52
2:F:313:GLN:HE21	2:F:331:MET:HG3	1.75	0.51
1:A:94:SER:HA	1:A:134:LEU:HA	1.93	0.51
3:G:145:LEU:HD22	3:G:168:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:239:VAL:HG22	2:F:240:SER:H	1.76	0.51
2:F:295:ARG:HE	3:G:306:GLY:H	1.59	0.51
1:A:9:LEU:HA	1:A:58:GLY:HA2	1.93	0.50
3:G:80:LEU:HD13	3:G:296:ILE:HG21	1.94	0.50
1:B:12:ALA:HB2	1:B:17:ARG:HD3	1.93	0.49
2:F:192:SER:HB2	2:F:208:ASN:HB2	1.94	0.49
1:A:100:MET:O	1:A:104:GLN:HG2	2.12	0.49
3:G:300:LEU:HA	3:G:308:ARG:HH22	1.78	0.49
3:G:64:ILE:HG21	3:G:121:GLY:HA3	1.93	0.49
3:G:15:ILE:HD11	3:G:80:LEU:HG	1.94	0.49
2:F:57:PRO:HB3	2:F:120:ALA:HB1	1.96	0.48
1:A:106:ARG:HE	1:A:106:ARG:HA	1.79	0.48
2:F:275:THR:HG21	2:F:310:PHE:HE1	1.79	0.48
3:G:215:THR:HG22	3:G:219:GLN:HE21	1.79	0.48
2:F:256:LYS:O	2:F:258:HIS:O	2.31	0.47
1:A:4:LEU:HD12	1:A:62:ILE:HA	1.97	0.47
1:B:85:GLN:HG3	1:B:163:GLU:HB2	1.96	0.47
2:F:206:THR:HA	2:F:230:TYR:O	2.15	0.47
3:G:276:TRP:HD1	3:G:337:PRO:HB2	1.79	0.47
2:F:117:VAL:HG22	2:F:269:ARG:HE	1.79	0.47
2:F:317:LYS:HZ2	2:F:327:PRO:HG3	1.80	0.47
1:B:83:LEU:HB3	1:B:161:LEU:HD23	1.96	0.47
1:B:6:ALA:HB1	1:B:9:LEU:HD13	1.96	0.47
2:F:295:ARG:HH21	3:G:306:GLY:HA3	1.79	0.46
2:F:35:LEU:HD22	3:G:328:PRO:HB2	1.96	0.46
3:G:180:PHE:HB3	3:G:184:ARG:HA	1.97	0.46
2:F:158:VAL:HG11	3:G:153:TRP:NE1	2.30	0.46
1:B:155:ASN:N	1:B:156:PRO:HD3	2.30	0.46
2:F:266:LEU:HD23	2:F:270:PHE:HB2	1.98	0.46
2:F:320:GLY:HA3	2:F:325:MET:HG2	1.98	0.46
2:F:311:LEU:HD21	3:G:33:ILE:HG13	1.98	0.46
1:A:210:VAL:HG12	1:A:215:LEU:HA	1.99	0.45
1:A:18:VAL:HG13	1:A:19:VAL:HG22	1.98	0.45
1:B:55:ARG:HD3	1:B:68:SER:HB2	1.98	0.45
2:F:193:GLY:HA2	2:F:207:LEU:HA	1.97	0.45
1:A:91:ARG:HG3	1:A:136:GLN:HA	1.99	0.45
2:F:15:GLN:O	2:F:19:LEU:HB2	2.17	0.45
1:A:89:ILE:HG23	1:A:147:GLU:HG3	1.99	0.45
1:B:31:ILE:HG21	1:B:203:VAL:HG13	1.99	0.45
1:A:159:ILE:HG21	1:A:183:LEU:HD23	1.99	0.45
3:G:29:LEU:HD12	3:G:32:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HA	1:A:180:ILE:HD12	2.00	0.44
2:F:80:TYR:HB2	2:F:288:VAL:HG12	1.98	0.44
2:F:267:HIS:O	2:F:271:THR:HB	2.16	0.44
1:A:14:LYS:HG3	1:A:16:ARG:HG3	2.00	0.44
1:B:110:THR:HB	1:B:113:GLN:HB2	2.00	0.44
3:G:298:GLY:HA2	3:G:359:LYS:HG3	1.99	0.43
1:B:4:LEU:HB3	1:B:26:VAL:HG13	1.99	0.43
1:A:221:PRO:HA	1:A:224:ILE:HD12	1.99	0.43
3:G:211:GLU:HG3	3:G:223:SER:HB3	2.01	0.43
2:F:31:LEU:HD13	2:F:52:LEU:HD13	2.00	0.42
2:F:51:LEU:HA	2:F:54:LEU:HB2	2.01	0.42
2:F:284:VAL:HG23	2:F:285:PRO:HD3	2.01	0.42
3:G:277:SER:HA	3:G:280:PHE:CD2	2.54	0.42
1:A:67:ILE:HA	1:A:70:LEU:HD13	2.02	0.41
1:B:129:HIS:CD2	1:B:130:LEU:HG	2.55	0.41
2:F:96:ALA:HA	2:F:99:ILE:HD12	2.01	0.41
1:A:67:ILE:HD12	1:A:75:ARG:HD3	2.02	0.41
2:F:133:ALA:HA	2:F:136:LYS:HG2	2.02	0.41
1:B:181:GLU:HG2	1:B:184:ARG:HH21	1.86	0.41
1:A:106:ARG:HB3	1:A:109:LEU:HD12	2.02	0.41
2:F:11:THR:HG21	2:F:72:LEU:HD12	2.02	0.41
2:F:191:ASP:HB2	2:F:209:LYS:HB3	2.02	0.41
1:B:127:ILE:HG22	1:B:130:LEU:HB2	2.02	0.41
2:F:138:ASN:HD21	2:F:237:GLN:HA	1.85	0.41
2:F:4:ILE:HD13	2:F:97:VAL:HG13	2.03	0.41
3:G:326:PHE:HA	3:G:329:LEU:HB2	2.01	0.41
3:G:80:LEU:HB3	3:G:296:ILE:HG12	2.03	0.41
3:G:98:THR:HB	3:G:101:GLN:H	1.86	0.41
1:A:209:ILE:HB	1:A:217:ALA:HB3	2.03	0.41
2:F:259:THR:O	2:F:259:THR:HG22	2.21	0.40
2:F:217:ALA:HB3	2:F:220:ARG:HB2	2.04	0.40
3:G:307:VAL:HA	3:G:310:VAL:HG22	2.03	0.40
1:A:9:LEU:HA	1:A:58:GLY:CA	2.52	0.40
2:F:4:ILE:HA	2:F:7:LEU:HD12	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:SER:CB	2:F:258:HIS:NE2[8_554]	1.39	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:SER:OG	2:F:258:HIS:NE2[8_554]	1.77	0.43
2:F:94:SER:OG	2:F:258:HIS:CD2[8_554]	1.93	0.27

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	233/241 (97%)	203 (87%)	23 (10%)	7 (3%)	4	32
1	B	235/241 (98%)	194 (83%)	37 (16%)	4 (2%)	9	42
2	F	313/365 (86%)	253 (81%)	41 (13%)	19 (6%)	1	18
3	G	332/360 (92%)	271 (82%)	51 (15%)	10 (3%)	4	32
All	All	1113/1207 (92%)	921 (83%)	152 (14%)	40 (4%)	3	29

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA
2	F	144	LEU
2	F	146	GLN
2	F	260	ASP
3	G	63	ASP
3	G	301	ARG
1	A	62	ILE
1	A	134	LEU
1	B	73	HIS
1	B	87	ALA
2	F	208	ASN
2	F	295	ARG
2	F	321	GLY
3	G	175	VAL
3	G	211	GLU

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Mol	Chain	Res	Type
3	G	219	GLN
3	G	302	SER
1	A	64	ASP
2	F	257	THR
2	F	261	ARG
3	G	199	SER
2	F	93	LEU
2	F	175	ALA
2	F	255	TRP
1	A	21	ASP
1	A	135	GLY
2	F	191	ASP
2	F	320	GLY
3	G	169	ASN
1	B	41	GLY
2	F	233	ILE
2	F	256	LYS
3	G	45	GLY
1	A	79	GLY
2	F	131	VAL
3	G	343	LEU
1	B	168	VAL
2	F	290	ASN
2	F	329	ILE
2	F	172	VAL

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	196/202 (97%)	167 (85%)	29 (15%)	3	18
1	B	198/202 (98%)	179 (90%)	19 (10%)	8	34
2	F	266/301 (88%)	220 (83%)	46 (17%)	2	12
3	G	283/300 (94%)	250 (88%)	33 (12%)	5	26
All	All	943/1005 (94%)	816 (86%)	127 (14%)	4	21

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	14	LYS
1	A	19	VAL
1	A	32	VAL
1	A	59	ASN
1	A	63	ASP
1	A	64	ASP
1	A	72	LEU
1	A	86	GLU
1	A	89	ILE
1	A	106	ARG
1	A	117	ARG
1	A	122	MET
1	A	132	ASP
1	A	136	GLN
1	A	169	ASP
1	A	176	ILE
1	A	181	GLU
1	A	190	VAL
1	A	191	LEU
1	A	197	VAL
1	A	198	ARG
1	A	203	VAL
1	A	206	ARG
1	A	212	GLN
1	A	226	GLU
1	A	229	GLN
1	A	230	VAL
1	A	231	LYS
1	B	8	ASN
1	B	21	ASP
1	B	24	LEU
1	B	38	ASN
1	B	69	LEU
1	B	85	GLN
1	B	86	GLU
1	B	102	VAL
1	B	107	ASP
1	B	108	ASP
1	B	110	THR
1	B	127	ILE
1	B	134	LEU

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Mol	Chain	Res	Type
1	B	169	ASP
1	B	175	ASP
1	B	191	LEU
1	B	226	GLU
1	B	229	GLN
1	B	235	LEU
2	F	3	ILE
2	F	5	ARG
2	F	21	ILE
2	F	27	PHE
2	F	35	LEU
2	F	39	VAL
2	F	40	ASP
2	F	47	LEU
2	F	54	LEU
2	F	62	LEU
2	F	85	ILE
2	F	87	VAL
2	F	98	LEU
2	F	104	ILE
2	F	105	LEU
2	F	131	VAL
2	F	138	ASN
2	F	144	LEU
2	F	170	HIS
2	F	173	PHE
2	F	191	ASP
2	F	207	LEU
2	F	222	PHE
2	F	224	ILE
2	F	227	PHE
2	F	231	GLN
2	F	254	LEU
2	F	265	GLU
2	F	266	LEU
2	F	267	HIS
2	F	271	THR
2	F	272	LEU
2	F	282	MET
2	F	284	VAL
2	F	293	GLN
2	F	297	LEU

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Mol	Chain	Res	Type
2	F	300	LEU
2	F	307	LEU
2	F	310	PHE
2	F	317	LYS
2	F	325	MET
2	F	330	TRP
2	F	332	TRP
2	F	335	ASN
2	F	344	LEU
2	F	348	TRP
3	G	7	LEU
3	G	9	ARG
3	G	24	PHE
3	G	33	ILE
3	G	50	LEU
3	G	55	TYR
3	G	63	ASP
3	G	68	PHE
3	G	73	LEU
3	G	86	ARG
3	G	89	LEU
3	G	98	THR
3	G	104	LEU
3	G	116	LEU
3	G	117	THR
3	G	139	GLN
3	G	141	TYR
3	G	150	GLN
3	G	152	LEU
3	G	167	LYS
3	G	184	ARG
3	G	198	ASP
3	G	216	ASP
3	G	234	LEU
3	G	244	LEU
3	G	249	LEU
3	G	275	MET
3	G	280	PHE
3	G	290	LEU
3	G	300	LEU
3	G	301	ARG
3	G	313	ILE

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Mol	Chain	Res	Type
3	G	357	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	126	HIS
1	B	196	ASN
1	B	229	GLN
2	F	138	ASN
2	F	151	GLN
2	F	237	GLN
2	F	313	GLN
3	G	38	GLN
3	G	219	GLN
3	G	233	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	179:ALA	C	180:PHE	N	3.86

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	235/241 (97%)	-0.14	5 (2%)	63	52	51, 93, 131, 162	0
1	B	237/241 (98%)	-0.34	2 (0%)	86	78	79, 126, 164, 195	0
2	F	323/365 (88%)	-0.20	18 (5%)	24	17	30, 113, 186, 252	0
3	G	340/360 (94%)	-0.04	20 (5%)	22	15	47, 96, 180, 254	0
All	All	1135/1207 (94%)	-0.17	45 (3%)	38	28	30, 107, 176, 254	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	324	LYS	8.1
1	B	1	MET	6.9
2	F	322	LYS	5.9
1	A	155	ASN	5.6
2	F	186	SER	5.4
3	G	360	ALA	5.3
3	G	176	SER	5.0
3	G	148	THR	4.9
1	B	81	GLY	4.7
2	F	240	SER	4.6
2	F	129	ASP	4.4
3	G	141	TYR	4.2
3	G	275	MET	3.8
3	G	239	LEU	3.6
2	F	236	HIS	3.5
1	A	154	ALA	3.5
3	G	359	LYS	3.4
2	F	325	MET	3.4
2	F	165	ASN	3.4
3	G	302	SER	3.0
3	G	260	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	153	ALA	3.0
1	A	151	ALA	3.0
2	F	323	GLY	3.0
3	G	211	GLU	2.8
3	G	271	TYR	2.8
2	F	164	VAL	2.8
2	F	128	GLN	2.7
2	F	241	ALA	2.7
3	G	190	ARG	2.7
3	G	140	MET	2.7
3	G	223	SER	2.6
2	F	141	MET	2.6
3	G	301	ARG	2.5
2	F	326	ASP	2.5
2	F	289	VAL	2.5
2	F	176	GLN	2.4
3	G	40	LYS	2.4
3	G	184	ARG	2.3
3	G	258	VAL	2.3
3	G	272	GLN	2.2
2	F	216	THR	2.2
3	G	248	ALA	2.2
2	F	175	ALA	2.1
1	A	81	GLY	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	PT	A	301	1/1	0.48	0.08	160,160,160,160	1
4	PT	G	401	1/1	0.90	0.35	236,236,236,236	1

6.5 Other polymers ⓘ

There are no such residues in this entry.