Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 09:49 PM JST

PDB ID	:	6JWP
Title	:	crystal structure of EGOC
Authors	:	Zhang, T.; Ding, J.
Deposited on	:	2019-04-21
Resolution	:	3.20 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:

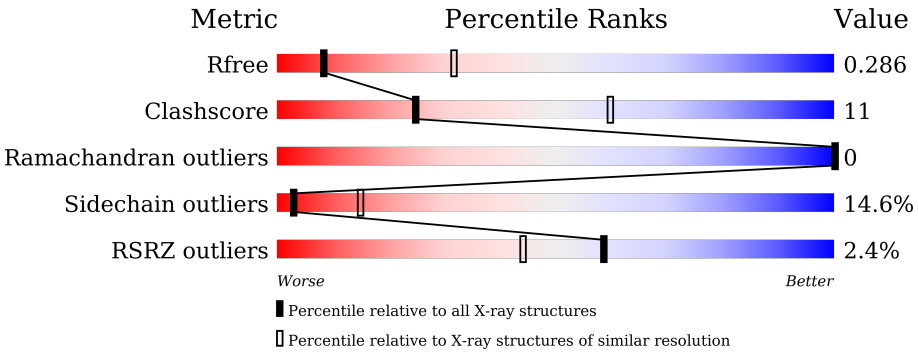
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	3% 58% 27% • 12%
1	F	312	63% 25% • 7%
2	B	345	% 55% 27% • 15%
2	G	345	% 41% 14% • 43%
3	C	129	6% 48% 21% 9% 22%
3	H	129	% 53% 16% • 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	75	72% 15% 11%
4	I	75	17% 51% 35% 13%
5	E	162	66% 21% 10%
5	J	162	65% 22% 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13142 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 GTP-binding protein GTR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2201	1425	361	398	17			
1	F	289	Total	C	N	O	S	0	0	0
			2342	1510	390	425	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q00582
A	0	HIS	-	expression tag	UNP Q00582
F	-1	SER	-	expression tag	UNP Q00582
F	0	HIS	-	expression tag	UNP Q00582

- Molecule 2 is a protein called GTP-binding protein GTR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	0	0	0
			2310	1479	367	450	14			
2	G	197	Total	C	N	O	S	0	0	0
			1396	886	230	274	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP P53290
B	-2	GLY	-	expression tag	UNP P53290
B	-1	ILE	-	expression tag	UNP P53290
B	0	ARG	-	expression tag	UNP P53290
G	-3	MET	-	initiating methionine	UNP P53290
G	-2	GLY	-	expression tag	UNP P53290
G	-1	ILE	-	expression tag	UNP P53290
G	0	ARG	-	expression tag	UNP P53290

- Molecule 3 is a protein called Protein MEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	100	Total	C	N	O	S	0	0	0
			780	488	138	153	1			
3	H	94	Total	C	N	O	S	0	0	0
			735	460	128	146	1			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	MET	-	initiating methionine	UNP Q02205
C	?	-	GLN	deletion	UNP Q02205
C	?	-	GLU	deletion	UNP Q02205
C	?	-	GLU	deletion	UNP Q02205
C	?	-	GLY	deletion	UNP Q02205
C	?	-	GLY	deletion	UNP Q02205
C	?	-	ASP	deletion	UNP Q02205
C	?	-	SER	deletion	UNP Q02205
C	?	-	ARG	deletion	UNP Q02205
C	?	-	GLU	deletion	UNP Q02205
C	?	-	ASP	deletion	UNP Q02205
C	?	-	GLU	deletion	UNP Q02205
C	?	-	ARG	deletion	UNP Q02205
C	?	-	SER	deletion	UNP Q02205
C	?	-	ALA	deletion	UNP Q02205
C	?	-	GLY	deletion	UNP Q02205
C	?	-	ASP	deletion	UNP Q02205
C	?	-	ASP	deletion	UNP Q02205
C	?	-	ASN	deletion	UNP Q02205
C	?	-	LEU	deletion	UNP Q02205
C	?	-	SER	deletion	UNP Q02205
C	?	-	GLY	deletion	UNP Q02205
C	?	-	HIS	deletion	UNP Q02205
C	?	-	SER	deletion	UNP Q02205
C	?	-	VAL	deletion	UNP Q02205
H	32	MET	-	initiating methionine	UNP Q02205
H	?	-	GLN	deletion	UNP Q02205
H	?	-	GLU	deletion	UNP Q02205
H	?	-	GLU	deletion	UNP Q02205
H	?	-	GLY	deletion	UNP Q02205
H	?	-	GLY	deletion	UNP Q02205
H	?	-	ASP	deletion	UNP Q02205
H	?	-	SER	deletion	UNP Q02205
H	?	-	ARG	deletion	UNP Q02205

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP Q02205
H	?	-	ASP	deletion	UNP Q02205
H	?	-	GLU	deletion	UNP Q02205
H	?	-	ARG	deletion	UNP Q02205
H	?	-	SER	deletion	UNP Q02205
H	?	-	ALA	deletion	UNP Q02205
H	?	-	GLY	deletion	UNP Q02205
H	?	-	ASP	deletion	UNP Q02205
H	?	-	ASP	deletion	UNP Q02205
H	?	-	ASN	deletion	UNP Q02205
H	?	-	LEU	deletion	UNP Q02205
H	?	-	SER	deletion	UNP Q02205
H	?	-	GLY	deletion	UNP Q02205
H	?	-	HIS	deletion	UNP Q02205
H	?	-	SER	deletion	UNP Q02205
H	?	-	VAL	deletion	UNP Q02205

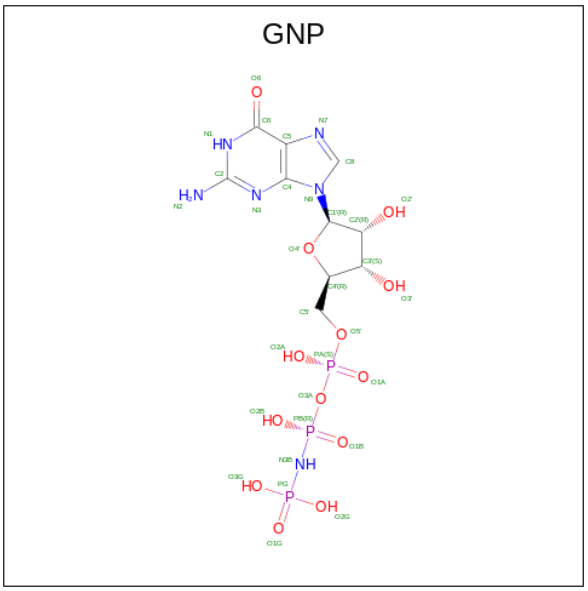
- Molecule 4 is a protein called Ego2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	67	Total	C	N	O	0	0	0
			503	314	85	104			
4	I	65	Total	C	N	O	0	0	0
			488	304	83	101			

- Molecule 5 is a protein called Protein SLM4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	146	Total	C	N	O	S	0	0	0
			1149	734	181	226	8			
5	J	144	Total	C	N	O	S	0	0	0
			1139	729	179	223	8			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
6	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
6	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

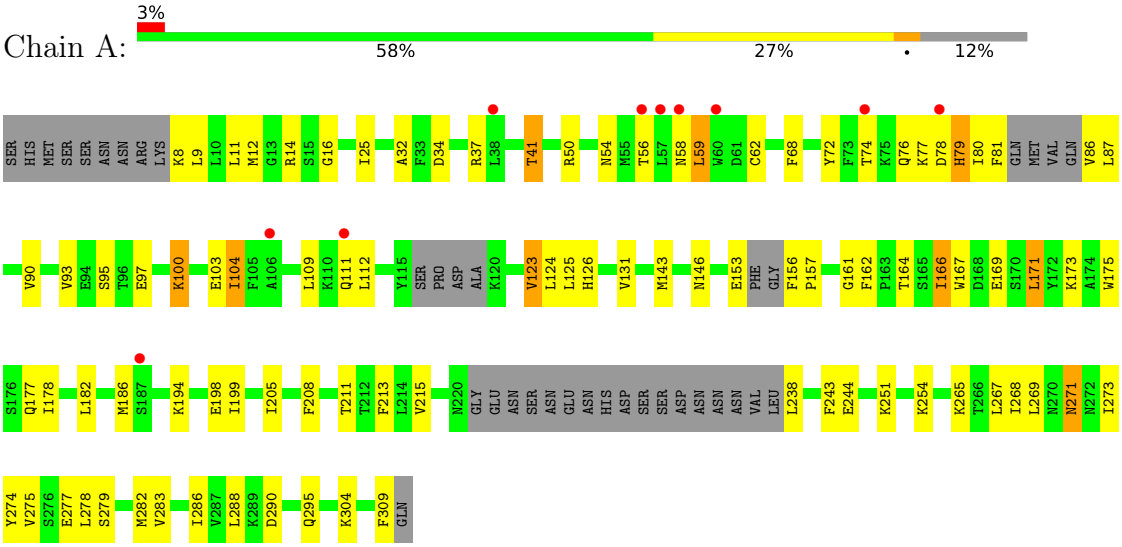
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

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.

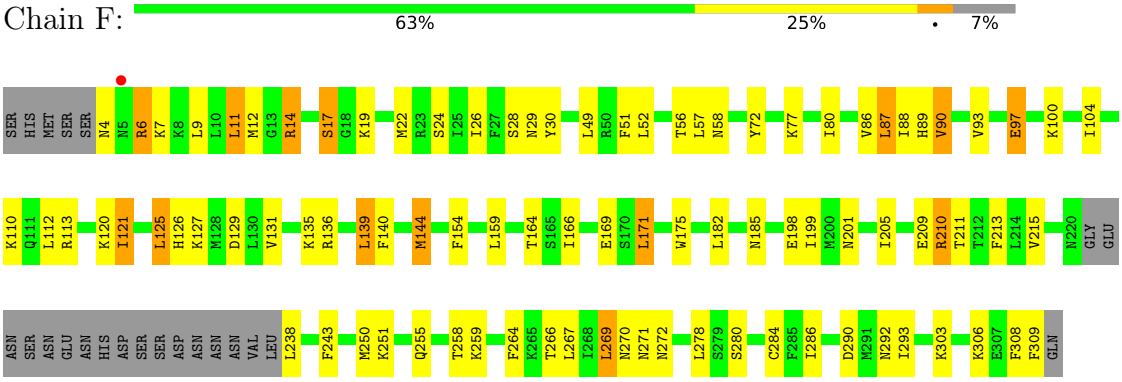
• Molecule 1: GTP-binding protein GTR1

Chain A:



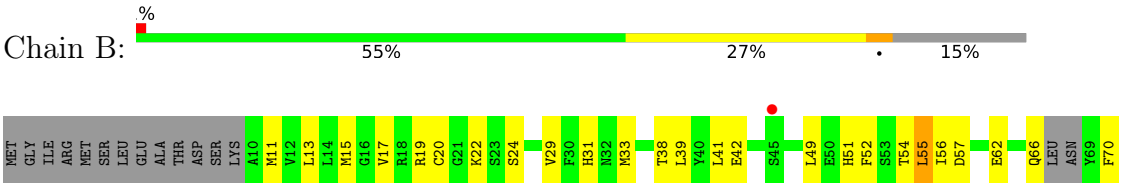
• Molecule 1: GTP-binding protein GTR1

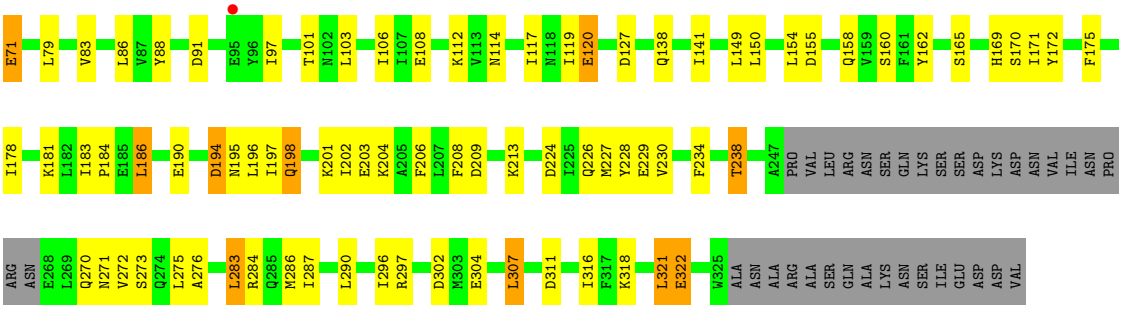
Chain F:



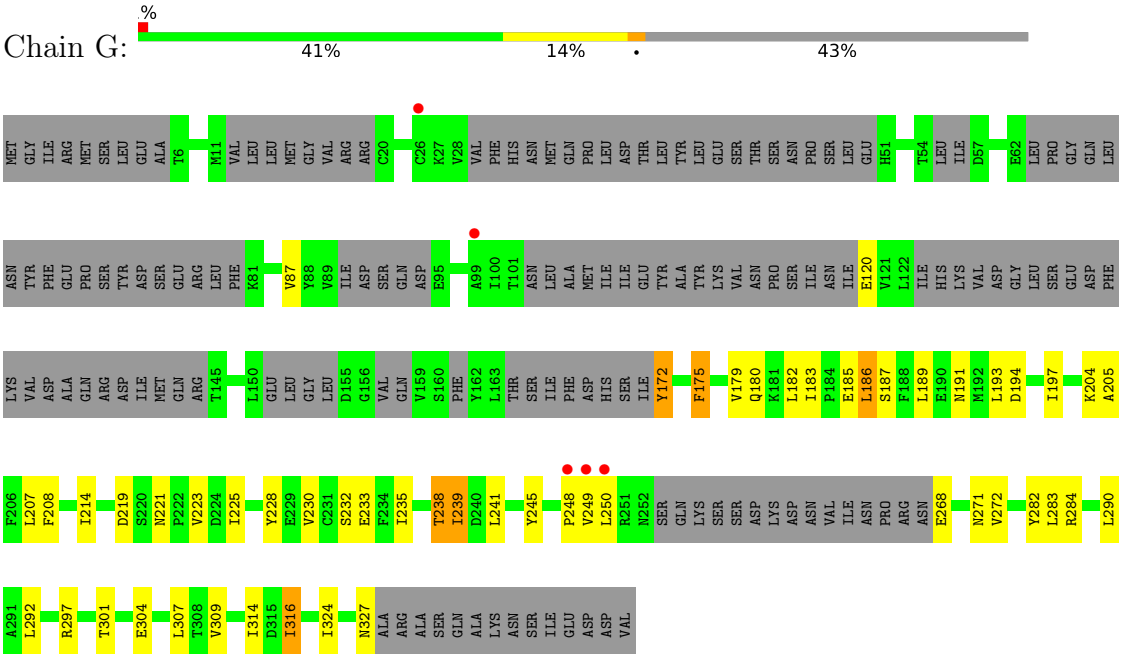
• Molecule 2: GTP-binding protein GTR2

Chain B:

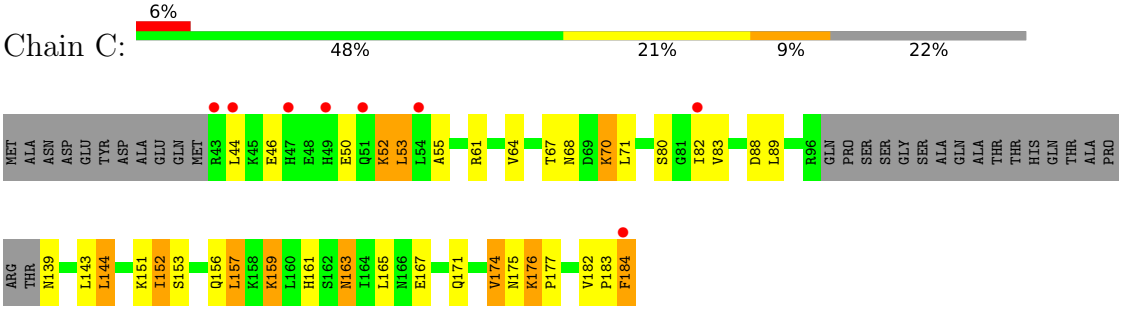




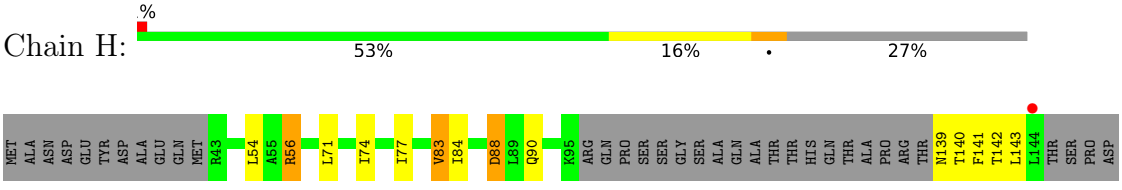
• Molecule 2: GTP-binding protein GTR2

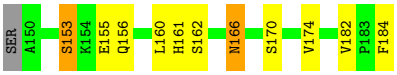


• Molecule 3: Protein MEH1



• Molecule 3: Protein MEH1



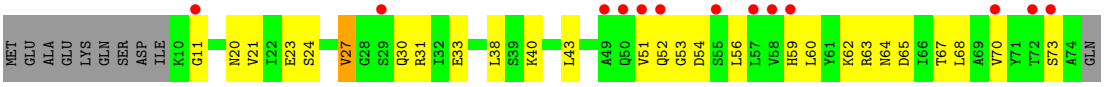


• Molecule 4: Ego2

Chain D:

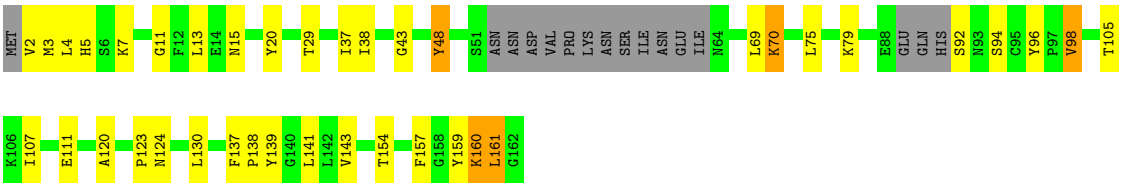
• Molecule 4: Ego2

Chain I:



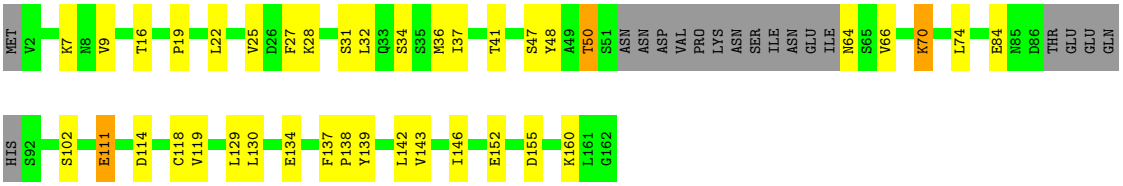
• Molecule 5: Protein SLM4

Chain E:



• Molecule 5: Protein SLM4

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.67Å 120.55Å 323.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.20 49.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	68.7 (49.24-3.20) 68.7 (49.19-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.230 , 0.285 0.230 , 0.286	Depositor DCC
R_{free} test set	1863 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13142	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: GNP, MG

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	0.26	0/2238	0.55	0/3004
1	F	0.25	0/2385	0.54	0/3201
2	B	0.26	0/2346	0.58	0/3180
2	G	0.30	0/1403	0.57	0/1897
3	C	0.27	0/788	0.53	0/1063
3	H	0.26	0/741	0.56	0/998
4	D	0.26	0/508	0.54	0/688
4	I	0.27	0/493	0.58	0/667
5	E	0.27	0/1168	0.56	0/1575
5	J	0.27	0/1158	0.54	0/1561
All	All	0.27	0/13228	0.55	0/17834

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2201	0	2215	60	0
1	F	2342	0	2384	50	0
2	B	2310	0	2279	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1396	0	1225	32	0
3	C	780	0	789	38	0
3	H	735	0	733	17	0
4	D	503	0	492	11	0
4	I	488	0	480	17	0
5	E	1149	0	1139	24	0
5	J	1139	0	1137	22	0
6	A	32	0	13	2	0
6	B	32	0	13	2	0
6	F	32	0	13	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
All	All	13142	0	12912	282	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 (282) 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:A:77:LYS:HB2	1:A:111:GLN:OE1	1.47	1.11
3:C:52:LYS:HE3	3:C:52:LYS:HA	1.41	1.02
3:C:50:GLU:HA	3:C:53:LEU:HD21	1.42	0.98
1:F:7:LYS:HD2	1:F:182:LEU:HD22	1.46	0.97
2:B:149:LEU:HD11	2:B:155:ASP:HA	1.51	0.91
1:A:173:LYS:HB2	1:A:244:GLU:HB3	1.54	0.89
3:C:182:VAL:HG12	3:C:183:PRO:HD2	1.57	0.87
3:C:50:GLU:HA	3:C:53:LEU:CD2	2.10	0.81
2:B:54:THR:HG23	2:B:55:LEU:H	1.49	0.78
2:B:120:GLU:HG2	2:B:178:ILE:HG12	1.66	0.77
5:J:66:VAL:O	5:J:70:LYS:HG3	1.85	0.75
5:E:124:ASN:O	5:E:160:LYS:HE3	1.87	0.75
2:G:238:THR:HB	2:G:271:ASN:HD22	1.50	0.75
3:C:183:PRO:O	3:C:184:PHE:CG	2.40	0.74
1:A:267:LEU:HD11	2:B:271:ASN:OD1	1.88	0.74
3:H:143:LEU:HA	4:I:51:VAL:HG12	1.70	0.73
1:F:272:ASN:HD21	2:G:249:VAL:HG21	1.53	0.73
1:A:8:LYS:HG2	1:A:58:ASN:H	1.55	0.71
2:B:160:SER:HB3	2:B:162:TYR:HE1	1.55	0.70
3:C:182:VAL:HG12	3:C:183:PRO:CD	2.21	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASP:O	2:B:197:ILE:HG13	1.91	0.69
2:G:232:SER:HA	2:G:235:ILE:HD12	1.74	0.69
3:C:52:LYS:HA	3:C:52:LYS:CE	2.21	0.68
1:A:81:PHE:CD2	1:A:112:LEU:HD13	2.28	0.68
1:A:76:GLN:O	1:A:80:ILE:HG12	1.94	0.68
2:B:19:ARG:HD2	6:B:401:GNP:HNB3	1.58	0.68
2:B:39:LEU:HA	6:B:401:GNP:O2'	1.94	0.68
1:A:304:LYS:HD2	5:E:159:TYR:OH	1.94	0.67
2:B:38:THR:HA	2:B:41:LEU:HD13	1.76	0.67
3:C:177:PRO:HG2	5:E:11:GLY:HA3	1.78	0.66
1:A:25:ILE:HD11	1:A:32:ALA:HA	1.78	0.66
2:B:20:CYS:HB2	2:B:91:ASP:HB2	1.79	0.65
2:B:202:ILE:HG12	2:B:296:ILE:HG12	1.79	0.64
4:D:21:VAL:HG13	5:E:138:PRO:HB3	1.80	0.64
1:A:123:VAL:HG23	1:A:161:GLY:HA3	1.80	0.64
1:A:267:LEU:CD1	2:B:273:SER:HB3	2.28	0.64
2:B:54:THR:HG23	2:B:55:LEU:N	2.13	0.63
5:E:98:VAL:HG23	5:E:105:THR:HG23	1.79	0.63
1:A:9:LEU:HG	1:A:86:VAL:HG22	1.80	0.63
3:C:183:PRO:O	3:C:184:PHE:CD2	2.52	0.62
2:G:197:ILE:HD13	2:G:219:ASP:HB3	1.80	0.62
1:A:267:LEU:HD13	2:B:273:SER:HB3	1.79	0.62
1:A:78:ASP:OD1	1:A:79:HIS:N	2.33	0.62
1:F:19:LYS:HG2	1:F:90:VAL:HG21	1.82	0.61
1:A:156:PHE:N	1:A:157:PRO:HD2	2.16	0.61
4:I:21:VAL:HG13	5:J:138:PRO:HB3	1.81	0.61
1:A:68:PHE:HB3	1:A:72:TYR:HE1	1.65	0.61
4:I:11:GLY:HA3	4:I:27:VAL:HG13	1.83	0.60
3:H:74:ILE:O	3:H:77:ILE:HG22	2.01	0.60
2:B:234:PHE:O	2:B:238:THR:HG23	2.02	0.60
2:G:238:THR:HG21	2:G:283:LEU:HD13	1.83	0.60
1:A:267:LEU:HB3	1:A:275:VAL:CG2	2.32	0.60
2:G:235:ILE:HG22	2:G:239:ILE:HD11	1.83	0.60
1:F:272:ASN:ND2	2:G:249:VAL:HG21	2.18	0.59
4:I:59:HIS:HB2	4:I:70:VAL:HG22	1.85	0.58
2:G:197:ILE:CD1	2:G:219:ASP:HB3	2.32	0.58
1:A:278:LEU:HD21	1:A:309:PHE:CE2	2.39	0.58
3:C:50:GLU:HA	3:C:53:LEU:CG	2.33	0.58
3:C:143:LEU:HA	4:D:51:VAL:HG12	1.86	0.58
1:A:25:ILE:HD12	1:A:166:ILE:HG13	1.85	0.57
3:C:183:PRO:C	3:C:184:PHE:CG	2.77	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:CD1	1:A:166:ILE:HG13	2.35	0.57
1:A:68:PHE:O	1:A:72:TYR:HD1	1.88	0.57
2:B:190:GLU:O	2:B:194:ASP:HB2	2.05	0.57
2:B:287:ILE:HG22	2:B:321:LEU:HD12	1.84	0.57
1:A:68:PHE:O	1:A:72:TYR:CD1	2.58	0.56
1:A:194:LYS:O	1:A:198:GLU:HG2	2.04	0.56
2:B:70:PHE:C	2:B:71:GLU:HG3	2.25	0.56
1:F:140:PHE:O	1:F:144:MET:HB2	2.06	0.56
5:J:70:LYS:NZ	5:J:70:LYS:HB3	2.19	0.55
5:J:129:LEU:HD23	5:J:146:ILE:HG13	1.88	0.55
2:B:203:GLU:HG3	2:B:204:LYS:HD2	1.88	0.55
2:B:29:VAL:HA	2:B:172:TYR:HE1	1.71	0.55
5:E:5:HIS:CE1	5:E:7:LYS:HB3	2.40	0.55
2:G:197:ILE:HD11	2:G:205:ALA:HB3	1.89	0.55
2:B:318:LYS:O	2:B:322:GLU:HB2	2.07	0.55
2:G:284:ARG:HD3	2:G:314:ILE:HG21	1.88	0.55
4:I:62:LYS:HE2	4:I:65:ASP:HA	1.88	0.55
3:C:182:VAL:CG1	3:C:183:PRO:CD	2.86	0.54
1:F:7:LYS:CD	1:F:182:LEU:HD22	2.31	0.54
2:B:208:PHE:O	2:B:290:LEU:HD23	2.08	0.54
1:A:265:LYS:HD3	2:B:276:ALA:HA	1.89	0.54
3:C:88:ASP:H	4:D:20:ASN:HB3	1.73	0.54
1:F:113:ARG:HD3	1:F:154:PHE:O	2.08	0.54
3:C:88:ASP:HB2	4:D:20:ASN:HA	1.90	0.54
2:B:15:MET:HE1	2:B:106:ILE:HG21	1.89	0.54
1:A:32:ALA:HB1	1:A:166:ILE:HG23	1.90	0.53
1:F:22:MET:O	1:F:26:ILE:HG12	2.08	0.53
1:A:16:GLY:H	6:A:401:GNP:HNB3	1.56	0.53
2:B:238:THR:HG21	2:B:283:LEU:HD23	1.90	0.53
2:G:316:ILE:HD12	3:H:71:LEU:HD23	1.91	0.53
1:A:205:ILE:HG12	1:A:286:ILE:HG23	1.91	0.53
2:B:226:GLN:O	2:B:230:VAL:HG23	2.09	0.53
2:B:195:ASN:HA	2:B:198:GLN:HB2	1.89	0.53
3:C:182:VAL:CG1	3:C:183:PRO:HD2	2.35	0.52
5:J:139:TYR:O	5:J:143:VAL:HG23	2.10	0.52
3:C:152:ILE:HD11	4:D:59:HIS:CD2	2.43	0.52
1:A:68:PHE:HB3	1:A:72:TYR:CE1	2.44	0.52
2:B:160:SER:HB3	2:B:162:TYR:CE1	2.40	0.52
1:F:125:LEU:HD12	1:F:140:PHE:HA	1.92	0.52
4:I:56:LEU:HD22	4:I:73:SER:HA	1.92	0.52
1:A:279:SER:HB2	1:A:282:MET:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:154:THR:HA	5:E:157:PHE:CD1	2.44	0.52
2:B:165:SER:H	2:B:170:SER:HB2	1.73	0.52
1:A:81:PHE:HD2	1:A:112:LEU:HD13	1.72	0.52
4:D:38:LEU:HD22	4:D:60:LEU:HD21	1.92	0.52
2:G:186:LEU:HG	2:G:187:SER:N	2.25	0.51
1:F:6:ARG:HG3	1:F:56:THR:HG23	1.93	0.51
1:F:278:LEU:HD11	1:F:284:CYS:HB3	1.93	0.51
3:C:82:ILE:HD12	5:E:75:LEU:HD21	1.93	0.51
5:E:13:LEU:HD21	5:E:37:ILE:HG13	1.92	0.51
5:J:119:VAL:HB	5:J:130:LEU:HD13	1.92	0.51
2:G:235:ILE:O	2:G:239:ILE:HG13	2.11	0.50
1:F:12:MET:O	1:F:89:HIS:HA	2.10	0.50
3:H:140:THR:O	4:I:53:GLY:HA3	2.12	0.50
4:I:21:VAL:CG1	5:J:138:PRO:HB3	2.42	0.50
1:F:131:VAL:HG23	1:F:136:ARG:HG2	1.93	0.50
2:G:87:VAL:HA	2:G:120:GLU:O	2.12	0.50
2:B:138:GLN:HA	2:B:141:ILE:HG22	1.93	0.50
1:A:50:ARG:HA	1:A:56:THR:HA	1.94	0.50
3:C:52:LYS:O	3:C:55:ALA:N	2.45	0.50
2:B:56:ILE:HB	2:B:183:ILE:HD11	1.94	0.49
3:C:82:ILE:HD12	5:E:75:LEU:CD2	2.42	0.49
1:F:267:LEU:C	1:F:267:LEU:HD23	2.31	0.49
3:C:159:LYS:O	3:C:163:ASN:HB2	2.13	0.49
1:A:79:HIS:C	1:A:79:HIS:CD2	2.86	0.49
2:B:304:GLU:OE2	5:E:70:LYS:NZ	2.42	0.49
5:J:22:LEU:HB2	5:J:27:PHE:HB3	1.94	0.49
1:A:81:PHE:HD2	1:A:112:LEU:HA	1.77	0.49
2:B:283:LEU:HD12	2:B:284:ARG:N	2.28	0.49
1:F:269:LEU:HD23	1:F:270:ASN:ND2	2.28	0.48
3:C:83:VAL:O	5:E:79:LYS:HD3	2.12	0.48
1:A:166:ILE:HA	1:A:171:LEU:HD12	1.95	0.48
1:A:269:LEU:HD22	1:A:273:ILE:HD12	1.95	0.48
5:J:22:LEU:HD13	5:J:27:PHE:HD2	1.78	0.48
1:A:175:TRP:HA	1:A:178:ILE:HB	1.95	0.48
2:B:88:TYR:CD1	2:B:103:LEU:HD12	2.48	0.48
4:I:21:VAL:HG21	4:I:24:SER:HB2	1.96	0.48
1:A:126:HIS:HA	1:A:164:THR:O	2.14	0.48
2:G:304:GLU:OE1	5:J:70:LYS:HE2	2.14	0.48
2:B:272:VAL:HG11	2:B:307:LEU:HD11	1.96	0.47
1:F:126:HIS:HA	1:F:164:THR:O	2.14	0.47
3:C:161:HIS:CE1	3:C:165:LEU:HD12	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LYS:NZ	2:G:233:GLU:OE1	2.47	0.47
1:F:9:LEU:HD13	1:F:86:VAL:HB	1.97	0.47
3:C:64:VAL:O	3:C:68:ASN:ND2	2.47	0.47
1:A:199:ILE:HD11	3:C:184:PHE:HD2	1.80	0.47
3:C:167:GLU:O	3:C:171:GLN:HB2	2.14	0.47
4:D:14:ALA:HB3	4:D:23:GLU:HG3	1.96	0.47
2:B:172:TYR:HB3	2:B:228:TYR:OH	2.15	0.47
4:D:59:HIS:HB2	4:D:70:VAL:HG22	1.97	0.46
2:B:120:GLU:HG3	2:B:162:TYR:CE1	2.50	0.46
4:D:54:ASP:O	4:D:56:LEU:HG	2.14	0.46
1:F:24:SER:HA	1:F:28:SER:OG	2.15	0.46
1:F:7:LYS:HD2	1:F:182:LEU:CD2	2.33	0.46
1:F:11:LEU:HD21	1:F:22:MET:HE2	1.97	0.46
1:F:250:MET:HE1	2:G:241:LEU:HD11	1.98	0.46
1:A:81:PHE:CD1	1:A:81:PHE:N	2.84	0.46
2:B:208:PHE:C	2:B:290:LEU:HD23	2.36	0.46
2:B:120:GLU:HG3	2:B:162:TYR:HE1	1.81	0.46
1:F:269:LEU:HD23	1:F:270:ASN:HD22	1.81	0.46
3:H:161:HIS:NE2	4:I:63:ARG:HB3	2.30	0.46
1:A:271:ASN:HD21	1:A:295:GLN:HG3	1.81	0.46
2:B:270:GLN:HB3	2:B:284:ARG:HG2	1.98	0.46
4:I:62:LYS:HB2	4:I:67:THR:HG23	1.97	0.46
3:C:151:LYS:H	4:D:59:HIS:CE1	2.34	0.46
2:G:324:ILE:O	3:H:56:ARG:NH2	2.48	0.46
1:A:90:VAL:HG12	1:A:124:LEU:HB2	1.97	0.45
1:A:267:LEU:HD12	2:B:272:VAL:O	2.16	0.45
5:J:19:PRO:HB3	5:J:31:SER:HA	1.99	0.45
3:H:153:SER:HB2	3:H:156:GLN:H	1.82	0.45
5:J:118:CYS:SG	5:J:142:LEU:HB3	2.56	0.45
1:A:304:LYS:HD2	5:E:159:TYR:HH	1.82	0.45
5:E:5:HIS:HE1	5:E:7:LYS:HB3	1.80	0.45
1:F:205:ILE:HG12	1:F:286:ILE:HG12	1.97	0.45
2:B:52:PHE:HE1	2:B:209:ASP:OD2	2.00	0.45
5:E:38:ILE:HD12	5:E:43:GLY:HA2	1.98	0.45
1:F:14:ARG:O	1:F:17:SER:OG	2.34	0.45
1:A:41:THR:N	6:A:401:GNP:O1G	2.49	0.45
3:C:176:LYS:H	3:C:176:LYS:HE3	1.82	0.45
5:E:105:THR:HB	5:E:123:PRO:HG3	1.98	0.45
1:A:97:GLU:HG2	1:F:139:LEU:HD11	1.99	0.45
5:E:139:TYR:O	5:E:143:VAL:HG23	2.17	0.45
1:F:121:ILE:HD13	1:F:159:LEU:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:74:ILE:O	3:H:77:ILE:CG2	2.64	0.45
1:F:113:ARG:CD	1:F:154:PHE:O	2.64	0.44
1:A:304:LYS:HD3	5:E:2:VAL:O	2.17	0.44
1:F:88:ILE:HD13	1:F:175:TRP:CH2	2.53	0.44
3:H:174:VAL:O	5:J:152:GLU:HG3	2.17	0.44
1:A:278:LEU:HD21	1:A:309:PHE:HE2	1.80	0.44
1:A:125:LEU:HD11	1:A:143:MET:HG2	1.99	0.44
2:B:206:PHE:HB2	2:B:208:PHE:CE1	2.52	0.44
1:F:308:PHE:HZ	3:H:184:PHE:C	2.21	0.44
1:F:201:ASN:HB2	5:J:7:LYS:HE3	1.99	0.43
2:G:238:THR:HB	2:G:271:ASN:ND2	2.25	0.43
2:G:172:TYR:HB3	2:G:228:TYR:OH	2.17	0.43
4:I:38:LEU:HD22	4:I:60:LEU:HD21	2.00	0.43
1:A:166:ILE:HG22	1:A:167:TRP:CD1	2.53	0.43
1:A:268:ILE:HG12	1:A:274:TYR:CE2	2.54	0.43
2:B:79:LEU:O	2:B:83:VAL:HG23	2.18	0.43
1:F:303:LYS:HG3	1:F:306:LYS:HD2	2.00	0.43
2:G:207:LEU:HD22	2:G:290:LEU:HB3	2.00	0.43
3:H:160:LEU:HD23	4:I:68:LEU:HD21	2.00	0.43
1:A:267:LEU:HD12	2:B:273:SER:HB3	2.00	0.43
2:B:15:MET:HE1	2:B:86:LEU:HD11	2.00	0.43
2:B:22:LYS:HB3	2:B:62:GLU:HG3	2.00	0.43
2:G:180:GLN:O	2:G:186:LEU:HD22	2.19	0.43
2:B:183:ILE:HG22	2:B:186:LEU:HB2	2.00	0.43
1:F:215:VAL:HG21	1:F:243:PHE:HB3	2.00	0.43
2:B:15:MET:CE	2:B:106:ILE:HG21	2.49	0.43
2:B:38:THR:O	2:B:41:LEU:HB2	2.19	0.43
2:B:224:ASP:OD1	2:B:224:ASP:N	2.52	0.43
2:B:316:ILE:HG21	3:C:70:LYS:HB3	2.00	0.43
1:F:125:LEU:HD23	1:F:125:LEU:HA	1.84	0.43
1:F:259:LYS:HB2	2:G:230:VAL:HG22	2.00	0.43
1:F:290:ASP:N	1:F:290:ASP:OD1	2.52	0.43
2:B:97:ILE:O	2:B:101:THR:OG1	2.35	0.43
3:C:151:LYS:H	4:D:59:HIS:HE1	1.67	0.43
1:F:11:LEU:HD22	1:F:19:LYS:HB3	2.00	0.42
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.87	0.42
2:B:154:LEU:HG	2:B:155:ASP:H	1.84	0.42
3:C:183:PRO:O	3:C:184:PHE:CB	2.67	0.42
1:F:164:THR:HG23	1:F:171:LEU:HA	1.99	0.42
3:C:68:ASN:HA	3:C:71:LEU:HD12	2.01	0.42
1:F:272:ASN:HD21	2:G:249:VAL:CG2	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:CYS:HB3	1:A:72:TYR:CE2	2.55	0.42
3:H:83:VAL:HA	5:J:111:GLU:O	2.20	0.42
2:B:169:HIS:ND1	2:B:229:GLU:HG2	2.35	0.42
1:F:278:LEU:HD13	1:F:309:PHE:CD2	2.54	0.42
2:G:245:TYR:C	2:G:248:PRO:HD2	2.40	0.42
3:H:162:SER:O	3:H:166:ASN:HB2	2.19	0.42
1:F:127:LYS:HE2	6:F:401:GNP:C4	2.49	0.42
5:J:34:SER:HB3	5:J:50:THR:HG23	2.02	0.42
1:F:97:GLU:HB2	1:F:100:LYS:HB3	2.02	0.42
5:J:9:VAL:HG13	5:J:37:ILE:HD12	2.01	0.42
2:G:208:PHE:CD2	2:G:235:ILE:HD11	2.55	0.42
3:H:88:ASP:OD2	5:J:139:TYR:N	2.47	0.42
4:I:33:GLU:CD	4:I:33:GLU:H	2.18	0.42
1:A:277:GLU:HA	1:A:283:VAL:HG22	2.02	0.41
2:B:183:ILE:HA	2:B:184:PRO:HD3	1.86	0.41
1:F:210:ARG:HD3	1:F:280:SER:O	2.20	0.41
2:G:239:ILE:HG13	2:G:239:ILE:H	1.71	0.41
2:B:33:MET:SD	2:B:38:THR:HG22	2.60	0.41
2:B:114:ASN:OD1	2:B:117:ILE:HG13	2.18	0.41
5:E:20:TYR:HD2	5:E:141:LEU:HD21	1.84	0.41
5:E:96:TYR:CE1	5:E:143:VAL:HG21	2.55	0.41
2:G:309:VAL:HG11	3:H:74:ILE:HG13	2.02	0.41
5:E:107:ILE:HG12	5:E:120:ALA:HB2	2.01	0.41
2:B:119:ILE:HB	2:B:158:GLN:CB	2.50	0.41
1:F:24:SER:HB3	1:F:30:TYR:HB2	2.02	0.41
1:F:51:PHE:CE2	1:F:209:GLU:HG3	2.56	0.41
1:F:270:ASN:HD22	1:F:270:ASN:N	2.18	0.41
5:E:161:LEU:HD12	5:E:161:LEU:HA	1.83	0.41
2:G:183:ILE:HG23	2:G:186:LEU:HB3	2.02	0.41
1:A:93:VAL:HG12	1:A:125:LEU:HD12	2.02	0.41
2:B:13:LEU:HD23	2:B:13:LEU:HA	1.90	0.41
5:J:70:LYS:HB3	5:J:70:LYS:HZ1	1.84	0.41
1:A:100:LYS:O	1:A:104:ILE:HG23	2.21	0.41
1:F:6:ARG:HA	1:F:56:THR:HG23	2.03	0.41
2:G:197:ILE:HD13	2:G:219:ASP:CB	2.50	0.41
3:H:88:ASP:HB2	4:I:20:ASN:HA	2.03	0.41
1:A:208:PHE:CD1	1:A:215:VAL:HA	2.56	0.41
1:A:277:GLU:O	1:A:282:MET:O	2.39	0.41
3:C:174:VAL:HG23	5:E:15:ASN:HB3	2.02	0.41
3:C:183:PRO:HB2	3:C:184:PHE:CE1	2.55	0.41
5:E:48:TYR:HD2	5:E:69:LEU:HD12	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:TYR:HB3	1:F:80:ILE:HG13	2.02	0.41
4:I:23:GLU:OE2	5:J:25:VAL:HG21	2.21	0.41
1:A:74:THR:O	1:A:77:LYS:CD	2.69	0.41
1:A:208:PHE:HE1	1:A:215:VAL:HG22	1.86	0.41
2:G:175:PHE:O	2:G:179:VAL:HG23	2.20	0.41
2:G:191:ASN:HA	2:G:194:ASP:HB2	2.03	0.41
3:C:153:SER:OG	3:C:156:GLN:HG3	2.20	0.40
5:J:16:THR:O	5:J:32:LEU:HD22	2.20	0.40
1:A:278:LEU:HD21	1:A:309:PHE:CD2	2.57	0.40
3:C:152:ILE:HG13	3:C:157:LEU:HD13	2.03	0.40
1:F:87:LEU:HD12	1:F:112:LEU:HD22	2.02	0.40
3:H:141:PHE:HA	4:I:53:GLY:HA3	2.03	0.40
5:J:37:ILE:HG12	5:J:129:LEU:HD12	2.02	0.40
3:C:68:ASN:HA	3:C:71:LEU:CD1	2.52	0.40
3:C:143:LEU:HD23	3:C:144:LEU:N	2.35	0.40
1:F:110:LYS:HB2	1:F:154:PHE:HE2	1.87	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	265/312 (85%)	248 (94%)	17 (6%)	0	100	100
1	F	285/312 (91%)	264 (93%)	21 (7%)	0	100	100
2	B	288/345 (84%)	267 (93%)	21 (7%)	0	100	100
2	G	171/345 (50%)	160 (94%)	11 (6%)	0	100	100
3	C	96/129 (74%)	93 (97%)	3 (3%)	0	100	100
3	H	88/129 (68%)	86 (98%)	2 (2%)	0	100	100
4	D	65/75 (87%)	58 (89%)	7 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	63/75 (84%)	60 (95%)	3 (5%)	0	100	100
5	E	140/162 (86%)	128 (91%)	12 (9%)	0	100	100
5	J	138/162 (85%)	129 (94%)	9 (6%)	0	100	100
All	All	1599/2046 (78%)	1493 (93%)	106 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	247/293 (84%)	212 (86%)	35 (14%)	3	15
1	F	268/293 (92%)	226 (84%)	42 (16%)	2	12
2	B	259/313 (83%)	223 (86%)	36 (14%)	3	16
2	G	127/313 (41%)	103 (81%)	24 (19%)	1	8
3	C	89/116 (77%)	70 (79%)	19 (21%)	1	5
3	H	83/116 (72%)	70 (84%)	13 (16%)	2	12
4	D	54/62 (87%)	50 (93%)	4 (7%)	13	46
4	I	53/62 (86%)	45 (85%)	8 (15%)	3	14
5	E	132/150 (88%)	119 (90%)	13 (10%)	8	31
5	J	132/150 (88%)	115 (87%)	17 (13%)	4	19
All	All	1444/1868 (77%)	1233 (85%)	211 (15%)	3	15

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	MET
1	A	14	ARG
1	A	34	ASP
1	A	37	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	41	THR
1	A	54	ASN
1	A	59	LEU
1	A	79	HIS
1	A	87	LEU
1	A	95	SER
1	A	100	LYS
1	A	103	GLU
1	A	104	ILE
1	A	109	LEU
1	A	123	VAL
1	A	131	VAL
1	A	146	ASN
1	A	153	GLU
1	A	162	PHE
1	A	166	ILE
1	A	169	GLU
1	A	171	LEU
1	A	177	GLN
1	A	182	LEU
1	A	186	MET
1	A	211	THR
1	A	213	PHE
1	A	238	LEU
1	A	243	PHE
1	A	251	LYS
1	A	254	LYS
1	A	271	ASN
1	A	288	LEU
1	A	290	ASP
2	B	11	MET
2	B	17	VAL
2	B	24	SER
2	B	31	HIS
2	B	42	GLU
2	B	49	LEU
2	B	51	HIS
2	B	55	LEU
2	B	57	ASP
2	B	66	GLN
2	B	71	GLU
2	B	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	112	LYS
2	B	120	GLU
2	B	127	ASP
2	B	150	LEU
2	B	171	ILE
2	B	175	PHE
2	B	181	LYS
2	B	186	LEU
2	B	194	ASP
2	B	196	LEU
2	B	198	GLN
2	B	201	LYS
2	B	213	LYS
2	B	227	MET
2	B	238	THR
2	B	275	LEU
2	B	283	LEU
2	B	286	MET
2	B	297	ARG
2	B	302	ASP
2	B	307	LEU
2	B	311	ASP
2	B	321	LEU
2	B	322	GLU
3	C	44	LEU
3	C	46	GLU
3	C	52	LYS
3	C	53	LEU
3	C	61	ARG
3	C	67	THR
3	C	70	LYS
3	C	80	SER
3	C	89	LEU
3	C	139	ASN
3	C	144	LEU
3	C	152	ILE
3	C	157	LEU
3	C	159	LYS
3	C	163	ASN
3	C	174	VAL
3	C	175	ASN
3	C	176	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	184	PHE
4	D	9	ILE
4	D	20	ASN
4	D	50	GLN
4	D	56	LEU
5	E	3	MET
5	E	4	LEU
5	E	29	THR
5	E	48	TYR
5	E	70	LYS
5	E	92	SER
5	E	94	SER
5	E	98	VAL
5	E	111	GLU
5	E	130	LEU
5	E	137	PHE
5	E	160	LYS
5	E	161	LEU
1	F	4	ASN
1	F	6	ARG
1	F	11	LEU
1	F	14	ARG
1	F	17	SER
1	F	29	ASN
1	F	49	LEU
1	F	52	LEU
1	F	57	LEU
1	F	58	ASN
1	F	77	LYS
1	F	87	LEU
1	F	90	VAL
1	F	93	VAL
1	F	97	GLU
1	F	104	ILE
1	F	120	LYS
1	F	121	ILE
1	F	125	LEU
1	F	129	ASP
1	F	135	LYS
1	F	139	LEU
1	F	144	MET
1	F	166	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	169	GLU
1	F	171	LEU
1	F	185	ASN
1	F	198	GLU
1	F	199	ILE
1	F	210	ARG
1	F	211	THR
1	F	213	PHE
1	F	238	LEU
1	F	251	LYS
1	F	255	GLN
1	F	258	THR
1	F	264	PHE
1	F	266	THR
1	F	269	LEU
1	F	271	ASN
1	F	292	ASN
1	F	293	ILE
2	G	172	TYR
2	G	175	PHE
2	G	182	LEU
2	G	185	GLU
2	G	186	LEU
2	G	189	LEU
2	G	193	LEU
2	G	204	LYS
2	G	214	ILE
2	G	221	ASN
2	G	223	VAL
2	G	225	ILE
2	G	238	THR
2	G	239	ILE
2	G	250	LEU
2	G	268	GLU
2	G	272	VAL
2	G	282	TYR
2	G	292	LEU
2	G	297	ARG
2	G	301	THR
2	G	307	LEU
2	G	316	ILE
2	G	327	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	54	LEU
3	H	56	ARG
3	H	83	VAL
3	H	84	ILE
3	H	88	ASP
3	H	90	GLN
3	H	139	ASN
3	H	142	THR
3	H	153	SER
3	H	155	GLU
3	H	166	ASN
3	H	170	SER
3	H	182	VAL
4	I	27	VAL
4	I	30	GLN
4	I	31	ARG
4	I	40	LYS
4	I	43	LEU
4	I	52	GLN
4	I	54	ASP
4	I	64	ASN
5	J	28	LYS
5	J	36	MET
5	J	41	THR
5	J	47	SER
5	J	48	TYR
5	J	50	THR
5	J	64	ASN
5	J	70	LYS
5	J	74	LEU
5	J	84	GLU
5	J	102	SER
5	J	111	GLU
5	J	114	ASP
5	J	134	GLU
5	J	137	PHE
5	J	155	ASP
5	J	160	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	271	ASN
3	C	51	GLN
4	D	59	HIS
5	E	5	HIS
1	F	54	ASN
1	F	158	ASN
1	F	270	ASN
1	F	272	ASN
2	G	271	ASN
2	G	327	ASN
3	H	139	ASN
5	J	67	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
6	GNP	B	401	7	29,34,34	1.38	4 (13%)	33,54,54	2.20	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GNP	A	401	7	29,34,34	1.33	5 (17%)	33,54,54	2.21	7 (21%)
6	GNP	F	401	7	29,34,34	1.40	6 (20%)	33,54,54	2.14	6 (18%)

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
6	GNP	B	401	7	-	5/14/38/38	0/3/3/3
6	GNP	A	401	7	-	6/14/38/38	0/3/3/3
6	GNP	F	401	7	-	8/14/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	GNP	C6-N1	4.02	1.40	1.33
6	A	401	GNP	C6-N1	3.94	1.39	1.33
6	F	401	GNP	C6-N1	3.84	1.39	1.33
6	F	401	GNP	PG-O1G	3.22	1.51	1.46
6	B	401	GNP	PG-O1G	3.11	1.51	1.46
6	F	401	GNP	PB-O1B	2.73	1.50	1.46
6	A	401	GNP	PB-O1B	2.63	1.50	1.46
6	B	401	GNP	PB-O1B	2.56	1.50	1.46
6	A	401	GNP	PG-O1G	2.51	1.50	1.46
6	F	401	GNP	PB-O2B	-2.14	1.51	1.56
6	F	401	GNP	PG-O2G	-2.10	1.51	1.56
6	A	401	GNP	PB-O2B	-2.07	1.51	1.56
6	B	401	GNP	PB-O2B	-2.04	1.51	1.56
6	F	401	GNP	PG-O3G	-2.01	1.51	1.56
6	A	401	GNP	PG-O2G	-2.00	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	401	GNP	C5-C6-N1	-8.01	112.47	123.43
6	A	401	GNP	C5-C6-N1	-8.00	112.49	123.43
6	B	401	GNP	C5-C6-N1	-7.91	112.62	123.43
6	A	401	GNP	C2-N1-C6	5.39	124.49	115.93
6	B	401	GNP	C2-N1-C6	5.32	124.38	115.93
6	F	401	GNP	C2-N1-C6	5.28	124.31	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	401	GNP	O2B-PB-O1B	4.12	118.56	109.92
6	A	401	GNP	O2B-PB-O1B	4.07	118.45	109.92
6	F	401	GNP	O2B-PB-O1B	3.93	118.16	109.92
6	A	401	GNP	C3'-C2'-C1'	3.22	105.83	100.98
6	B	401	GNP	C3'-C2'-C1'	3.20	105.80	100.98
6	F	401	GNP	C3'-C2'-C1'	3.11	105.65	100.98
6	A	401	GNP	N3-C2-N1	-2.95	123.29	127.22
6	B	401	GNP	N3-C2-N1	-2.92	123.33	127.22
6	F	401	GNP	N3-C2-N1	-2.77	123.52	127.22
6	A	401	GNP	O2G-PG-O1G	-2.35	107.54	113.45
6	F	401	GNP	O2G-PG-O1G	-2.34	107.57	113.45
6	A	401	GNP	O3G-PG-O1G	-2.28	107.72	113.45
6	B	401	GNP	O2G-PG-O1G	-2.05	108.29	113.45

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	GNP	PB-N3B-PG-O1G
6	A	401	GNP	PG-N3B-PB-O1B
6	A	401	GNP	PA-O3A-PB-O1B
6	A	401	GNP	PA-O3A-PB-O2B
6	B	401	GNP	PG-N3B-PB-O1B
6	B	401	GNP	PG-N3B-PB-O3A
6	B	401	GNP	PA-O3A-PB-O1B
6	B	401	GNP	PA-O3A-PB-O2B
6	F	401	GNP	PB-N3B-PG-O1G
6	F	401	GNP	PG-N3B-PB-O1B
6	F	401	GNP	PA-O3A-PB-O1B
6	F	401	GNP	PA-O3A-PB-O2B
6	F	401	GNP	C5'-O5'-PA-O3A
6	F	401	GNP	C5'-O5'-PA-O1A
6	F	401	GNP	O4'-C4'-C5'-O5'
6	A	401	GNP	C5'-O5'-PA-O1A
6	F	401	GNP	C5'-O5'-PA-O2A
6	A	401	GNP	O4'-C4'-C5'-O5'
6	B	401	GNP	PB-N3B-PG-O1G

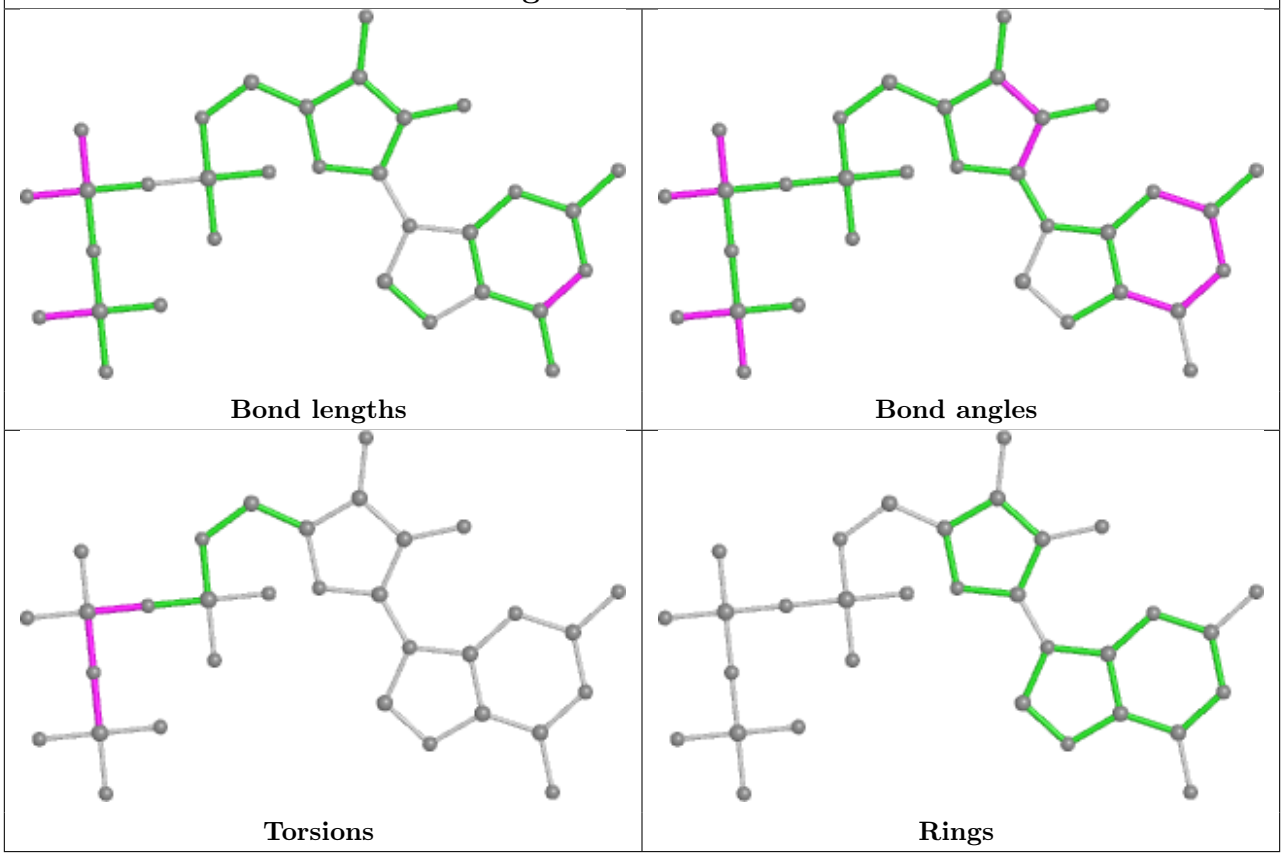
There are no ring outliers.

3 monomers are involved in 5 short contacts:

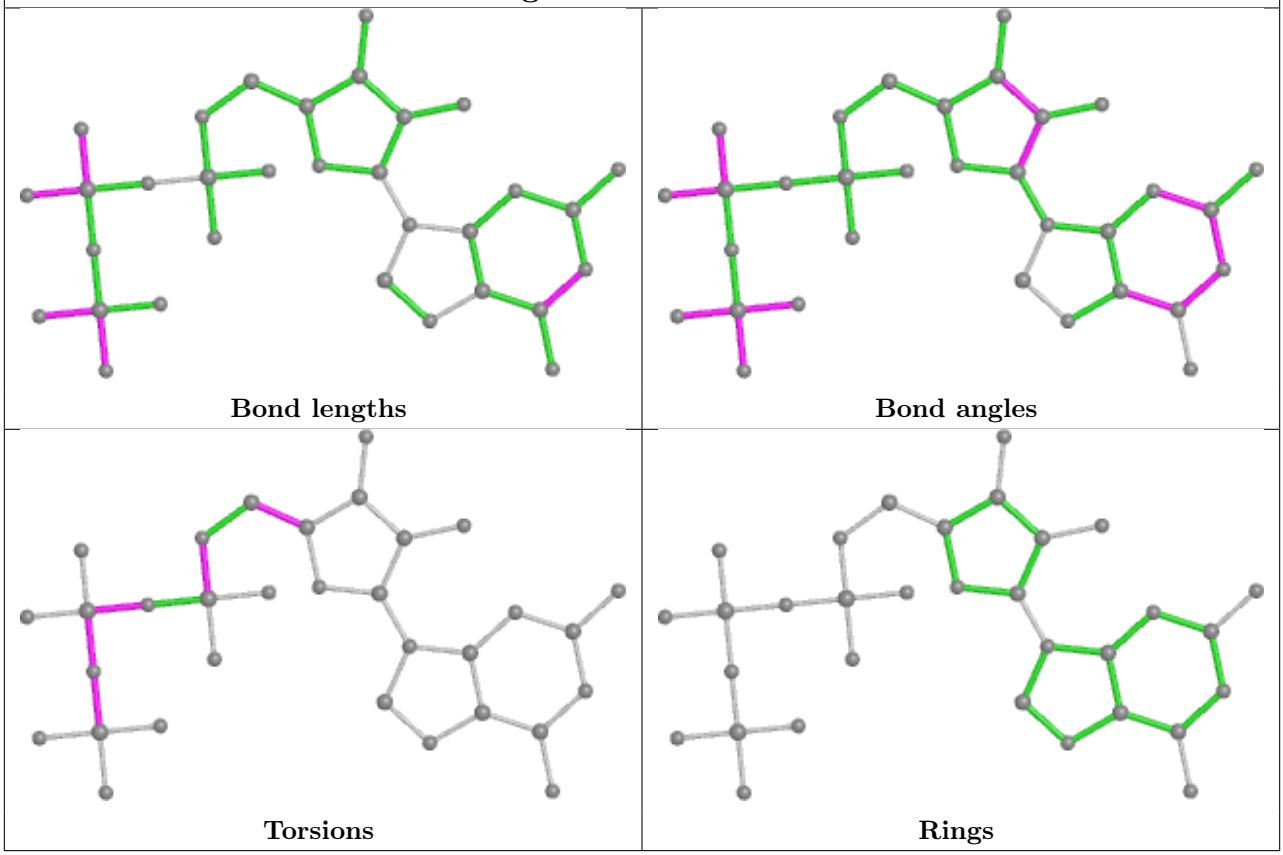
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	401	GNP	2	0
6	A	401	GNP	2	0
6	F	401	GNP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

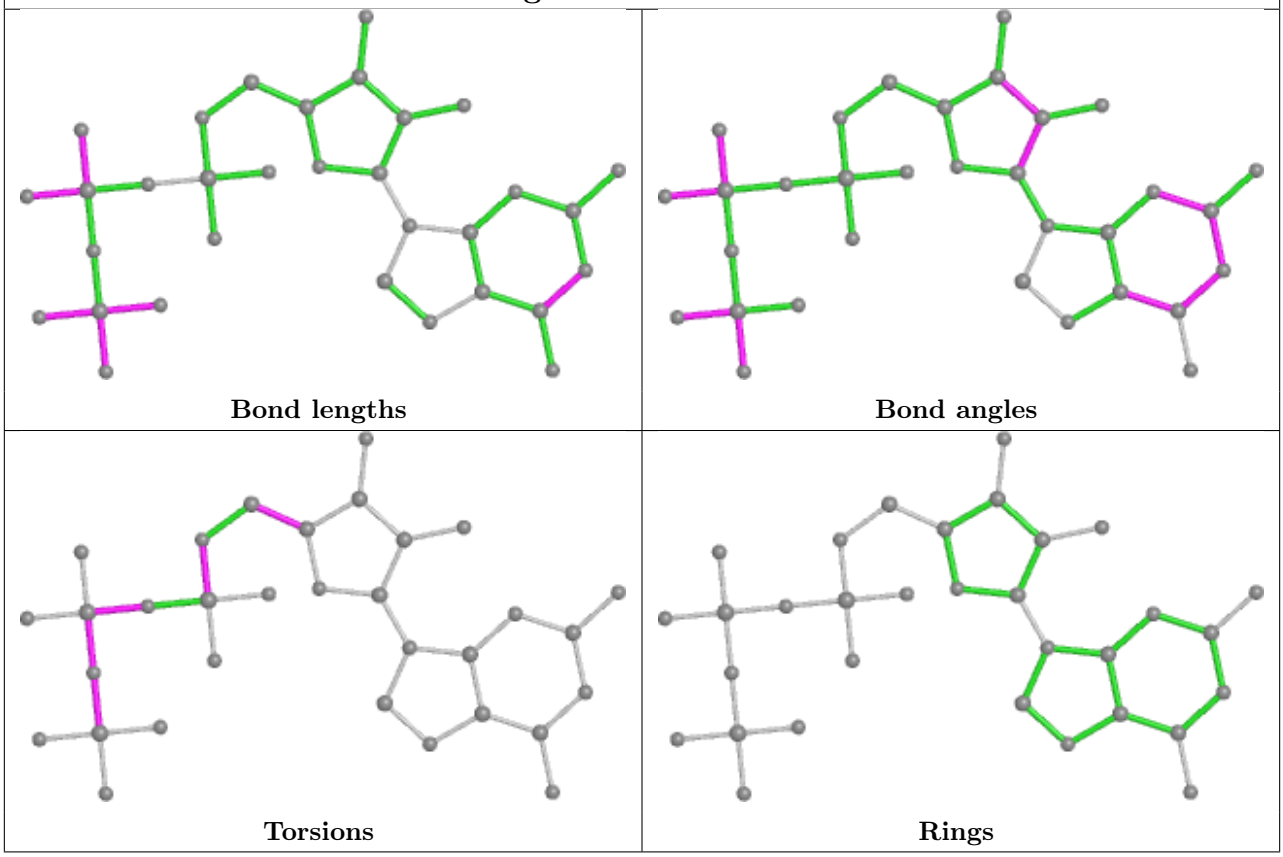
Ligand GNP B 401



Ligand GNP A 401



Ligand GNP F 401



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	A	275/312 (88%)	0.14	10 (3%) 42 27	51, 81, 128, 160	0
1	F	289/312 (92%)	-0.27	1 (0%) 94 92	32, 58, 86, 99	0
2	B	294/345 (85%)	-0.04	2 (0%) 87 81	52, 80, 113, 130	0
2	G	197/345 (57%)	-0.07	5 (2%) 57 43	28, 63, 122, 139	0
3	C	100/129 (77%)	0.47	8 (8%) 12 6	38, 78, 156, 192	0
3	H	94/129 (72%)	-0.11	1 (1%) 80 69	48, 75, 117, 128	0
4	D	67/75 (89%)	0.07	0 100 100	37, 51, 84, 94	0
4	I	65/75 (86%)	0.69	13 (20%) 1 1	59, 93, 127, 146	0
5	E	146/162 (90%)	-0.30	0 100 100	33, 55, 80, 119	0
5	J	144/162 (88%)	-0.25	0 100 100	32, 54, 83, 100	0
All	All	1671/2046 (81%)	-0.03	40 (2%) 59 44	28, 69, 118, 192	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ASP	4.2
3	C	47	HIS	3.9
4	I	59	HIS	3.8
3	C	44	LEU	3.5
4	I	73	SER	3.4
1	A	56	THR	3.3
3	C	51	GLN	3.3
4	I	72	THR	3.3
4	I	57	LEU	3.2
3	C	54	LEU	3.2
3	C	49	HIS	3.0
2	G	26	CYS	3.0
4	I	11	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	I	55	SER	2.8
1	A	57	LEU	2.8
3	C	184	PHE	2.8
2	G	249	VAL	2.8
1	A	58	ASN	2.7
4	I	51	VAL	2.7
3	H	144	LEU	2.6
4	I	50	GLN	2.6
1	A	74	THR	2.6
1	A	60	TRP	2.4
1	A	106	ALA	2.3
2	G	248	PRO	2.3
3	C	43	ARG	2.3
4	I	58	VAL	2.3
1	A	38	LEU	2.2
4	I	70	VAL	2.2
2	G	250	LEU	2.2
4	I	49	ALA	2.2
3	C	82	ILE	2.2
1	A	111	GLN	2.2
1	A	187	SER	2.1
2	B	95	GLU	2.1
2	G	99	ALA	2.1
2	B	45	SER	2.1
4	I	29	SER	2.1
4	I	52	GLN	2.1
1	F	5	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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,

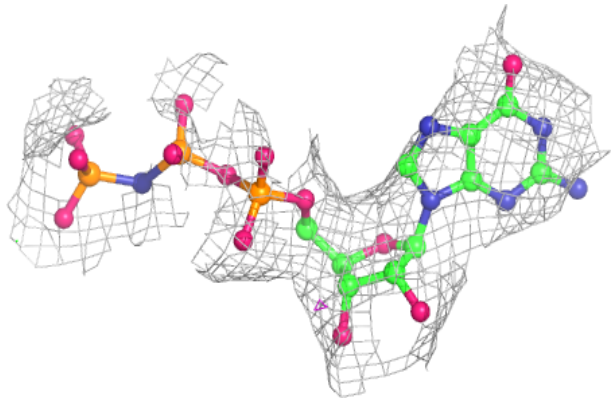
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

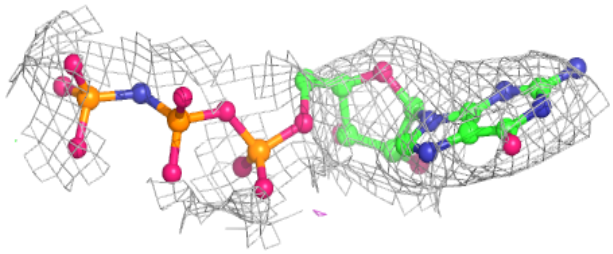
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	402	1/1	0.79	0.17	88,88,88,88	0
6	GNP	B	401	32/32	0.96	0.17	80,91,99,100	0
6	GNP	A	401	32/32	0.96	0.17	67,74,95,95	0
7	MG	B	402	1/1	0.96	0.07	70,70,70,70	0
6	GNP	F	401	32/32	0.97	0.18	44,48,55,56	0
7	MG	F	402	1/1	0.98	0.15	44,44,44,44	0

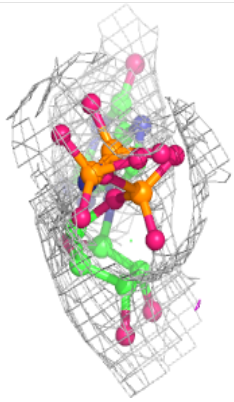
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GNP B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

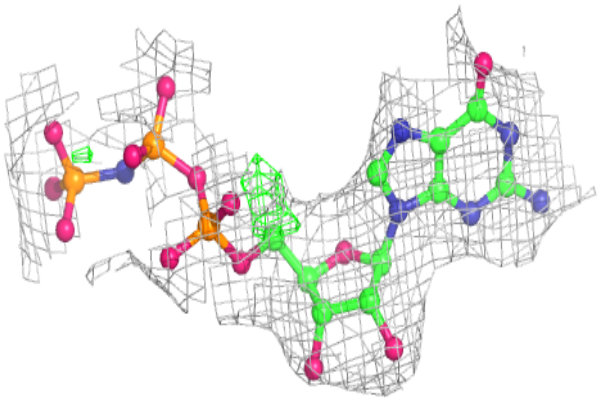


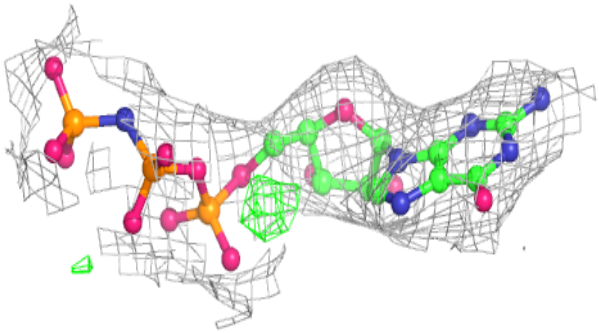


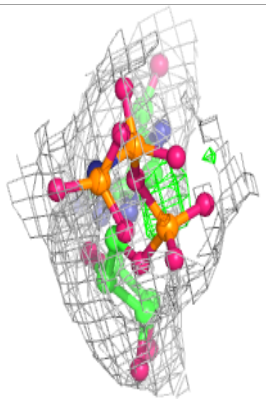


Electron density around GNP A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

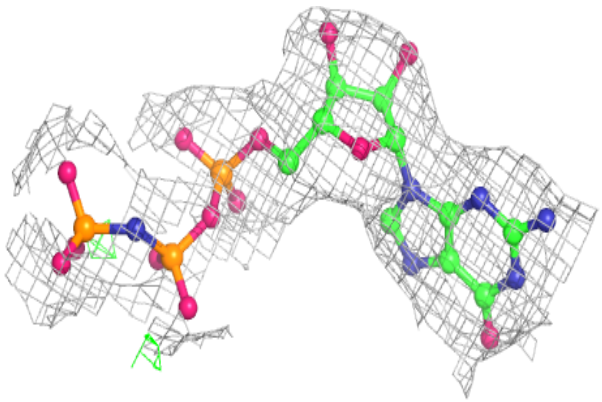


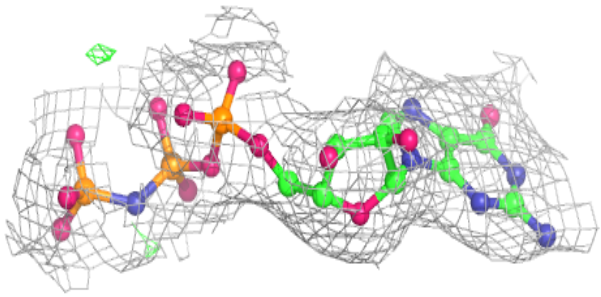


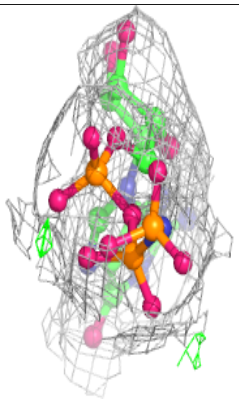


Electron density around GNP F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.