



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 PM GMT

PDB ID : 3ZJC
Title : Crystal structure of GMPPNP-bound human GIMAP7 L100Q variant
Authors : Schwefel, D.; Daumke, O.
Deposited on : 2013-01-17
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

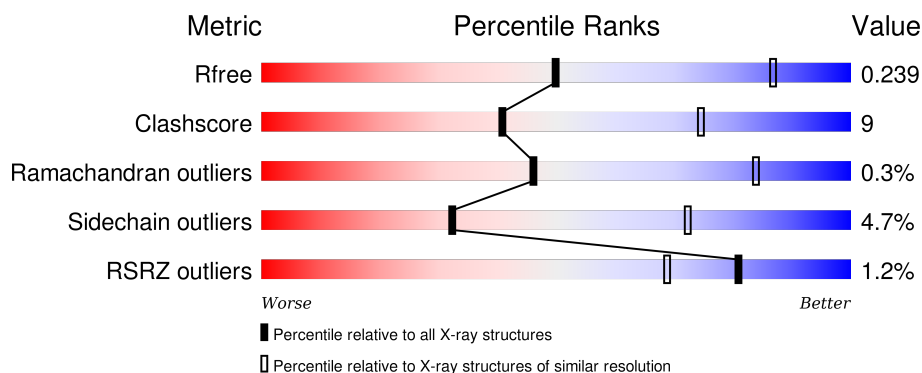
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	
1	C	305	
1	D	305	
1	E	305	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	305	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	1296	-	-	-	X
2	MG	B	1294	-	-	-	X
2	MG	C	1294	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12623 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 GTPASE IMAP FAMILY MEMBER 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	266	0	0
			2275	1429	392	441	13			
1	B	257	Total	C	N	O	S	146	0	0
			2054	1287	360	395	12			
1	C	254	Total	C	N	O	S	183	0	0
			2022	1268	352	390	12			
1	D	223	Total	C	N	O	S	218	0	0
			1752	1109	298	333	12			
1	E	286	Total	C	N	O	S	313	0	0
			2304	1450	398	443	13			
1	F	252	Total	C	N	O	S	285	0	0
			2016	1275	346	383	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q8NHV1
A	-3	PRO	-	EXPRESSION TAG	UNP Q8NHV1
A	-2	LEU	-	EXPRESSION TAG	UNP Q8NHV1
A	-1	GLY	-	EXPRESSION TAG	UNP Q8NHV1
A	0	SER	-	EXPRESSION TAG	UNP Q8NHV1
A	100	GLN	LEU	ENGINEERED MUTATION	UNP Q8NHV1
B	-4	GLY	-	EXPRESSION TAG	UNP Q8NHV1
B	-3	PRO	-	EXPRESSION TAG	UNP Q8NHV1
B	-2	LEU	-	EXPRESSION TAG	UNP Q8NHV1
B	-1	GLY	-	EXPRESSION TAG	UNP Q8NHV1
B	0	SER	-	EXPRESSION TAG	UNP Q8NHV1
B	100	GLN	LEU	ENGINEERED MUTATION	UNP Q8NHV1
C	-4	GLY	-	EXPRESSION TAG	UNP Q8NHV1
C	-3	PRO	-	EXPRESSION TAG	UNP Q8NHV1
C	-2	LEU	-	EXPRESSION TAG	UNP Q8NHV1
C	-1	GLY	-	EXPRESSION TAG	UNP Q8NHV1
C	0	SER	-	EXPRESSION TAG	UNP Q8NHV1

Continued on next page...

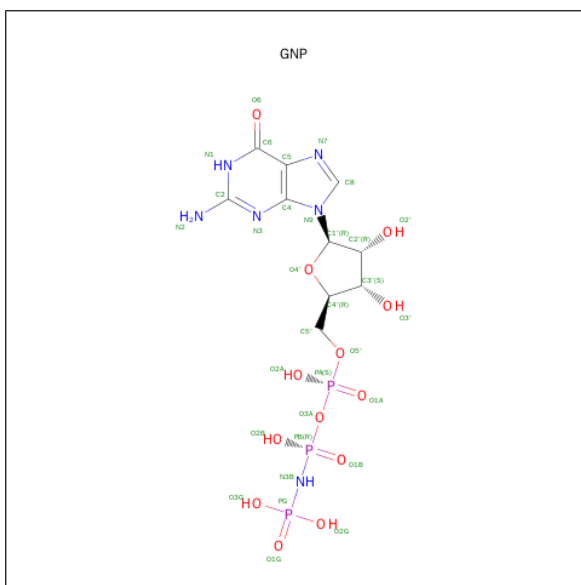
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	GLN	LEU	ENGINEERED MUTATION	UNP Q8NHV1
D	-4	GLY	-	EXPRESSION TAG	UNP Q8NHV1
D	-3	PRO	-	EXPRESSION TAG	UNP Q8NHV1
D	-2	LEU	-	EXPRESSION TAG	UNP Q8NHV1
D	-1	GLY	-	EXPRESSION TAG	UNP Q8NHV1
D	0	SER	-	EXPRESSION TAG	UNP Q8NHV1
D	100	GLN	LEU	ENGINEERED MUTATION	UNP Q8NHV1
E	-4	GLY	-	EXPRESSION TAG	UNP Q8NHV1
E	-3	PRO	-	EXPRESSION TAG	UNP Q8NHV1
E	-2	LEU	-	EXPRESSION TAG	UNP Q8NHV1
E	-1	GLY	-	EXPRESSION TAG	UNP Q8NHV1
E	0	SER	-	EXPRESSION TAG	UNP Q8NHV1
E	100	GLN	LEU	ENGINEERED MUTATION	UNP Q8NHV1
F	-4	GLY	-	EXPRESSION TAG	UNP Q8NHV1
F	-3	PRO	-	EXPRESSION TAG	UNP Q8NHV1
F	-2	LEU	-	EXPRESSION TAG	UNP Q8NHV1
F	-1	GLY	-	EXPRESSION TAG	UNP Q8NHV1
F	0	SER	-	EXPRESSION TAG	UNP Q8NHV1
F	100	GLN	LEU	ENGINEERED MUTATION	UNP Q8NHV1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

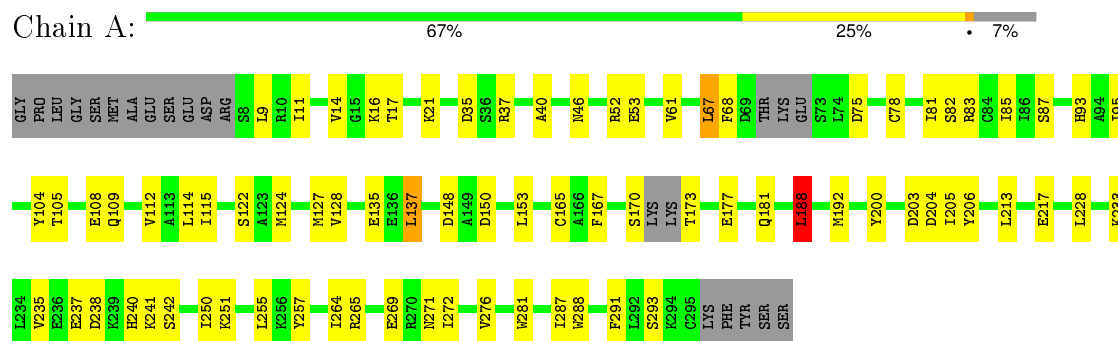
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0

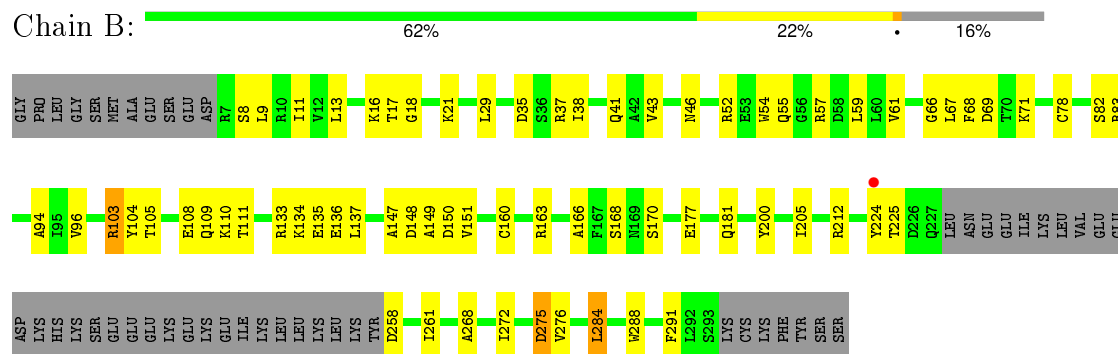
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

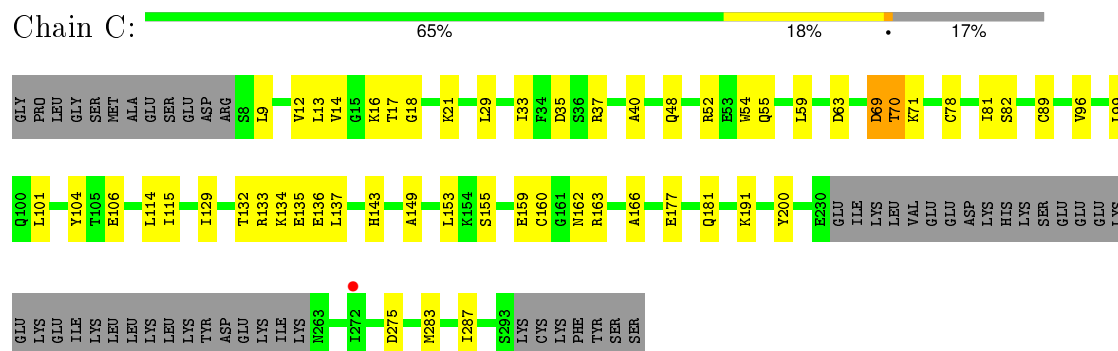
• Molecule 1: GTPASE IMAP FAMILY MEMBER 7



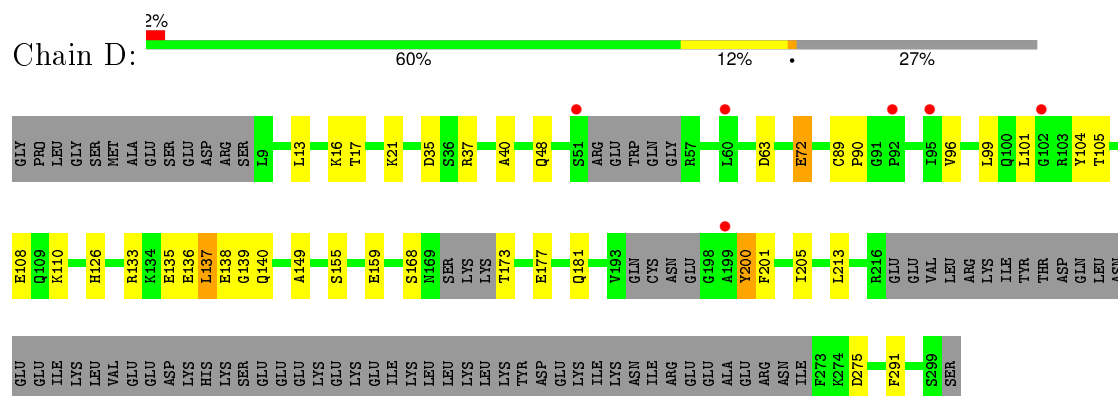
• Molecule 1: GTPASE IMAP FAMILY MEMBER 7



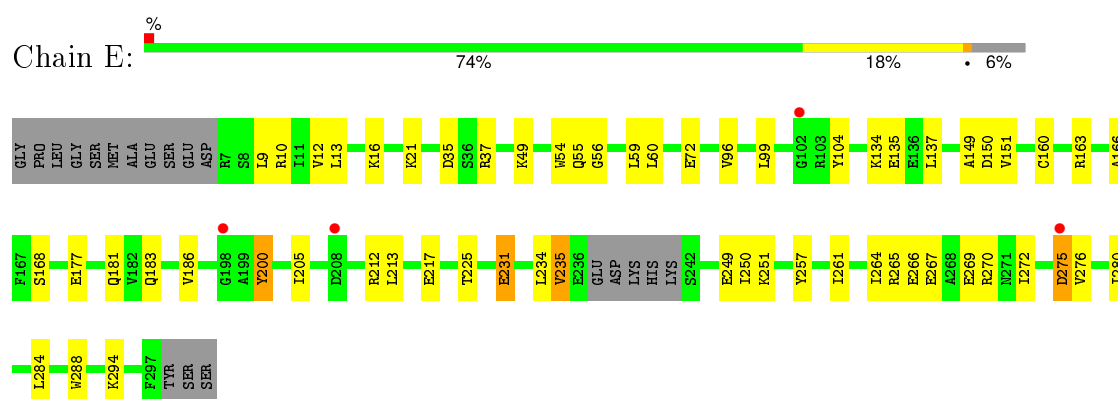
• Molecule 1: GTPASE IMAP FAMILY MEMBER 7



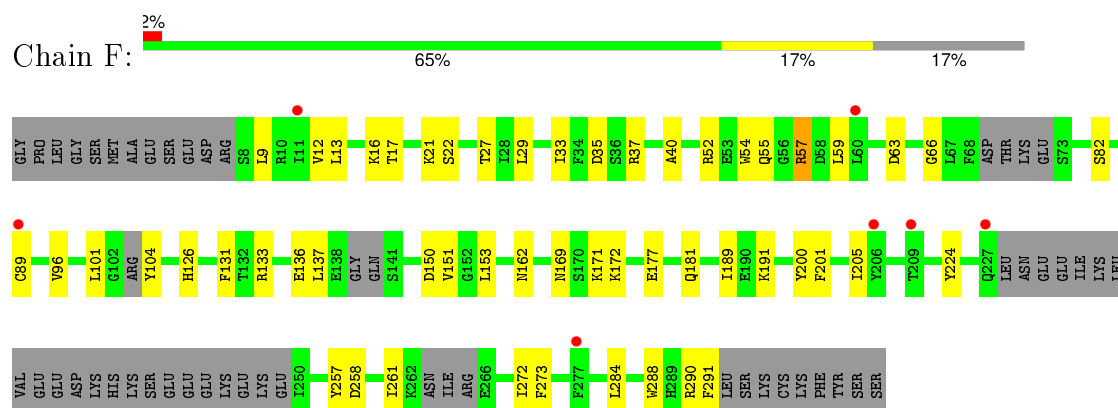
- Molecule 1: GTPASE IMAP FAMILY MEMBER 7



- Molecule 1: GTPASE IMAP FAMILY MEMBER 7



- Molecule 1: GTPASE IMAP FAMILY MEMBER 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.85Å 90.94Å 114.55Å 77.30° 85.23° 89.23°	Depositor
Resolution (Å)	32.44 – 3.15 45.69 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (32.44-3.15) 88.8 (45.69-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.234 , 0.305 0.238 , 0.239	Depositor DCC
R_{free} test set	1496 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 29779 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12623	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.27	0/2302	0.52	1/3080 (0.0%)
1	B	0.29	0/2080	0.49	0/2787
1	C	0.28	0/2048	0.49	0/2747
1	D	0.25	0/1774	0.45	0/2375
1	E	0.27	0/2332	0.49	0/3119
1	F	0.25	0/2039	0.45	0/2726
All	All	0.27	0/12575	0.48	1/16834 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LEU	CA-CB-CG	5.49	127.92	115.30

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	2275	0	2306	44	0
1	B	2054	0	2080	41	0
1	C	2022	0	2038	29	0
1	D	1752	0	1770	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2304	0	2351	35	0
1	F	2016	0	2055	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	32	0	13	1	0
3	B	32	0	13	2	0
3	C	32	0	13	3	0
3	D	32	0	13	1	0
3	E	32	0	13	1	0
3	F	32	0	13	2	0
4	A	2	0	0	2	0
All	All	12623	0	12678	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (187) 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:35:ASP:OD2	1:A:37:ARG:NH1	2.12	0.83
1:A:240:HIS:HA	1:E:251:LYS:HG2	1.63	0.81
1:B:18:GLY:H	3:B:1295:GNP:HNB3	1.31	0.79
1:C:18:GLY:H	3:C:1295:GNP:HNB3	1.32	0.77
1:E:135:GLU:OE2	3:E:1299:GNP:N2	2.20	0.72
1:A:46:ASN:OD1	1:A:83:ARG:NH1	2.22	0.72
1:B:16:LYS:O	1:B:21:LYS:NZ	2.22	0.71
1:C:136:GLU:OE2	1:D:133:ARG:NH1	2.18	0.71
1:E:16:LYS:O	1:E:21:LYS:NZ	2.24	0.70
1:B:105:THR:OG1	1:B:108:GLU:OE1	2.07	0.70
1:A:203:ASP:OD1	1:A:204:ASP:N	2.23	0.70
1:E:35:ASP:OD2	1:E:37:ARG:NH1	2.25	0.69
1:A:135:GLU:OE2	3:A:1297:GNP:N2	2.23	0.67
1:E:217:GLU:OE2	1:E:265:ARG:NE	2.28	0.67
1:A:105:THR:OG1	1:A:108:GLU:OE1	2.11	0.66
1:A:16:LYS:O	1:A:21:LYS:NZ	2.28	0.66
1:B:52:ARG:NH1	1:B:54:TRP:HD1	1.93	0.66
1:E:54:TRP:O	1:E:56:GLY:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:OD2	1:B:37:ARG:NH1	2.30	0.65
1:A:11:ILE:HD11	1:A:61:VAL:HG22	1.78	0.65
1:E:267:GLU:OE1	1:E:270:ARG:NH2	2.30	0.64
1:A:82:SER:HB3	1:A:276:VAL:HG23	1.79	0.64
1:C:16:LYS:O	1:C:21:LYS:NZ	2.30	0.63
1:B:133:ARG:HB3	1:B:136:GLU:HG3	1.80	0.62
1:B:11:ILE:HG22	1:B:94:ALA:HB3	1.82	0.62
4:A:2002:HOH:O	1:B:103:ARG:NH1	2.32	0.62
1:B:9:LEU:HD22	1:B:59:LEU:HD22	1.81	0.62
1:A:170:SER:O	1:A:173:THR:N	2.32	0.62
1:C:21:LYS:N	3:C:1295:GNP:O1B	2.33	0.61
1:A:81:ILE:HD11	1:A:114:LEU:HD21	1.80	0.61
1:F:9:LEU:HD23	1:F:59:LEU:HD22	1.81	0.61
1:E:235:VAL:HG11	1:E:250:ILE:HG13	1.83	0.61
1:B:54:TRP:O	1:B:57:ARG:N	2.27	0.61
1:D:133:ARG:HB3	1:D:136:GLU:HG3	1.84	0.60
1:B:67:LEU:HG	1:B:111:THR:HG23	1.85	0.59
1:B:147:ALA:O	1:F:171:LYS:HB3	2.03	0.59
1:F:35:ASP:OD2	1:F:37:ARG:NH1	2.35	0.59
1:D:35:ASP:OD2	1:D:37:ARG:NH1	2.34	0.59
1:F:16:LYS:O	1:F:21:LYS:NZ	2.35	0.58
1:C:135:GLU:OE2	3:C:1295:GNP:N2	2.21	0.58
1:D:16:LYS:O	1:D:21:LYS:NZ	2.35	0.58
1:C:133:ARG:HB3	1:C:136:GLU:HG3	1.86	0.58
1:D:135:GLU:OE2	3:D:1301:GNP:N2	2.34	0.58
1:B:224:TYR:O	1:B:258:ASP:N	2.36	0.58
1:A:93:HIS:CD2	1:A:200:TYR:HB3	2.38	0.57
1:E:294:LYS:HB2	1:F:290:ARG:O	2.05	0.56
1:B:52:ARG:HH12	1:B:54:TRP:HD1	1.53	0.55
1:E:49:LYS:HD2	1:E:60:LEU:HD21	1.88	0.55
1:F:104:TYR:HB2	1:F:153:LEU:HD13	1.90	0.54
1:D:101:LEU:HD21	1:D:137:LEU:HD23	1.90	0.54
1:B:212:ARG:HB3	1:B:272:ILE:HD12	1.91	0.53
1:F:177:GLU:O	1:F:181:GLN:HG3	2.08	0.53
1:A:150:ASP:OD1	1:B:41:GLN:HB3	2.09	0.53
1:A:85:ILE:HD13	1:A:205:ILE:HG21	1.91	0.53
1:A:287:ILE:HG22	1:A:291:PHE:HE1	1.74	0.53
1:B:17:THR:HG23	1:B:66:GLY:HA3	1.92	0.52
1:F:224:TYR:HB3	1:F:257:TYR:HE1	1.75	0.52
1:C:134:LYS:HD2	1:C:166:ALA:HB3	1.92	0.52
1:C:35:ASP:OD2	1:C:37:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:HD23	1:E:96:VAL:HB	1.93	0.51
1:A:238:ASP:OD2	1:A:241:LYS:NZ	2.35	0.51
1:B:46:ASN:OD1	1:B:83:ARG:NH1	2.43	0.51
1:B:11:ILE:HD11	1:B:61:VAL:HG22	1.92	0.51
1:E:213:LEU:HD23	1:E:265:ARG:HH11	1.76	0.51
1:E:213:LEU:HD23	1:E:265:ARG:HD2	1.93	0.51
1:C:153:LEU:HD23	1:D:40:ALA:HB1	1.93	0.50
1:F:54:TRP:O	1:F:57:ARG:N	2.33	0.50
1:A:78:CYS:O	1:A:82:SER:OG	2.23	0.50
1:C:69:ASP:N	1:C:69:ASP:OD1	2.25	0.50
1:E:9:LEU:HD23	1:E:59:LEU:HD22	1.93	0.50
1:D:48:GLN:HG3	1:D:63:ASP:HB3	1.93	0.50
1:A:203:ASP:H	1:A:206:TYR:HB2	1.75	0.50
1:A:104:TYR:HB2	1:A:153:LEU:HD13	1.93	0.50
1:E:275:ASP:OD1	1:E:275:ASP:N	2.45	0.50
1:C:40:ALA:HB3	1:D:149:ALA:HA	1.94	0.50
1:C:106:GLU:OE2	1:D:110:LYS:NZ	2.40	0.49
1:B:17:THR:CG2	1:B:66:GLY:HA3	2.42	0.49
1:F:133:ARG:HB3	1:F:136:GLU:HG3	1.94	0.49
1:C:9:LEU:HD22	1:C:59:LEU:HD22	1.94	0.49
1:B:69:ASP:HB3	1:B:71:LYS:O	2.12	0.49
1:F:22:SER:OG	1:F:63:ASP:OD2	2.17	0.49
1:B:135:GLU:OE1	1:B:168:SER:OG	2.18	0.49
1:C:78:CYS:O	1:C:82:SER:OG	2.30	0.49
1:F:126:HIS:ND1	1:F:201:PHE:HB2	2.28	0.48
1:B:160:CYS:O	1:B:163:ARG:NE	2.46	0.48
1:A:177:GLU:O	1:A:181:GLN:HG3	2.13	0.48
1:C:13:LEU:HD23	1:C:96:VAL:HB	1.96	0.48
1:A:228:LEU:HD22	1:A:257:TYR:CG	2.48	0.48
1:A:9:LEU:HD23	1:A:93:HIS:ND1	2.28	0.48
1:D:90:PRO:HG2	1:D:200:TYR:CE2	2.48	0.48
1:F:17:THR:HB	1:F:66:GLY:HA3	1.95	0.48
1:B:135:GLU:OE2	3:B:1295:GNP:N2	2.37	0.47
1:C:177:GLU:O	1:C:181:GLN:HG3	2.14	0.47
1:D:177:GLU:O	1:D:181:GLN:HG3	2.15	0.47
1:E:257:TYR:CZ	1:E:261:ILE:HD11	2.50	0.47
1:D:137:LEU:O	1:D:139:GLY:N	2.48	0.46
1:A:112:VAL:HG13	1:A:124:MET:HE3	1.96	0.46
1:F:13:LEU:HD23	1:F:96:VAL:HB	1.97	0.46
1:F:150:ASP:OD1	1:F:151:VAL:N	2.41	0.46
1:C:14:VAL:HG21	1:C:115:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HA	1:A:272:ILE:HD11	1.98	0.46
1:C:104:TYR:HB2	1:C:153:LEU:HD13	1.97	0.46
1:A:67:LEU:HD11	1:A:114:LEU:HD23	1.96	0.46
1:B:148:ASP:OD1	1:F:172:LYS:HG2	2.15	0.46
1:F:29:LEU:HD13	1:F:33:ILE:HD12	1.98	0.46
1:A:52:ARG:HG2	1:A:53:GLU:N	2.29	0.46
1:B:13:LEU:HD23	1:B:96:VAL:HB	1.98	0.46
1:E:261:ILE:HA	1:E:264:ILE:HG13	1.98	0.45
1:E:212:ARG:HB3	1:E:272:ILE:HD11	1.97	0.45
1:A:105:THR:O	1:A:109:GLN:HG3	2.16	0.45
1:D:72:GLU:HG2	1:D:72:GLU:H	1.41	0.45
1:C:101:LEU:HB2	1:C:132:THR:O	2.16	0.45
1:B:275:ASP:OD1	1:B:275:ASP:N	2.50	0.45
1:A:233:LYS:O	1:A:237:GLU:HG2	2.16	0.45
1:C:70:THR:OG1	1:C:71:LYS:N	2.49	0.45
1:F:131:PHE:HZ	1:F:153:LEU:HD11	1.81	0.45
1:C:81:ILE:HD11	1:C:114:LEU:HD21	1.98	0.45
1:A:95:ILE:O	1:A:127:MET:HA	2.16	0.45
1:A:271:ASN:HA	1:E:183:GLN:NE2	2.31	0.45
1:D:13:LEU:HD23	1:D:96:VAL:HB	1.98	0.45
1:C:48:GLN:HG3	1:C:63:ASP:HB3	1.98	0.45
1:F:21:LYS:NZ	3:F:1293:GNP:O1B	2.48	0.45
1:B:68:PHE:CZ	1:B:110:LYS:HB3	2.52	0.45
1:B:177:GLU:O	1:B:181:GLN:HG3	2.16	0.45
1:C:149:ALA:HA	1:D:40:ALA:HB3	1.99	0.45
1:F:101:LEU:HD21	1:F:137:LEU:HD23	1.98	0.45
1:B:258:ASP:HA	1:B:261:ILE:HG13	1.99	0.44
1:B:268:ALA:O	1:B:272:ILE:HG12	2.17	0.44
1:E:10:ARG:HH21	1:E:200:TYR:HD2	1.65	0.44
1:E:265:ARG:O	1:E:269:GLU:HG3	2.16	0.44
1:D:137:LEU:H	1:D:137:LEU:HG	1.57	0.44
1:D:99:LEU:HD21	1:D:104:TYR:HD1	1.82	0.44
1:E:150:ASP:OD1	1:E:151:VAL:N	2.41	0.44
1:E:54:TRP:CZ3	1:E:186:VAL:HG11	2.54	0.43
1:B:37:ARG:NH1	1:B:43:VAL:HG13	2.32	0.43
1:D:168:SER:HB3	1:D:173:THR:HG21	1.99	0.43
1:D:105:THR:OG1	1:D:108:GLU:OE1	2.25	0.43
1:F:284:LEU:O	1:F:288:TRP:HB2	2.18	0.43
1:C:29:LEU:HA	1:C:52:ARG:HD2	2.00	0.43
1:A:93:HIS:HD2	1:A:200:TYR:HB3	1.80	0.43
1:B:134:LYS:HD2	1:B:166:ALA:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:HIS:ND1	1:D:201:PHE:HB2	2.34	0.43
1:C:155:SER:O	1:C:159:GLU:HG3	2.18	0.43
1:E:213:LEU:HD11	1:E:272:ILE:HG21	2.01	0.43
1:E:99:LEU:HD21	1:E:104:TYR:HD1	1.84	0.43
1:A:251:LYS:O	1:A:255:LEU:HG	2.18	0.43
1:A:265:ARG:O	1:A:269:GLU:HG3	2.19	0.43
1:A:137:LEU:HA	1:B:38:ILE:HG21	1.99	0.43
1:B:29:LEU:O	1:B:52:ARG:HD2	2.19	0.43
1:E:284:LEU:O	1:E:288:TRP:HB2	2.19	0.43
1:A:228:LEU:HD13	1:A:257:TYR:HB2	2.00	0.42
1:A:271:ASN:ND2	4:A:2001:HOH:O	2.49	0.42
1:C:160:CYS:O	1:C:163:ARG:NE	2.52	0.42
1:A:9:LEU:HA	1:A:93:HIS:ND1	2.35	0.42
1:F:52:ARG:NH1	1:F:54:TRP:HD1	2.18	0.42
1:A:14:VAL:HG21	1:A:115:ILE:HD11	2.02	0.42
1:E:231:GLU:O	1:E:234:LEU:HB2	2.20	0.42
1:B:272:ILE:HG22	1:B:276:VAL:HG23	2.02	0.42
1:E:177:GLU:O	1:E:181:GLN:HG3	2.20	0.42
1:A:67:LEU:HD12	1:A:68:PHE:CE2	2.55	0.41
1:E:99:LEU:HD21	1:E:104:TYR:CD1	2.55	0.41
1:E:134:LYS:HD2	1:E:166:ALA:HB3	2.01	0.41
1:F:9:LEU:HD11	1:F:189:ILE:HG21	2.02	0.41
1:D:213:LEU:HA	1:D:213:LEU:HD23	1.92	0.41
1:A:40:ALA:HB3	1:B:149:ALA:HA	2.02	0.41
1:C:29:LEU:HD13	1:C:33:ILE:HD12	2.02	0.41
1:B:284:LEU:O	1:B:288:TRP:N	2.52	0.41
1:A:235:VAL:HG11	1:A:250:ILE:HG13	2.02	0.41
1:E:149:ALA:HA	1:F:40:ALA:HB3	2.01	0.41
1:F:258:ASP:O	1:F:261:ILE:HG22	2.21	0.41
1:A:217:GLU:HG2	1:A:264:ILE:HG22	2.02	0.41
1:E:135:GLU:OE1	1:E:168:SER:OG	2.23	0.41
1:F:27:THR:HG21	1:F:169:ASN:HA	2.02	0.41
1:E:276:VAL:O	1:E:280:ILE:HG12	2.20	0.41
1:D:137:LEU:HD13	1:D:140:GLN:O	2.21	0.41
1:C:99:LEU:HD13	1:C:129:ILE:HG23	2.03	0.41
1:B:150:ASP:OD1	1:B:151:VAL:N	2.49	0.41
1:B:78:CYS:O	1:B:82:SER:OG	2.26	0.41
1:B:104:TYR:CE2	1:B:109:GLN:HG2	2.56	0.41
1:A:81:ILE:O	1:A:85:ILE:HG13	2.21	0.40
1:A:165:CYS:SG	1:A:188:LEU:HD21	2.62	0.40
1:C:283:MET:O	1:C:287:ILE:HG13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:CYS:O	1:E:163:ARG:NE	2.55	0.40
1:E:213:LEU:O	1:E:217:GLU:HG3	2.22	0.40
1:D:155:SER:O	1:D:159:GLU:HG3	2.21	0.40
1:F:82:SER:HB2	1:F:273:PHE:HE1	1.87	0.40
1:F:169:ASN:ND2	3:F:1293:GNP:N7	2.58	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	277/305 (91%)	270 (98%)	7 (2%)	0	100	100
1	B	253/305 (83%)	246 (97%)	6 (2%)	1 (0%)	39	79
1	C	250/305 (82%)	242 (97%)	7 (3%)	1 (0%)	39	79
1	D	213/305 (70%)	208 (98%)	4 (2%)	1 (0%)	34	76
1	E	282/305 (92%)	274 (97%)	7 (2%)	1 (0%)	39	79
1	F	240/305 (79%)	237 (99%)	2 (1%)	1 (0%)	39	79
All	All	1515/1830 (83%)	1477 (98%)	33 (2%)	5 (0%)	46	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	E	55	GLN
1	F	55	GLN
1	C	55	GLN
1	D	138	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/273 (93%)	239 (94%)	15 (6%)	24	63
1	B	228/273 (84%)	218 (96%)	10 (4%)	35	73
1	C	224/273 (82%)	212 (95%)	12 (5%)	27	67
1	D	194/273 (71%)	186 (96%)	8 (4%)	37	75
1	E	257/273 (94%)	246 (96%)	11 (4%)	35	74
1	F	224/273 (82%)	215 (96%)	9 (4%)	38	76
All	All	1381/1638 (84%)	1316 (95%)	65 (5%)	32	72

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	67	LEU
1	A	75	ASP
1	A	87	SER
1	A	122	SER
1	A	128	VAL
1	A	137	LEU
1	A	148	ASP
1	A	167	PHE
1	A	188	LEU
1	A	192	MET
1	A	242	SER
1	A	281	TRP
1	A	288	TRP
1	A	293	SER
1	B	8	SER
1	B	103	ARG
1	B	137	LEU
1	B	170	SER
1	B	200	TYR
1	B	205	ILE
1	B	225	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	275	ASP
1	B	284	LEU
1	B	291	PHE
1	C	12	VAL
1	C	17	THR
1	C	54	TRP
1	C	69	ASP
1	C	70	THR
1	C	89	CYS
1	C	137	LEU
1	C	143	HIS
1	C	162	ASN
1	C	191	LYS
1	C	200	TYR
1	C	275	ASP
1	D	17	THR
1	D	72	GLU
1	D	89	CYS
1	D	137	LEU
1	D	200	TYR
1	D	205	ILE
1	D	275	ASP
1	D	291	PHE
1	E	12	VAL
1	E	72	GLU
1	E	137	LEU
1	E	200	TYR
1	E	205	ILE
1	E	225	THR
1	E	231	GLU
1	E	235	VAL
1	E	249	GLU
1	E	266	GLU
1	E	275	ASP
1	F	12	VAL
1	F	57	ARG
1	F	89	CYS
1	F	162	ASN
1	F	191	LYS
1	F	200	TYR
1	F	205	ILE
1	F	272	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	291	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	D	48	GLN
1	F	196	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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	GNP	A	1297	2	28,34,34	1.88	5 (17%)	33,54,54	2.38	6 (18%)
3	GNP	B	1295	2	28,34,34	1.84	5 (17%)	33,54,54	2.33	7 (21%)
3	GNP	C	1295	2	28,34,34	1.89	4 (14%)	33,54,54	2.31	6 (18%)
3	GNP	D	1301	2	28,34,34	1.88	5 (17%)	33,54,54	2.48	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GNP	E	1299	2	28,34,34	1.84	4 (14%)	33,54,54	2.41	6 (18%)
3	GNP	F	1293	2	28,34,34	1.90	4 (14%)	33,54,54	2.33	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
3	GNP	A	1297	2	-	0/12/38/38	0/3/3/3
3	GNP	B	1295	2	-	1/12/38/38	0/3/3/3
3	GNP	C	1295	2	-	1/12/38/38	0/3/3/3
3	GNP	D	1301	2	-	0/12/38/38	0/3/3/3
3	GNP	E	1299	2	-	1/12/38/38	0/3/3/3
3	GNP	F	1293	2	-	0/12/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1293	GNP	PB-O3A	-5.65	1.52	1.59
3	A	1297	GNP	PB-O3A	-5.49	1.52	1.59
3	C	1295	GNP	PB-O3A	-5.33	1.52	1.59
3	D	1301	GNP	PB-O3A	-5.29	1.52	1.59
3	E	1299	GNP	PB-O3A	-5.09	1.52	1.59
3	B	1295	GNP	PB-O3A	-4.86	1.53	1.59
3	D	1301	GNP	PB-O2B	-3.06	1.48	1.56
3	F	1293	GNP	PB-O2B	-2.96	1.48	1.56
3	E	1299	GNP	PB-O2B	-2.95	1.48	1.56
3	A	1297	GNP	PB-O2B	-2.95	1.48	1.56
3	C	1295	GNP	PB-O2B	-2.94	1.48	1.56
3	B	1295	GNP	PB-O2B	-2.89	1.48	1.56
3	A	1297	GNP	PB-N3B	-2.03	1.58	1.63
3	D	1301	GNP	C8-N7	-2.02	1.30	1.34
3	B	1295	GNP	C8-N7	-2.01	1.30	1.34
3	B	1295	GNP	C6-N1	3.42	1.39	1.33
3	A	1297	GNP	C6-N1	3.49	1.39	1.33
3	D	1301	GNP	C6-N1	3.50	1.39	1.33
3	F	1293	GNP	C6-N1	3.60	1.39	1.33
3	E	1299	GNP	C6-N1	3.62	1.39	1.33
3	C	1295	GNP	C6-N1	3.64	1.39	1.33
3	F	1293	GNP	PG-O1G	4.34	1.51	1.46
3	A	1297	GNP	PG-O1G	4.38	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1299	GNP	PG-O1G	4.43	1.51	1.46
3	D	1301	GNP	PG-O1G	4.46	1.51	1.46
3	C	1295	GNP	PG-O1G	4.64	1.51	1.46
3	B	1295	GNP	PG-O1G	4.86	1.51	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1301	GNP	C5-C6-N1	-8.94	111.36	123.59
3	B	1295	GNP	C5-C6-N1	-8.82	111.53	123.59
3	F	1293	GNP	C5-C6-N1	-8.64	111.78	123.59
3	E	1299	GNP	C5-C6-N1	-8.62	111.81	123.59
3	A	1297	GNP	C5-C6-N1	-8.56	111.88	123.59
3	C	1295	GNP	C5-C6-N1	-8.42	112.08	123.59
3	D	1301	GNP	O1G-PG-N3B	-4.62	104.81	111.90
3	E	1299	GNP	O1G-PG-N3B	-4.60	104.84	111.90
3	D	1301	GNP	PA-O3A-PB	-4.15	118.75	132.67
3	A	1297	GNP	O1G-PG-N3B	-4.11	105.59	111.90
3	A	1297	GNP	PA-O3A-PB	-3.66	120.41	132.67
3	C	1295	GNP	O1G-PG-N3B	-3.64	106.31	111.90
3	B	1295	GNP	O1G-PG-N3B	-3.56	106.44	111.90
3	F	1293	GNP	PA-O3A-PB	-3.39	121.30	132.67
3	E	1299	GNP	PA-O3A-PB	-3.30	121.59	132.67
3	F	1293	GNP	O1G-PG-N3B	-3.18	107.01	111.90
3	B	1295	GNP	O1B-PB-N3B	-2.63	107.86	111.90
3	C	1295	GNP	PA-O3A-PB	-2.63	123.85	132.67
3	C	1295	GNP	N3-C2-N1	-2.44	123.72	127.44
3	E	1299	GNP	N3-C2-N1	-2.27	123.98	127.44
3	A	1297	GNP	N3-C2-N1	-2.26	124.01	127.44
3	B	1295	GNP	N3-C2-N1	-2.13	124.19	127.44
3	B	1295	GNP	PA-O3A-PB	-2.13	125.53	132.67
3	D	1301	GNP	N3-C2-N1	-2.13	124.21	127.44
3	F	1293	GNP	N3-C2-N1	-2.12	124.22	127.44
3	D	1301	GNP	O3A-PA-O5'	2.05	108.39	102.94
3	B	1295	GNP	O2B-PB-O1B	3.39	117.08	110.00
3	E	1299	GNP	O2B-PB-O1B	3.61	117.54	110.00
3	C	1295	GNP	O2B-PB-O1B	3.72	117.76	110.00
3	A	1297	GNP	O2B-PB-O1B	3.89	118.11	110.00
3	D	1301	GNP	O2B-PB-O1B	3.89	118.12	110.00
3	F	1293	GNP	O2B-PB-O1B	4.25	118.88	110.00
3	F	1293	GNP	C6-N1-C2	6.28	124.66	115.94
3	C	1295	GNP	C6-N1-C2	6.32	124.72	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1297	GNP	C6-N1-C2	6.38	124.79	115.94
3	E	1299	GNP	C6-N1-C2	6.42	124.85	115.94
3	B	1295	GNP	C6-N1-C2	6.45	124.89	115.94
3	D	1301	GNP	C6-N1-C2	6.54	125.01	115.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1295	GNP	O1G-PG-N3B-PB
3	B	1295	GNP	O1G-PG-N3B-PB
3	E	1299	GNP	O1B-PB-N3B-PG

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1297	GNP	1	0
3	B	1295	GNP	2	0
3	C	1295	GNP	3	0
3	D	1301	GNP	1	0
3	E	1299	GNP	1	0
3	F	1293	GNP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	283/305 (92%)	-0.33	0	100 100	27, 66, 105, 126	60 (21%)
1	B	257/305 (84%)	-0.42	1 (0%)	93 90	27, 53, 96, 170	34 (13%)
1	C	254/305 (83%)	-0.36	1 (0%)	93 90	25, 56, 99, 130	40 (15%)
1	D	223/305 (73%)	-0.07	6 (2%)	58 42	29, 79, 120, 152	45 (20%)
1	E	286/305 (93%)	-0.24	4 (1%)	78 64	38, 70, 106, 137	69 (24%)
1	F	252/305 (82%)	0.02	7 (2%)	56 40	46, 89, 131, 157	60 (23%)
All	All	1555/1830 (84%)	-0.24	19 (1%)	81 69	25, 69, 114, 170	308 (19%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	224	TYR	2.9
1	F	60	LEU	2.8
1	F	89	CYS	2.7
1	F	11	ILE	2.6
1	E	198	GLY	2.6
1	D	95	ILE	2.5
1	D	102	GLY	2.5
1	F	209	THR	2.5
1	D	199	ALA	2.4
1	F	206	TYR	2.3
1	D	60	LEU	2.2
1	C	272	ILE	2.2
1	E	208	ASP	2.1
1	E	275	ASP	2.1
1	E	102	GLY	2.1
1	F	227	GLN	2.1
1	D	92	PRO	2.1
1	D	51	SER	2.0
1	F	277	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	1296	1/1	0.88	0.73	35.69	279,279,279,279	0
2	MG	C	1294	1/1	0.89	0.72	23.78	215,215,215,215	0
2	MG	B	1294	1/1	0.82	0.23	2.99	37,37,37,37	0
2	MG	F	1292	1/1	0.96	0.21	0.10	79,79,79,79	0
3	GNP	C	1295	32/32	0.96	0.17	-0.11	6,52,68,82	0
3	GNP	B	1295	32/32	0.96	0.17	-0.20	17,54,68,88	0
3	GNP	F	1293	32/32	0.93	0.18	-0.36	43,64,97,104	0
3	GNP	D	1301	32/32	0.96	0.18	-0.37	28,74,97,173	0
3	GNP	A	1297	32/32	0.96	0.16	-0.55	6,56,82,86	0
2	MG	D	1300	1/1	0.93	0.12	-1.85	34,34,34,34	0
3	GNP	E	1299	32/32	0.96	0.14	-2.03	39,66,82,164	0
2	MG	E	1298	1/1	0.98	0.05	-4.47	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.