Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 07:35 PM EDT

PDB ID	:	1TU3
Title	:	Crystal Structure of Rab5 complex with Rabaptin5 C-terminal Domain
Authors	:	Zhu, G.; Zhai, P.; Liu, J.; Terzyan, S.; Li, G.; Zhang, X.C.
Deposited on	:	2004-06-24
Resolution	:	2.31 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

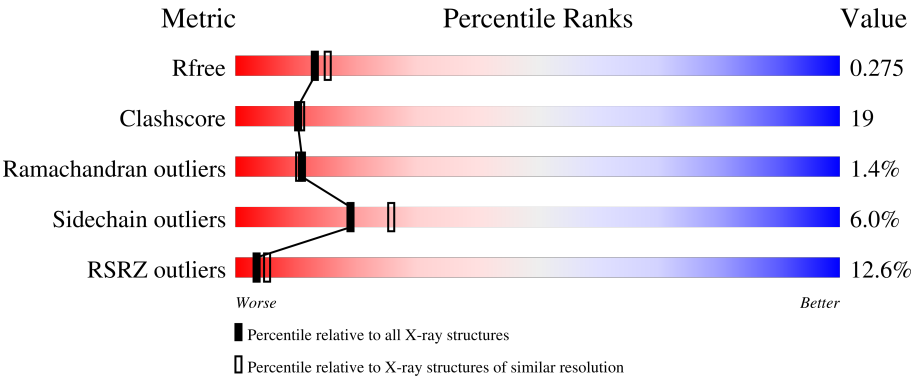
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	171	8% 65% 29%
1	B	171	8% 65% 28%
1	C	171	12% 57% 37%
1	D	171	20% 39% 41% 6% 14%
1	E	171	6% 74% 22%

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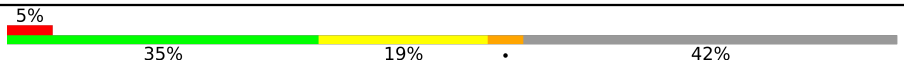
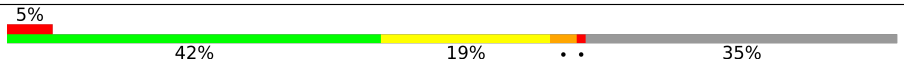
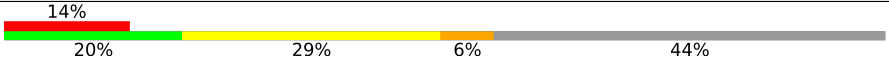
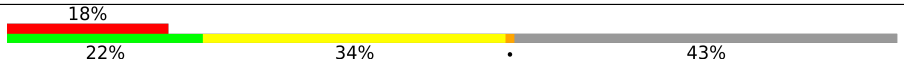
Mol	Chain	Length	Quality of chain
2	F	79	
2	G	79	
2	H	79	
2	I	79	
2	J	79	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8735 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 Ras-related protein Rab-5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1296	825	218	247	6			
1	B	166	Total	C	N	O	S	0	0	0
			1305	831	220	248	6			
1	C	166	Total	C	N	O	S	0	0	0
			1305	829	221	249	6			
1	D	147	Total	C	N	O	S	0	0	0
			1141	726	190	220	5			
1	E	167	Total	C	N	O	S	0	0	0
			1313	835	222	250	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	cloning artifact	UNP P20339
B	14	MET	-	cloning artifact	UNP P20339
C	14	MET	-	cloning artifact	UNP P20339
D	14	MET	-	cloning artifact	UNP P20339
E	14	MET	-	cloning artifact	UNP P20339

- Molecule 2 is a protein called Rab GTPase binding effector protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	46	Total	C	N	O	0	0	0
			381	233	74	74			
2	G	51	Total	C	N	O	0	0	0
			422	257	82	83			
2	H	44	Total	C	N	O	0	0	0
			367	225	71	71			
2	I	45	Total	C	N	O	0	0	0
			375	230	73	72			
2	J	53	Total	C	N	O	0	0	0
			437	267	84	86			

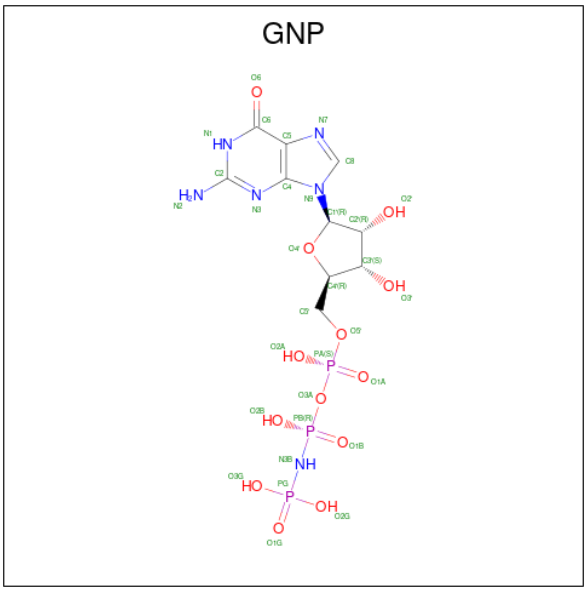
There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	784	GLY	-	cloning artifact	UNP Q15276
F	785	PRO	-	cloning artifact	UNP Q15276
F	786	LEU	-	cloning artifact	UNP Q15276
F	787	GLY	-	cloning artifact	UNP Q15276
F	788	SER	-	cloning artifact	UNP Q15276
G	784	GLY	-	cloning artifact	UNP Q15276
G	785	PRO	-	cloning artifact	UNP Q15276
G	786	LEU	-	cloning artifact	UNP Q15276
G	787	GLY	-	cloning artifact	UNP Q15276
G	788	SER	-	cloning artifact	UNP Q15276
H	784	GLY	-	cloning artifact	UNP Q15276
H	785	PRO	-	cloning artifact	UNP Q15276
H	786	LEU	-	cloning artifact	UNP Q15276
H	787	GLY	-	cloning artifact	UNP Q15276
H	788	SER	-	cloning artifact	UNP Q15276
I	784	GLY	-	cloning artifact	UNP Q15276
I	785	PRO	-	cloning artifact	UNP Q15276
I	786	LEU	-	cloning artifact	UNP Q15276
I	787	GLY	-	cloning artifact	UNP Q15276
I	788	SER	-	cloning artifact	UNP Q15276
J	784	GLY	-	cloning artifact	UNP Q15276
J	785	PRO	-	cloning artifact	UNP Q15276
J	786	LEU	-	cloning artifact	UNP Q15276
J	787	GLY	-	cloning artifact	UNP Q15276
J	788	SER	-	cloning artifact	UNP Q15276

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	24	Total	O	0	0
			24	24		
5	C	17	Total	O	0	0
			17	17		
5	D	20	Total	O	0	0
			20	20		
5	E	61	Total	O	0	0
			61	61		
5	F	9	Total	O	0	0
			9	9		
5	G	13	Total	O	0	0
			13	13		

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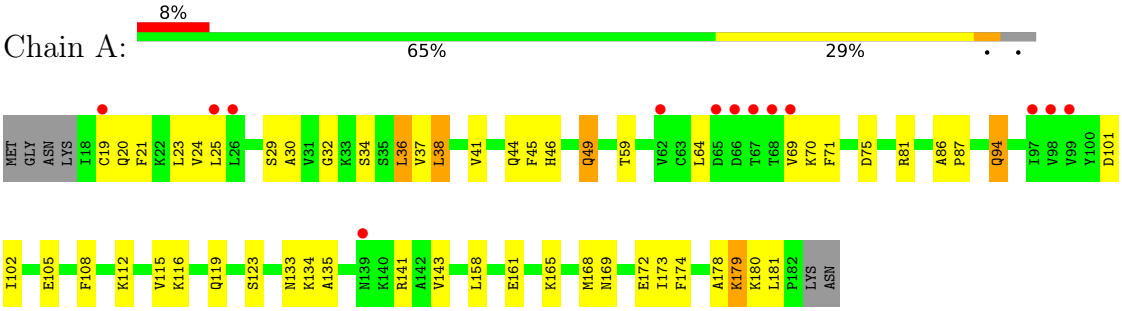
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	5	Total O 5 5	0	0
5	I	2	Total O 2 2	0	0
5	J	15	Total O 15 15	0	0

3 Residue-property plots (i)

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

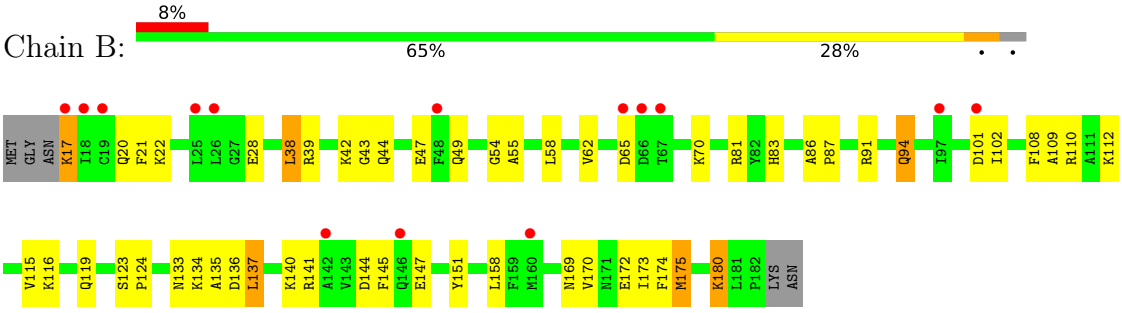
• Molecule 1: Ras-related protein Rab-5A

Chain A:



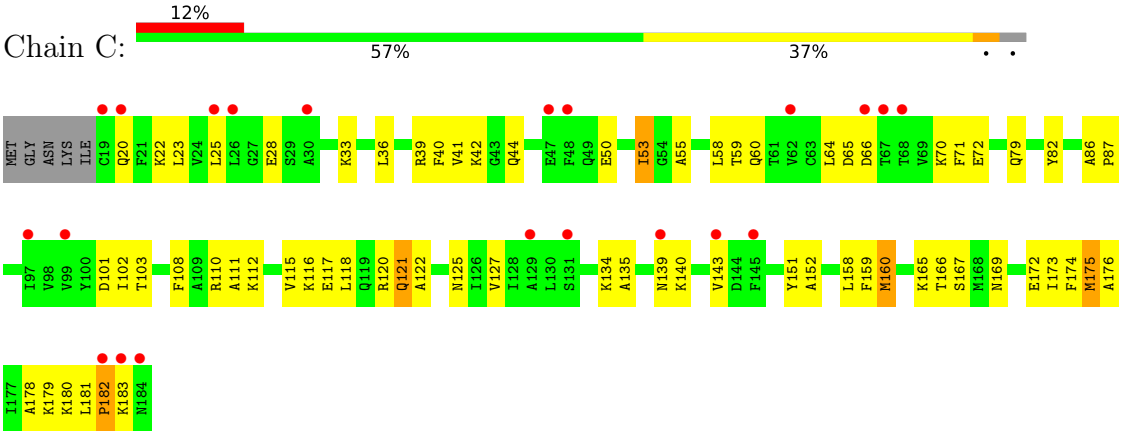
• Molecule 1: Ras-related protein Rab-5A

Chain B:

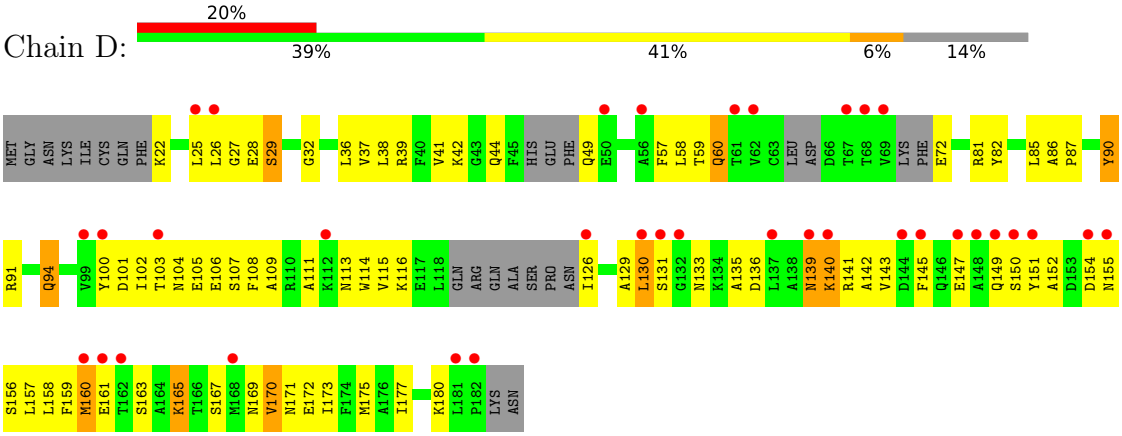


• Molecule 1: Ras-related protein Rab-5A

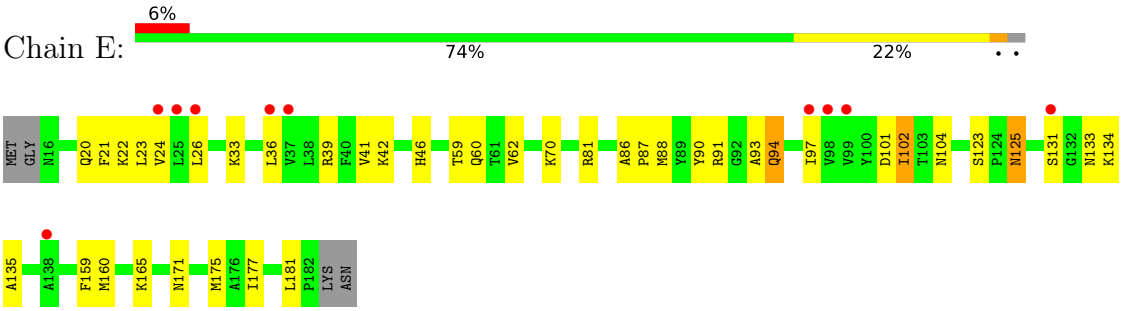
Chain C:



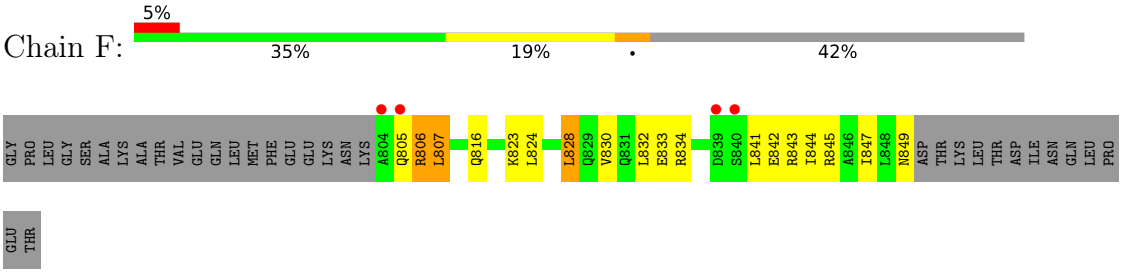
• Molecule 1: Ras-related protein Rab-5A



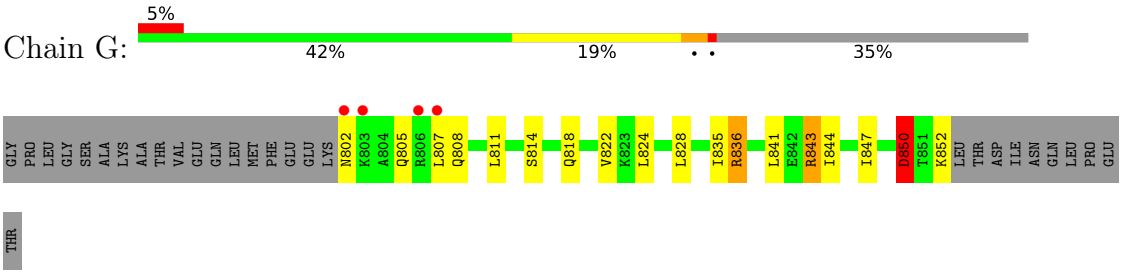
• Molecule 1: Ras-related protein Rab-5A



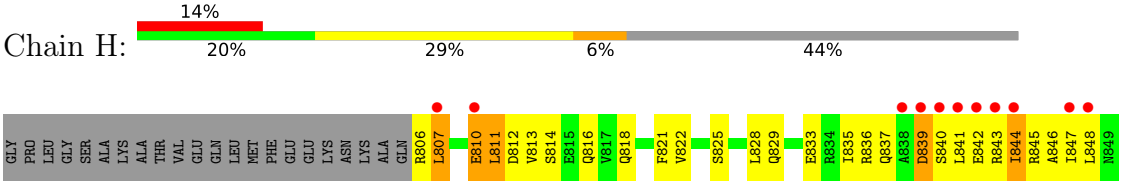
• Molecule 2: Rab GTPase binding effector protein 1



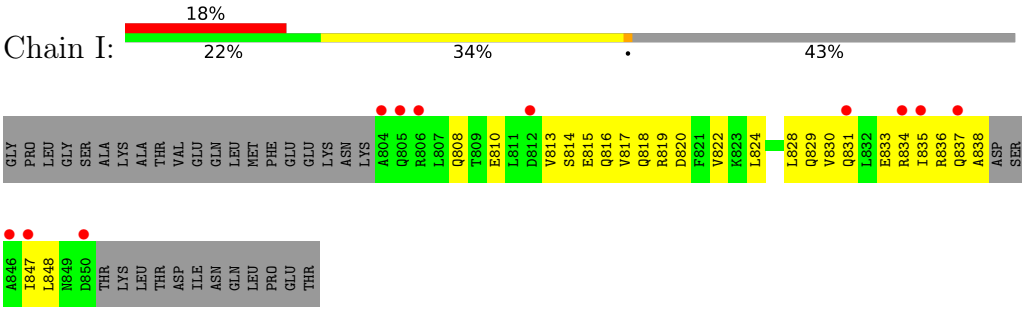
• Molecule 2: Rab GTPase binding effector protein 1



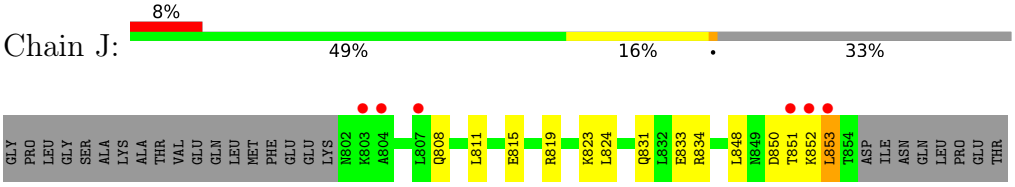
• Molecule 2: Rab GTPase binding effector protein 1



• Molecule 2: Rab GTPase binding effector protein 1



• Molecule 2: Rab GTPase binding effector protein 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.40Å 83.50Å 144.90Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	29.72 – 2.31 29.71 – 2.32	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.72-2.31) 90.8 (29.71-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.277 0.218 , 0.275	Depositor DCC
R_{free} test set	1078 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.6	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	0.94	EDS
Total number of atoms	8735	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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	0.54	0/1319	0.64	0/1782
1	B	0.48	0/1328	0.56	0/1793
1	C	0.44	0/1328	0.52	0/1793
1	D	0.41	0/1155	0.53	0/1555
1	E	0.56	0/1336	0.64	0/1804
2	F	0.48	0/381	0.59	0/511
2	G	0.48	0/422	0.54	0/565
2	H	0.40	0/367	0.47	0/492
2	I	0.37	0/374	0.48	0/500
2	J	0.52	0/437	0.62	0/586
All	All	0.48	0/8447	0.57	0/11381

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	90	TYR	Sidechain

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	1296	0	1285	39	0
1	B	1305	0	1298	50	0
1	C	1305	0	1293	41	0
1	D	1141	0	1138	74	0
1	E	1313	0	1304	30	0
2	F	381	0	395	20	0
2	G	422	0	438	19	0
2	H	367	0	382	39	0
2	I	375	0	389	33	0
2	J	437	0	456	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	32	0	13	0	0
4	B	32	0	13	0	0
4	C	32	0	13	0	0
4	D	32	0	13	1	0
4	E	32	0	13	0	0
5	A	62	0	0	1	0
5	B	24	0	0	1	0
5	C	17	0	0	1	0
5	D	20	0	0	2	0
5	E	61	0	0	0	0
5	F	9	0	0	0	0
5	G	13	0	0	1	0
5	H	5	0	0	0	0
5	I	2	0	0	0	0
5	J	15	0	0	2	0
All	All	8735	0	8443	317	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 19.

All (317) 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:21:PHE:HB2	1:A:94:GLN:HG3	1.40	1.00
1:B:38:LEU:HD22	1:B:44:GLN:HB2	1.48	0.94
1:A:38:LEU:HD12	1:A:44:GLN:HB2	1.54	0.90
2:H:843:ARG:HH21	2:H:846:ALA:HB3	1.38	0.89
1:B:158:LEU:HD11	1:B:180:LYS:HZ3	1.38	0.89
1:E:21:PHE:HB2	1:E:94:GLN:HG3	1.58	0.84
1:B:158:LEU:HD11	1:B:180:LYS:NZ	1.93	0.84
1:C:116:LYS:HD2	1:C:120:ARG:HH22	1.48	0.78
1:B:81:ARG:NH1	2:F:816:GLN:HE21	1.82	0.78
1:D:169:ASN:HA	1:D:172:GLU:HG2	1.68	0.76
2:I:834:ARG:HH11	2:I:847:ILE:HD11	1.52	0.75
2:H:841:LEU:HA	2:H:844:ILE:HG22	1.71	0.72
2:H:841:LEU:HD12	2:I:841:LEU:HD23	1.72	0.71
1:E:42:LYS:HA	2:G:843:ARG:NH2	2.04	0.71
2:H:844:ILE:HD13	2:I:844:ILE:HD13	1.74	0.70
1:D:171:ASN:O	1:D:175:MET:HG2	1.92	0.69
2:H:848:LEU:HD11	2:I:836:ARG:HB3	1.72	0.69
1:A:20:GLN:HE21	1:A:70:LYS:HE3	1.58	0.68
1:A:20:GLN:NE2	1:A:70:LYS:HE3	2.09	0.68
1:D:100:TYR:HB3	1:D:111:ALA:HB2	1.74	0.67
2:G:843:ARG:HE	2:G:843:ARG:HA	1.59	0.67
1:C:41:VAL:HA	1:C:60:GLN:NE2	2.10	0.67
1:D:41:VAL:HG12	1:D:42:LYS:HE3	1.76	0.66
1:D:86:ALA:HB3	1:D:87:PRO:HD3	1.76	0.66
1:D:170:VAL:O	1:D:173:ILE:HG22	1.95	0.66
1:A:102:ILE:HD13	1:A:135:ALA:HA	1.78	0.66
1:E:21:PHE:HB2	1:E:94:GLN:CG	2.26	0.66
1:A:21:PHE:CE2	1:A:181:LEU:HD11	2.31	0.65
1:E:102:ILE:HD13	1:E:135:ALA:HA	1.78	0.65
1:E:91:ARG:O	1:E:91:ARG:HG3	1.98	0.64
1:D:32:GLY:HA3	1:D:133:ASN:HD22	1.62	0.64
2:J:851:THR:HG22	2:J:852:LYS:H	1.64	0.63
1:D:42:LYS:HA	1:D:42:LYS:HE2	1.80	0.63
1:A:169:ASN:HA	1:A:172:GLU:OE2	1.99	0.62
1:A:179:LYS:HB2	1:A:179:LYS:NZ	2.14	0.62
1:C:41:VAL:HA	1:C:60:GLN:HE21	1.63	0.62
1:B:38:LEU:CD2	1:B:44:GLN:HB2	2.25	0.61
1:D:94:GLN:CD	1:D:94:GLN:H	2.04	0.61
1:B:116:LYS:HD3	2:H:812:ASP:OD1	1.99	0.61
1:D:158:LEU:HD21	1:D:180:LYS:HD2	1.81	0.61
1:D:158:LEU:HD12	1:D:158:LEU:N	2.15	0.61
1:B:81:ARG:HH11	2:F:816:GLN:HE21	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:842:GLU:O	2:H:845:ARG:HB3	2.01	0.60
1:A:46:HIS:HB2	1:A:49:GLN:HG2	1.84	0.60
1:C:169:ASN:HA	1:C:172:GLU:HG2	1.83	0.60
1:C:178:ALA:HA	1:C:181:LEU:HD12	1.83	0.60
1:D:32:GLY:HA3	1:D:133:ASN:ND2	2.15	0.60
2:F:833:GLU:HA	2:F:833:GLU:OE1	2.00	0.60
2:H:836:ARG:HH21	2:I:848:LEU:HB3	1.66	0.60
1:E:88:MET:SD	2:J:819:ARG:HG3	2.42	0.60
1:B:21:PHE:HB2	1:B:94:GLN:CG	2.31	0.59
2:H:848:LEU:HD21	2:I:836:ARG:HA	1.83	0.59
2:I:841:LEU:O	2:I:845:ARG:HG3	2.02	0.59
1:B:158:LEU:HD12	1:B:158:LEU:H	1.68	0.59
1:E:42:LYS:HA	2:G:843:ARG:HH22	1.67	0.59
2:I:818:GLN:O	2:I:822:VAL:HG23	2.03	0.59
1:D:38:LEU:HD12	1:D:49:GLN:HE22	1.68	0.59
2:F:807:LEU:HD22	2:G:807:LEU:CD2	2.33	0.59
1:C:58:LEU:HD23	2:H:833:GLU:OE1	2.03	0.59
1:D:22:LYS:HA	1:D:72:GLU:HB2	1.83	0.58
1:D:136:ASP:HB3	1:D:163:SER:OG	2.03	0.58
1:B:20:GLN:CB	1:B:70:LYS:HB3	2.33	0.58
1:A:23:LEU:HD23	1:A:23:LEU:C	2.24	0.57
1:A:81:ARG:HB3	5:A:413:HOH:O	2.04	0.57
1:C:169:ASN:HA	1:C:172:GLU:CG	2.34	0.57
1:A:115:VAL:O	1:A:119:GLN:HG3	2.03	0.57
1:A:102:ILE:HG23	1:A:133:ASN:O	2.05	0.57
1:E:101:ASP:HB3	1:E:104:ASN:HB3	1.86	0.57
2:G:843:ARG:HA	2:G:843:ARG:NE	2.20	0.57
2:H:843:ARG:C	2:H:845:ARG:H	2.08	0.56
1:B:115:VAL:O	1:B:119:GLN:HG3	2.05	0.56
2:H:811:LEU:HD11	2:I:810:GLU:OE2	2.05	0.56
2:H:814:SER:HG	2:I:814:SER:HG	1.54	0.56
2:H:813:VAL:O	2:H:816:GLN:HG2	2.06	0.56
1:E:21:PHE:CE2	1:E:181:LEU:HD11	2.40	0.56
1:B:158:LEU:HD12	1:B:158:LEU:N	2.19	0.56
2:H:843:ARG:NH2	2:H:846:ALA:HB3	2.17	0.56
1:D:105:GLU:HB2	1:D:142:ALA:HB1	1.88	0.56
1:C:117:GLU:O	1:C:121:GLN:HB2	2.06	0.56
2:F:807:LEU:HD22	2:G:807:LEU:HD23	1.88	0.56
1:B:102:ILE:CD1	1:B:135:ALA:HA	2.37	0.55
2:H:818:GLN:O	2:H:822:VAL:HG23	2.06	0.55
1:B:136:ASP:OD1	1:B:137:LEU:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:824:LEU:O	2:I:828:LEU:HG	2.06	0.55
1:D:141:ARG:NH2	1:D:145:PHE:H	2.05	0.55
1:D:41:VAL:HA	1:D:60:GLN:HG3	1.88	0.55
1:D:37:VAL:O	1:D:41:VAL:HG23	2.07	0.55
1:B:81:ARG:NH1	2:F:816:GLN:NE2	2.52	0.54
1:E:41:VAL:HA	1:E:60:GLN:HE21	1.71	0.54
1:E:102:ILE:CD1	1:E:135:ALA:HA	2.37	0.54
2:I:831:GLN:HA	2:I:834:ARG:HG2	1.88	0.54
1:B:38:LEU:HD23	1:B:42:LYS:HB2	1.88	0.54
1:D:102:ILE:HG12	1:D:135:ALA:HA	1.90	0.54
2:H:807:LEU:HA	2:H:810:GLU:OE2	2.08	0.54
1:A:141:ARG:NH1	1:A:161:GLU:OE2	2.40	0.54
1:B:81:ARG:HH11	2:F:816:GLN:NE2	2.04	0.54
1:C:182:PRO:HG2	1:C:183:LYS:H	1.72	0.54
2:H:836:ARG:HH21	2:I:848:LEU:CB	2.21	0.54
2:F:807:LEU:HD11	2:G:808:GLN:HG2	1.89	0.54
2:F:842:GLU:O	2:F:845:ARG:HG2	2.07	0.54
2:G:802:ASN:N	2:G:805:GLN:HG3	2.23	0.54
1:A:105:GLU:OE1	1:A:143:VAL:HG22	2.07	0.54
1:B:17:LYS:HD2	1:B:17:LYS:N	2.22	0.54
1:D:141:ARG:HH22	1:D:145:PHE:H	1.54	0.54
1:B:108:PHE:CE2	1:B:112:LYS:HE3	2.43	0.54
1:D:105:GLU:HA	1:D:143:VAL:HG12	1.90	0.54
1:C:102:ILE:HG13	1:C:103:THR:N	2.23	0.53
1:D:39:ARG:HG3	1:D:170:VAL:HG11	1.90	0.53
1:D:139:ASN:HA	5:D:551:HOH:O	2.06	0.53
1:C:59:THR:HA	1:C:71:PHE:O	2.08	0.53
1:D:156:SER:O	1:D:157:LEU:HD23	2.08	0.53
1:D:59:THR:HG22	1:D:72:GLU:N	2.23	0.53
2:F:844:ILE:HD13	2:G:844:ILE:HD13	1.91	0.53
1:C:139:ASN:OD1	1:C:140:LYS:HG3	2.09	0.53
1:B:101:ASP:OD2	1:B:134:LYS:HD2	2.07	0.53
1:E:20:GLN:CB	1:E:70:LYS:HB3	2.39	0.53
1:D:165:LYS:HB2	4:D:4202:GNP:N1	2.24	0.53
1:B:20:GLN:HB2	1:B:70:LYS:HB3	1.90	0.53
2:I:813:VAL:HA	2:I:816:GLN:HE21	1.73	0.53
1:B:169:ASN:HA	1:B:172:GLU:OE1	2.09	0.53
1:C:112:LYS:HG2	1:C:151:TYR:CZ	2.43	0.53
2:H:839:ASP:HB2	2:H:843:ARG:HB2	1.89	0.53
1:A:29:SER:O	1:A:30:ALA:HB3	2.08	0.52
1:D:39:ARG:NH2	1:D:165:LYS:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:TYR:O	1:D:85:LEU:HB2	2.10	0.52
1:D:94:GLN:H	1:D:94:GLN:NE2	2.08	0.52
1:C:172:GLU:CD	1:C:172:GLU:H	2.12	0.52
1:B:112:LYS:HG2	1:B:151:TYR:CZ	2.44	0.51
1:D:90:TYR:O	1:D:90:TYR:HD1	1.91	0.51
1:D:152:ALA:CB	1:D:159:PHE:HB2	2.41	0.51
1:E:22:LYS:HB3	1:E:93:ALA:HA	1.91	0.51
1:C:20:GLN:HB3	1:C:70:LYS:HB3	1.92	0.51
2:J:851:THR:O	2:J:852:LYS:HD3	2.11	0.51
2:J:853:LEU:HD13	5:J:504:HOH:O	2.10	0.51
1:C:101:ASP:OD2	1:C:134:LYS:HD2	2.11	0.51
1:D:100:TYR:HB3	1:D:111:ALA:CB	2.41	0.51
1:D:169:ASN:HA	1:D:172:GLU:CG	2.39	0.51
1:D:111:ALA:O	1:D:115:VAL:HG23	2.11	0.51
1:B:83:HIS:HE1	1:B:110:ARG:HH22	1.56	0.50
2:J:811:LEU:O	2:J:815:GLU:HG2	2.11	0.50
2:H:840:SER:HA	2:I:841:LEU:HD21	1.92	0.50
1:B:21:PHE:HB2	1:B:94:GLN:HG3	1.94	0.50
1:D:25:LEU:O	1:D:26:LEU:HD23	2.11	0.50
1:D:159:PHE:O	1:D:160:MET:HB2	2.11	0.50
1:A:101:ASP:OD2	1:A:134:LYS:HD2	2.12	0.50
1:A:178:ALA:HA	1:A:181:LEU:HD12	1.94	0.50
1:C:152:ALA:HB2	1:C:159:PHE:HB2	1.94	0.50
2:I:834:ARG:HA	2:I:837:GLN:HB3	1.93	0.50
2:I:844:ILE:O	2:I:847:ILE:HG22	2.11	0.50
1:A:59:THR:HA	1:A:71:PHE:O	2.12	0.49
2:G:818:GLN:O	2:G:822:VAL:HG23	2.13	0.49
1:D:147:GLU:O	1:D:150:SER:HB2	2.13	0.49
1:D:158:LEU:HD12	1:D:158:LEU:H	1.77	0.49
2:H:841:LEU:HA	2:H:844:ILE:CG2	2.42	0.49
1:D:145:PHE:HD1	1:D:161:GLU:HG3	1.77	0.49
1:B:21:PHE:HB2	1:B:94:GLN:OE1	2.13	0.49
1:B:112:LYS:HG2	1:B:151:TYR:CE1	2.48	0.49
1:C:39:ARG:NH2	1:C:165:LYS:O	2.45	0.49
1:D:155:ASN:O	1:D:156:SER:HB3	2.13	0.48
2:I:838:ALA:HB1	2:I:843:ARG:HH11	1.78	0.48
1:A:86:ALA:N	1:A:87:PRO:CD	2.76	0.48
1:D:28:GLU:HG2	1:D:29:SER:N	2.28	0.48
1:C:166:THR:O	1:C:167:SER:HB3	2.12	0.48
1:B:38:LEU:HD12	1:B:49:GLN:OE1	2.14	0.48
1:B:112:LYS:HA	1:B:151:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HD13	1:B:135:ALA:HA	1.96	0.48
1:C:118:LEU:O	1:C:122:ALA:HB3	2.13	0.48
2:H:844:ILE:CD1	2:I:844:ILE:HD13	2.40	0.48
1:A:141:ARG:HH12	1:A:161:GLU:CD	2.17	0.48
1:D:152:ALA:HB1	1:D:159:PHE:HB2	1.96	0.48
1:D:167:SER:HA	1:D:170:VAL:HG21	1.96	0.48
1:B:101:ASP:CG	1:B:134:LYS:HD2	2.34	0.48
2:F:834:ARG:HG3	2:F:834:ARG:HH11	1.79	0.48
1:A:158:LEU:HD11	1:A:180:LYS:HD2	1.95	0.48
1:C:28:GLU:HB2	1:C:110:ARG:HG2	1.96	0.48
1:D:160:MET:HB3	1:D:173:ILE:HD13	1.96	0.48
2:I:817:VAL:HA	2:I:820:ASP:OD2	2.14	0.48
1:B:158:LEU:H	1:B:158:LEU:CD1	2.27	0.47
1:A:19:CYS:O	1:A:69:VAL:HA	2.14	0.47
1:B:173:ILE:HG23	1:B:174:PHE:N	2.29	0.47
1:E:23:LEU:C	1:E:23:LEU:HD23	2.35	0.47
1:A:173:ILE:HG23	1:A:174:PHE:N	2.28	0.47
1:D:129:ALA:CB	1:D:177:ILE:HD11	2.44	0.47
1:E:97:ILE:HG12	1:E:177:ILE:HD11	1.96	0.47
1:E:125:ASN:C	1:E:125:ASN:HD22	2.18	0.47
1:A:101:ASP:CG	1:A:134:LYS:HD2	2.34	0.47
1:D:139:ASN:HB2	1:D:140:LYS:HD3	1.97	0.47
1:E:20:GLN:HB3	1:E:70:LYS:HB3	1.96	0.47
1:B:86:ALA:N	1:B:87:PRO:CD	2.78	0.47
1:C:25:LEU:HD12	1:C:25:LEU:N	2.30	0.47
1:C:176:ALA:O	1:C:179:LYS:HG2	2.15	0.47
2:H:841:LEU:HD11	2:I:841:LEU:HB2	1.97	0.47
1:A:32:GLY:HA3	1:A:133:ASN:ND2	2.30	0.47
2:F:841:LEU:HD23	2:G:841:LEU:HD12	1.97	0.47
1:D:32:GLY:O	1:D:36:LEU:HB2	2.15	0.46
1:B:83:HIS:CE1	1:B:110:ARG:HH12	2.32	0.46
1:C:127:VAL:HG13	1:C:180:LYS:HD3	1.97	0.46
1:B:58:LEU:HD22	2:G:836:ARG:NH2	2.30	0.46
2:H:848:LEU:HD13	2:I:835:ILE:HG22	1.96	0.46
1:D:81:ARG:HG2	5:D:550:HOH:O	2.16	0.46
2:F:843:ARG:HE	2:F:847:ILE:HD11	1.80	0.46
1:D:27:GLY:HA2	1:D:114:TRP:CD1	2.50	0.46
1:D:106:GLU:O	1:D:109:ALA:HB3	2.15	0.46
1:C:42:LYS:HB2	1:C:44:GLN:HG2	1.97	0.45
1:D:155:ASN:HB2	1:D:157:LEU:HG	1.98	0.45
1:A:173:ILE:CG2	1:A:174:PHE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:832:LEU:HD12	2:G:828:LEU:HD22	1.99	0.45
2:H:825:SER:O	2:H:829:GLN:HG3	2.16	0.45
1:D:100:TYR:HE1	1:D:143:VAL:HG21	1.81	0.45
1:E:171:ASN:O	1:E:175:MET:HG2	2.16	0.45
1:C:64:LEU:HD21	1:C:175:MET:HG3	1.98	0.45
1:C:102:ILE:O	1:C:143:VAL:HG23	2.17	0.45
1:D:101:ASP:HB3	1:D:104:ASN:HB3	1.98	0.45
1:B:54:GLY:O	1:B:55:ALA:HB2	2.16	0.45
1:D:130:LEU:HD23	1:D:131:SER:H	1.81	0.45
1:B:109:ALA:HA	1:B:112:LYS:HD2	1.99	0.44
1:B:141:ARG:HH12	1:B:145:PHE:HB2	1.81	0.44
1:C:22:LYS:HA	1:C:72:GLU:HB2	1.98	0.44
2:H:835:ILE:HD13	2:I:835:ILE:HD13	1.99	0.44
1:E:81:ARG:HH11	1:E:81:ARG:HG2	1.82	0.44
2:H:828:LEU:HD13	2:I:829:GLN:HG3	1.99	0.44
1:D:90:TYR:O	1:D:90:TYR:CD1	2.70	0.44
1:E:59:THR:HG23	2:J:833:GLU:HG2	1.98	0.44
2:G:835:ILE:HG13	2:G:847:ILE:HG21	2.00	0.44
2:H:821:PHE:CE2	2:I:822:VAL:HG22	2.53	0.44
2:J:851:THR:HA	5:J:611:HOH:O	2.18	0.44
1:D:141:ARG:HH22	1:D:145:PHE:N	2.14	0.44
1:D:102:ILE:HA	1:D:143:VAL:CG2	2.48	0.44
1:E:24:VAL:HG11	1:E:90:TYR:HB3	1.99	0.44
1:C:111:ALA:O	1:C:115:VAL:HG23	2.18	0.43
1:A:21:PHE:CD2	1:A:181:LEU:HD11	2.53	0.43
1:D:113:ASN:HA	1:D:116:LYS:HE3	1.99	0.43
2:H:836:ARG:NH2	2:I:848:LEU:HB3	2.33	0.43
2:I:815:GLU:HA	2:I:818:GLN:HE21	1.83	0.43
2:J:831:GLN:HG2	2:J:834:ARG:HH21	1.82	0.43
1:C:40:PHE:CE2	1:C:60:GLN:HG2	2.53	0.43
5:C:541:HOH:O	2:H:833:GLU:HG3	2.17	0.43
2:G:802:ASN:HA	2:G:805:GLN:OE1	2.18	0.43
2:G:852:LYS:HD2	2:G:852:LYS:N	2.33	0.43
1:B:28:GLU:HB2	1:B:110:ARG:HG2	1.99	0.43
1:C:159:PHE:CG	1:C:160:MET:N	2.87	0.43
1:A:32:GLY:HA3	1:A:133:ASN:HD22	1.84	0.43
1:D:151:TYR:O	1:D:154:ASP:HB2	2.18	0.43
2:G:802:ASN:HB2	5:G:560:HOH:O	2.19	0.43
1:A:34:SER:OG	1:A:75:ASP:OD2	2.36	0.43
1:D:85:LEU:HD22	2:I:822:VAL:HG21	2.00	0.43
2:F:832:LEU:HA	2:F:832:LEU:HD23	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:835:ILE:HG13	2:H:847:ILE:HG21	2.00	0.43
1:A:102:ILE:CD1	1:A:135:ALA:HA	2.48	0.43
1:B:102:ILE:HD11	1:B:135:ALA:HA	1.99	0.43
1:D:167:SER:HA	1:D:170:VAL:CG2	2.49	0.43
1:B:47:GLU:HG3	5:B:422:HOH:O	2.19	0.43
1:D:158:LEU:N	1:D:158:LEU:CD1	2.82	0.43
2:H:806:ARG:HB2	2:H:806:ARG:CZ	2.49	0.43
1:B:123:SER:OG	1:B:124:PRO:HD2	2.19	0.43
1:B:170:VAL:O	1:B:173:ILE:HG22	2.18	0.43
1:C:86:ALA:N	1:C:87:PRO:CD	2.82	0.42
1:D:108:PHE:O	1:D:111:ALA:HB3	2.19	0.42
1:E:133:ASN:O	1:E:134:LYS:HB2	2.19	0.42
1:E:26:LEU:C	1:E:33:LYS:HD3	2.40	0.42
1:D:104:ASN:HB3	1:D:107:SER:HB2	2.01	0.42
1:E:39:ARG:NH2	1:E:165:LYS:O	2.51	0.42
2:I:819:ARG:CZ	2:I:819:ARG:HB2	2.49	0.42
1:A:158:LEU:HD11	1:A:180:LYS:CD	2.49	0.42
1:C:173:ILE:HG23	1:C:174:PHE:N	2.35	0.42
1:B:39:ARG:O	1:B:43:GLY:HA2	2.20	0.42
1:C:158:LEU:HD21	1:C:176:ALA:HB1	2.01	0.42
1:D:130:LEU:HD12	1:D:157:LEU:HD12	2.01	0.42
2:F:830:VAL:HG13	2:F:834:ARG:NH1	2.34	0.42
2:H:843:ARG:C	2:H:845:ARG:N	2.73	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.90	0.42
1:C:108:PHE:CZ	1:C:112:LYS:HE3	2.55	0.42
1:A:25:LEU:HD12	1:A:25:LEU:N	2.35	0.42
1:B:22:LYS:NZ	1:B:91:ARG:O	2.52	0.42
1:B:109:ALA:O	1:B:112:LYS:HB2	2.20	0.42
1:D:87:PRO:O	1:D:91:ARG:HB2	2.20	0.42
1:E:159:PHE:O	1:E:160:MET:HG3	2.20	0.42
2:J:831:GLN:CG	2:J:834:ARG:HH21	2.33	0.42
1:D:94:GLN:NE2	1:D:94:GLN:N	2.67	0.42
2:H:844:ILE:O	2:H:844:ILE:HG23	2.19	0.41
1:A:108:PHE:CE2	1:A:112:LYS:HE3	2.55	0.41
1:D:102:ILE:HA	1:D:143:VAL:HG21	2.02	0.41
1:D:126:ILE:O	1:D:126:ILE:HG23	2.21	0.41
1:E:62:VAL:HG11	1:E:175:MET:SD	2.61	0.41
2:F:806:ARG:NH1	2:F:807:LEU:HB2	2.36	0.41
1:B:62:VAL:HG11	1:B:175:MET:SD	2.61	0.41
1:D:57:PHE:O	1:D:58:LEU:HD23	2.20	0.41
2:F:843:ARG:O	2:F:847:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:847:ILE:C	2:F:849:ASN:H	2.24	0.41
1:A:23:LEU:HD23	1:A:24:VAL:N	2.35	0.41
1:A:168:MET:O	1:A:169:ASN:HB2	2.21	0.41
1:C:55:ALA:O	2:H:829:GLN:NE2	2.50	0.41
1:A:45:PHE:CE2	1:A:165:LYS:HD3	2.56	0.41
1:E:23:LEU:HD23	1:E:24:VAL:N	2.35	0.41
1:E:62:VAL:HG21	1:E:175:MET:HE1	2.03	0.41
2:F:824:LEU:O	2:F:828:LEU:HD22	2.20	0.41
1:C:53:ILE:O	1:C:82:TYR:CZ	2.73	0.41
2:H:848:LEU:HD21	2:I:836:ARG:CB	2.51	0.41
2:J:848:LEU:HD23	2:J:848:LEU:HA	1.91	0.41
1:A:37:VAL:O	1:A:41:VAL:HG23	2.21	0.41
1:B:133:ASN:O	1:B:134:LYS:HB2	2.21	0.41
1:D:149:GLN:O	1:D:152:ALA:HB3	2.21	0.41
1:E:86:ALA:N	1:E:87:PRO:CD	2.84	0.41
2:H:848:LEU:CD1	2:I:836:ARG:HB3	2.48	0.41
2:J:819:ARG:O	2:J:823:LYS:HD3	2.21	0.41
1:D:38:LEU:HD22	1:D:44:GLN:NE2	2.35	0.40
1:E:46:HIS:NE2	2:G:850:ASP:OD1	2.54	0.40
2:G:811:LEU:O	2:G:814:SER:HB3	2.21	0.40
2:J:851:THR:HG22	2:J:852:LYS:N	2.32	0.40
1:C:59:THR:HG23	2:H:833:GLU:HG2	2.02	0.40
2:I:830:VAL:O	2:I:833:GLU:HB3	2.21	0.40
1:B:141:ARG:NH1	1:B:145:PHE:HB2	2.37	0.40
1:C:102:ILE:HD13	1:C:135:ALA:HA	2.04	0.40
1:C:116:LYS:HD2	1:C:120:ARG:NH2	2.24	0.40
1:D:158:LEU:H	1:D:158:LEU:CD1	2.34	0.40
1:C:79:GLN:HE21	1:C:79:GLN:HB2	1.68	0.40
2:H:828:LEU:CD1	2:I:829:GLN:HG3	2.51	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	163/171 (95%)	147 (90%)	15 (9%)	1 (1%)	25 30
1	B	164/171 (96%)	155 (94%)	8 (5%)	1 (1%)	25 30
1	C	164/171 (96%)	147 (90%)	13 (8%)	4 (2%)	6 4
1	D	137/171 (80%)	118 (86%)	16 (12%)	3 (2%)	6 5
1	E	165/171 (96%)	156 (94%)	8 (5%)	1 (1%)	25 30
2	F	44/79 (56%)	42 (96%)	2 (4%)	0	100 100
2	G	49/79 (62%)	45 (92%)	3 (6%)	1 (2%)	7 6
2	H	42/79 (53%)	37 (88%)	3 (7%)	2 (5%)	2 1
2	I	41/79 (52%)	35 (85%)	6 (15%)	0	100 100
2	J	51/79 (65%)	48 (94%)	2 (4%)	1 (2%)	7 6
All	All	1020/1250 (82%)	930 (91%)	76 (8%)	14 (1%)	11 10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	182	PRO
1	A	64	LEU
1	B	65	ASP
1	D	165	LYS
2	G	850	ASP
1	C	65	ASP
1	C	160	MET
1	D	160	MET
1	C	53	ILE
2	H	839	ASP
2	H	844	ILE
2	J	853	LEU
1	D	170	VAL
1	E	102	ILE

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	138/143 (96%)	131 (95%)	7 (5%)	24 33
1	B	139/143 (97%)	130 (94%)	9 (6%)	17 22
1	C	139/143 (97%)	131 (94%)	8 (6%)	20 27
1	D	121/143 (85%)	114 (94%)	7 (6%)	20 27
1	E	140/143 (98%)	135 (96%)	5 (4%)	35 48
2	F	43/72 (60%)	38 (88%)	5 (12%)	5 5
2	G	48/72 (67%)	44 (92%)	4 (8%)	11 13
2	H	42/72 (58%)	38 (90%)	4 (10%)	8 9
2	I	42/72 (58%)	40 (95%)	2 (5%)	25 35
2	J	50/72 (69%)	47 (94%)	3 (6%)	19 26
All	All	902/1075 (84%)	848 (94%)	54 (6%)	19 26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	38	LEU
1	A	49	GLN
1	A	94	GLN
1	A	116	LYS
1	A	123	SER
1	A	179	LYS
1	B	17	LYS
1	B	38	LEU
1	B	94	GLN
1	B	137	LEU
1	B	140	LYS
1	B	144	ASP
1	B	147	GLU
1	B	175	MET
1	B	180	LYS
1	C	23	LEU
1	C	33	LYS
1	C	36	LEU
1	C	50	GLU
1	C	66	ASP
1	C	121	GLN
1	C	125	ASN
1	C	175	MET

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Mol	Chain	Res	Type
1	D	29	SER
1	D	60	GLN
1	D	94	GLN
1	D	103	THR
1	D	130	LEU
1	D	139	ASN
1	D	140	LYS
1	E	36	LEU
1	E	94	GLN
1	E	123	SER
1	E	125	ASN
1	E	131	SER
2	F	805	GLN
2	F	806	ARG
2	F	807	LEU
2	F	823	LYS
2	F	828	LEU
2	G	824	LEU
2	G	836	ARG
2	G	843	ARG
2	G	850	ASP
2	H	807	LEU
2	H	810	GLU
2	H	811	LEU
2	H	837	GLN
2	I	808	GLN
2	I	841	LEU
2	J	808	GLN
2	J	824	LEU
2	J	850	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	49	GLN
1	A	94	GLN
1	A	146	GLN
1	B	46	HIS
1	B	121	GLN
1	B	125	ASN
1	C	60	GLN

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Mol	Chain	Res	Type
1	C	79	GLN
1	C	113	ASN
1	C	119	GLN
1	C	121	GLN
1	C	146	GLN
1	D	44	GLN
1	D	49	GLN
1	D	94	GLN
1	D	155	ASN
1	E	125	ASN
2	F	805	GLN
2	F	816	GLN
2	F	849	ASN
2	G	808	GLN
2	H	816	GLN
2	H	818	GLN
2	I	816	GLN
2	I	818	GLN
2	I	831	GLN

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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	GNP	D	4202	3	29,34,34	2.50	12 (41%)	33,54,54	2.82	7 (21%)
4	GNP	C	3202	3	29,34,34	2.26	10 (34%)	33,54,54	3.00	9 (27%)
4	GNP	E	5202	3	29,34,34	2.26	11 (37%)	33,54,54	2.78	8 (24%)
4	GNP	A	1202	3	29,34,34	2.28	10 (34%)	33,54,54	2.88	7 (21%)
4	GNP	B	2202	3	29,34,34	2.19	11 (37%)	33,54,54	2.75	7 (21%)

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
4	GNP	D	4202	3	-	4/14/38/38	0/3/3/3
4	GNP	C	3202	3	-	4/14/38/38	0/3/3/3
4	GNP	E	5202	3	-	3/14/38/38	0/3/3/3
4	GNP	A	1202	3	-	3/14/38/38	0/3/3/3
4	GNP	B	2202	3	-	4/14/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4202	GNP	PB-O3A	5.71	1.66	1.59
4	E	5202	GNP	PB-O3A	5.64	1.66	1.59
4	A	1202	GNP	C2-N2	5.23	1.44	1.33
4	D	4202	GNP	C2-N2	5.23	1.44	1.33
4	B	2202	GNP	C2-N2	5.03	1.44	1.33
4	C	3202	GNP	C2-N2	4.80	1.43	1.33
4	E	5202	GNP	C2-N2	4.79	1.43	1.33
4	D	4202	GNP	PG-N3B	4.43	1.74	1.63
4	C	3202	GNP	PG-N3B	4.35	1.74	1.63
4	A	1202	GNP	C6-N1	4.34	1.40	1.33
4	A	1202	GNP	PB-O3A	4.34	1.64	1.59
4	C	3202	GNP	PB-O3A	4.28	1.64	1.59
4	B	2202	GNP	C6-N1	4.11	1.40	1.33
4	E	5202	GNP	C6-N1	3.80	1.39	1.33
4	A	1202	GNP	PG-N3B	3.76	1.73	1.63
4	C	3202	GNP	C5-C6	3.74	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4202	GNP	C6-N1	3.71	1.39	1.33
4	C	3202	GNP	C6-N1	3.61	1.39	1.33
4	B	2202	GNP	PG-N3B	3.58	1.72	1.63
4	A	1202	GNP	C5-C6	3.46	1.47	1.41
4	D	4202	GNP	C5-C6	3.43	1.47	1.41
4	B	2202	GNP	PB-O3A	3.41	1.63	1.59
4	E	5202	GNP	C5-C6	3.37	1.47	1.41
4	B	2202	GNP	PG-O3G	-3.04	1.48	1.56
4	D	4202	GNP	PG-O3G	-3.03	1.48	1.56
4	E	5202	GNP	C2'-C1'	-2.96	1.49	1.53
4	B	2202	GNP	C5-C6	2.92	1.46	1.41
4	B	2202	GNP	O4'-C4'	-2.83	1.38	1.45
4	D	4202	GNP	O6-C6	-2.80	1.17	1.24
4	A	1202	GNP	O6-C6	-2.77	1.17	1.24
4	E	5202	GNP	O6-C6	-2.75	1.17	1.24
4	D	4202	GNP	PB-O2B	-2.72	1.49	1.56
4	B	2202	GNP	O6-C6	-2.70	1.17	1.24
4	C	3202	GNP	O6-C6	-2.69	1.17	1.24
4	C	3202	GNP	PB-N3B	2.64	1.70	1.63
4	D	4202	GNP	PB-N3B	2.63	1.70	1.63
4	D	4202	GNP	O4'-C4'	-2.60	1.39	1.45
4	C	3202	GNP	PG-O1G	2.53	1.50	1.46
4	A	1202	GNP	C2'-C1'	-2.53	1.49	1.53
4	A	1202	GNP	O4'-C4'	-2.51	1.39	1.45
4	D	4202	GNP	PG-O1G	2.50	1.50	1.46
4	C	3202	GNP	PG-O3G	-2.49	1.50	1.56
4	E	5202	GNP	PG-N3B	2.43	1.69	1.63
4	E	5202	GNP	PG-O2G	-2.29	1.50	1.56
4	E	5202	GNP	O4'-C4'	-2.26	1.40	1.45
4	B	2202	GNP	PG-O2G	-2.25	1.50	1.56
4	D	4202	GNP	PB-O1B	2.25	1.49	1.46
4	B	2202	GNP	C3'-C4'	2.23	1.58	1.53
4	A	1202	GNP	C2-N1	2.22	1.39	1.35
4	A	1202	GNP	PG-O2G	-2.20	1.50	1.56
4	B	2202	GNP	PG-O1G	2.14	1.49	1.46
4	E	5202	GNP	PB-O2B	-2.11	1.51	1.56
4	E	5202	GNP	PG-O3G	-2.10	1.51	1.56
4	C	3202	GNP	C8-N7	-2.08	1.31	1.34

All (38) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1202	GNP	C5-C6-N1	-9.14	110.93	123.43
4	E	5202	GNP	C5-C6-N1	-9.00	111.13	123.43
4	C	3202	GNP	C5-C6-N1	-8.99	111.13	123.43
4	D	4202	GNP	C5-C6-N1	-8.91	111.25	123.43
4	B	2202	GNP	C5-C6-N1	-8.82	111.37	123.43
4	C	3202	GNP	O1G-PG-N3B	-7.43	100.83	111.77
4	E	5202	GNP	C2-N3-C4	-7.37	106.94	115.36
4	C	3202	GNP	C2-N3-C4	-7.29	107.03	115.36
4	B	2202	GNP	C2-N3-C4	-7.11	107.23	115.36
4	D	4202	GNP	C2-N3-C4	-6.99	107.37	115.36
4	A	1202	GNP	C2-N3-C4	-6.95	107.41	115.36
4	D	4202	GNP	O1G-PG-N3B	-6.86	101.67	111.77
4	A	1202	GNP	O1G-PG-N3B	-6.61	102.04	111.77
4	B	2202	GNP	N2-C2-N1	-5.74	108.32	117.25
4	C	3202	GNP	N2-C2-N1	-5.42	108.82	117.25
4	E	5202	GNP	N2-C2-N1	-5.25	109.08	117.25
4	B	2202	GNP	O1G-PG-N3B	-5.18	104.14	111.77
4	D	4202	GNP	N2-C2-N1	-5.12	109.29	117.25
4	C	3202	GNP	N3-C2-N1	5.06	133.98	127.22
4	A	1202	GNP	N2-C2-N1	-5.01	109.47	117.25
4	A	1202	GNP	N3-C2-N1	4.94	133.82	127.22
4	E	5202	GNP	N3-C2-N1	4.94	133.82	127.22
4	B	2202	GNP	N3-C2-N1	4.92	133.79	127.22
4	D	4202	GNP	N3-C2-N1	4.84	133.69	127.22
4	E	5202	GNP	O2B-PB-O1B	4.77	119.92	109.92
4	A	1202	GNP	O2B-PB-O1B	4.71	119.79	109.92
4	C	3202	GNP	O2B-PB-O1B	4.69	119.76	109.92
4	E	5202	GNP	O1G-PG-N3B	-4.62	104.97	111.77
4	D	4202	GNP	O2B-PB-O1B	3.85	117.98	109.92
4	B	2202	GNP	O2B-PB-O1B	3.39	117.03	109.92
4	C	3202	GNP	O1B-PB-N3B	-2.44	108.17	111.77
4	A	1202	GNP	O4'-C4'-C5'	2.42	117.34	109.37
4	D	4202	GNP	O4'-C4'-C5'	2.24	116.75	109.37
4	E	5202	GNP	O4'-C4'-C5'	2.19	116.58	109.37
4	C	3202	GNP	O4'-C4'-C5'	2.16	116.48	109.37
4	C	3202	GNP	C2-N1-C6	2.09	119.24	115.93
4	E	5202	GNP	C2-N1-C6	2.08	119.24	115.93
4	B	2202	GNP	C2-N1-C6	2.05	119.19	115.93

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1202	GNP	PG-N3B-PB-O1B
4	A	1202	GNP	PA-O3A-PB-O1B
4	A	1202	GNP	PA-O3A-PB-O2B
4	B	2202	GNP	PG-N3B-PB-O1B
4	B	2202	GNP	PA-O3A-PB-O1B
4	B	2202	GNP	PA-O3A-PB-O2B
4	C	3202	GNP	PG-N3B-PB-O1B
4	C	3202	GNP	PA-O3A-PB-O1B
4	C	3202	GNP	PA-O3A-PB-O2B
4	D	4202	GNP	PG-N3B-PB-O1B
4	D	4202	GNP	PG-N3B-PB-O3A
4	D	4202	GNP	PA-O3A-PB-O1B
4	D	4202	GNP	PA-O3A-PB-O2B
4	E	5202	GNP	PG-N3B-PB-O1B
4	E	5202	GNP	PA-O3A-PB-O1B
4	E	5202	GNP	PA-O3A-PB-O2B
4	B	2202	GNP	PG-N3B-PB-O3A
4	C	3202	GNP	PG-N3B-PB-O3A

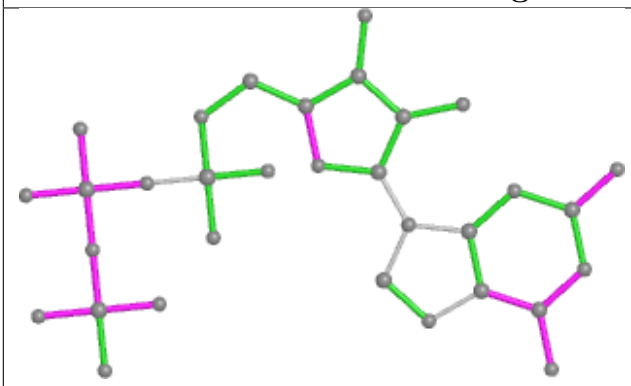
There are no ring outliers.

1 monomer is involved in 1 short contact:

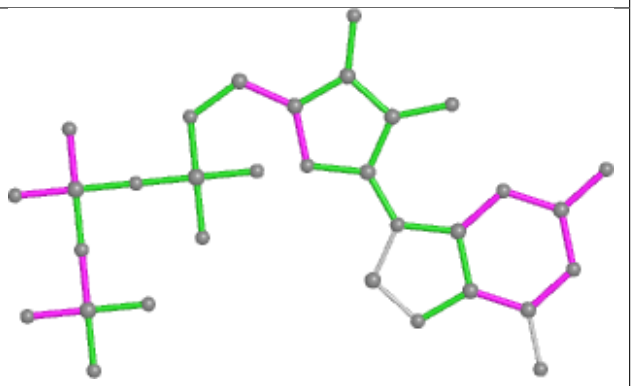
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4202	GNP	1	0

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.

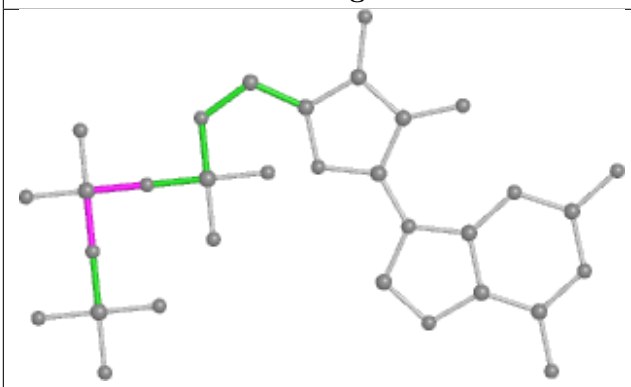
Ligand GNP D 4202



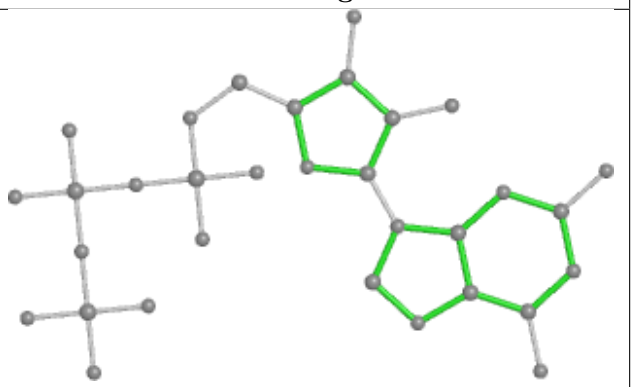
Bond lengths



Bond angles

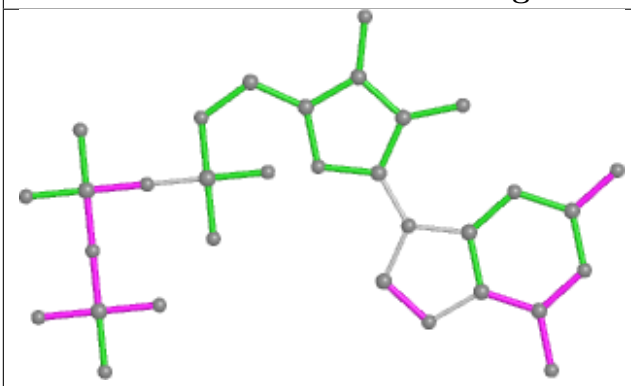


Torsions

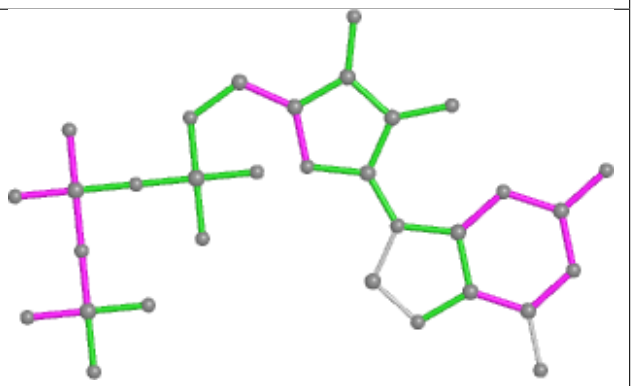


Rings

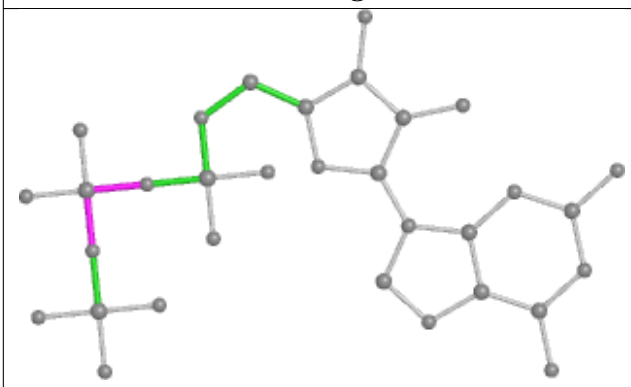
Ligand GNP C 3202



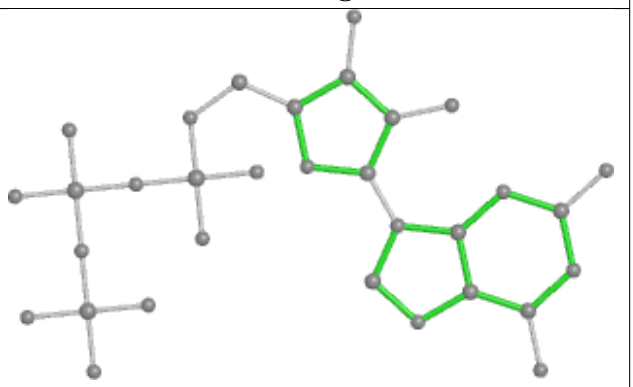
Bond lengths



Bond angles

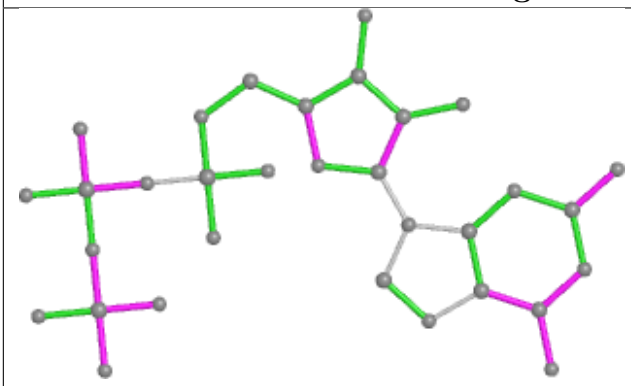


Torsions

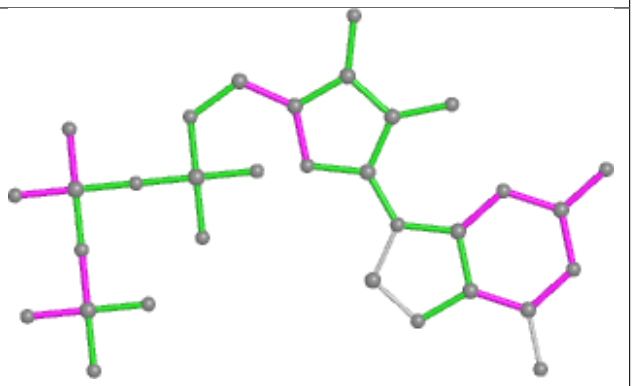


Rings

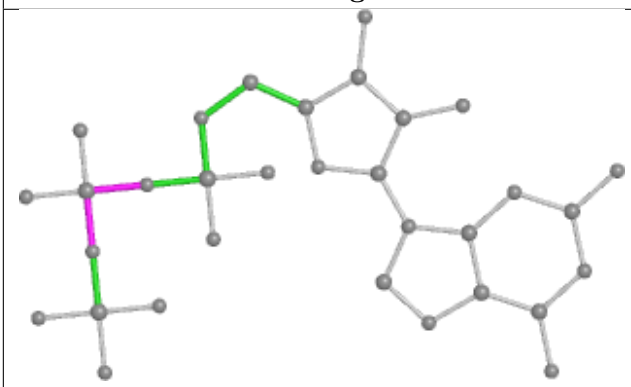
Ligand GNP E 5202



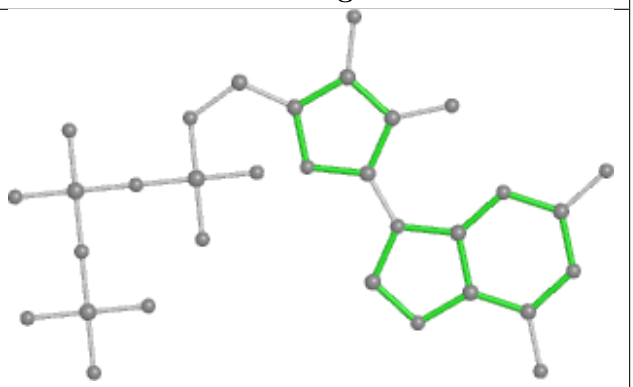
Bond lengths



Bond angles

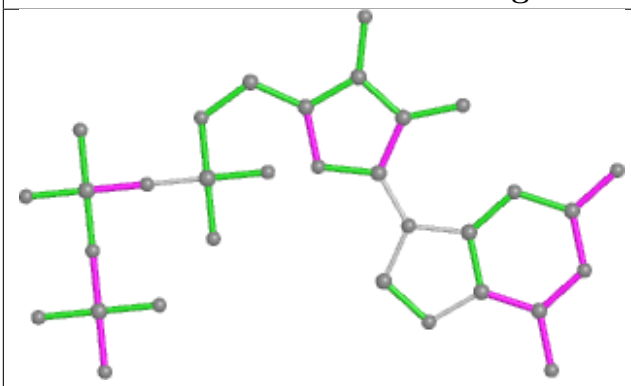


Torsions

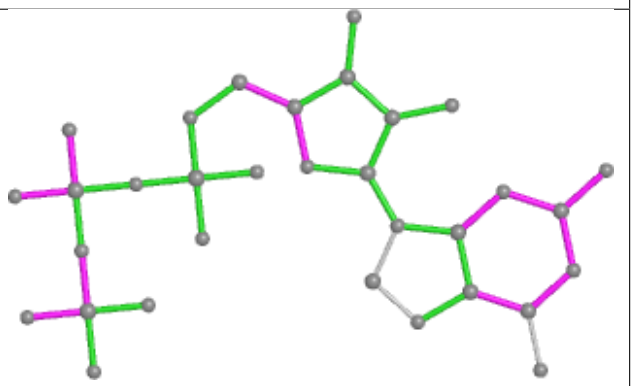


Rings

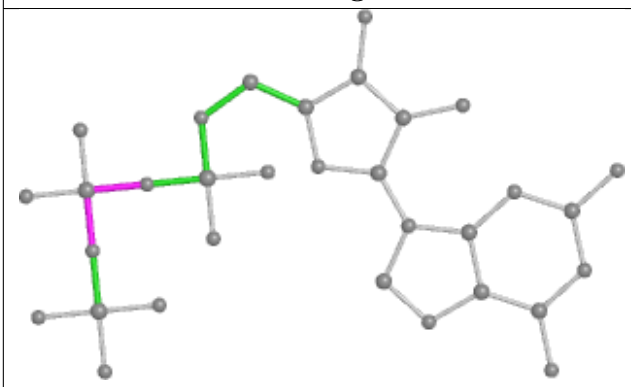
Ligand GNP A 1202



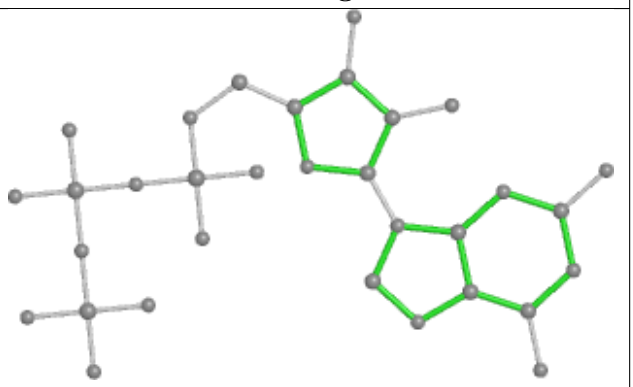
Bond lengths



Bond angles

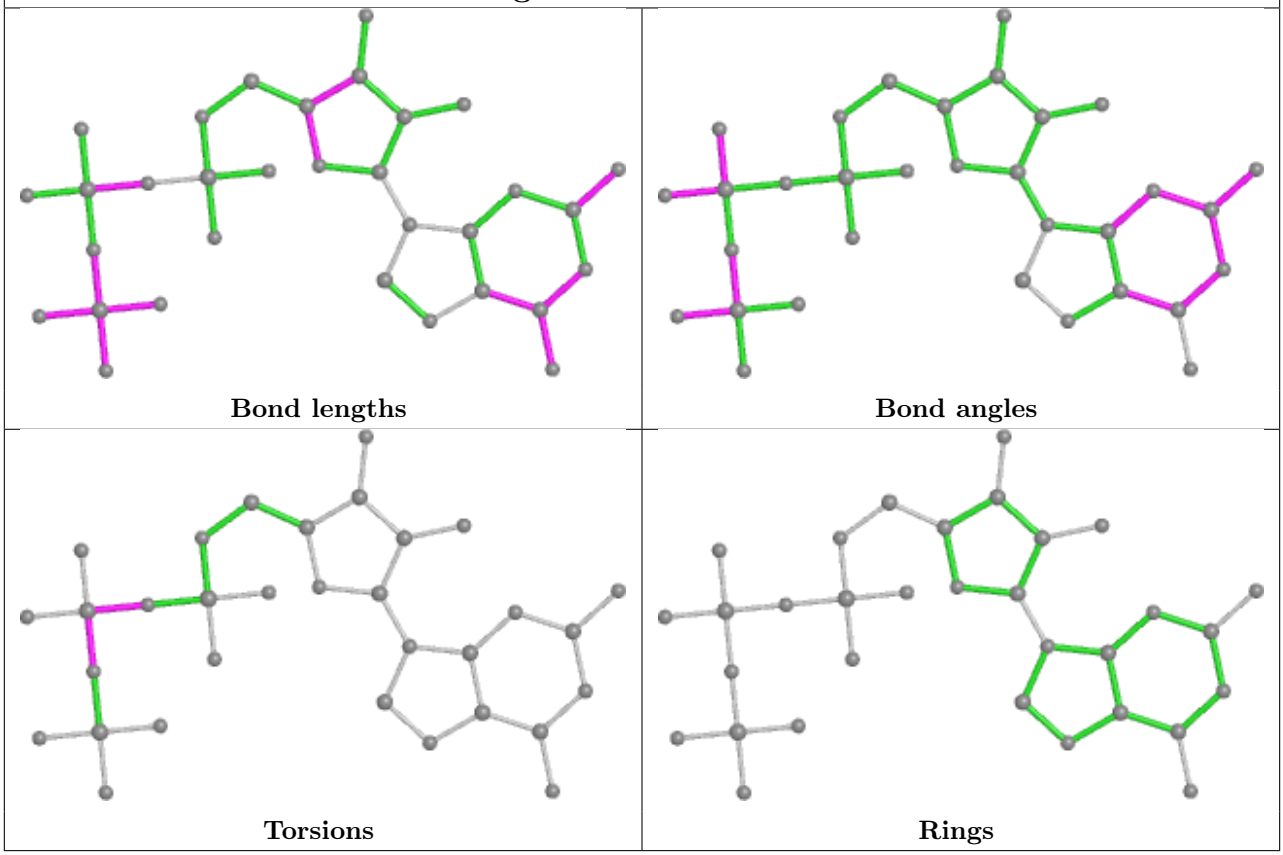


Torsions



Rings

Ligand GNP B 2202



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	165/171 (96%)	0.45	13 (7%) 12 17	26, 47, 84, 117	0
1	B	166/171 (97%)	0.55	14 (8%) 11 15	35, 61, 94, 117	0
1	C	166/171 (97%)	0.80	21 (12%) 3 5	40, 70, 107, 121	0
1	D	147/171 (85%)	1.26	35 (23%) 0 1	48, 84, 111, 118	0
1	E	167/171 (97%)	0.40	10 (5%) 21 28	26, 46, 76, 88	0
2	F	46/79 (58%)	0.23	4 (8%) 10 14	27, 55, 99, 101	0
2	G	51/79 (64%)	0.34	4 (7%) 13 17	32, 60, 108, 118	0
2	H	44/79 (55%)	1.05	11 (25%) 0 1	45, 79, 119, 127	0
2	I	45/79 (56%)	1.21	14 (31%) 0 0	55, 92, 115, 123	0
2	J	53/79 (67%)	0.43	6 (11%) 5 7	26, 56, 108, 117	0
All	All	1050/1250 (84%)	0.67	132 (12%) 3 5	26, 62, 111, 127	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	LEU	6.1
1	C	183	LYS	5.2
2	G	803	LYS	5.0
1	D	62	VAL	4.8
1	C	182	PRO	4.6
1	D	151	TYR	4.6
1	C	48	PHE	4.5
1	C	66	ASP	4.5
1	D	68	THR	4.3
1	E	99	VAL	4.2
1	C	47	GLU	4.1
2	H	847	ILE	4.1
1	C	62	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	840	SER	3.9
1	B	66	ASP	3.8
1	A	99	VAL	3.8
1	E	98	VAL	3.7
1	D	131	SER	3.7
2	J	853	LEU	3.7
1	D	150	SER	3.7
1	C	184	ASN	3.7
1	D	140	LYS	3.6
1	E	97	ILE	3.6
2	H	841	LEU	3.6
2	H	838	ALA	3.5
2	J	803	LYS	3.5
2	I	837	GLN	3.5
1	A	67	THR	3.5
2	H	843	ARG	3.5
1	B	48	PHE	3.4
2	H	839	ASP	3.4
2	G	802	ASN	3.4
2	G	807	LEU	3.4
1	D	137	LEU	3.3
1	A	25	LEU	3.3
1	D	139	ASN	3.3
1	D	182	PRO	3.3
1	B	67	THR	3.2
1	B	97	ILE	3.2
2	H	842	GLU	3.2
1	B	65	ASP	3.2
1	A	97	ILE	3.1
1	C	67	THR	3.1
2	I	804	ALA	3.1
1	D	132	GLY	3.1
1	C	19	CYS	3.1
1	C	25	LEU	3.1
2	I	842	GLU	3.1
1	B	26	LEU	3.0
1	D	160	MET	3.0
1	E	26	LEU	3.0
2	G	806	ARG	3.0
1	D	126	ILE	3.0
1	D	154	ASP	3.0
2	H	807	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	147	GLU	2.9
1	A	66	ASP	2.9
1	B	19	CYS	2.9
2	J	852	LYS	2.9
2	J	807	LEU	2.9
1	B	146	GLN	2.8
1	D	144	ASP	2.8
1	D	168	MET	2.8
1	E	138	ALA	2.8
2	I	846	ALA	2.8
1	B	18	ILE	2.8
1	C	99	VAL	2.8
1	C	143	VAL	2.7
2	I	806	ARG	2.7
2	I	843	ARG	2.7
2	H	848	LEU	2.7
1	C	97	ILE	2.7
1	D	100	TYR	2.7
1	D	67	THR	2.7
1	D	69	VAL	2.6
2	I	831	GLN	2.6
1	D	148	ALA	2.6
2	I	850	ASP	2.6
1	A	26	LEU	2.6
1	A	62	VAL	2.6
1	C	68	THR	2.5
1	D	50	GLU	2.5
2	I	845	ARG	2.5
2	F	840	SER	2.5
1	D	149	GLN	2.5
1	E	131	SER	2.5
1	B	160	MET	2.4
2	J	851	THR	2.4
1	E	24	VAL	2.4
2	H	844	ILE	2.4
1	D	162	THR	2.4
2	H	810	GLU	2.4
1	D	25	LEU	2.4
1	B	142	ALA	2.4
1	D	145	PHE	2.4
1	B	25	LEU	2.4
1	D	130	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	847	ILE	2.3
1	C	20	GLN	2.3
1	D	61	THR	2.3
1	C	131	SER	2.3
1	A	139	ASN	2.3
1	E	25	LEU	2.3
2	J	804	ALA	2.3
1	A	68	THR	2.3
1	C	26	LEU	2.3
2	F	839	ASP	2.3
1	D	112	LYS	2.2
2	I	812	ASP	2.2
1	A	19	CYS	2.2
2	I	805	GLN	2.2
1	A	69	VAL	2.2
1	C	30	ALA	2.2
1	C	129	ALA	2.2
1	C	139	ASN	2.2
1	D	155	ASN	2.2
1	A	98	VAL	2.2
1	C	145	PHE	2.1
1	D	103	THR	2.1
2	I	835	ILE	2.1
1	D	26	LEU	2.1
1	E	36	LEU	2.1
2	F	805	GLN	2.1
1	D	56	ALA	2.1
2	F	804	ALA	2.1
1	E	37	VAL	2.1
1	B	17	LYS	2.0
1	A	65	ASP	2.0
1	D	99	VAL	2.0
1	D	161	GLU	2.0
1	B	101	ASP	2.0
2	I	834	ARG	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)

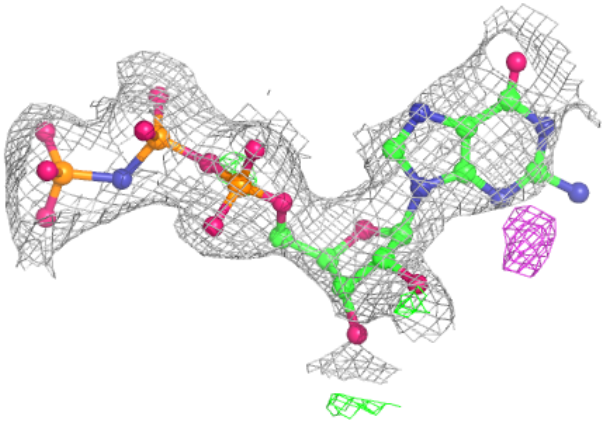
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

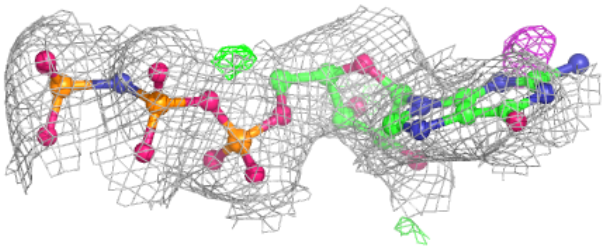
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	3201	1/1	0.93	0.09	45,45,45,45	0
4	GNP	D	4202	32/32	0.94	0.15	42,97,116,120	0
4	GNP	C	3202	32/32	0.96	0.11	29,75,81,82	0
4	GNP	B	2202	32/32	0.97	0.12	39,50,64,64	0
3	MG	B	2201	1/1	0.98	0.13	40,40,40,40	0
3	MG	A	1201	1/1	0.98	0.09	28,28,28,28	0
3	MG	E	5201	1/1	0.98	0.10	39,39,39,39	0
4	GNP	E	5202	32/32	0.98	0.12	26,53,73,77	0
3	MG	D	4201	1/1	0.99	0.07	51,51,51,51	0
4	GNP	A	1202	32/32	0.99	0.12	20,46,57,69	0

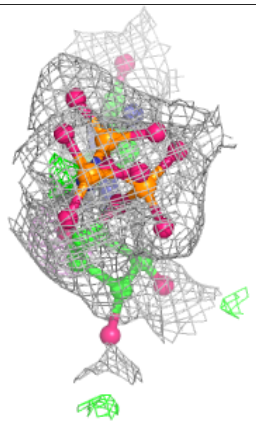
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP D 4202:

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

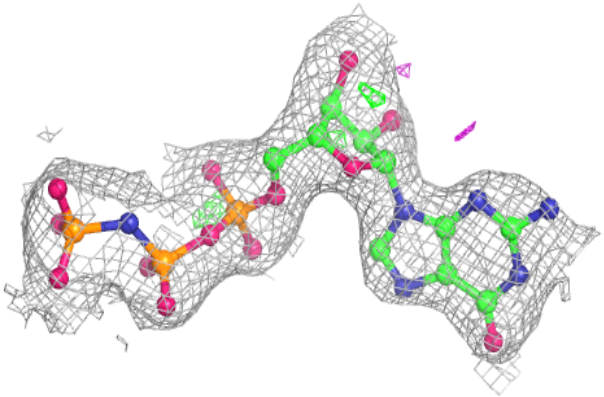


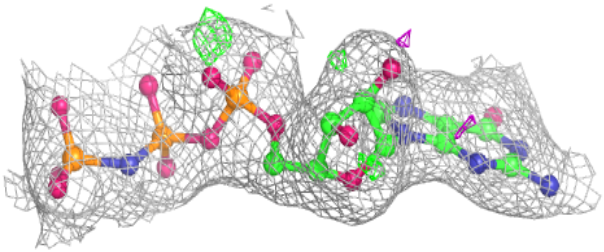


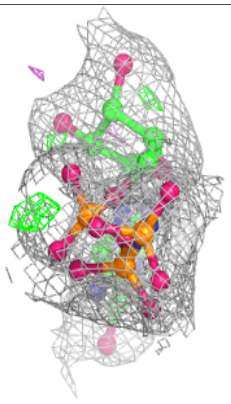


Electron density around GNP C 3202:

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

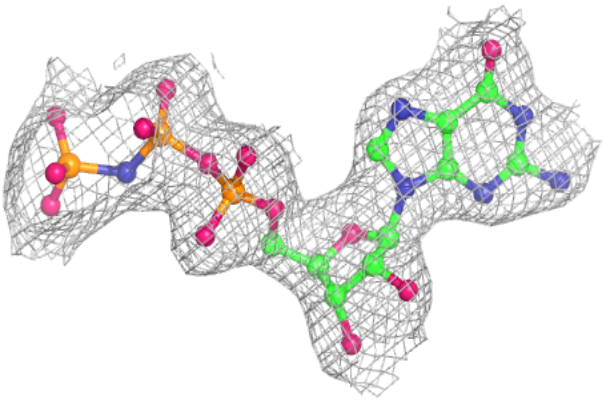


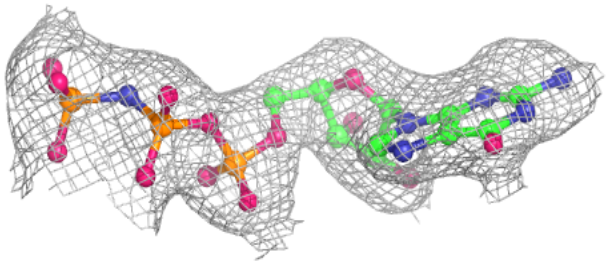


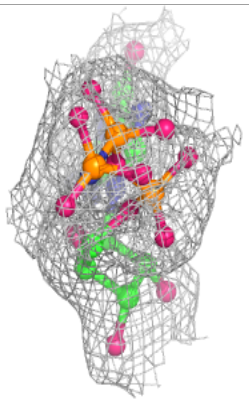


Electron density around GNP B 2202:

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

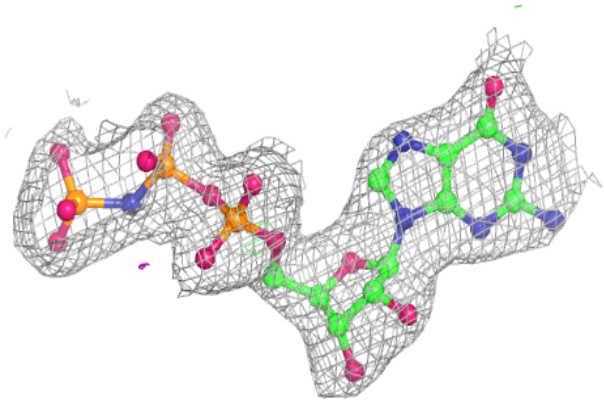


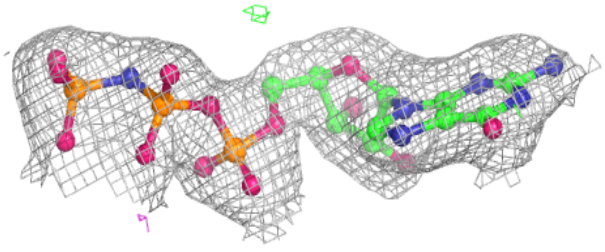


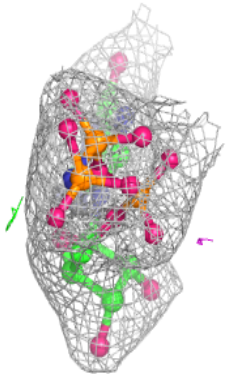


Electron density around GNP E 5202:

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

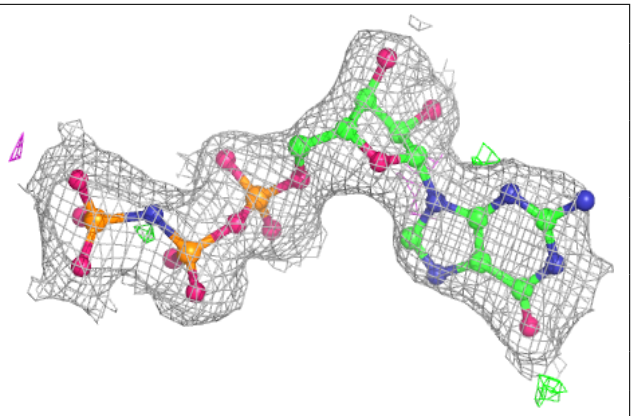


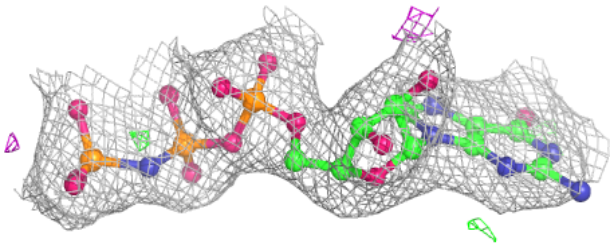


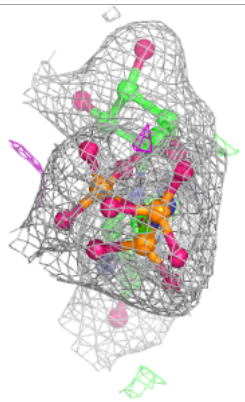


Electron density around GNP A 1202:

$2mF_o$-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

There are no such residues in this entry.