



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:30 PM UTC

PDB ID : 4Q66 / pdb_00004q66
Title : Structure of Exomer bound to Arf1.
Authors : Paczkowski, J.E.; Fromme, J.C.
Deposited on : 2014-04-21
Resolution : 3.35 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

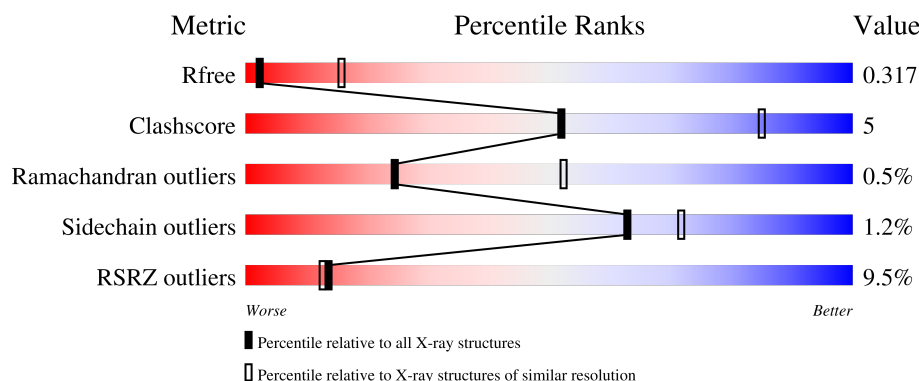
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.



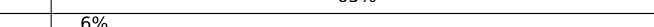
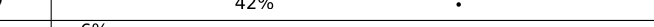
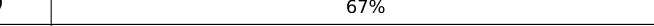
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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	368	5% 52% 8% 39%
1	D	368	7% 41% 6% 54%
1	G	368	5% 49% 9% 43%
1	J	368	6% 36% 6% 57%
2	B	739	5% 61% 7% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	739	
2	H	739	
2	K	739	
3	C	175	
3	F	175	
3	I	175	
3	L	175	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26303 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 Chs5p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1788	1149	309	323	7			
1	J	158	Total	C	N	O	S	0	0	0
			1240	801	210	226	3			
1	G	211	Total	C	N	O	S	0	0	0
			1655	1064	281	304	6			
1	D	171	Total	C	N	O	S	0	0	0
			1357	878	230	245	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP W7PD87
A	-2	ASP	-	expression tag	UNP W7PD87
A	-1	PRO	-	expression tag	UNP W7PD87
A	0	GLU	-	expression tag	UNP W7PD87
A	1	PHE	-	expression tag	UNP W7PD87
J	-3	MET	-	initiating methionine	UNP W7PD87
J	-2	ASP	-	expression tag	UNP W7PD87
J	-1	PRO	-	expression tag	UNP W7PD87
J	0	GLU	-	expression tag	UNP W7PD87
J	1	PHE	-	expression tag	UNP W7PD87
G	-3	MET	-	initiating methionine	UNP W7PD87
G	-2	ASP	-	expression tag	UNP W7PD87
G	-1	PRO	-	expression tag	UNP W7PD87
G	0	GLU	-	expression tag	UNP W7PD87
G	1	PHE	-	expression tag	UNP W7PD87
D	-3	MET	-	initiating methionine	UNP W7PD87
D	-2	ASP	-	expression tag	UNP W7PD87
D	-1	PRO	-	expression tag	UNP W7PD87
D	0	GLU	-	expression tag	UNP W7PD87
D	1	PHE	-	expression tag	UNP W7PD87

- Molecule 2 is a protein called Protein BCH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	593	Total	C	N	O	S	0	0	0
			4809	3106	792	888	23			
2	E	557	Total	C	N	O	S	0	0	0
			4493	2903	738	830	22			
2	B	507	Total	C	N	O	S	0	0	0
			4108	2656	673	758	21			
2	H	338	Total	C	N	O	S	0	0	0
			2711	1747	447	499	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	725	GLY	-	expression tag	UNP Q05029
K	726	THR	-	expression tag	UNP Q05029
K	727	GLU	-	expression tag	UNP Q05029
K	728	ASN	-	expression tag	UNP Q05029
K	729	LEU	-	expression tag	UNP Q05029
K	730	TYR	-	expression tag	UNP Q05029
K	731	PHE	-	expression tag	UNP Q05029
K	732	GLN	-	expression tag	UNP Q05029
K	733	GLY	-	expression tag	UNP Q05029
K	734	HIS	-	expression tag	UNP Q05029
K	735	HIS	-	expression tag	UNP Q05029
K	736	HIS	-	expression tag	UNP Q05029
K	737	HIS	-	expression tag	UNP Q05029
K	738	HIS	-	expression tag	UNP Q05029
K	739	HIS	-	expression tag	UNP Q05029
E	725	GLY	-	expression tag	UNP Q05029
E	726	THR	-	expression tag	UNP Q05029
E	727	GLU	-	expression tag	UNP Q05029
E	728	ASN	-	expression tag	UNP Q05029
E	729	LEU	-	expression tag	UNP Q05029
E	730	TYR	-	expression tag	UNP Q05029
E	731	PHE	-	expression tag	UNP Q05029
E	732	GLN	-	expression tag	UNP Q05029
E	733	GLY	-	expression tag	UNP Q05029
E	734	HIS	-	expression tag	UNP Q05029
E	735	HIS	-	expression tag	UNP Q05029
E	736	HIS	-	expression tag	UNP Q05029
E	737	HIS	-	expression tag	UNP Q05029
E	738	HIS	-	expression tag	UNP Q05029
E	739	HIS	-	expression tag	UNP Q05029

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLY	-	expression tag	UNP Q05029
B	726	THR	-	expression tag	UNP Q05029
B	727	GLU	-	expression tag	UNP Q05029
B	728	ASN	-	expression tag	UNP Q05029
B	729	LEU	-	expression tag	UNP Q05029
B	730	TYR	-	expression tag	UNP Q05029
B	731	PHE	-	expression tag	UNP Q05029
B	732	GLN	-	expression tag	UNP Q05029
B	733	GLY	-	expression tag	UNP Q05029
B	734	HIS	-	expression tag	UNP Q05029
B	735	HIS	-	expression tag	UNP Q05029
B	736	HIS	-	expression tag	UNP Q05029
B	737	HIS	-	expression tag	UNP Q05029
B	738	HIS	-	expression tag	UNP Q05029
B	739	HIS	-	expression tag	UNP Q05029
H	725	GLY	-	expression tag	UNP Q05029
H	726	THR	-	expression tag	UNP Q05029
H	727	GLU	-	expression tag	UNP Q05029
H	728	ASN	-	expression tag	UNP Q05029
H	729	LEU	-	expression tag	UNP Q05029
H	730	TYR	-	expression tag	UNP Q05029
H	731	PHE	-	expression tag	UNP Q05029
H	732	GLN	-	expression tag	UNP Q05029
H	733	GLY	-	expression tag	UNP Q05029
H	734	HIS	-	expression tag	UNP Q05029
H	735	HIS	-	expression tag	UNP Q05029
H	736	HIS	-	expression tag	UNP Q05029
H	737	HIS	-	expression tag	UNP Q05029
H	738	HIS	-	expression tag	UNP Q05029
H	739	HIS	-	expression tag	UNP Q05029

- Molecule 3 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	146	Total	C	N	O	S	0	0	0
			1173	745	205	217	6			
3	L	139	Total	C	N	O	S	0	0	0
			1115	711	195	203	6			
3	C	134	Total	C	N	O	S	0	0	0
			1056	673	177	202	4			
3	I	86	Total	C	N	O	S	0	0	0
			666	426	113	123	4			

There are 48 discrepancies between the modelled and reference sequences:

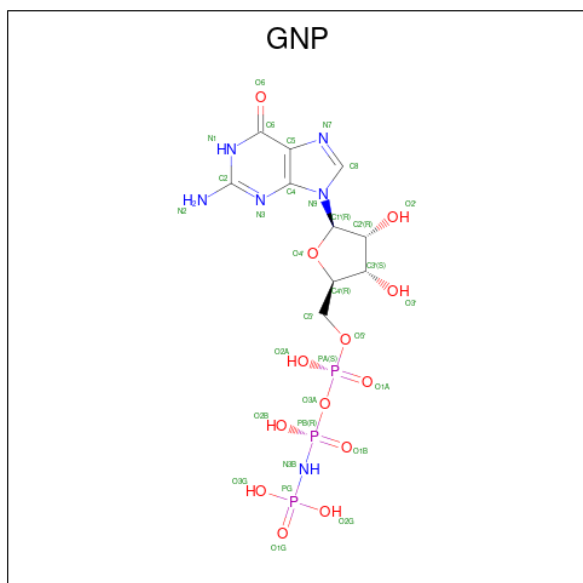
Chain	Residue	Modelled	Actual	Comment	Reference
F	7	MET	-	expression tag	UNP P11076
F	8	THR	-	expression tag	UNP P11076
F	9	GLU	-	expression tag	UNP P11076
F	10	ASN	-	expression tag	UNP P11076
F	11	LEU	-	expression tag	UNP P11076
F	12	TYR	-	expression tag	UNP P11076
F	13	PHE	-	expression tag	UNP P11076
F	14	GLN	-	expression tag	UNP P11076
F	15	GLY	-	expression tag	UNP P11076
F	16	SER	-	expression tag	UNP P11076
F	17	GLY	-	expression tag	UNP P11076
F	71	LEU	GLN	engineered mutation	UNP P11076
L	7	MET	-	expression tag	UNP P11076
L	8	THR	-	expression tag	UNP P11076
L	9	GLU	-	expression tag	UNP P11076
L	10	ASN	-	expression tag	UNP P11076
L	11	LEU	-	expression tag	UNP P11076
L	12	TYR	-	expression tag	UNP P11076
L	13	PHE	-	expression tag	UNP P11076
L	14	GLN	-	expression tag	UNP P11076
L	15	GLY	-	expression tag	UNP P11076
L	16	SER	-	expression tag	UNP P11076
L	17	GLY	-	expression tag	UNP P11076
L	71	LEU	GLN	engineered mutation	UNP P11076
C	7	MET	-	expression tag	UNP P11076
C	8	THR	-	expression tag	UNP P11076
C	9	GLU	-	expression tag	UNP P11076
C	10	ASN	-	expression tag	UNP P11076
C	11	LEU	-	expression tag	UNP P11076
C	12	TYR	-	expression tag	UNP P11076
C	13	PHE	-	expression tag	UNP P11076
C	14	GLN	-	expression tag	UNP P11076
C	15	GLY	-	expression tag	UNP P11076
C	16	SER	-	expression tag	UNP P11076
C	17	GLY	-	expression tag	UNP P11076
C	71	LEU	GLN	engineered mutation	UNP P11076
I	7	MET	-	expression tag	UNP P11076
I	8	THR	-	expression tag	UNP P11076
I	9	GLU	-	expression tag	UNP P11076
I	10	ASN	-	expression tag	UNP P11076
I	11	LEU	-	expression tag	UNP P11076
I	12	TYR	-	expression tag	UNP P11076

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	13	PHE	-	expression tag	UNP P11076
I	14	GLN	-	expression tag	UNP P11076
I	15	GLY	-	expression tag	UNP P11076
I	16	SER	-	expression tag	UNP P11076
I	17	GLY	-	expression tag	UNP P11076
I	71	LEU	GLN	engineered mutation	UNP P11076

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	L	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	I	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

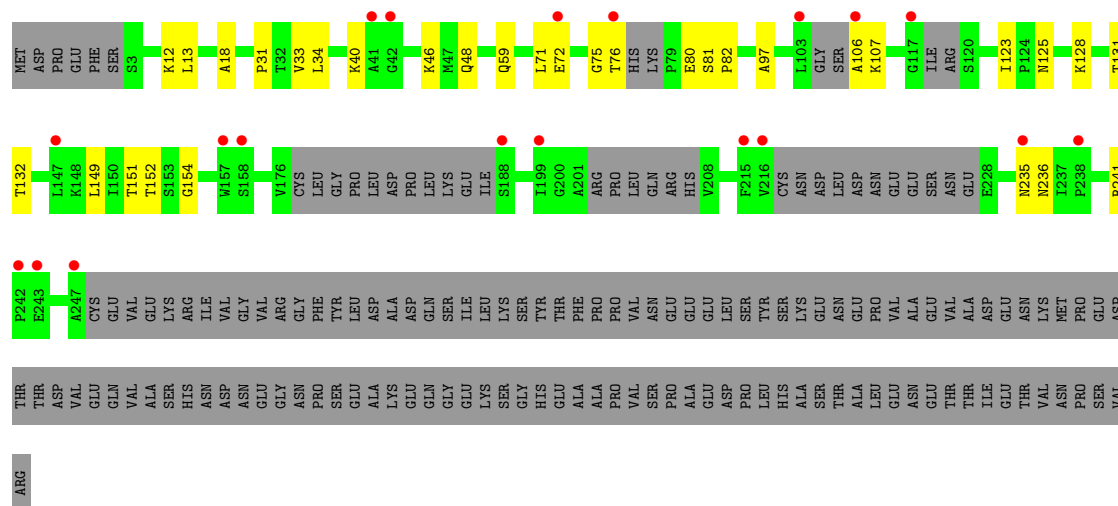
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Mg	0	0
			1	1		

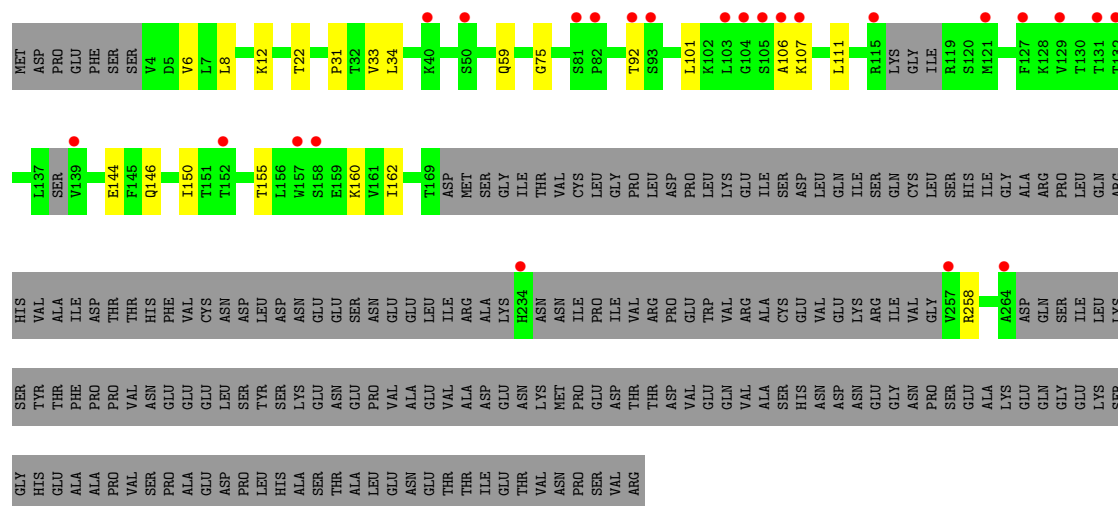
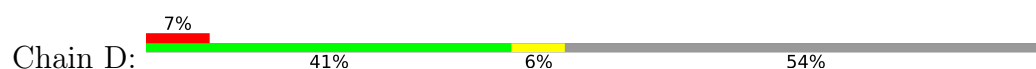
Continued on next page...

Continued from previous page...

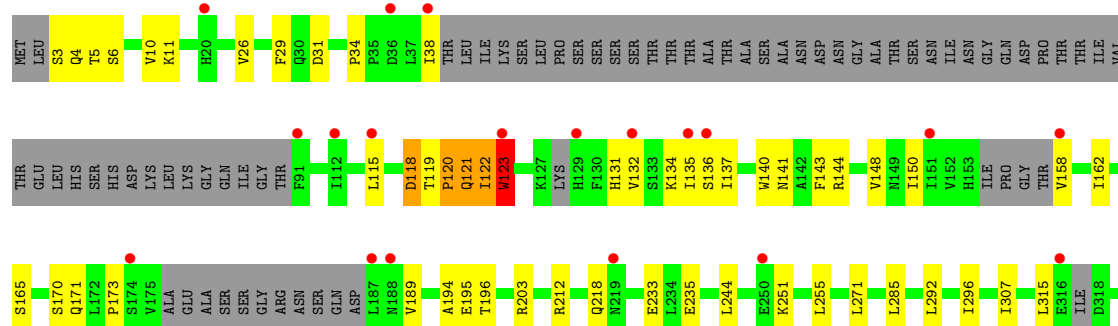
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	I	1	Total 1	Mg 1	0	0

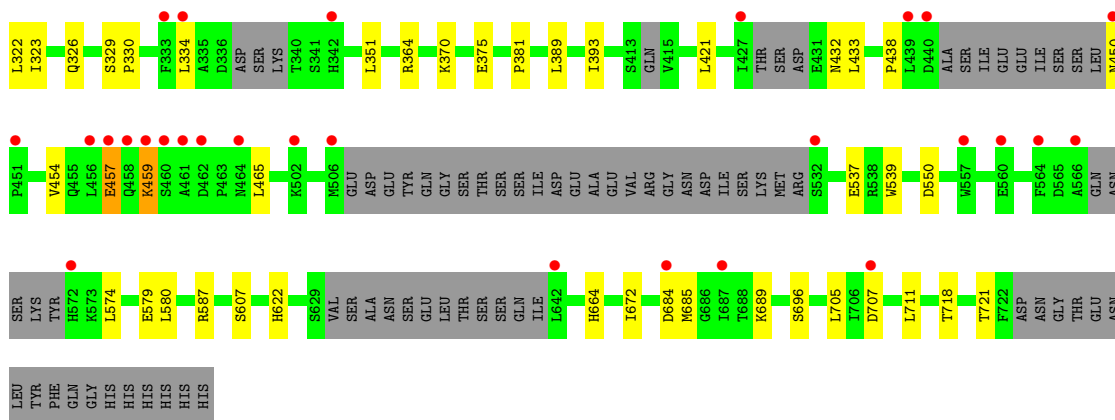


- Molecule 1: Chs5p

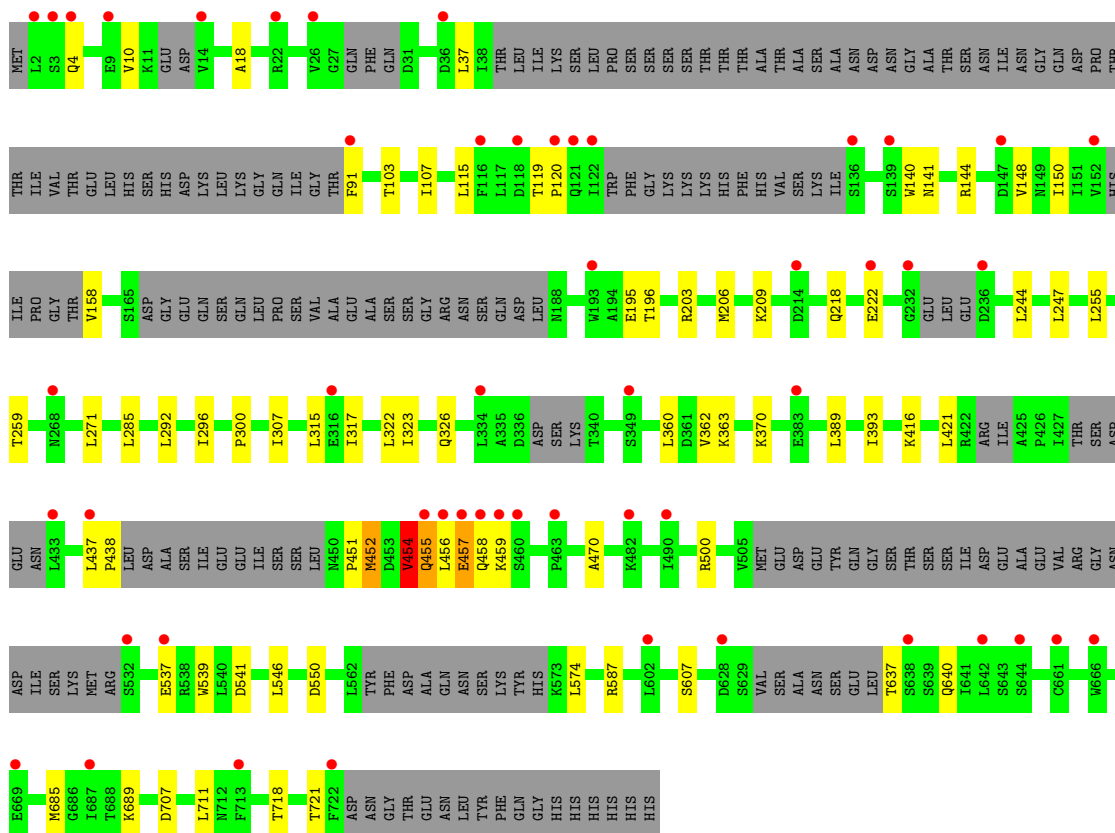


- Molecule 2: Protein BCH1



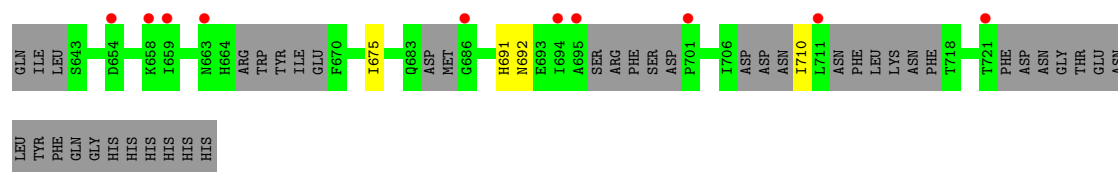


- Molecule 2: Protein BCH1

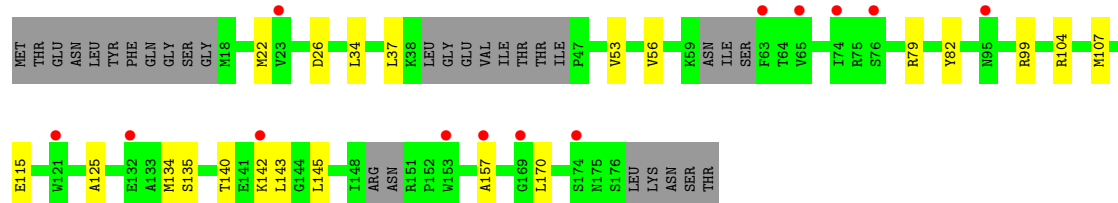


- Molecule 2: Protein BCH1

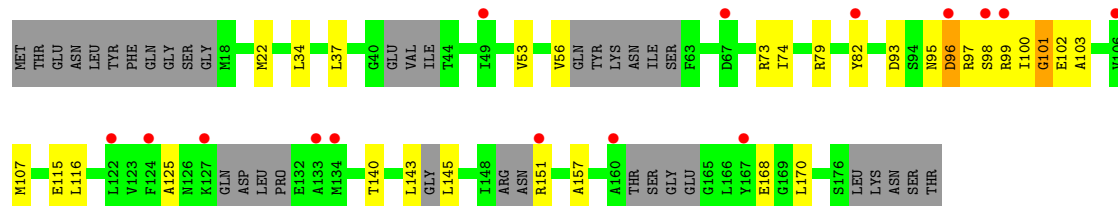




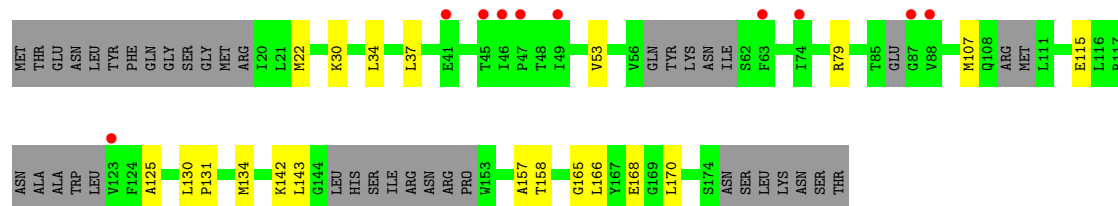
• Molecule 3: ADP-ribosylation factor 1



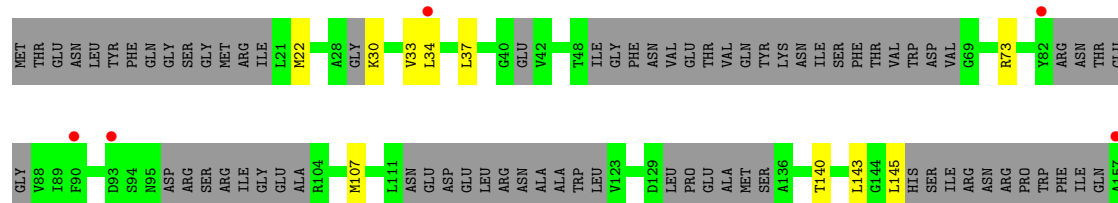
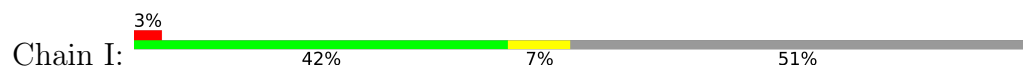
• Molecule 3: ADP-ribosylation factor 1



• Molecule 3: ADP-ribosylation factor 1



• Molecule 3: ADP-ribosylation factor 1



A160	
L166	
Y167	
E168	
G169	
LEU	
GLU	
TRP	
LEU	
SER	
ASN	
SER	
LEU	
LYS	
ASN	
SER	
THR	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.66Å 208.17Å 155.08Å 90.00° 105.48° 90.00°	Depositor
Resolution (Å)	43.17 – 3.35 43.17 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.17-3.35) 91.1 (43.17-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.279 , 0.310 0.286 , 0.317	Depositor DCC
R_{free} test set	2557 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	93.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	26303	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% 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, 0.333 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	0.25	0/1818	0.72	2/2456 (0.1%)
1	D	0.25	0/1379	0.69	0/1862
1	G	0.25	0/1679	0.71	1/2269 (0.0%)
1	J	0.24	0/1258	0.67	0/1699
2	B	0.26	0/4175	0.67	0/5634
2	E	0.26	0/4571	0.69	1/6183 (0.0%)
2	H	0.23	0/2740	0.62	0/3682
2	K	0.26	0/4901	0.69	2/6630 (0.0%)
3	C	0.24	0/1070	0.65	0/1442
3	F	0.24	0/1194	0.66	0/1609
3	I	0.22	0/667	0.57	0/887
3	L	0.26	0/1131	0.65	1/1521 (0.1%)
All	All	0.25	0/26583	0.68	7/35874 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	CB-CA-C	-6.33	108.26	115.79
3	L	95	ASN	N-CA-C	6.19	117.70	111.07
2	K	457	GLU	CB-CA-C	-5.81	109.89	116.63
1	A	40	LYS	CB-CA-C	-5.57	110.14	116.54
1	G	40	LYS	CB-CA-C	-5.48	110.27	116.63
2	E	457	GLU	CB-CA-C	-5.28	110.51	116.63
2	K	123	TRP	CB-CA-C	-5.23	109.57	115.79

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	1788	0	1872	20	0
1	D	1357	0	1435	14	0
1	G	1655	0	1743	23	0
1	J	1240	0	1325	17	0
2	B	4108	0	4150	52	0
2	E	4493	0	4560	40	0
2	H	2711	0	2781	15	0
2	K	4809	0	4841	48	0
3	C	1056	0	1042	12	0
3	F	1173	0	1158	12	0
3	I	666	0	681	8	0
3	L	1115	0	1109	23	0
4	C	32	0	13	1	0
4	F	32	0	13	0	0
4	I	32	0	13	1	0
4	L	32	0	13	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
All	All	26303	0	26749	270	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 5.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:VAL:O	2:B:28:GLN:N	1.72	1.19
3:L:100:ILE:O	3:L:103:ALA:N	1.85	1.09
2:B:22:ARG:O	2:B:23:ARG:NE	1.88	1.06
3:L:100:ILE:HG23	3:L:101:GLY:H	1.31	0.96
3:L:100:ILE:HG23	3:L:101:GLY:N	1.81	0.93
3:L:100:ILE:CG2	3:L:101:GLY:H	1.83	0.90
1:A:151:THR:HG22	1:A:153:SER:H	1.42	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:GLN:HE22	2:B:22:ARG:HD3	1.42	0.81
3:L:100:ILE:O	3:L:102:GLU:N	2.15	0.79
2:B:24:ALA:O	2:B:26:VAL:HG23	1.88	0.74
1:D:75:GLY:HA2	2:E:317:ILE:HG23	1.69	0.73
2:K:218:GLN:HE22	2:K:421:LEU:HD12	1.53	0.73
1:G:72:GLU:O	1:G:76:THR:OG1	2.06	0.73
2:B:24:ALA:O	2:B:26:VAL:N	2.21	0.73
2:E:362:VAL:HG13	2:E:363:LYS:HG2	1.73	0.70
2:B:26:VAL:HG12	2:B:27:GLY:N	2.06	0.70
3:L:96:ASP:OD2	3:L:96:ASP:N	2.25	0.69
2:K:162:ILE:HB	2:K:170:SER:HB3	1.74	0.69
3:L:100:ILE:O	3:L:101:GLY:C	2.37	0.68
1:G:241:ARG:H	1:G:241:ARG:HD3	1.60	0.67
2:B:21:GLN:OE1	2:B:22:ARG:HB3	1.96	0.66
2:B:21:GLN:HE22	2:B:22:ARG:CD	2.08	0.65
1:G:71:LEU:O	1:G:76:THR:HG23	1.97	0.64
2:E:685:MET:HB2	2:E:689:LYS:HD3	1.80	0.64
3:L:99:ARG:O	3:L:99:ARG:HG3	1.97	0.64
2:K:459:LYS:HE3	2:K:574:LEU:HD13	1.79	0.64
1:G:33:VAL:HG13	1:G:34:LEU:HD12	1.81	0.63
2:B:21:GLN:NE2	2:B:22:ARG:HG2	2.13	0.62
3:L:73:ARG:HG3	3:L:74:ILE:HG12	1.80	0.62
1:A:71:LEU:O	1:A:76:THR:OG1	2.17	0.62
2:E:452:MET:SD	2:E:452:MET:N	2.72	0.61
3:L:100:ILE:C	3:L:102:GLU:N	2.59	0.61
2:E:637:THR:OG1	2:E:640:GLN:OE1	2.18	0.61
3:L:93:ASP:CG	3:L:96:ASP:OD2	2.43	0.61
1:A:166:HIS:ND1	1:A:170:ASP:OD2	2.34	0.60
1:A:34:LEU:HD22	1:D:6:VAL:HG11	1.82	0.60
2:B:26:VAL:C	2:B:28:GLN:H	2.03	0.60
3:C:125:ALA:HB3	3:C:157:ALA:HA	1.82	0.60
1:A:35:LEU:HB3	1:A:39:VAL:HG21	1.84	0.60
2:E:144:ARG:NH1	2:E:195:GLU:OE2	2.34	0.60
2:E:218:GLN:HE22	2:E:421:LEU:HD12	1.67	0.60
2:E:550:ASP:OD2	2:E:587:ARG:NH1	2.35	0.59
2:E:4:GLN:H	2:E:115:LEU:HD11	1.68	0.59
2:B:459:LYS:HD3	2:B:574:LEU:HD13	1.85	0.59
2:K:144:ARG:NH1	2:K:195:GLU:OE2	2.36	0.59
3:F:37:LEU:HB3	3:F:56:VAL:HG11	1.85	0.59
1:J:59:GLN:NE2	2:K:375:GLU:OE2	2.35	0.58
2:B:26:VAL:C	2:B:28:GLN:N	2.56	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:HG13	1:D:34:LEU:HD12	1.84	0.58
3:L:140:THR:HG22	3:L:145:LEU:HD12	1.86	0.58
2:K:118:ASP:OD1	2:K:118:ASP:N	2.37	0.58
2:E:500:ARG:NH2	2:E:541:ASP:OD1	2.36	0.58
3:C:22:MET:HE1	3:C:34:LEU:HB2	1.86	0.58
2:B:25:ARG:HG3	2:B:25:ARG:O	2.04	0.57
2:K:3:SER:O	2:K:5:THR:N	2.35	0.57
3:L:107:MET:HE1	3:L:143:LEU:HB3	1.86	0.57
3:L:22:MET:HE1	3:L:34:LEU:HB2	1.86	0.57
1:A:22:THR:OG1	1:A:24:ASP:OD1	2.19	0.57
2:K:685:MET:HB2	2:K:689:LYS:HD3	1.86	0.57
1:A:75:GLY:HA2	2:B:317:ILE:HG23	1.87	0.57
2:K:140:TRP:O	2:K:203:ARG:NH1	2.36	0.57
2:H:307:ILE:HD13	2:H:323:ILE:HG12	1.87	0.57
1:G:75:GLY:HA2	2:H:317:ILE:HG23	1.87	0.57
2:B:500:ARG:NH2	2:B:541:ASP:OD1	2.38	0.57
1:A:109:LYS:HE3	1:A:152:THR:HB	1.88	0.56
1:A:176:VAL:HG12	1:A:214:HIS:HB2	1.88	0.56
3:F:104:ARG:NH1	3:F:142:LYS:O	2.39	0.56
1:J:144:GLU:OE1	1:J:160:LYS:NZ	2.39	0.55
2:H:255:LEU:HD12	2:H:271:LEU:HB2	1.88	0.55
1:J:103:LEU:HD21	1:J:108:LEU:HB3	1.87	0.55
3:I:30:LYS:NZ	4:I:201:GNP:O3G	2.39	0.55
2:B:685:MET:HB2	2:B:689:LYS:HD3	1.89	0.55
2:B:550:ASP:OD2	2:B:587:ARG:NH1	2.40	0.54
3:C:30:LYS:NZ	4:C:201:GNP:O1B	2.36	0.54
2:B:457:GLU:OE2	2:B:458:GLN:N	2.41	0.54
3:F:107:MET:HE1	3:F:143:LEU:HD13	1.90	0.54
2:K:148:VAL:HG21	2:K:196:THR:HG21	1.89	0.53
3:C:37:LEU:HD21	3:C:166:LEU:HB3	1.89	0.53
2:E:459:LYS:HD2	2:E:574:LEU:HD13	1.90	0.53
2:B:144:ARG:NH1	2:B:195:GLU:OE2	2.42	0.53
1:G:71:LEU:O	1:G:76:THR:CG2	2.57	0.53
2:K:696:SER:HB3	3:L:79:ARG:HD2	1.90	0.53
1:D:8:LEU:HD22	1:D:22:THR:HG22	1.90	0.53
3:F:125:ALA:HB3	3:F:157:ALA:HA	1.91	0.53
3:I:37:LEU:HD21	3:I:166:LEU:HB3	1.91	0.53
2:E:18:ALA:HB1	2:E:37:LEU:HD21	1.91	0.52
3:L:125:ALA:HB3	3:L:157:ALA:HA	1.90	0.52
1:J:54:GLU:HA	1:J:57:LYS:HZ3	1.73	0.52
2:K:120:PRO:O	2:K:122:ILE:HG13	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLN:HE22	2:B:421:LEU:HD12	1.75	0.52
2:B:307:ILE:HD13	2:B:323:ILE:HG12	1.91	0.52
2:B:21:GLN:CG	2:B:22:ARG:N	2.73	0.52
3:F:26:ASP:O	3:F:99:ARG:NH2	2.42	0.52
3:F:22:MET:HE1	3:F:34:LEU:HB2	1.92	0.52
2:E:259:THR:HA	2:E:416:LYS:HD2	1.92	0.51
2:B:21:GLN:NE2	2:B:22:ARG:CG	2.73	0.51
2:B:696:SER:O	3:C:79:ARG:NE	2.44	0.51
2:B:244:LEU:HD12	2:B:247:LEU:HD12	1.91	0.51
2:B:537:GLU:O	2:B:539:TRP:N	2.43	0.51
1:J:83:VAL:HG12	1:J:159:GLU:HG3	1.91	0.51
1:G:12:LYS:HG3	2:K:381:PRO:HD2	1.93	0.51
1:A:54:GLU:HA	1:A:57:LYS:HE2	1.91	0.50
2:B:255:LEU:HD12	2:B:271:LEU:HB2	1.92	0.50
2:K:195:GLU:OE2	2:K:251:LYS:NZ	2.44	0.50
2:B:21:GLN:HG3	2:B:22:ARG:H	1.77	0.50
2:K:550:ASP:OD2	2:K:587:ARG:NH1	2.44	0.50
2:H:692:ASN:HD22	3:I:73:ARG:HB3	1.76	0.50
3:F:37:LEU:HD13	3:F:170:LEU:HD11	1.94	0.49
1:D:144:GLU:HB3	1:D:162:ILE:HG22	1.94	0.49
2:H:370:LYS:HB2	2:H:393:ILE:HG21	1.94	0.49
2:H:396:LYS:NZ	2:H:486:GLU:OE2	2.43	0.49
1:D:101:LEU:HD11	1:D:111:LEU:HD22	1.94	0.49
2:E:454:VAL:HG22	2:E:455:GLN:H	1.77	0.49
2:E:244:LEU:HD12	2:E:247:LEU:HD12	1.95	0.49
3:C:37:LEU:HD13	3:C:170:LEU:HD11	1.95	0.49
2:E:707:ASP:HA	2:E:711:LEU:HB3	1.94	0.49
2:K:38:ILE:HG12	2:K:137:ILE:HG23	1.95	0.48
2:K:322:LEU:O	2:K:326:GLN:HG2	2.14	0.48
2:B:21:GLN:HE22	2:B:22:ARG:HG2	1.78	0.48
3:I:107:MET:HE1	3:I:143:LEU:HB3	1.96	0.48
1:A:106:ALA:O	1:A:153:SER:OG	2.27	0.48
2:K:307:ILE:HD13	2:K:323:ILE:HG12	1.96	0.48
2:K:194:ALA:HA	2:K:244:LEU:HD21	1.95	0.48
2:K:664:HIS:CG	2:K:705:LEU:HD11	2.49	0.48
2:K:255:LEU:HD12	2:K:271:LEU:HB2	1.95	0.47
2:E:4:GLN:HA	2:E:115:LEU:HD21	1.95	0.47
2:E:457:GLU:HA	2:E:459:LYS:HE2	1.96	0.47
2:B:3:SER:O	2:B:5:THR:N	2.45	0.47
2:B:427:ILE:HG21	2:B:433:LEU:HD11	1.96	0.47
1:G:151:THR:OG1	1:G:154:GLY:O	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:26:VAL:HG12	2:K:165:SER:HA	1.97	0.47
2:E:307:ILE:HD13	2:E:323:ILE:HG12	1.96	0.47
2:E:370:LYS:HB2	2:E:393:ILE:HG21	1.95	0.47
2:B:21:GLN:HE22	2:B:22:ARG:CG	2.26	0.47
2:B:707:ASP:HA	2:B:711:LEU:HB3	1.97	0.47
3:I:22:MET:HE1	3:I:34:LEU:HB2	1.95	0.47
1:G:13:LEU:HD23	1:G:18:ALA:HB2	1.96	0.47
2:K:389:LEU:O	2:K:393:ILE:HG12	2.14	0.47
2:B:622:HIS:NE2	2:B:684:ASP:OD2	2.46	0.47
2:B:21:GLN:CD	2:B:22:ARG:N	2.73	0.47
2:B:304:ILE:HG12	2:B:351:LEU:HD21	1.95	0.47
3:I:140:THR:HG23	3:I:145:LEU:HB2	1.96	0.47
2:E:437:LEU:HD12	2:E:438:PRO:HD2	1.95	0.47
3:L:115:GLU:OE1	3:L:115:GLU:N	2.46	0.47
2:K:173:PRO:HG2	2:K:189:VAL:HG22	1.97	0.47
2:E:255:LEU:HD12	2:E:271:LEU:HB2	1.97	0.47
2:B:389:LEU:O	2:B:393:ILE:HG12	2.15	0.46
1:A:44:ILE:HD11	1:D:59:GLN:HG3	1.97	0.46
2:K:292:LEU:O	2:K:296:ILE:HG13	2.15	0.46
2:K:718:THR:O	2:K:721:THR:OG1	2.28	0.46
1:J:106:ALA:HB1	1:J:107:LYS:HB2	1.96	0.46
2:H:229:PHE:HE1	2:H:278:ILE:HG23	1.80	0.46
1:J:14:ASP:OD1	1:J:15:ALA:N	2.40	0.46
1:G:106:ALA:N	1:G:107:LYS:HA	2.31	0.46
1:J:44:ILE:HD11	1:G:59:GLN:HG3	1.98	0.46
1:G:235:ASN:O	1:G:236:ASN:HB2	2.15	0.46
2:B:21:GLN:HG3	2:B:22:ARG:N	2.31	0.46
1:A:77:HIS:O	1:A:79:PRO:HD3	2.16	0.46
1:D:106:ALA:HA	1:D:107:LYS:HA	1.77	0.46
2:K:622:HIS:NE2	2:K:684:ASP:OD2	2.46	0.46
2:B:21:GLN:OE1	2:B:22:ARG:HD2	2.16	0.45
2:K:131:HIS:HA	2:K:134:LYS:HD2	1.97	0.45
2:H:389:LEU:O	2:H:393:ILE:HG12	2.17	0.45
2:K:537:GLU:O	2:K:539:TRP:N	2.44	0.45
1:A:106:ALA:HB1	1:A:151:THR:CG2	2.47	0.45
1:A:233:LYS:HB3	1:A:234:HIS:H	1.56	0.45
1:D:106:ALA:HB1	1:D:107:LYS:HB2	1.99	0.45
2:K:707:ASP:HA	2:K:711:LEU:HB3	1.99	0.45
2:H:207:ILE:HG23	2:H:208:MET:HG2	1.98	0.45
1:G:75:GLY:C	1:G:76:THR:HG23	2.42	0.45
2:K:170:SER:OG	2:K:171:GLN:N	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:718:THR:O	2:E:721:THR:OG1	2.31	0.45
3:F:140:THR:HG23	3:F:145:LEU:HD12	1.99	0.45
1:J:113:LEU:O	1:J:120:SER:HB2	2.17	0.44
1:D:31:PRO:HG2	1:D:34:LEU:HD13	1.99	0.44
2:B:23:ARG:HA	2:B:23:ARG:HD3	1.72	0.44
3:L:116:LEU:O	3:L:151:ARG:NH1	2.49	0.44
2:E:537:GLU:O	2:E:539:TRP:N	2.45	0.44
1:G:82:PRO:HG3	1:G:149:LEU:HB2	1.98	0.44
2:E:389:LEU:O	2:E:393:ILE:HG12	2.16	0.44
3:L:37:LEU:HB3	3:L:56:VAL:HG11	1.99	0.44
2:K:465:LEU:HG	2:K:580:LEU:HD23	2.00	0.44
2:E:148:VAL:HG21	2:E:196:THR:HG21	1.98	0.44
2:K:334:LEU:HD11	2:K:351:LEU:HD12	1.99	0.44
2:E:296:ILE:HG23	2:E:300:PRO:HA	2.00	0.44
3:F:134:MET:HE1	3:F:142:LYS:HG3	2.00	0.44
2:B:558:GLN:HE21	2:B:581:PHE:HZ	1.65	0.44
2:B:21:GLN:NE2	2:B:22:ARG:CD	2.77	0.44
1:G:31:PRO:HG2	1:G:34:LEU:HD13	2.00	0.44
3:C:115:GLU:OE1	3:C:115:GLU:N	2.46	0.44
2:B:194:ALA:HA	2:B:244:LEU:HD21	2.00	0.43
1:J:6:VAL:HG21	1:G:34:LEU:HG	1.99	0.43
1:G:97:ALA:HB2	1:G:131:THR:HG22	2.00	0.43
2:K:579:GLU:OE2	2:K:607:SER:OG	2.31	0.43
2:E:206:MET:HE1	2:E:209:LYS:HD3	2.00	0.43
2:H:537:GLU:O	2:H:539:TRP:N	2.47	0.43
3:C:107:MET:HE1	3:C:143:LEU:HB3	2.00	0.43
1:A:231:ARG:HB2	1:A:233:LYS:HG2	2.00	0.43
3:F:79:ARG:HA	3:F:82:TYR:CD2	2.53	0.43
1:A:106:ALA:HB1	1:A:151:THR:HG21	2.00	0.43
2:K:134:LYS:HB3	2:K:135:ILE:HA	1.99	0.43
2:K:233:GLU:C	2:K:235:GLU:H	2.26	0.43
2:E:119:THR:HA	2:E:120:PRO:HD2	1.94	0.43
2:E:292:LEU:O	2:E:296:ILE:HG13	2.18	0.43
2:K:11:LYS:HB2	2:K:432:ASN:HD21	1.83	0.43
2:K:212:ARG:HH22	2:K:672:ILE:HG21	1.83	0.43
2:H:675:ILE:HG12	2:H:710:ILE:HG23	2.01	0.43
1:D:146:GLN:HB3	1:D:160:LYS:HA	2.01	0.43
2:B:21:GLN:NE2	2:B:22:ARG:HD3	2.21	0.43
2:K:11:LYS:HE2	2:K:123:TRP:HE1	1.84	0.42
3:C:134:MET:HE1	3:C:142:LYS:HG3	2.00	0.42
3:C:168:GLU:OE1	3:C:168:GLU:N	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ILE:HG23	1:D:155:THR:HG22	2.00	0.42
2:B:23:ARG:HG3	2:B:424:ILE:HG22	2.00	0.42
2:B:6:SER:HA	2:B:667:TYR:HD1	1.83	0.42
2:K:329:SER:HA	2:K:330:PRO:HD3	1.84	0.42
2:E:470:ALA:HA	2:E:546:LEU:HD23	2.00	0.42
1:J:106:ALA:HA	1:J:107:LYS:HA	1.77	0.42
2:E:140:TRP:O	2:E:203:ARG:NH1	2.50	0.42
2:E:360:LEU:HD13	2:E:393:ILE:HD13	2.02	0.42
1:J:135:SER:CB	3:L:99:ARG:HD2	2.49	0.42
1:G:123:ILE:HD12	1:G:132:THR:HG21	2.01	0.42
1:D:258:ARG:HD3	3:F:135:SER:HB3	2.02	0.42
2:K:143:PHE:CZ	2:K:255:LEU:HD11	2.54	0.42
2:H:360:LEU:HD13	2:H:393:ILE:HD13	2.00	0.42
3:F:115:GLU:OE1	3:F:115:GLU:N	2.46	0.42
2:K:6:SER:HB3	2:K:438:PRO:HB3	2.01	0.42
2:E:285:LEU:HD21	2:E:315:LEU:HD11	2.01	0.42
1:A:113:LEU:O	1:A:120:SER:OG	2.36	0.41
2:K:29:PHE:CZ	2:K:34:PRO:HG3	2.54	0.41
2:K:141:ASN:HB3	2:K:196:THR:HA	2.01	0.41
2:E:141:ASN:HB3	2:E:196:THR:HA	2.00	0.41
2:B:29:PHE:HD1	2:B:29:PHE:HA	1.77	0.41
2:E:103:THR:O	2:E:107:ILE:HG13	2.20	0.41
1:G:46:LYS:HE2	1:G:48:GLN:HE21	1.84	0.41
1:G:72:GLU:C	1:G:76:THR:OG1	2.62	0.41
3:L:37:LEU:HD13	3:L:170:LEU:HD11	2.01	0.41
1:A:101:LEU:HD11	1:A:111:LEU:HD22	2.02	0.41
1:J:109:LYS:HB2	1:J:150:ILE:HG22	2.01	0.41
3:L:100:ILE:HG22	3:L:101:GLY:H	1.80	0.41
1:D:12:LYS:HE2	1:D:12:LYS:HB3	1.91	0.41
2:B:32:LEU:HB2	2:B:419:TYR:CE1	2.56	0.41
2:B:140:TRP:O	2:B:203:ARG:NH1	2.42	0.41
2:B:259:THR:HA	2:B:416:LYS:HD2	2.01	0.41
2:H:304:ILE:HG12	2:H:351:LEU:HD21	2.01	0.41
1:A:215:PHE:CZ	1:A:233:LYS:HE2	2.56	0.41
2:K:285:LEU:HD21	2:K:315:LEU:HD11	2.03	0.41
2:H:551:LEU:HD23	2:H:588:LEU:HD13	2.03	0.41
3:C:130:LEU:HA	3:C:131:PRO:HD3	1.92	0.41
3:L:79:ARG:HA	3:L:82:TYR:CD2	2.54	0.41
2:E:222:GLU:OE1	2:E:222:GLU:N	2.50	0.41
2:B:21:GLN:O	2:B:22:ARG:HB3	2.21	0.41
2:E:322:LEU:O	2:E:326:GLN:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:457:GLU:HB3	2:E:458:GLN:H	1.62	0.41
2:B:718:THR:O	2:B:721:THR:OG1	2.28	0.41
3:I:168:GLU:OE1	3:I:168:GLU:N	2.49	0.41
1:J:13:LEU:HD22	1:J:40:LYS:O	2.22	0.40
2:K:10:VAL:HG22	2:K:433:LEU:HB3	2.02	0.40
2:K:370:LYS:HB2	2:K:393:ILE:HG21	2.01	0.40
1:G:125:ASN:HB3	1:G:128:LYS:HB2	2.04	0.40
2:H:292:LEU:O	2:H:296:ILE:HG13	2.20	0.40
3:C:158:THR:HG22	3:C:165:GLY:O	2.22	0.40
3:I:33:VAL:HG22	3:I:160:ALA:HB2	2.03	0.40
1:J:109:LYS:N	1:J:150:ILE:O	2.46	0.40
1:G:107:LYS:HE3	1:G:107:LYS:HB2	1.90	0.40
2:K:4:GLN:H	2:K:115:LEU:HD13	1.86	0.40
1:J:71:LEU:O	1:J:76:THR:OG1	2.30	0.40
1:J:150:ILE:HG23	1:J:155:THR:HG22	2.02	0.40
1:G:81:SER:HA	1:G:82:PRO:HD3	1.91	0.40
2:E:10:VAL:HB	2:E:91:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/368 (58%)	190 (90%)	22 (10%)	0	100	100
1	D	162/368 (44%)	152 (94%)	10 (6%)	0	100	100
1	G	197/368 (54%)	183 (93%)	13 (7%)	1 (0%)	24	52
1	J	150/368 (41%)	139 (93%)	11 (7%)	0	100	100
2	B	469/739 (64%)	446 (95%)	19 (4%)	4 (1%)	14	41
2	E	527/739 (71%)	503 (95%)	21 (4%)	3 (1%)	21	49
2	H	300/739 (41%)	290 (97%)	10 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	567/739 (77%)	536 (94%)	25 (4%)	6 (1%)	11	36
3	C	122/175 (70%)	120 (98%)	2 (2%)	0	100	100
3	F	138/175 (79%)	136 (99%)	2 (1%)	0	100	100
3	I	68/175 (39%)	66 (97%)	2 (3%)	0	100	100
3	L	125/175 (71%)	119 (95%)	5 (4%)	1 (1%)	16	44
All	All	3037/5128 (59%)	2880 (95%)	142 (5%)	15 (0%)	24	52

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	454	VAL
2	B	22	ARG
2	B	25	ARG
2	B	27	GLY
2	E	451	PRO
3	L	101	GLY
1	G	80	GLU
2	K	31	ASP
2	E	607	SER
2	K	119	THR
2	K	120	PRO
2	K	121	GLN
2	K	136	SER
2	K	364	ARG
2	B	26	VAL

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	207/333 (62%)	202 (98%)	5 (2%)	43	62
1	D	157/333 (47%)	156 (99%)	1 (1%)	78	79
1	G	193/333 (58%)	192 (100%)	1 (0%)	81	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	145/333 (44%)	143 (99%)	2 (1%)	59	69
2	B	467/672 (70%)	465 (100%)	2 (0%)	84	82
2	E	512/672 (76%)	506 (99%)	6 (1%)	63	72
2	H	307/672 (46%)	306 (100%)	1 (0%)	86	84
2	K	545/672 (81%)	534 (98%)	11 (2%)	48	65
3	C	113/150 (75%)	112 (99%)	1 (1%)	70	75
3	F	124/150 (83%)	123 (99%)	1 (1%)	73	76
3	I	71/150 (47%)	71 (100%)	0	100	100
3	L	118/150 (79%)	113 (96%)	5 (4%)	26	52
All	All	2959/4620 (64%)	2923 (99%)	36 (1%)	63	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	151	THR
1	A	230	ILE
1	A	233	LYS
1	A	262	LEU
1	J	76	THR
1	J	160	LYS
1	G	152	THR
1	D	92	THR
2	K	118	ASP
2	K	121	GLN
2	K	122	ILE
2	K	123	TRP
2	K	132	VAL
2	K	150	ILE
2	K	158	VAL
2	K	450	ASN
2	K	454	VAL
2	K	457	GLU
2	K	459	LYS
2	E	150	ILE
2	E	158	VAL
2	E	452	MET
2	E	454	VAL
2	E	455	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	456	LEU
2	B	22	ARG
2	B	23	ARG
2	H	691	HIS
3	F	53	VAL
3	L	53	VAL
3	L	96	ASP
3	L	97	ARG
3	L	98	SER
3	L	168	GLU
3	C	53	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	J	146	GLN
1	G	25	HIS
1	D	125	ASN
1	D	166	HIS
2	K	21	GLN
2	K	28	GLN
2	K	218	GLN
2	K	326	GLN
2	K	342	HIS
2	K	432	ASN
2	K	464	ASN
2	K	478	GLN
2	K	495	GLN
2	K	590	HIS
2	K	604	GLN
2	K	664	HIS
2	K	704	GLN
2	E	211	ASN
2	E	218	GLN
2	E	299	HIS
2	E	326	GLN
2	E	342	HIS
2	E	478	GLN
2	E	495	GLN
2	E	704	GLN
2	B	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	324	ASN
2	B	326	GLN
2	B	342	HIS
2	B	478	GLN
2	B	558	GLN
2	B	604	GLN
2	B	616	GLN
2	B	640	GLN
2	B	664	HIS
2	B	704	GLN
2	B	716	ASN
2	H	326	GLN
2	H	478	GLN
2	H	495	GLN
2	H	616	GLN
2	H	664	HIS
2	H	692	ASN
2	H	704	GLN
3	F	80	HIS
3	F	95	ASN
3	L	175	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	F	201	5	34,34,34	1.85	6 (17%)	47,54,54	1.03	4 (8%)
4	GNP	C	201	5	34,34,34	1.84	6 (17%)	47,54,54	1.02	4 (8%)
4	GNP	I	201	5	34,34,34	1.82	6 (17%)	47,54,54	1.04	4 (8%)
4	GNP	L	201	5	34,34,34	1.83	6 (17%)	47,54,54	1.01	4 (8%)

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	F	201	5	-	2/18/38/38	0/3/3/3
4	GNP	C	201	5	-	2/18/38/38	0/3/3/3
4	GNP	I	201	5	-	7/18/38/38	0/3/3/3
4	GNP	L	201	5	-	2/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	GNP	PA-O3A	-6.58	1.52	1.59
4	F	201	GNP	PA-O3A	-6.55	1.52	1.59
4	L	201	GNP	PA-O3A	-6.47	1.52	1.59
4	I	201	GNP	PA-O3A	-6.41	1.52	1.59
4	C	201	GNP	PB-O3A	-5.30	1.52	1.59
4	F	201	GNP	PB-O3A	-5.29	1.52	1.59
4	L	201	GNP	PB-O3A	-5.24	1.52	1.59
4	I	201	GNP	PB-O3A	-5.16	1.52	1.59
4	F	201	GNP	PG-O1G	3.48	1.51	1.46
4	I	201	GNP	PG-O1G	3.45	1.51	1.46
4	L	201	GNP	PG-O1G	3.43	1.51	1.46
4	C	201	GNP	PG-O1G	3.41	1.51	1.46
4	I	201	GNP	PB-O2B	-3.14	1.48	1.56
4	C	201	GNP	PB-O2B	-3.13	1.48	1.56
4	F	201	GNP	PB-O2B	-3.13	1.48	1.56
4	L	201	GNP	PB-O2B	-3.10	1.48	1.56
4	L	201	GNP	PG-O3G	-2.05	1.51	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	201	GNP	PG-O3G	-2.04	1.51	1.56
4	C	201	GNP	PG-O3G	-2.04	1.51	1.56
4	L	201	GNP	PG-O2G	-2.01	1.51	1.56
4	C	201	GNP	PG-O2G	-2.01	1.51	1.56
4	F	201	GNP	PG-O2G	-2.01	1.51	1.56
4	F	201	GNP	PG-O3G	-2.00	1.51	1.56
4	I	201	GNP	PG-O2G	-2.00	1.51	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	GNP	O2B-PB-O1B	3.86	118.14	109.87
4	C	201	GNP	O2B-PB-O1B	3.80	118.01	109.87
4	L	201	GNP	O2B-PB-O1B	3.79	118.00	109.87
4	I	201	GNP	O2B-PB-O1B	3.75	117.92	109.87
4	I	201	GNP	O3G-PG-O1G	-3.34	105.08	113.45
4	C	201	GNP	O3G-PG-O1G	-3.34	105.08	113.45
4	F	201	GNP	O3G-PG-O1G	-3.32	105.14	113.45
4	L	201	GNP	O3G-PG-O1G	-3.29	105.21	113.45
4	C	201	GNP	O2G-PG-O3G	3.07	115.84	107.59
4	L	201	GNP	O2G-PG-O3G	3.06	115.81	107.59
4	F	201	GNP	O2G-PG-O3G	3.06	115.80	107.59
4	I	201	GNP	O2G-PG-O3G	3.05	115.79	107.59
4	F	201	GNP	O1G-PG-N3B	-2.27	108.42	111.77
4	I	201	GNP	O1G-PG-N3B	-2.22	108.50	111.77
4	L	201	GNP	O1G-PG-N3B	-2.14	108.62	111.77
4	C	201	GNP	O1G-PG-N3B	-2.07	108.73	111.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	GNP	PB-N3B-PG-O1G
4	F	201	GNP	PG-N3B-PB-O1B
4	L	201	GNP	PB-N3B-PG-O1G
4	L	201	GNP	PG-N3B-PB-O1B
4	C	201	GNP	PB-N3B-PG-O1G
4	C	201	GNP	PG-N3B-PB-O1B
4	I	201	GNP	PB-N3B-PG-O1G
4	I	201	GNP	PG-N3B-PB-O1B
4	I	201	GNP	PG-N3B-PB-O3A
4	I	201	GNP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	201	GNP	C5'-O5'-PA-O3A
4	I	201	GNP	C5'-O5'-PA-O2A
4	I	201	GNP	PA-O3A-PB-O1B

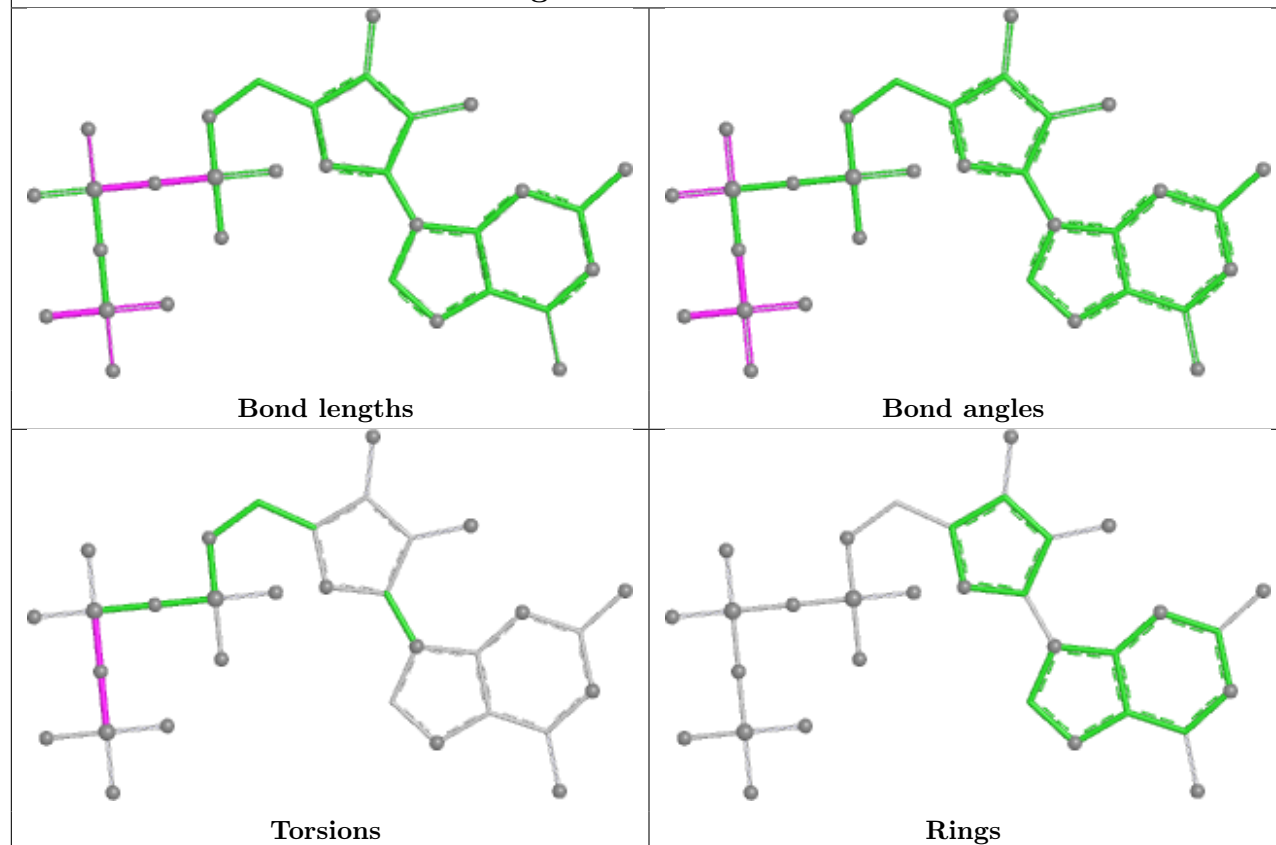
There are no ring outliers.

2 monomers are involved in 2 short contacts:

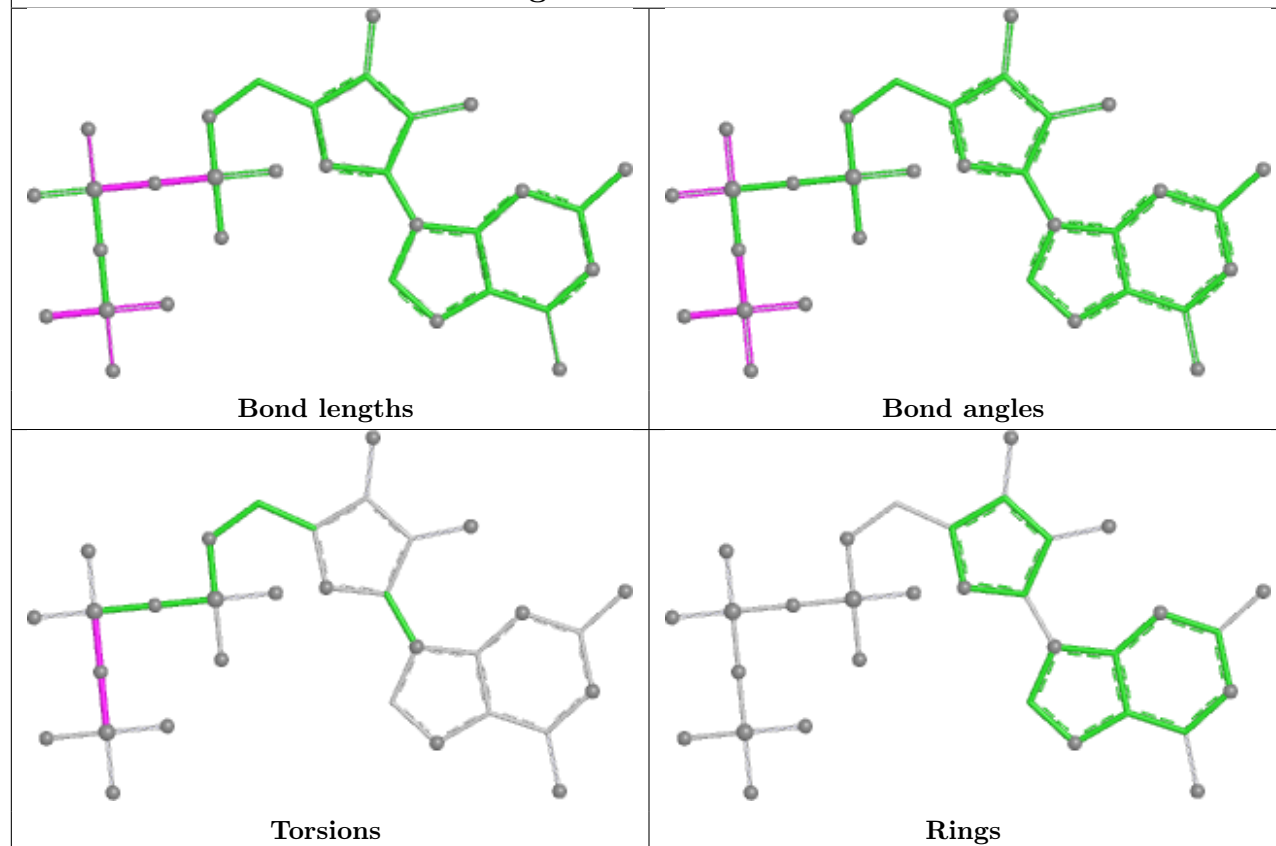
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	GNP	1	0
4	I	201	GNP	1	0

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 than 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.

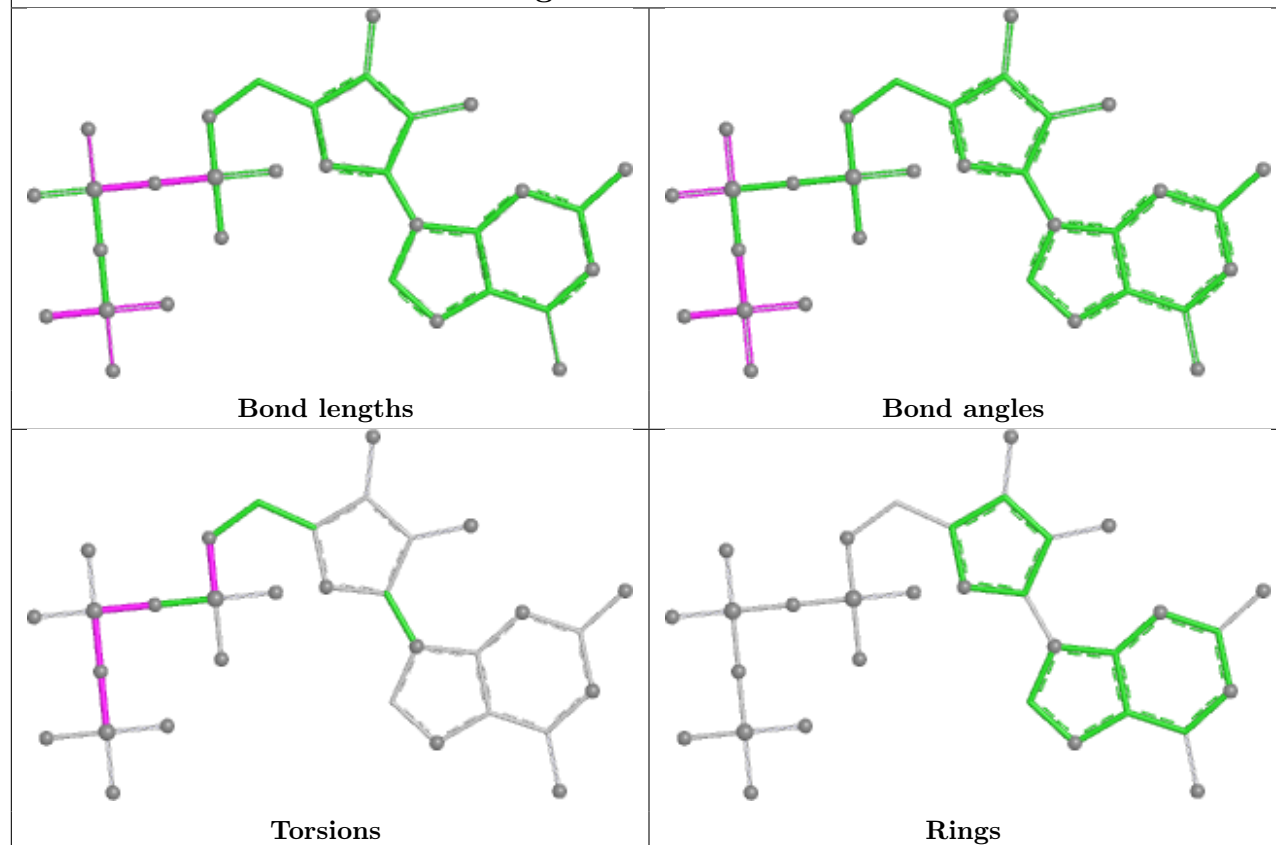
Ligand GNP F 201



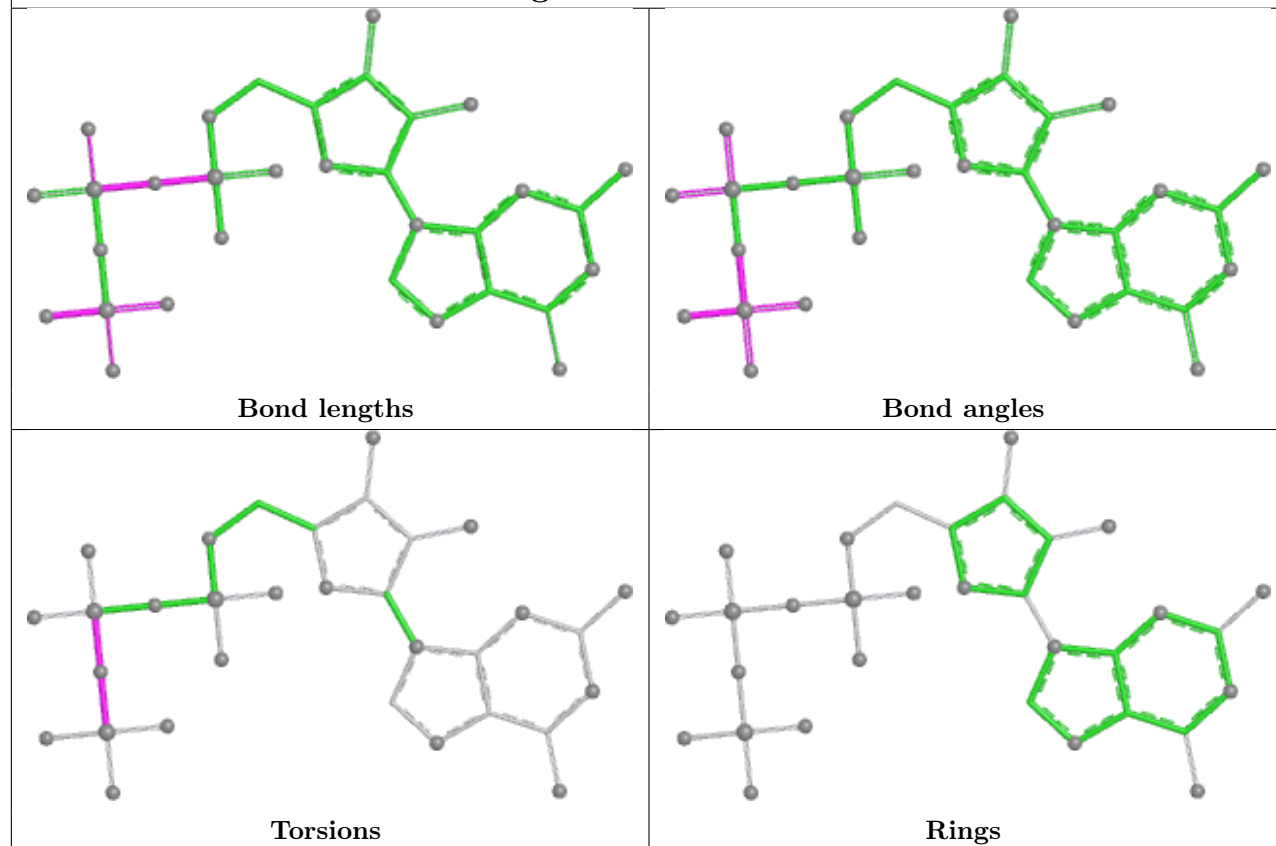
Ligand GNP C 201



Ligand GNP I 201



Ligand GNP L 201



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	226/368 (61%)	0.66	20 (8%) 15 14	63, 102, 153, 199	0
1	D	171/368 (46%)	0.79	24 (14%) 6 7	58, 103, 174, 290	0
1	G	211/368 (57%)	0.69	19 (9%) 15 13	61, 108, 176, 203	0
1	J	158/368 (42%)	0.83	23 (14%) 6 6	62, 93, 159, 233	0
2	B	507/739 (68%)	0.50	40 (7%) 18 15	24, 102, 149, 204	0
2	E	557/739 (75%)	0.51	52 (9%) 14 13	53, 90, 147, 273	0
2	H	338/739 (45%)	0.82	42 (12%) 8 8	86, 133, 179, 213	0
2	K	593/739 (80%)	0.39	47 (7%) 18 15	53, 79, 143, 231	0
3	C	134/175 (76%)	0.52	10 (7%) 20 16	79, 123, 176, 197	0
3	F	146/175 (83%)	0.66	13 (8%) 15 13	76, 118, 157, 185	0
3	I	86/175 (49%)	0.64	5 (5%) 29 21	92, 127, 179, 204	0
3	L	139/175 (79%)	0.87	15 (10%) 11 10	24, 115, 147, 174	0
All	All	3266/5128 (63%)	0.60	310 (9%) 14 13	24, 103, 163, 290	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	ALA	6.4
1	A	105	SER	6.3
1	A	104	GLY	6.2
1	G	243	GLU	5.6
1	G	42	GLY	5.4
2	E	669	GLU	5.0
2	K	566	ALA	4.9
2	H	202	VAL	4.9
2	H	501	SER	4.8
2	B	97	ILE	4.7
2	B	456	LEU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	267	SER	4.5
2	H	610	CYS	4.5
2	K	250	GLU	4.4
1	J	118	ILE	4.4
1	A	158	SER	4.4
1	G	106	ALA	4.3
2	B	686	GLY	4.3
1	A	103	LEU	4.2
1	J	106	ALA	4.2
1	J	136	GLY	4.2
2	K	642	LEU	4.2
2	B	666	TRP	4.2
2	K	456	LEU	4.1
2	E	232	GLY	4.0
2	K	136	SER	4.0
3	I	93	ASP	4.0
2	H	260	HIS	4.0
1	J	145	PHE	3.9
2	K	187	LEU	3.9
3	F	121	TRP	3.8
3	F	63	PHE	3.8
2	K	135	ILE	3.7
1	D	82	PRO	3.7
2	E	139	SER	3.7
2	K	427	ILE	3.7
2	K	36	ASP	3.6
2	E	2	LEU	3.6
2	H	663	ASN	3.6
2	E	118	ASP	3.6
2	B	147	ASP	3.5
2	K	557	TRP	3.5
2	K	219	ASN	3.5
2	E	458	GLN	3.5
2	H	553	THR	3.5
3	F	65	VAL	3.5
2	H	659	ILE	3.5
2	E	91	PHE	3.5
2	H	196	THR	3.5
2	E	214	ASP	3.4
2	B	250	GLU	3.4
1	G	117	GLY	3.4
2	K	451	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	609	VAL	3.4
2	E	116	PHE	3.4
2	B	494	GLU	3.4
2	K	458	GLN	3.4
2	B	501	SER	3.4
1	D	104	GLY	3.3
1	A	63	PHE	3.3
1	A	118	ILE	3.3
3	L	106	VAL	3.3
1	J	107	LYS	3.2
2	E	628	ASP	3.2
2	K	129	HIS	3.2
1	G	242	PRO	3.2
1	A	121	MET	3.2
2	H	625	ILE	3.2
2	H	686	GLY	3.2
2	K	91	PHE	3.2
3	L	96	ASP	3.2
2	E	316	GLU	3.2
2	K	439	LEU	3.1
2	B	226	PHE	3.1
2	B	35	PRO	3.1
3	F	74	ILE	3.1
1	J	166	HIS	3.1
2	K	459	LYS	3.1
1	J	105	SER	3.1
2	K	707	ASP	3.1
2	K	334	LEU	3.1
2	K	20	HIS	3.1
2	B	238	ALA	3.1
2	H	500	ARG	3.1
2	H	535	LEU	3.0
1	J	135	SER	3.0
2	K	316	GLU	3.0
1	J	157	TRP	3.0
1	J	121	MET	3.0
2	E	638	SER	3.0
2	E	459	LYS	3.0
1	D	139	VAL	3.0
1	D	157	TRP	3.0
1	J	112	ILE	3.0
2	B	343	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	654	ASP	3.0
1	D	132	THR	3.0
2	E	136	SER	2.9
1	D	129	VAL	2.9
1	A	230	ILE	2.9
1	D	121	MET	2.9
2	H	502	LYS	2.9
2	E	644	SER	2.9
2	B	146	TYR	2.9
2	E	687	ILE	2.9
2	H	486	GLU	2.9
2	B	140	TRP	2.9
1	J	153	SER	2.9
1	D	81	SER	2.9
2	K	532	SER	2.9
1	G	199	ILE	2.9
2	H	275	LEU	2.9
3	L	124	PHE	2.9
1	A	229	LEU	2.9
1	J	96	LEU	2.9
3	C	74	ILE	2.9
2	B	613	ASN	2.8
3	L	99	ARG	2.8
3	L	167	TYR	2.8
1	A	2	SER	2.8
1	J	158	SER	2.8
1	D	257	VAL	2.8
1	J	117	GLY	2.8
2	B	427	ILE	2.8
1	D	92	THR	2.8
2	B	234	LEU	2.8
3	L	122	LEU	2.8
2	K	132	VAL	2.8
1	G	103	LEU	2.8
2	B	3	SER	2.8
2	E	722	PHE	2.7
2	B	109	ALA	2.7
2	B	96	GLY	2.7
2	K	123	TRP	2.7
2	K	684	ASP	2.7
2	H	344	GLN	2.7
2	H	701	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	105	SER	2.7
2	E	349	SER	2.7
2	E	383	GLU	2.7
2	H	589	GLY	2.7
3	L	127	LYS	2.7
2	E	642	LEU	2.7
1	A	116	LYS	2.6
1	G	76	THR	2.6
1	J	7	LEU	2.6
2	B	10	VAL	2.6
3	L	67	ASP	2.6
3	C	41	GLU	2.6
2	H	272	VAL	2.6
2	K	572	HIS	2.6
2	E	36	ASP	2.6
2	E	437	LEU	2.6
2	B	535	LEU	2.6
3	F	142	LYS	2.6
2	K	38	ILE	2.6
2	H	490	ILE	2.6
1	A	135	SER	2.6
1	A	153	SER	2.6
2	B	108	PHE	2.6
2	B	139	SER	2.6
2	H	324	ASN	2.6
2	K	115	LEU	2.6
2	K	158	VAL	2.6
1	A	155	THR	2.6
2	K	564	PHE	2.5
3	F	76	SER	2.5
1	A	245	VAL	2.5
1	G	235	ASN	2.5
2	K	560	GLU	2.5
1	A	157	TRP	2.5
1	G	158	SER	2.5
2	E	455	GLN	2.5
2	B	21	GLN	2.5
3	F	95	ASN	2.5
3	L	133	ALA	2.5
3	L	134	MET	2.5
2	E	463	PRO	2.5
2	H	694	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	493	TRP	2.5
2	E	433	LEU	2.5
1	A	210	ILE	2.5
2	K	112	ILE	2.5
2	K	687	ILE	2.5
1	D	131	THR	2.5
2	H	721	THR	2.5
3	C	45	THR	2.5
1	G	247	ALA	2.4
1	D	158	SER	2.4
3	F	132	GLU	2.4
1	G	215	PHE	2.4
3	I	90	PHE	2.4
2	B	98	ASP	2.4
1	A	46	LYS	2.4
3	C	63	PHE	2.4
2	H	255	LEU	2.4
2	B	263	ASN	2.4
2	E	26	VAL	2.4
2	H	400	MET	2.4
2	E	532	SER	2.4
2	B	654	ASP	2.4
2	H	611	ALA	2.4
2	K	502	LYS	2.4
2	K	506	MET	2.4
2	B	344	GLN	2.4
3	F	174	SER	2.4
2	K	440	ASP	2.4
1	G	188	SER	2.4
2	E	482	LYS	2.3
3	I	34	LEU	2.3
1	G	72	GLU	2.3
2	E	152	VAL	2.3
1	J	92	THR	2.3
1	D	93	SER	2.3
3	L	98	SER	2.3
2	B	91	PHE	2.3
1	G	238	PRO	2.3
3	L	82	TYR	2.3
2	K	333	PHE	2.3
2	E	713	PHE	2.3
2	K	188	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	39	VAL	2.3
2	E	457	GLU	2.3
2	K	151	ILE	2.3
3	F	157	ALA	2.3
3	C	87	GLY	2.3
2	B	433	LEU	2.3
2	E	460	SER	2.3
3	I	82	TYR	2.3
2	E	236	ASP	2.3
2	K	457	GLU	2.2
2	K	461	ALA	2.2
2	E	222	GLU	2.2
3	C	49	ILE	2.2
1	D	127	PHE	2.2
1	J	38	ASN	2.2
2	E	147	ASP	2.2
2	B	24	ALA	2.2
3	L	160	ALA	2.2
2	H	192	ILE	2.2
1	G	41	ALA	2.2
2	B	239	ASN	2.2
2	H	658	LYS	2.2
1	J	140	ASP	2.2
2	E	666	TRP	2.2
1	G	216	VAL	2.1
1	D	152	THR	2.1
2	H	201	ILE	2.1
3	L	49	ILE	2.1
1	D	103	LEU	2.1
2	K	460	SER	2.1
2	B	460	SER	2.1
2	H	475	SER	2.1
2	H	586	LYS	2.1
2	E	22	ARG	2.1
2	K	450	ASN	2.1
2	K	462	ASP	2.1
1	G	157	TRP	2.1
3	F	153	TRP	2.1
2	E	490	ILE	2.1
2	B	548	TYR	2.1
2	E	9	GLU	2.1
3	F	169	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	123	VAL	2.1
1	D	234	HIS	2.1
1	J	134	ILE	2.1
2	E	334	LEU	2.1
2	E	602	LEU	2.1
1	J	119	ARG	2.1
1	D	264	ALA	2.1
2	E	121	GLN	2.1
2	H	199	SER	2.1
2	E	268	ASN	2.1
2	E	14	VAL	2.1
3	F	23	VAL	2.1
3	C	88	VAL	2.1
2	E	537	GLU	2.1
2	K	464	ASN	2.1
1	G	147	LEU	2.1
2	E	456	LEU	2.1
2	B	665	ARG	2.1
2	H	364	ARG	2.1
2	H	375	GLU	2.1
1	D	40	LYS	2.0
2	B	424	ILE	2.0
3	L	151	ARG	2.0
2	H	256	ASP	2.0
2	E	661	CYS	2.0
2	H	695	ALA	2.0
2	E	4	GLN	2.0
3	C	47	PRO	2.0
1	D	107	LYS	2.0
2	H	253	VAL	2.0
1	J	137	LEU	2.0
2	H	711	LEU	2.0
1	D	50	SER	2.0
2	K	174	SER	2.0
2	E	3	SER	2.0
2	E	122	ILE	2.0
2	B	138	SER	2.0
2	K	342	HIS	2.0
2	E	193	TRP	2.0
2	H	622	HIS	2.0
1	A	169	THR	2.0
2	B	425	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	157	ALA	2.0
2	B	440	ASP	2.0
2	E	120	PRO	2.0
1	D	115	ARG	2.0
3	C	46	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

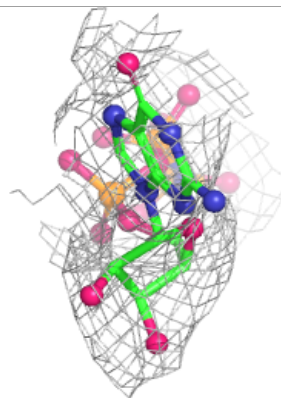
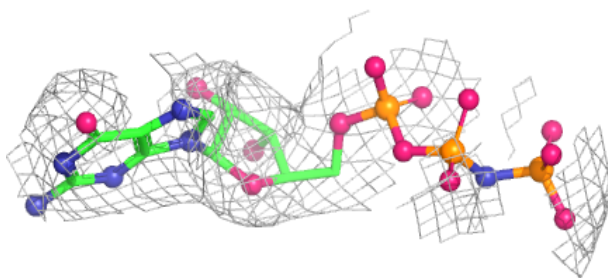
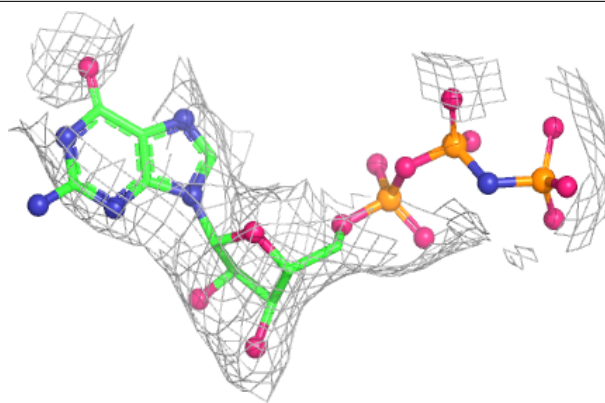
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GNP	F	201	32/32	0.90	0.10	98,129,153,381	0
4	GNP	C	201	32/32	0.91	0.08	53,82,103,108	0
4	GNP	L	201	32/32	0.92	0.10	86,112,138,201	0
5	MG	C	202	1/1	0.92	0.09	60,60,60,60	0
5	MG	I	202	1/1	0.94	0.06	83,83,83,83	0
4	GNP	I	201	32/32	0.95	0.06	50,94,122,244	0
5	MG	L	202	1/1	0.96	0.11	51,51,51,51	0
5	MG	F	202	1/1	0.97	0.12	59,59,59,59	0

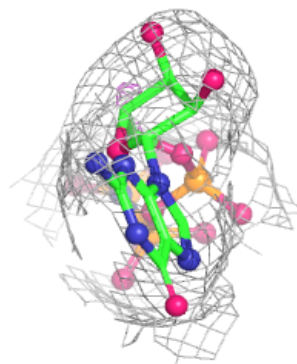
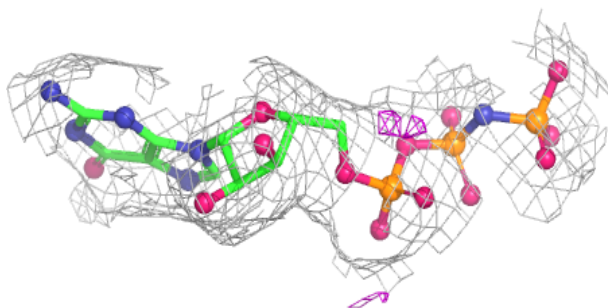
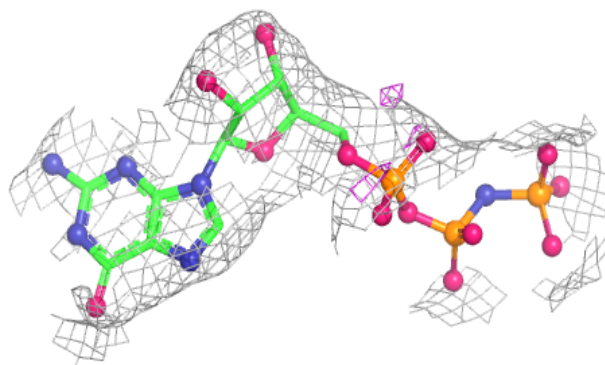
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP F 201:

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

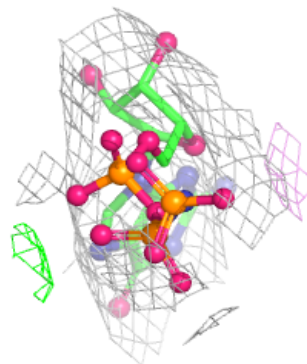
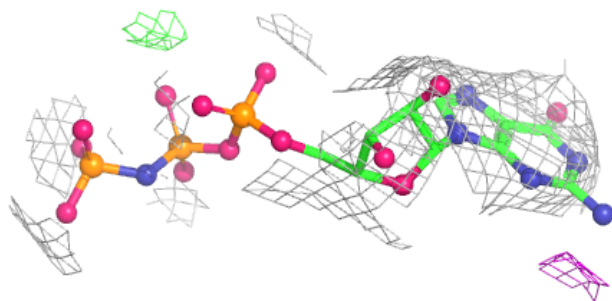
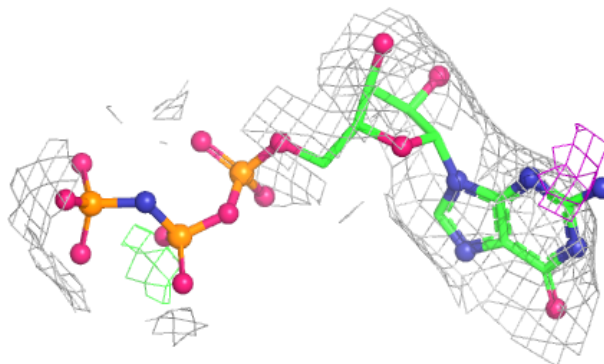
**Electron density around GNP C 201:**

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

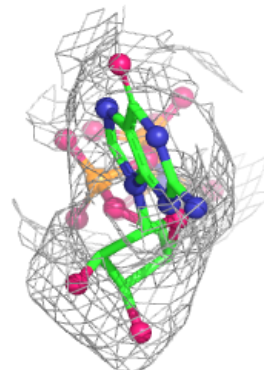
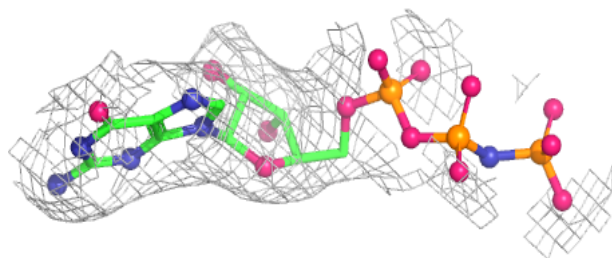
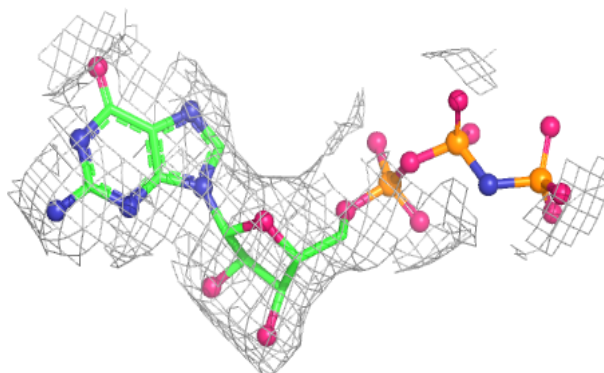


Electron density around GNP L 201:

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

**Electron density around GNP I 201:**

$2mF_o-DF_c$ (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.