Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 01:12 AM EST

PDB ID	:	4M8N
Title	:	Crystal Structure of PlexinC1/Rap1B Complex
Authors	:	Pascoe, H.G.; Wang, Y.; Brautigam, C.A.; He, H.; Zhang, X.
Deposited on	:	2013-08-13
Resolution	:	3.29 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:

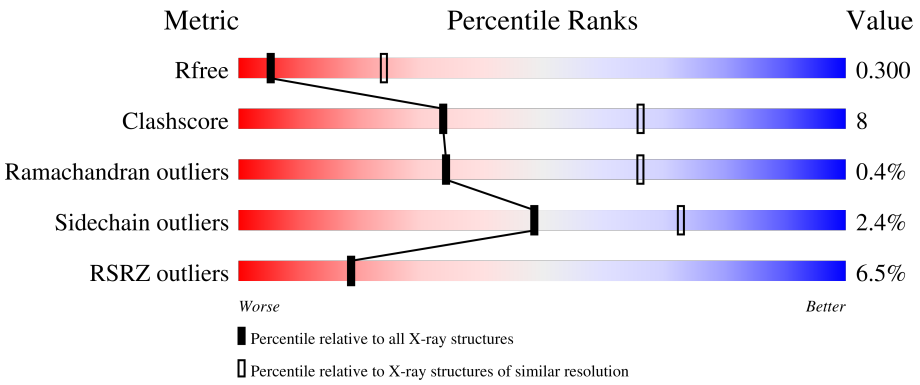
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	599	3%, 78%, 17%, •
1	B	599	5%, 71%, 22%, • 5%
1	C	599	3%, 74%, 18%, • 7%
1	D	599	7%, 72%, 20%, • 7%
2	E	199	6%, 70%, 14%, • 16%

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Mol	Chain	Length	Quality of chain
2	F	199	9% 64% 18% • 17%
2	G	199	16% 66% 18% 16%
2	H	199	12% 69% 15% 16%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22228 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 PlexinC1 Intracellular Region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	574	4356	2818	717	801	20	0	0	0
1	B	571	4262	2756	702	784	20	0	0	0
1	C	560	4218	2719	699	780	20	0	0	0
1	D	560	4230	2738	695	777	20	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	549	GLY	-	expression tag	UNP Q5RGW1
A	550	GLY	-	expression tag	UNP Q5RGW1
A	551	SER	-	expression tag	UNP Q5RGW1
B	549	GLY	-	expression tag	UNP Q5RGW1
B	550	GLY	-	expression tag	UNP Q5RGW1
B	551	SER	-	expression tag	UNP Q5RGW1
C	549	GLY	-	expression tag	UNP Q5RGW1
C	550	GLY	-	expression tag	UNP Q5RGW1
C	551	SER	-	expression tag	UNP Q5RGW1
D	549	GLY	-	expression tag	UNP Q5RGW1
D	550	GLY	-	expression tag	UNP Q5RGW1
D	551	SER	-	expression tag	UNP Q5RGW1

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	168	1277	805	215	250	7	0	0	0
2	F	166	1262	797	213	245	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	168	1258	793	211	247	7	0	0	0
			Total	C	N	O	S			
2	H	167	1223	779	206	232	6	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P61224
E	-1	PRO	-	expression tag	UNP P61224
E	0	HIS	-	expression tag	UNP P61224
E	167	SER	-	expression tag	UNP P61224
E	168	GLY	-	expression tag	UNP P61224
E	169	GLY	-	expression tag	UNP P61224
E	170	SER	-	expression tag	UNP P61224
E	171	GLY	-	expression tag	UNP P61224
E	172	SER	-	expression tag	UNP P61224
E	173	GLY	-	expression tag	UNP P61224
E	174	SER	-	expression tag	UNP P61224
E	175	SER	-	expression tag	UNP P61224
E	176	GLY	-	expression tag	UNP P61224
E	177	GLY	-	expression tag	UNP P61224
E	178	SER	-	expression tag	UNP P61224
E	179	GLY	-	expression tag	UNP P61224
E	180	SER	-	expression tag	UNP P61224
E	181	GLY	-	expression tag	UNP P61224
E	182	GLY	-	expression tag	UNP P61224
E	183	GLY	-	expression tag	UNP P61224
E	184	SER	-	expression tag	UNP P61224
E	185	GLY	-	expression tag	UNP P61224
E	186	SER	-	expression tag	UNP P61224
E	187	GLY	-	expression tag	UNP P61224
E	188	SER	-	expression tag	UNP P61224
E	189	SER	-	expression tag	UNP P61224
E	190	GLY	-	expression tag	UNP P61224
E	191	LEU	-	expression tag	UNP P61224
E	192	PRO	-	expression tag	UNP P61224
E	193	GLU	-	expression tag	UNP P61224
E	194	THR	-	expression tag	UNP P61224
E	195	GLY	-	expression tag	UNP P61224
E	196	GLY	-	expression tag	UNP P61224
F	-2	GLY	-	expression tag	UNP P61224

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	PRO	-	expression tag	UNP P61224
F	0	HIS	-	expression tag	UNP P61224
F	167	SER	-	expression tag	UNP P61224
F	168	GLY	-	expression tag	UNP P61224
F	169	GLY	-	expression tag	UNP P61224
F	170	SER	-	expression tag	UNP P61224
F	171	GLY	-	expression tag	UNP P61224
F	172	SER	-	expression tag	UNP P61224
F	173	GLY	-	expression tag	UNP P61224
F	174	SER	-	expression tag	UNP P61224
F	175	SER	-	expression tag	UNP P61224
F	176	GLY	-	expression tag	UNP P61224
F	177	GLY	-	expression tag	UNP P61224
F	178	SER	-	expression tag	UNP P61224
F	179	GLY	-	expression tag	UNP P61224
F	180	SER	-	expression tag	UNP P61224
F	181	GLY	-	expression tag	UNP P61224
F	182	GLY	-	expression tag	UNP P61224
F	183	GLY	-	expression tag	UNP P61224
F	184	SER	-	expression tag	UNP P61224
F	185	GLY	-	expression tag	UNP P61224
F	186	SER	-	expression tag	UNP P61224
F	187	GLY	-	expression tag	UNP P61224
F	188	SER	-	expression tag	UNP P61224
F	189	SER	-	expression tag	UNP P61224
F	190	GLY	-	expression tag	UNP P61224
F	191	LEU	-	expression tag	UNP P61224
F	192	PRO	-	expression tag	UNP P61224
F	193	GLU	-	expression tag	UNP P61224
F	194	THR	-	expression tag	UNP P61224
F	195	GLY	-	expression tag	UNP P61224
F	196	GLY	-	expression tag	UNP P61224
G	-2	GLY	-	expression tag	UNP P61224
G	-1	PRO	-	expression tag	UNP P61224
G	0	HIS	-	expression tag	UNP P61224
G	167	SER	-	expression tag	UNP P61224
G	168	GLY	-	expression tag	UNP P61224
G	169	GLY	-	expression tag	UNP P61224
G	170	SER	-	expression tag	UNP P61224
G	171	GLY	-	expression tag	UNP P61224
G	172	SER	-	expression tag	UNP P61224
G	173	GLY	-	expression tag	UNP P61224

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Chain	Residue	Modelled	Actual	Comment	Reference
G	174	SER	-	expression tag	UNP P61224
G	175	SER	-	expression tag	UNP P61224
G	176	GLY	-	expression tag	UNP P61224
G	177	GLY	-	expression tag	UNP P61224
G	178	SER	-	expression tag	UNP P61224
G	179	GLY	-	expression tag	UNP P61224
G	180	SER	-	expression tag	UNP P61224
G	181	GLY	-	expression tag	UNP P61224
G	182	GLY	-	expression tag	UNP P61224
G	183	GLY	-	expression tag	UNP P61224
G	184	SER	-	expression tag	UNP P61224
G	185	GLY	-	expression tag	UNP P61224
G	186	SER	-	expression tag	UNP P61224
G	187	GLY	-	expression tag	UNP P61224
G	188	SER	-	expression tag	UNP P61224
G	189	SER	-	expression tag	UNP P61224
G	190	GLY	-	expression tag	UNP P61224
G	191	LEU	-	expression tag	UNP P61224
G	192	PRO	-	expression tag	UNP P61224
G	193	GLU	-	expression tag	UNP P61224
G	194	THR	-	expression tag	UNP P61224
G	195	GLY	-	expression tag	UNP P61224
G	196	GLY	-	expression tag	UNP P61224
H	-2	GLY	-	expression tag	UNP P61224
H	-1	PRO	-	expression tag	UNP P61224
H	0	HIS	-	expression tag	UNP P61224
H	167	SER	-	expression tag	UNP P61224
H	168	GLY	-	expression tag	UNP P61224
H	169	GLY	-	expression tag	UNP P61224
H	170	SER	-	expression tag	UNP P61224
H	171	GLY	-	expression tag	UNP P61224
H	172	SER	-	expression tag	UNP P61224
H	173	GLY	-	expression tag	UNP P61224
H	174	SER	-	expression tag	UNP P61224
H	175	SER	-	expression tag	UNP P61224
H	176	GLY	-	expression tag	UNP P61224
H	177	GLY	-	expression tag	UNP P61224
H	178	SER	-	expression tag	UNP P61224
H	179	GLY	-	expression tag	UNP P61224
H	180	SER	-	expression tag	UNP P61224
H	181	GLY	-	expression tag	UNP P61224
H	182	GLY	-	expression tag	UNP P61224

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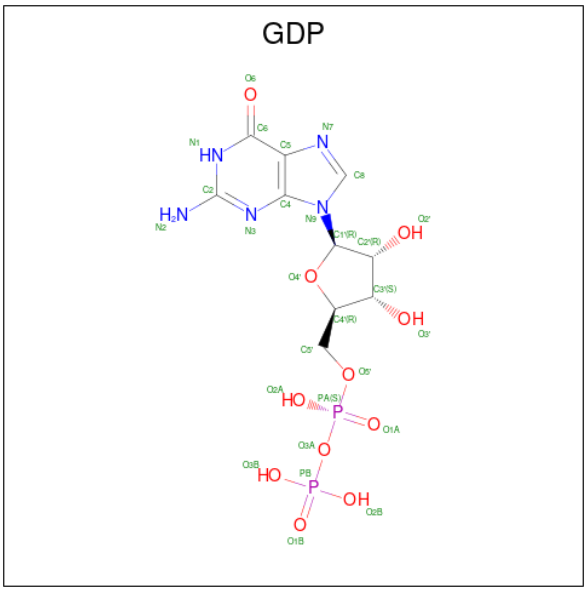
Chain	Residue	Modelled	Actual	Comment	Reference
H	183	GLY	-	expression tag	UNP P61224
H	184	SER	-	expression tag	UNP P61224
H	185	GLY	-	expression tag	UNP P61224
H	186	SER	-	expression tag	UNP P61224
H	187	GLY	-	expression tag	UNP P61224
H	188	SER	-	expression tag	UNP P61224
H	189	SER	-	expression tag	UNP P61224
H	190	GLY	-	expression tag	UNP P61224
H	191	LEU	-	expression tag	UNP P61224
H	192	PRO	-	expression tag	UNP P61224
H	193	GLU	-	expression tag	UNP P61224
H	194	THR	-	expression tag	UNP P61224
H	195	GLY	-	expression tag	UNP P61224
H	196	GLY	-	expression tag	UNP P61224

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

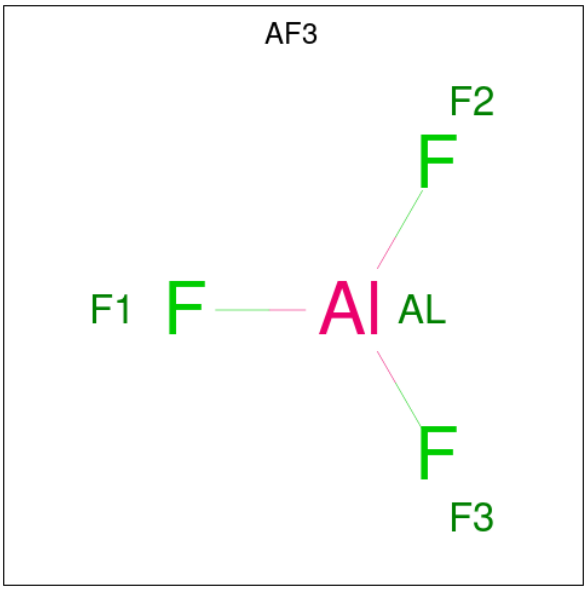
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	E	1	1	1	0	0
3	F	1	1	1	0	0
3	G	1	1	1	0	0
3	H	1	1	1	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	E	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
4	F	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
4	G	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
4	H	1	28	10	5	11	2	0	0

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
5	E	1	4	1	3	0	0
5	F	1	4	1	3	0	0
5	G	1	4	1	3	0	0
5	H	1	4	1	3	0	0

- Molecule 6 is water.

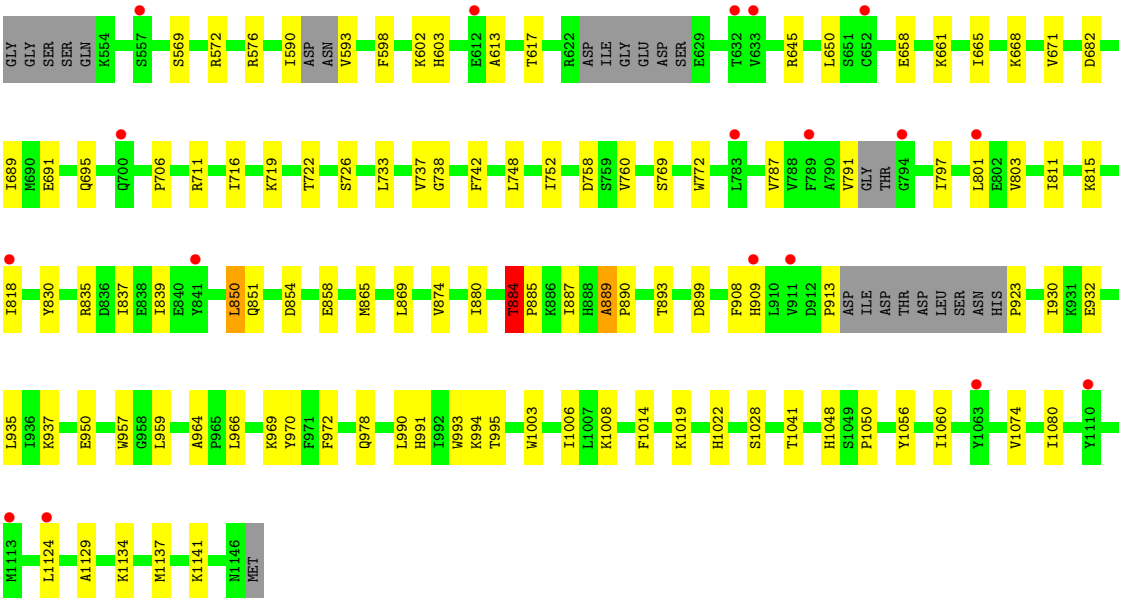
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	4	4	4	0	0
6	B	1	1	1	0	0
6	C	3	3	3	0	0
6	D	1	1	1	0	0
6	H	1	1	1	0	0

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.

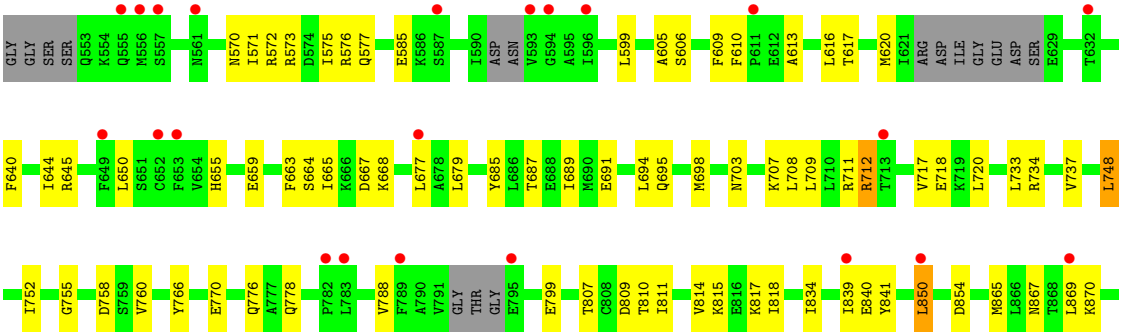
• Molecule 1: PlexinC1 Intracellular Region

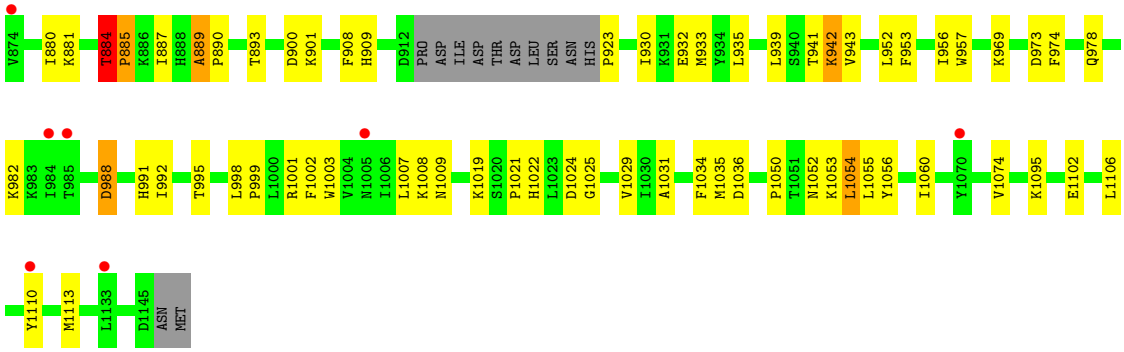
Chain A:



• Molecule 1: PlexinC1 Intracellular Region

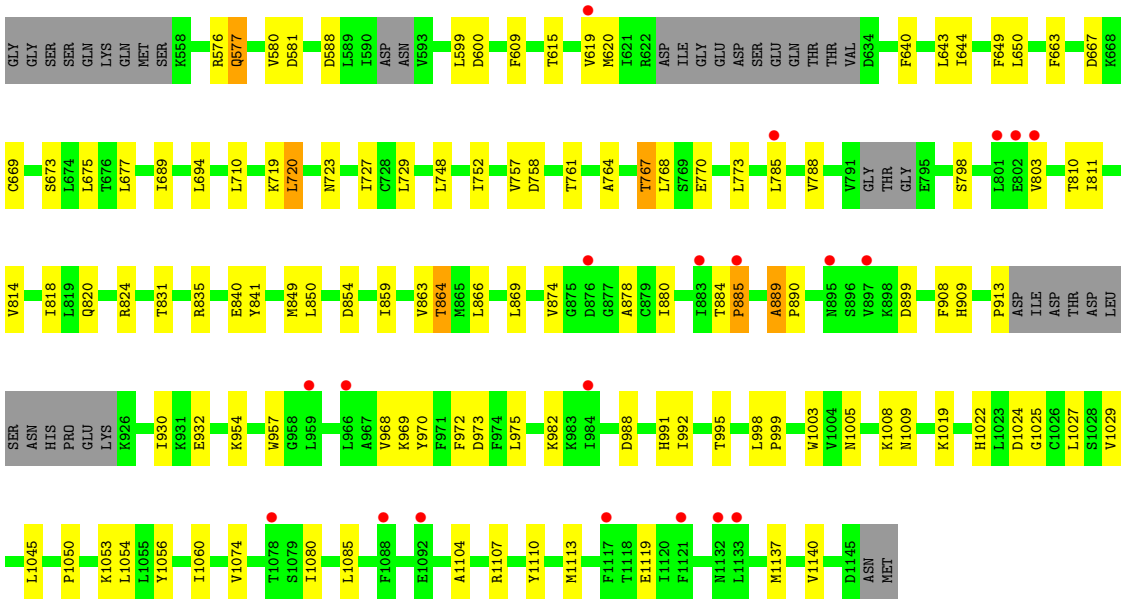
Chain B:





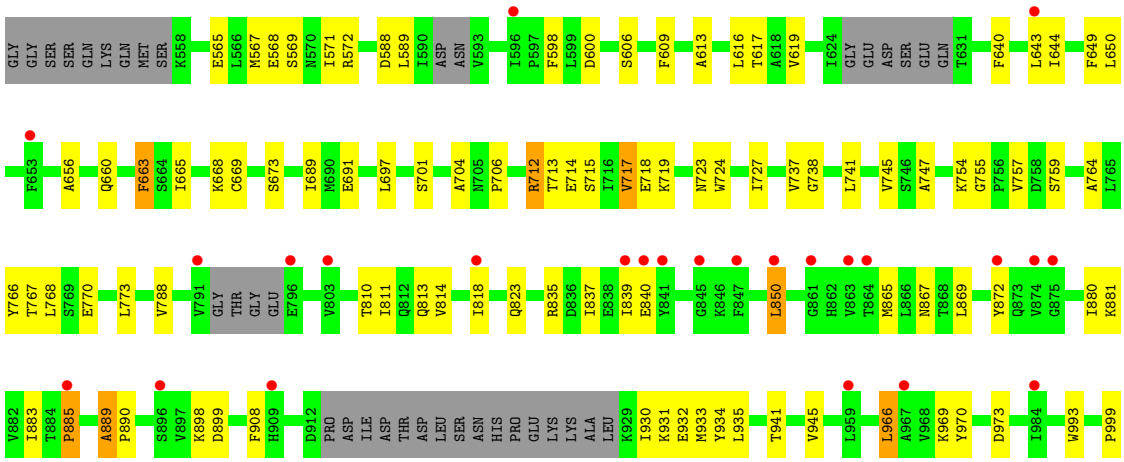
• Molecule 1: PlexinC1 Intracellular Region

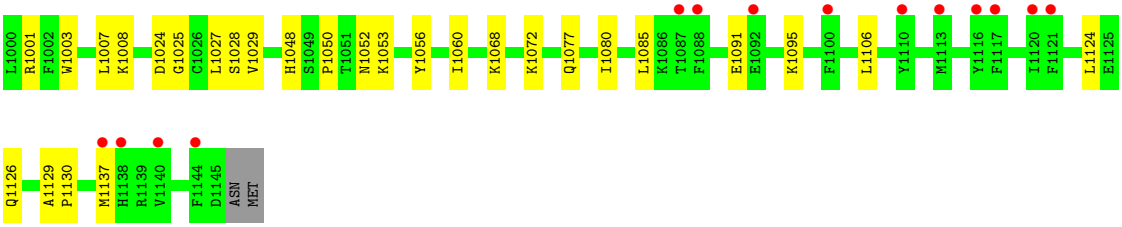
Chain C:



• Molecule 1: PlexinC1 Intracellular Region

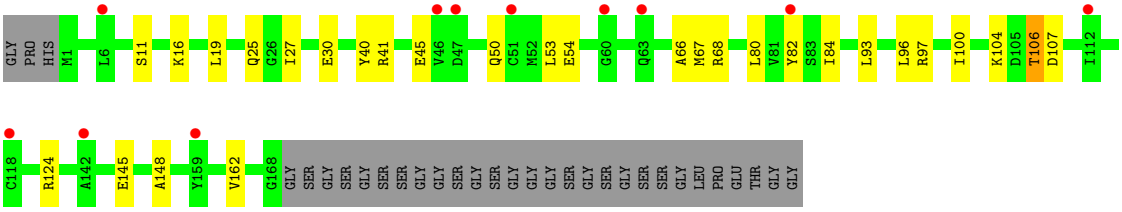
Chain D:





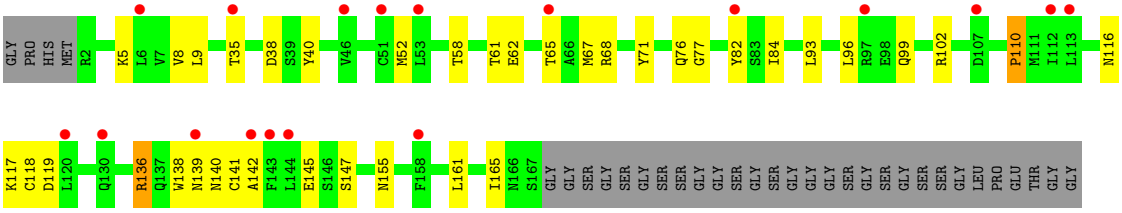
• Molecule 2: Ras-related protein Rap-1b

Chain E:



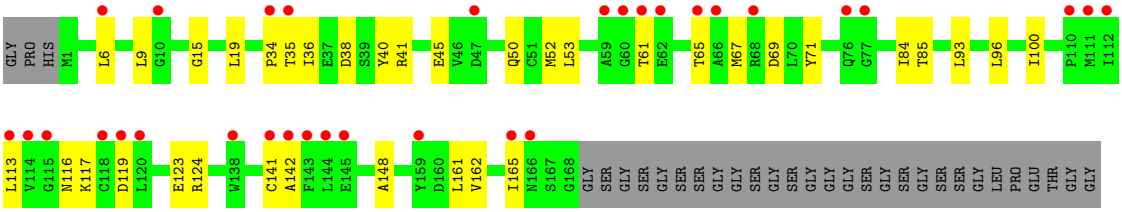
• Molecule 2: Ras-related protein Rap-1b

Chain F:



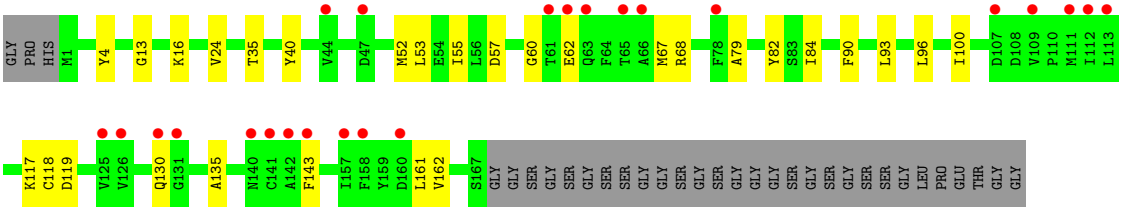
• Molecule 2: Ras-related protein Rap-1b

Chain G:



• Molecule 2: Ras-related protein Rap-1b

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.28Å 84.73Å 138.75Å 91.09° 95.15° 90.32°	Depositor
Resolution (Å)	41.05 – 3.29 42.36 – 3.29	Depositor EDS
% Data completeness (in resolution range)	90.2 (41.05-3.29) 90.3 (42.36-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.243 , 0.299 0.243 , 0.300	Depositor DCC
R_{free} test set	1804 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å^2)	111.8	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 91.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h,k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22228	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.70% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, MG, GDP

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	0.28	0/4437	0.45	4/6023 (0.1%)
1	B	0.28	0/4341	0.45	3/5905 (0.1%)
1	C	0.26	0/4298	0.43	3/5845 (0.1%)
1	D	0.26	0/4312	0.41	2/5861 (0.0%)
2	E	0.25	0/1293	0.40	0/1750
2	F	0.25	0/1278	0.41	0/1730
2	G	0.24	0/1274	0.39	0/1729
2	H	0.25	0/1239	0.41	0/1682
All	All	0.26	0/22472	0.43	12/30525 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	890	PRO	N-CA-CB	6.15	110.68	103.30
1	C	890	PRO	N-CA-CB	6.08	110.59	103.30
1	B	890	PRO	N-CA-CB	6.04	110.55	103.30
1	C	913	PRO	N-CA-CB	5.98	110.48	103.30
1	B	923	PRO	N-CA-CB	5.98	110.47	103.30
1	A	913	PRO	N-CA-CB	5.94	110.43	103.30
1	A	923	PRO	N-CA-CB	5.93	110.42	103.30
1	A	890	PRO	N-CA-CB	5.92	110.41	103.30
1	A	885	PRO	N-CA-CB	5.90	110.38	103.30
1	B	885	PRO	N-CA-CB	5.88	110.35	103.30
1	C	885	PRO	N-CA-CB	5.81	110.27	103.30
1	D	885	PRO	N-CA-CB	5.74	110.19	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4356	0	4143	58	0
1	B	4262	0	3980	95	0
1	C	4218	0	3952	71	0
1	D	4230	0	3971	79	0
2	E	1277	0	1229	16	0
2	F	1262	0	1212	27	0
2	G	1258	0	1188	22	0
2	H	1223	0	1153	22	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	E	28	0	12	0	0
4	F	28	0	12	3	0
4	G	28	0	12	2	0
4	H	28	0	12	5	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0
5	G	4	0	0	0	0
5	H	4	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
All	All	22228	0	20876	365	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 8.

All (365) 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:C:577:GLN:NE2	1:C:581:ASP:OD2	2.21	0.74
1:C:811:ILE:HD12	1:C:850:LEU:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:NH1	1:A:899:ASP:OD2	2.22	0.72
1:B:811:ILE:HD12	1:B:850:LEU:HD13	1.70	0.72
2:H:60:GLY:O	2:H:68:ARG:NH1	2.22	0.71
2:G:45:GLU:HA	2:G:50:GLN:HA	1.73	0.71
1:C:859:ILE:HG12	1:C:864:THR:HG23	1.72	0.71
1:A:691:GLU:OE2	1:A:970:TYR:OH	2.06	0.70
1:A:932:GLU:HA	1:A:935:LEU:HG	1.74	0.69
1:D:835:ARG:NH2	1:D:899:ASP:OD2	2.24	0.69
1:B:1110:TYR:HA	1:B:1113:MET:HB3	1.76	0.68
1:B:695:GLN:HG3	1:B:978:GLN:HE22	1.59	0.68
1:D:1091:GLU:HG2	1:D:1095:LYS:HD3	1.76	0.67
1:B:1095:LYS:HE3	1:D:1130:PRO:HG3	1.78	0.66
1:D:1008:LYS:NZ	1:D:1024:ASP:OD1	2.28	0.66
1:A:760:VAL:HG21	1:A:908:PHE:HA	1.75	0.66
1:B:576:ARG:NH2	1:C:770:GLU:OE2	2.28	0.66
1:A:811:ILE:HD12	1:A:850:LEU:HD13	1.78	0.66
1:B:841:TYR:HB2	1:B:850:LEU:HD23	1.78	0.65
2:H:82:TYR:HB3	2:H:93:LEU:HD11	1.79	0.65
1:D:932:GLU:HA	1:D:935:LEU:HD13	1.78	0.65
2:F:82:TYR:HB3	2:F:93:LEU:HD11	1.78	0.65
1:D:1050:PRO:HG2	1:D:1053:LYS:HB2	1.77	0.64
1:D:706:PRO:O	1:D:993:TRP:NE1	2.28	0.64
1:D:718:GLU:OE1	1:D:1001:ARG:NH1	2.31	0.64
1:A:803:VAL:HG11	1:A:818:ILE:HG22	1.80	0.64
1:C:885:PRO:HA	1:C:889:ALA:HB3	1.80	0.64
1:A:969:LYS:NZ	1:A:1074:VAL:O	2.24	0.64
1:B:809:ASP:OD2	1:B:817:LYS:NZ	2.22	0.64
1:D:650:LEU:HD23	1:D:689:ILE:HG12	1.79	0.64
1:B:570:ASN:OD1	1:B:573:ARG:NH2	2.30	0.63
2:E:106:THR:OG1	2:E:107:ASP:N	2.27	0.63
1:D:669:CYS:HA	1:D:719:LYS:HG2	1.80	0.63
1:A:811:ILE:HG22	1:A:815:LYS:HE3	1.81	0.63
1:B:885:PRO:HA	1:B:889:ALA:HB3	1.79	0.63
2:E:25:GLN:HB2	2:E:27:ILE:HG22	1.81	0.63
2:H:40:TYR:HB2	2:H:55:ILE:HB	1.79	0.63
1:C:640:PHE:HD1	1:C:1140:VAL:HG11	1.64	0.62
1:B:999:PRO:HA	1:B:1003:TRP:HB2	1.81	0.62
2:F:9:LEU:HB3	2:F:96:LEU:HD23	1.81	0.62
2:F:77:GLY:HA2	2:F:110:PRO:HB2	1.82	0.61
1:C:767:THR:OG1	1:C:768:LEU:N	2.33	0.61
1:A:966:LEU:HD12	1:A:1080:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:LEU:HD23	1:B:689:ILE:HG12	1.81	0.61
1:D:840:GLU:HB2	1:D:881:LYS:HB2	1.81	0.61
1:A:1056:TYR:O	1:A:1060:ILE:HG12	2.01	0.60
1:C:999:PRO:HA	1:C:1003:TRP:HB2	1.83	0.60
2:G:141:CYS:SG	2:G:142:ALA:N	2.75	0.60
1:B:606:SER:HB2	1:B:617:THR:HB	1.83	0.60
1:D:606:SER:HB2	1:D:617:THR:HB	1.83	0.60
1:D:1001:ARG:NH2	2:H:62:GLU:O	2.33	0.60
1:B:1054:LEU:HD21	1:C:580:VAL:HG22	1.84	0.60
1:B:640:PHE:HD2	1:B:1106:LEU:HD22	1.67	0.60
2:E:82:TYR:HB3	2:E:93:LEU:HD11	1.83	0.59
2:G:93:LEU:HD13	2:G:113:LEU:HD11	1.85	0.59
2:G:85:THR:HG23	2:G:123:GLU:HB3	1.84	0.59
1:D:770:GLU:HG2	1:D:931:LYS:HE2	1.84	0.58
1:D:613:ALA:HB1	1:D:616:LEU:HB2	1.85	0.58
1:D:588:ASP:OD1	1:D:754:LYS:NZ	2.30	0.58
1:B:810:THR:HG23	1:B:909:HIS:CE1	2.39	0.58
1:D:598:PHE:HE1	1:D:738:GLY:HA3	1.69	0.58
1:C:863:VAL:HG12	1:C:908:PHE:HD1	1.69	0.58
1:B:748:LEU:O	1:B:752:ILE:HG13	2.03	0.58
1:D:811:ILE:HD12	1:D:850:LEU:HD13	1.85	0.58
1:B:734:ARG:HH21	1:D:1126:GLN:HA	1.69	0.58
1:C:600:ASP:OD1	1:C:600:ASP:N	2.37	0.57
1:B:807:THR:HB	1:B:870:LYS:HG3	1.85	0.57
2:F:61:THR:O	2:F:68:ARG:NH2	2.37	0.57
1:A:590:ILE:HG23	1:A:593:VAL:HG23	1.87	0.57
1:D:759:SER:O	1:D:898:LYS:NZ	2.37	0.57
1:B:576:ARG:HB2	1:C:932:GLU:HG2	1.86	0.57
1:B:1036:ASP:OD2	1:B:1053:LYS:NZ	2.37	0.57
2:G:84:ILE:HD12	2:G:124:ARG:HE	1.68	0.56
1:D:1056:TYR:O	1:D:1060:ILE:HG12	2.05	0.56
1:A:576:ARG:HB2	1:D:932:GLU:HG2	1.86	0.56
1:C:988:ASP:O	1:C:992:ILE:HG12	2.06	0.56
1:B:707:LYS:HA	1:B:992:ILE:HG21	1.87	0.56
1:A:990:LEU:HD22	1:A:994:LYS:HE3	1.87	0.56
1:C:1008:LYS:NZ	1:C:1024:ASP:OD1	2.39	0.56
2:F:84:ILE:HD11	2:F:118:CYS:HA	1.88	0.56
1:B:644:ILE:O	1:B:685:TYR:OH	2.22	0.55
1:B:703:ASN:HD22	1:B:712:ARG:NH1	2.04	0.55
1:A:737:VAL:HG21	1:A:1003:TRP:HH2	1.70	0.55
1:A:1129:ALA:HB3	1:A:1134:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1019:LYS:HE3	1:C:1024:ASP:HB2	1.88	0.55
1:D:966:LEU:HD23	1:D:1080:ILE:HD13	1.89	0.55
1:A:851:GLN:HE21	1:A:854:ASP:HB3	1.71	0.55
2:E:45:GLU:HA	2:E:50:GLN:HA	1.89	0.55
2:G:53:LEU:HD11	2:G:162:VAL:HG21	1.89	0.54
1:C:972:PHE:HD2	1:C:1074:VAL:HG11	1.72	0.54
2:H:117:LYS:HG2	4:H:201:GDP:C5	2.43	0.54
2:E:41:ARG:NH1	2:E:54:GLU:OE2	2.39	0.54
1:C:748:LEU:O	1:C:752:ILE:HG13	2.08	0.54
1:D:867:ASN:ND2	1:D:872:TYR:OH	2.40	0.54
2:E:11:SER:O	2:E:16:LYS:NZ	2.41	0.54
2:H:53:LEU:HD23	2:H:55:ILE:HD11	1.89	0.54
1:D:713:THR:HG21	2:H:62:GLU:HB3	1.90	0.53
2:F:35:THR:HB	5:F:202:AF3:F2	1.97	0.53
2:F:99:GLN:HG3	2:F:102:ARG:HH21	1.73	0.53
1:B:605:ALA:HB1	1:B:609:PHE:CE2	2.43	0.53
1:C:969:LYS:NZ	1:C:1074:VAL:O	2.27	0.53
2:E:19:LEU:HD23	2:E:148:ALA:HB2	1.90	0.53
2:F:118:CYS:HB3	2:F:145:GLU:HG2	1.91	0.53
1:D:885:PRO:HA	1:D:889:ALA:HB3	1.90	0.53
1:C:1009:ASN:HD21	2:F:65:THR:HB	1.74	0.53
1:D:609:PHE:HB3	1:D:673:SER:HB3	1.90	0.52
1:D:767:THR:OG1	1:D:768:LEU:N	2.42	0.52
1:B:900:ASP:OD1	1:B:901:LYS:N	2.43	0.52
1:B:942:LYS:HG3	1:B:1055:LEU:HD22	1.91	0.52
2:H:119:ASP:OD1	2:H:119:ASP:N	2.43	0.52
1:C:991:HIS:O	1:C:995:THR:HG23	2.09	0.52
1:D:643:LEU:HD11	1:D:1137:MET:HA	1.92	0.52
2:H:119:ASP:OD2	4:H:201:GDP:N2	2.40	0.52
1:A:645:ARG:NE	1:A:682:ASP:OD2	2.41	0.52
1:B:942:LYS:HE3	1:B:1056:TYR:CE2	2.45	0.51
1:A:1050:PRO:HD3	2:E:40:TYR:CE2	2.45	0.51
1:B:1007:LEU:HD23	1:B:1031:ALA:HA	1.92	0.51
1:A:671:VAL:HG11	1:A:716:ILE:HD13	1.93	0.51
1:C:620:MET:HB3	1:C:677:LEU:HD21	1.92	0.51
1:A:706:PRO:O	1:A:993:TRP:NE1	2.42	0.51
1:A:1124:LEU:HG	1:A:1129:ALA:HB2	1.92	0.51
1:C:729:LEU:HD21	1:C:968:VAL:HG23	1.91	0.51
1:C:810:THR:O	1:C:814:VAL:HG23	2.10	0.51
1:A:1008:LYS:O	1:A:1019:LYS:NZ	2.39	0.51
1:B:969:LYS:HE3	1:B:973:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:LYS:HB2	2:F:76:GLN:HG3	1.92	0.51
1:B:655:HIS:O	1:B:659:GLU:HG2	2.11	0.51
1:D:589:LEU:HD13	1:D:747:ALA:HB1	1.93	0.51
1:B:737:VAL:HG11	1:B:1003:TRP:CZ3	2.46	0.51
1:B:620:MET:HB3	1:B:677:LEU:HD21	1.91	0.50
1:D:837:ILE:HA	1:D:883:ILE:O	2.11	0.50
1:A:752:ILE:HD13	1:A:1022:HIS:CE1	2.46	0.50
1:B:884:THR:H	1:B:887:ILE:HD12	1.76	0.50
1:B:889:ALA:O	1:B:893:THR:OG1	2.28	0.50
1:D:668:LYS:HZ1	1:D:715:SER:HA	1.76	0.50
1:B:953:PHE:CZ	1:B:1034:PHE:HB2	2.47	0.50
1:B:1035:MET:HE2	2:G:36:ILE:HG13	1.92	0.50
1:A:748:LEU:O	1:A:752:ILE:HG13	2.11	0.50
1:B:770:GLU:OE2	1:C:576:ARG:NH2	2.44	0.50
1:B:760:VAL:HG21	1:B:908:PHE:HA	1.94	0.50
2:G:69:ASP:OD1	2:G:69:ASP:N	2.42	0.50
1:A:884:THR:H	1:A:887:ILE:HD12	1.77	0.50
1:D:941:THR:O	1:D:945:VAL:HG22	2.12	0.50
1:D:1048:HIS:HB3	2:H:24:VAL:HG12	1.94	0.50
1:A:1048:HIS:HB3	2:E:25:GLN:HG2	1.94	0.49
1:B:737:VAL:HG21	1:B:1003:TRP:HH2	1.76	0.49
1:D:715:SER:HB2	1:D:717:VAL:HG23	1.93	0.49
2:G:19:LEU:HD23	2:G:148:ALA:HB2	1.93	0.49
1:A:791:VAL:H	1:A:797:ILE:HB	1.76	0.49
2:F:118:CYS:SG	2:F:147:SER:HB2	2.52	0.49
1:C:835:ARG:NH1	1:C:899:ASP:OD2	2.33	0.49
1:C:841:TYR:HB2	1:C:850:LEU:HD23	1.95	0.49
1:C:954:LYS:HG2	1:C:957:TRP:HE1	1.77	0.49
1:C:1025:GLY:O	1:C:1029:VAL:HG23	2.13	0.49
1:B:752:ILE:HD13	1:B:1022:HIS:CE1	2.47	0.48
1:B:1056:TYR:O	1:B:1060:ILE:HG12	2.13	0.48
1:B:865:MET:HB2	1:B:908:PHE:CZ	2.48	0.48
1:D:1068:LYS:O	1:D:1072:LYS:HG2	2.13	0.48
1:A:602:LYS:HG3	1:A:603:HIS:CD2	2.49	0.48
2:E:124:ARG:NH1	2:E:145:GLU:OE2	2.41	0.48
1:B:854:ASP:OD1	1:B:867:ASN:ND2	2.36	0.48
1:C:650:LEU:HD23	1:C:689:ILE:HG12	1.96	0.48
1:C:969:LYS:HE3	1:C:973:ASP:OD2	2.13	0.48
2:G:15:GLY:HA3	2:G:116:ASN:HD22	1.77	0.48
2:G:9:LEU:HD21	2:G:71:TYR:CE1	2.49	0.48
1:B:815:LYS:HB3	1:B:834:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:ALA:HA	1:D:712:ARG:HH22	1.79	0.48
1:A:711:ARG:NE	5:E:202:AF3:F3	2.37	0.48
1:A:737:VAL:HG11	1:A:1003:TRP:CZ3	2.49	0.48
1:B:952:LEU:HD21	1:B:1007:LEU:HD11	1.95	0.48
1:B:969:LYS:NZ	1:B:1074:VAL:O	2.34	0.48
1:D:600:ASP:N	1:D:600:ASP:OD1	2.46	0.48
2:H:16:LYS:NZ	4:H:201:GDP:O1B	2.41	0.48
1:C:1110:TYR:HA	1:C:1113:MET:HB3	1.95	0.48
1:B:758:ASP:OD1	1:B:909:HIS:HB3	2.13	0.47
1:A:722:THR:O	1:A:726:SER:OG	2.32	0.47
1:C:752:ILE:HD13	1:C:1022:HIS:CE1	2.49	0.47
1:B:687:THR:O	1:B:691:GLU:HG3	2.13	0.47
1:C:1104:ALA:HA	1:C:1107:ARG:HD2	1.97	0.47
2:F:8:VAL:O	2:F:58:THR:OG1	2.22	0.47
1:C:669:CYS:SG	2:F:62:GLU:HG2	2.55	0.47
1:D:814:VAL:HG21	1:D:869:LEU:HD21	1.95	0.47
1:B:839:ILE:HG23	1:B:880:ILE:HG23	1.96	0.47
2:F:119:ASP:OD1	2:F:119:ASP:N	2.47	0.47
1:D:660:GLN:HB2	1:D:663:PHE:HB2	1.97	0.47
1:D:1025:GLY:O	1:D:1028:SER:OG	2.25	0.47
1:B:613:ALA:O	1:B:617:THR:HG23	2.15	0.47
1:C:609:PHE:HB3	1:C:673:SER:HB3	1.96	0.47
1:A:733:LEU:HD21	1:A:1006:ILE:HG12	1.97	0.46
1:D:773:LEU:HD21	1:D:934:TYR:HB2	1.96	0.46
1:B:733:LEU:HD12	1:B:737:VAL:HB	1.96	0.46
1:B:1050:PRO:HD3	2:G:40:TYR:CE2	2.51	0.46
1:D:640:PHE:O	1:D:644:ILE:HG12	2.16	0.46
1:B:998:LEU:O	1:B:1002:PHE:HB3	2.16	0.46
1:C:758:ASP:OD2	1:C:761:THR:OG1	2.23	0.46
2:H:79:ALA:HB2	2:H:161:LEU:HD11	1.96	0.46
1:D:613:ALA:O	1:D:617:THR:HG23	2.15	0.46
2:E:84:ILE:HD12	2:E:124:ARG:HG3	1.96	0.46
1:A:658:GLU:OE2	1:A:716:ILE:N	2.34	0.46
1:A:889:ALA:O	1:A:893:THR:OG1	2.34	0.46
1:D:644:ILE:HG23	1:D:650:LEU:HD13	1.98	0.46
1:D:999:PRO:HA	1:D:1003:TRP:HB2	1.98	0.46
2:H:117:LYS:HE2	4:H:201:GDP:C8	2.51	0.46
1:A:665:ILE:HA	1:A:668:LYS:HD2	1.98	0.46
1:D:970:TYR:HB2	1:D:1080:ILE:HD12	1.98	0.46
1:C:1119:GLU:OE1	1:C:1119:GLU:N	2.49	0.45
1:D:1124:LEU:HG	1:D:1129:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ILE:HG21	1:B:679:LEU:HD21	1.98	0.45
1:B:663:PHE:CE1	1:B:667:ASP:HB3	2.52	0.45
2:H:135:ALA:HB2	2:H:143:PHE:HB2	1.97	0.45
1:D:788:VAL:N	1:D:880:ILE:O	2.40	0.45
1:D:930:ILE:HB	1:D:933:MET:HE3	1.99	0.45
1:A:650:LEU:HD23	1:A:689:ILE:HG12	1.99	0.45
1:D:724:TRP:HA	1:D:727:ILE:HD12	1.99	0.45
2:F:136:ARG:HD3	2:F:140:ASN:HA	1.98	0.45
1:A:830:TYR:HD2	1:A:837:ILE:HD11	1.82	0.45
2:F:119:ASP:OD2	4:F:201:GDP:N2	2.42	0.45
1:A:758:ASP:OD1	1:A:909:HIS:HB3	2.17	0.45
2:F:161:LEU:O	2:F:165:ILE:HG13	2.17	0.45
1:B:664:SER:O	1:B:668:LYS:HG3	2.16	0.44
1:C:785:LEU:HD13	1:C:880:ILE:HD12	1.99	0.44
1:C:840:GLU:HA	1:C:849:MET:HA	1.99	0.44
1:C:1056:TYR:O	1:C:1060:ILE:HG12	2.17	0.44
1:D:713:THR:HA	1:D:718:GLU:OE1	2.16	0.44
1:A:972:PHE:HD2	1:A:1074:VAL:HG11	1.82	0.44
1:B:694:LEU:HD22	1:B:974:PHE:HE2	1.83	0.44
2:E:96:LEU:O	2:E:100:ILE:HG12	2.17	0.44
2:F:116:ASN:OD1	2:F:117:LYS:N	2.48	0.44
1:A:613:ALA:O	1:A:617:THR:HG23	2.18	0.44
1:A:839:ILE:HG23	1:A:880:ILE:HG23	2.00	0.44
1:C:788:VAL:HG13	1:C:798:SER:HA	1.99	0.44
2:G:96:LEU:O	2:G:100:ILE:HG12	2.17	0.44
1:A:930:ILE:HG23	1:D:572:ARG:HG2	1.99	0.44
1:A:937:LYS:HA	1:A:937:LYS:HD3	1.66	0.44
1:B:708:LEU:HD23	1:B:712:ARG:HH21	1.82	0.44
1:B:869:LEU:HA	1:B:869:LEU:HD23	1.85	0.44
1:C:669:CYS:HA	1:C:719:LYS:HG2	2.00	0.44
1:C:675:LEU:HD23	1:C:720:LEU:HD11	1.99	0.44
1:B:571:ILE:O	1:B:575:ILE:HG13	2.18	0.44
1:C:663:PHE:CE1	1:C:667:ASP:HB3	2.53	0.44
2:E:104:LYS:HD3	2:E:104:LYS:HA	1.82	0.44
1:B:991:HIS:O	1:B:995:THR:HG23	2.17	0.44
1:D:1050:PRO:HB2	1:D:1052:ASN:OD1	2.16	0.44
1:D:865:MET:HB2	1:D:908:PHE:CZ	2.53	0.43
1:B:814:VAL:O	1:B:818:ILE:HG13	2.18	0.43
1:C:1050:PRO:HD3	2:F:40:TYR:CE1	2.53	0.43
2:F:139:ASN:O	2:F:139:ASN:ND2	2.51	0.43
1:D:723:ASN:O	1:D:727:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:O	1:B:956:ILE:HG13	2.19	0.43
1:B:1008:LYS:O	1:B:1019:LYS:NZ	2.30	0.43
1:C:820:GLN:O	1:C:824:ARG:HB2	2.19	0.43
1:D:567:MET:O	1:D:571:ILE:HG13	2.18	0.43
2:F:141:CYS:SG	2:F:142:ALA:N	2.91	0.43
1:A:991:HIS:O	1:A:995:THR:HG23	2.18	0.43
2:G:35:THR:HG23	2:G:38:ASP:OD2	2.18	0.43
2:H:96:LEU:O	2:H:100:ILE:HG12	2.19	0.43
1:B:988:ASP:O	1:B:992:ILE:HG12	2.18	0.43
1:C:803:VAL:HG11	1:C:818:ILE:HG12	2.00	0.43
1:C:970:TYR:CE1	1:C:1085:LEU:HD11	2.54	0.43
1:C:1045:LEU:HD13	1:C:1054:LEU:HD12	2.01	0.43
2:F:117:LYS:HG2	4:F:201:GDP:C6	2.53	0.43
1:B:1025:GLY:O	1:B:1029:VAL:HG23	2.19	0.43
1:C:1027:LEU:HD23	1:C:1027:LEU:HA	1.85	0.43
2:G:6:LEU:HD22	2:G:161:LEU:HD13	2.01	0.43
1:B:734:ARG:NH2	1:D:1126:GLN:HA	2.33	0.43
1:D:668:LYS:HZ3	1:D:714:GLU:C	2.22	0.43
1:B:1009:ASN:HD21	2:G:65:THR:HB	1.84	0.42
1:D:691:GLU:OE2	1:D:970:TYR:OH	2.28	0.42
2:H:40:TYR:N	2:H:55:ILE:O	2.48	0.42
1:A:869:LEU:HD22	1:A:874:VAL:HG21	2.01	0.42
1:C:841:TYR:HE1	1:C:878:ALA:HB1	1.84	0.42
1:D:656:ALA:O	1:D:660:GLN:NE2	2.30	0.42
1:D:697:LEU:O	1:D:701:SER:HB3	2.19	0.42
1:D:757:VAL:HG22	1:D:764:ALA:HB2	2.00	0.42
2:F:9:LEU:HD21	2:F:71:TYR:HE1	1.83	0.42
1:B:1008:LYS:HE3	1:B:1008:LYS:HB3	1.91	0.42
1:B:1050:PRO:HB2	1:B:1052:ASN:OD1	2.20	0.42
1:C:694:LEU:HD11	1:C:710:LEU:HD21	2.01	0.42
2:F:9:LEU:HD21	2:F:71:TYR:CE1	2.54	0.42
2:F:138:TRP:HB2	2:F:141:CYS:HB2	2.01	0.42
2:H:4:TYR:CE2	2:H:162:VAL:HG13	2.55	0.42
1:A:598:PHE:HZ	1:A:738:GLY:HA3	1.84	0.42
1:B:703:ASN:O	1:B:712:ARG:NH1	2.53	0.42
1:C:640:PHE:O	1:C:644:ILE:HG12	2.20	0.42
2:E:80:LEU:HB3	2:E:93:LEU:HD22	2.00	0.42
2:F:117:LYS:HG2	4:F:201:GDP:C5	2.54	0.42
2:G:117:LYS:HE2	4:G:201:GDP:C4	2.54	0.42
1:A:959:LEU:HD22	1:A:964:ALA:HA	2.02	0.42
1:B:613:ALA:HB1	1:B:616:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ARG:HH21	2:G:34:PRO:HA	1.85	0.42
1:B:930:ILE:HB	1:B:933:MET:HE3	2.00	0.42
1:C:599:LEU:HD23	1:C:599:LEU:HA	1.91	0.42
1:C:643:LEU:HD11	1:C:1137:MET:HA	2.01	0.42
1:C:758:ASP:OD1	1:C:909:HIS:HB3	2.20	0.42
1:D:588:ASP:OD1	1:D:588:ASP:N	2.53	0.42
1:A:695:GLN:HG3	1:A:978:GLN:HE22	1.84	0.42
1:A:787:VAL:HB	1:A:801:LEU:HB3	2.01	0.42
1:B:1102:GLU:N	1:B:1102:GLU:OE1	2.52	0.42
1:A:858:GLU:HG2	1:A:865:MET:HE2	2.01	0.42
1:A:1141:LYS:HB3	1:A:1141:LYS:HE2	1.79	0.42
1:B:932:GLU:HA	1:B:935:LEU:HG	2.01	0.42
1:D:766:TYR:HB3	1:D:941:THR:OG1	2.20	0.42
2:G:161:LEU:O	2:G:165:ILE:HG13	2.20	0.42
1:B:640:PHE:CE2	1:B:644:ILE:HD11	2.55	0.42
1:C:854:ASP:OD1	1:C:854:ASP:N	2.52	0.42
1:C:869:LEU:HD22	1:C:874:VAL:HG21	2.01	0.42
2:H:84:ILE:HD11	2:H:118:CYS:HA	2.02	0.42
1:A:966:LEU:HD11	1:A:1080:ILE:HG21	2.01	0.42
1:B:572:ARG:HG2	1:C:930:ILE:HG23	2.00	0.42
1:D:741:LEU:O	1:D:745:VAL:HG23	2.19	0.42
1:A:769:SER:HB3	1:A:772:TRP:HB2	2.02	0.42
1:B:694:LEU:O	1:B:698:MET:HG2	2.20	0.41
1:D:640:PHE:HD2	1:D:1106:LEU:HD22	1.85	0.41
1:D:755:GLY:HA3	1:D:766:TYR:CD1	2.54	0.41
2:H:90:PHE:HE2	2:H:130:GLN:HE21	1.66	0.41
1:A:966:LEU:CD1	1:A:1080:ILE:HD13	2.48	0.41
1:C:850:LEU:HD12	1:C:850:LEU:O	2.20	0.41
1:D:565:GLU:O	1:D:569:SER:OG	2.22	0.41
1:D:810:THR:O	1:D:814:VAL:HG23	2.20	0.41
1:B:788:VAL:HA	1:B:799:GLU:O	2.21	0.41
1:C:972:PHE:HD1	1:C:975:LEU:HD12	1.86	0.41
1:A:719:LYS:HA	1:A:719:LYS:HD2	1.84	0.41
1:D:1007:LEU:O	1:D:1027:LEU:HD13	2.21	0.41
1:B:776:GLN:HG2	1:B:778:GLN:HE21	1.86	0.41
1:C:757:VAL:HG22	1:C:764:ALA:HB2	2.02	0.41
1:C:1053:LYS:NZ	2:F:38:ASP:OD1	2.53	0.41
2:G:117:LYS:HG2	4:G:201:GDP:C6	2.56	0.41
2:H:35:THR:HG21	2:H:57:ASP:OD2	2.21	0.41
1:B:645:ARG:HA	1:B:685:TYR:CZ	2.55	0.41
1:C:588:ASP:OD1	1:C:588:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1024:ASP:OD2	2:H:67:MET:HB3	2.20	0.41
2:H:13:GLY:HA2	4:H:201:GDP:O3A	2.21	0.41
1:A:742:PHE:HB2	1:A:1014:PHE:CZ	2.55	0.41
1:A:569:SER:HA	1:A:572:ARG:HD2	2.03	0.41
1:B:665:ILE:HD12	2:G:61:THR:HG21	2.03	0.41
1:B:766:TYR:HB3	1:B:941:THR:OG1	2.21	0.41
1:C:970:TYR:HB2	1:C:1080:ILE:HG13	2.03	0.41
1:D:814:VAL:O	1:D:818:ILE:HG13	2.21	0.41
1:A:737:VAL:HG21	1:A:1003:TRP:CH2	2.53	0.41
1:B:1021:PRO:O	1:B:1024:ASP:HB3	2.21	0.41
1:C:810:THR:HG21	1:C:866:LEU:HD12	2.02	0.41
1:D:969:LYS:HD3	1:D:1077:GLN:HB3	2.03	0.41
1:D:1008:LYS:HE3	1:D:1008:LYS:HB3	1.89	0.41
1:B:610:PHE:HB2	1:B:617:THR:HG22	2.03	0.41
1:B:982:LYS:HE3	1:B:982:LYS:HB3	1.85	0.41
1:C:723:ASN:O	1:C:727:ILE:HG13	2.21	0.41
2:E:53:LEU:HD11	2:E:162:VAL:HG21	2.03	0.41
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.93	0.40
1:B:1003:TRP:O	1:B:1007:LEU:HB2	2.21	0.40
1:B:1055:LEU:HD23	1:B:1055:LEU:HA	1.86	0.40
1:C:677:LEU:HD12	1:C:677:LEU:HA	1.95	0.40
1:D:737:VAL:HG11	1:D:1003:TRP:CZ3	2.55	0.40
2:E:66:ALA:HB3	2:E:68:ARG:CZ	2.51	0.40
1:B:840:GLU:HB2	1:B:881:LYS:HB3	2.04	0.40
1:D:1027:LEU:HD23	1:D:1027:LEU:HA	1.89	0.40
2:G:119:ASP:OD1	2:G:119:ASP:N	2.52	0.40
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.96	0.40
1:C:643:LEU:HB3	1:C:649:PHE:CE2	2.57	0.40
1:C:982:LYS:HE2	1:C:982:LYS:HB3	1.81	0.40
1:D:839:ILE:HG23	1:D:880:ILE:HG23	2.03	0.40
1:B:718:GLU:HB3	1:B:1001:ARG:CZ	2.51	0.40
1:B:755:GLY:HA3	1:B:766:TYR:CE1	2.56	0.40
1:B:939:LEU:O	1:B:943:VAL:HG23	2.22	0.40
1:C:767:THR:HG22	1:C:773:LEU:HD13	2.04	0.40
1:D:643:LEU:HD13	1:D:649:PHE:CZ	2.56	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	564/599 (94%)	522 (93%)	40 (7%)	2 (0%)	34	66
1	B	561/599 (94%)	527 (94%)	31 (6%)	3 (0%)	29	61
1	C	550/599 (92%)	514 (94%)	34 (6%)	2 (0%)	34	66
1	D	550/599 (92%)	505 (92%)	43 (8%)	2 (0%)	34	66
2	E	166/199 (83%)	152 (92%)	13 (8%)	1 (1%)	25	57
2	F	164/199 (82%)	153 (93%)	10 (6%)	1 (1%)	25	57
2	G	166/199 (83%)	157 (95%)	9 (5%)	0	100	100
2	H	165/199 (83%)	151 (92%)	14 (8%)	0	100	100
All	All	2886/3192 (90%)	2681 (93%)	194 (7%)	11 (0%)	34	66

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	889	ALA
1	D	889	ALA
1	A	889	ALA
1	A	884	THR
1	B	585	GLU
1	D	663	PHE
1	C	889	ALA
2	E	30	GLU
1	B	884	THR
1	C	998	LEU
2	F	110	PRO

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	439/552 (80%)	431 (98%)	8 (2%)	59	78
1	B	418/552 (76%)	406 (97%)	12 (3%)	42	69
1	C	420/552 (76%)	411 (98%)	9 (2%)	53	75
1	D	421/552 (76%)	409 (97%)	12 (3%)	42	69
2	E	133/163 (82%)	130 (98%)	3 (2%)	50	73
2	F	131/163 (80%)	127 (97%)	4 (3%)	40	67
2	G	128/163 (78%)	125 (98%)	3 (2%)	50	73
2	H	118/163 (72%)	117 (99%)	1 (1%)	81	89
All	All	2208/2860 (77%)	2156 (98%)	52 (2%)	49	73

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	661	LYS
1	A	850	LEU
1	A	884	THR
1	A	950	GLU
1	A	957	TRP
1	A	1028	SER
1	A	1041	THR
1	A	1137	MET
1	B	577	GLN
1	B	709	LEU
1	B	712	ARG
1	B	717	VAL
1	B	720	LEU
1	B	748	LEU
1	B	850	LEU
1	B	884	THR
1	B	942	LYS
1	B	957	TRP
1	B	988	ASP
1	B	1054	LEU
1	C	577	GLN
1	C	615	THR
1	C	619	VAL
1	C	720	LEU

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Mol	Chain	Res	Type
1	C	767	THR
1	C	831	THR
1	C	864	THR
1	C	884	THR
1	C	1005	ASN
1	D	568	GLU
1	D	619	VAL
1	D	665	ILE
1	D	712	ARG
1	D	717	VAL
1	D	813	GLN
1	D	823	GLN
1	D	850	LEU
1	D	966	LEU
1	D	973	ASP
1	D	1029	VAL
1	D	1085	LEU
2	E	67	MET
2	E	97	ARG
2	E	106	THR
2	F	52	MET
2	F	67	MET
2	F	136	ARG
2	F	155	ASN
2	G	41	ARG
2	G	52	MET
2	G	67	MET
2	H	52	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	HIS
1	A	813	GLN
1	A	823	GLN
1	A	867	ASN
1	A	946	HIS
1	A	978	GLN
1	A	1009	ASN
1	A	1136	ASN
1	B	703	ASN
1	B	894	GLN

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Mol	Chain	Res	Type
1	B	978	GLN
1	C	577	GLN
1	C	695	GLN
1	C	1005	ASN
1	C	1009	ASN
1	C	1090	GLN
1	C	1101	ASN
1	D	867	ASN
1	D	946	HIS
1	D	978	GLN
2	F	91	ASN
2	F	94	GLN
2	G	49	GLN
2	H	22	GLN
2	H	153	ASN
2	H	164	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
5	AF3	H	202	-	0,3,3	-	-	-		
4	GDP	G	201	3	24,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
5	AF3	G	202	-	0,3,3	-	-	-		
5	AF3	F	202	-	0,3,3	-	-	-		
4	GDP	F	201	3	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
5	AF3	E	202	-	0,3,3	-	-	-		
4	GDP	H	201	3	24,30,30	0.93	1 (4%)	30,47,47	1.33	5 (16%)
4	GDP	E	201	3	24,30,30	0.94	1 (4%)	30,47,47	1.27	5 (16%)

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	GDP	G	201	3	-	8/12/32/32	0/3/3/3
4	GDP	H	201	3	-	0/12/32/32	0/3/3/3
4	GDP	F	201	3	-	5/12/32/32	0/3/3/3
4	GDP	E	201	3	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	201	GDP	C6-N1	-2.42	1.34	1.37
4	G	201	GDP	C6-N1	-2.38	1.34	1.37
4	F	201	GDP	C6-N1	-2.35	1.34	1.37
4	H	201	GDP	C6-N1	-2.19	1.34	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	201	GDP	PA-O3A-PB	-3.42	121.09	132.83
4	H	201	GDP	C3'-C2'-C1'	3.35	106.02	100.98
4	E	201	GDP	C3'-C2'-C1'	3.05	105.56	100.98
4	F	201	GDP	C3'-C2'-C1'	2.95	105.42	100.98
4	F	201	GDP	PA-O3A-PB	-2.94	122.73	132.83
4	H	201	GDP	PA-O3A-PB	-2.94	122.74	132.83
4	G	201	GDP	C3'-C2'-C1'	2.90	105.34	100.98
4	E	201	GDP	PA-O3A-PB	-2.86	123.02	132.83
4	F	201	GDP	C5-C6-N1	2.41	118.20	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	201	GDP	C8-N7-C5	2.35	107.47	102.99
4	F	201	GDP	C8-N7-C5	2.35	107.46	102.99
4	E	201	GDP	C5-C6-N1	2.31	118.04	113.95
4	H	201	GDP	C5-C6-N1	2.31	118.03	113.95
4	G	201	GDP	C8-N7-C5	2.31	107.39	102.99
4	H	201	GDP	C8-N7-C5	2.26	107.29	102.99
4	G	201	GDP	C5-C6-N1	2.24	117.91	113.95
4	H	201	GDP	O6-C6-C5	-2.02	120.42	124.37
4	E	201	GDP	O6-C6-C5	-2.01	120.45	124.37

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	GDP	PA-O3A-PB-O2B
4	F	201	GDP	PA-O3A-PB-O2B
4	G	201	GDP	PA-O3A-PB-O2B
4	G	201	GDP	C5'-O5'-PA-O1A
4	G	201	GDP	C5'-O5'-PA-O2A
4	G	201	GDP	O4'-C4'-C5'-O5'
4	G	201	GDP	C3'-C4'-C5'-O5'
4	E	201	GDP	C5'-O5'-PA-O3A
4	F	201	GDP	C5'-O5'-PA-O3A
4	F	201	GDP	C5'-O5'-PA-O1A
4	E	201	GDP	PA-O3A-PB-O1B
4	F	201	GDP	PA-O3A-PB-O1B
4	F	201	GDP	PA-O3A-PB-O3B
4	G	201	GDP	PA-O3A-PB-O3B
4	G	201	GDP	C5'-O5'-PA-O3A
4	E	201	GDP	C5'-O5'-PA-O1A
4	G	201	GDP	PA-O3A-PB-O1B

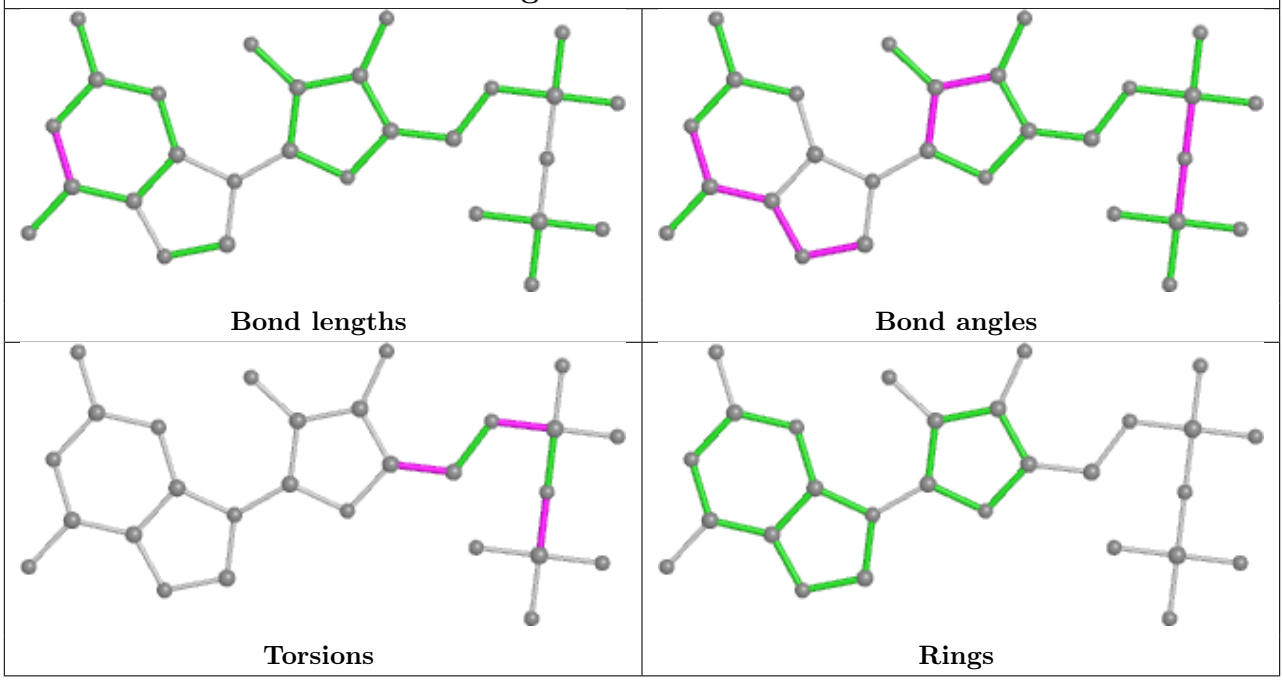
There are no ring outliers.

5 monomers are involved in 12 short contacts:

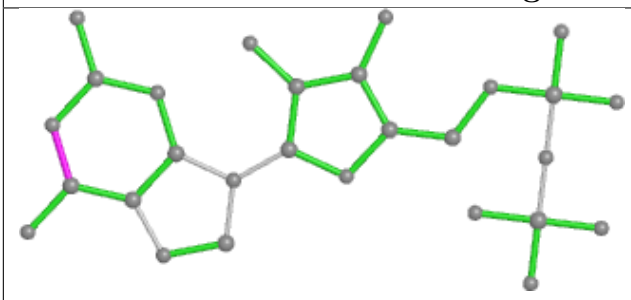
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	201	GDP	2	0
5	F	202	AF3	1	0
4	F	201	GDP	3	0
5	E	202	AF3	1	0
4	H	201	GDP	5	0

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.

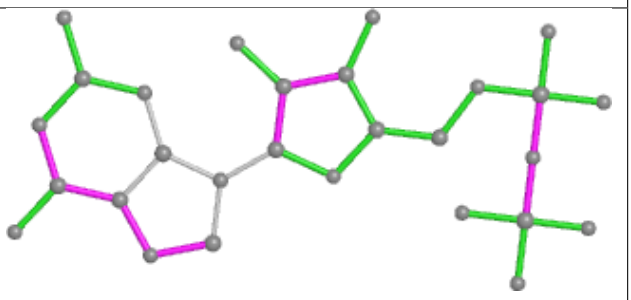
Ligand GDP G 201



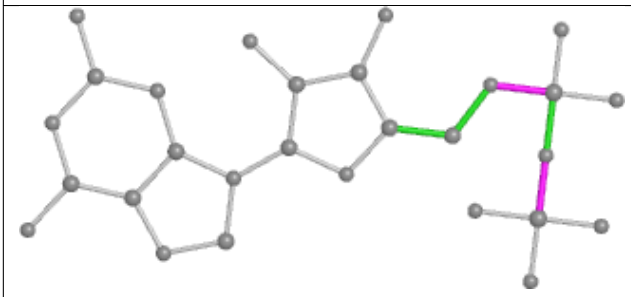
Ligand GDP F 201



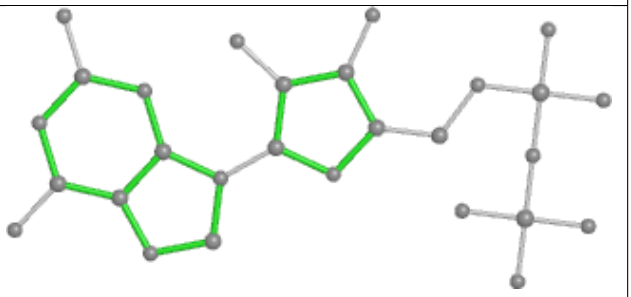
Bond lengths



Bond angles

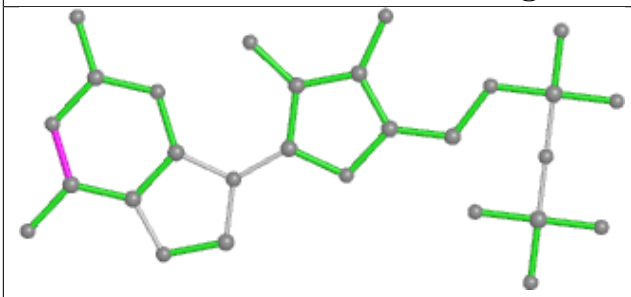


Torsions

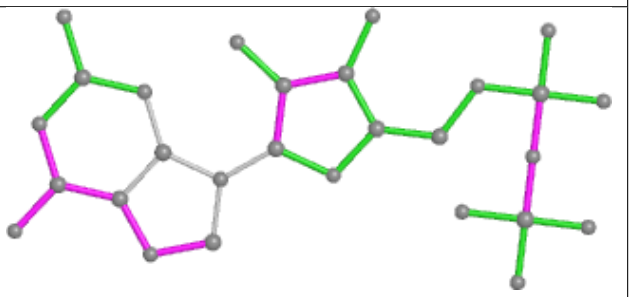


Rings

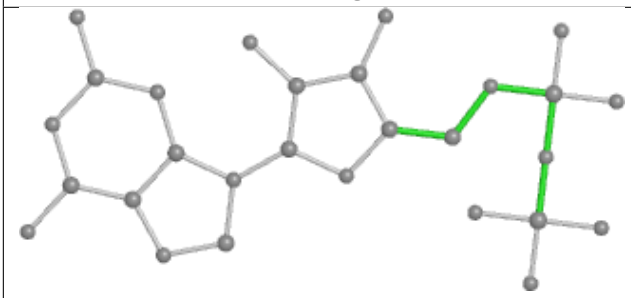
Ligand GDP H 201



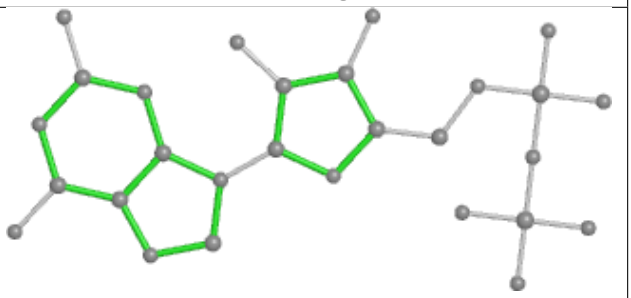
Bond lengths



Bond angles

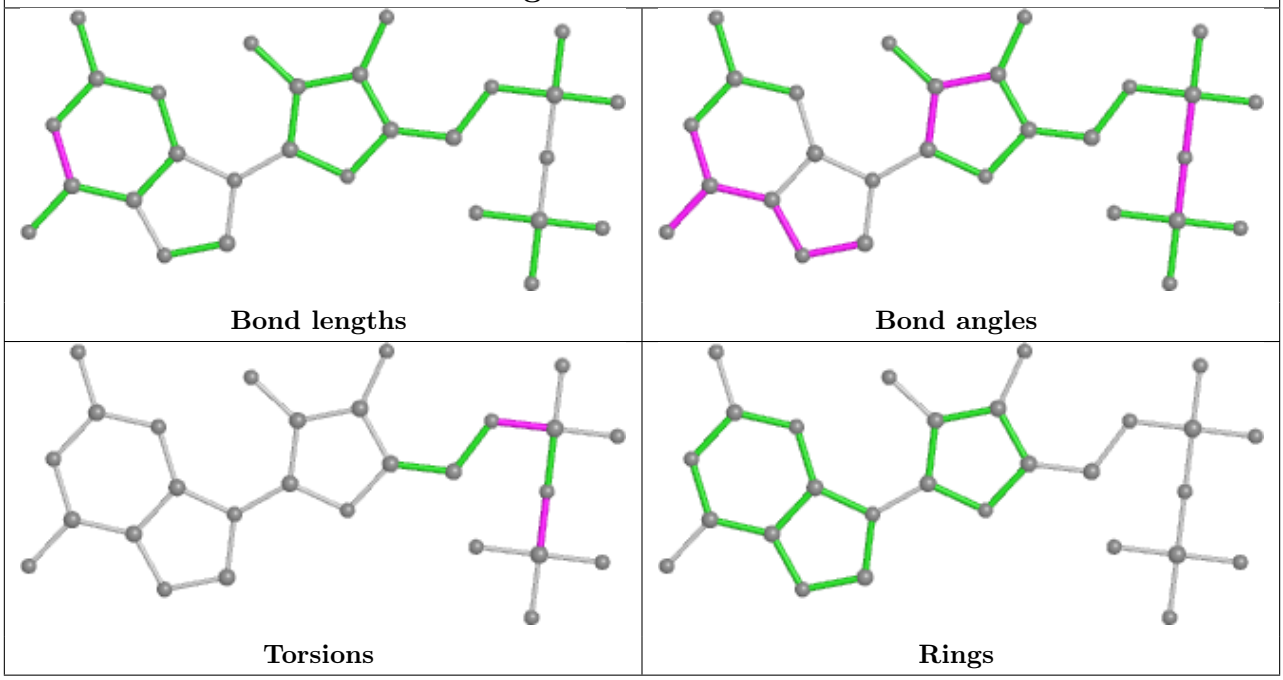


Torsions



Rings

Ligand GDP E 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	574/599 (95%)	0.12	18 (3%)	49	48	66, 132, 194, 219	0
1	B	571/599 (95%)	0.23	29 (5%)	28	26	62, 135, 220, 277	0
1	C	560/599 (93%)	0.06	20 (3%)	42	40	70, 134, 189, 214	0
1	D	560/599 (93%)	0.33	39 (6%)	16	16	83, 153, 223, 253	0
2	E	168/199 (84%)	0.43	11 (6%)	18	18	91, 139, 179, 208	0
2	F	166/199 (83%)	0.68	18 (10%)	5	5	94, 147, 186, 205	0
2	G	168/199 (84%)	0.95	32 (19%)	1	1	95, 166, 214, 234	0
2	H	167/199 (83%)	0.80	24 (14%)	2	2	110, 168, 222, 243	0
All	All	2934/3192 (91%)	0.31	191 (6%)	18	18	62, 143, 207, 277	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	76	GLN	8.7
2	H	113	LEU	5.6
1	D	847	PHE	5.4
2	H	141	CYS	5.1
2	G	142	ALA	5.1
1	D	1140	VAL	5.0
1	D	1121	PHE	5.0
1	B	652	CYS	4.8
2	H	142	ALA	4.7
2	G	118	CYS	4.6
1	B	985	THR	4.5
2	G	59	ALA	4.4
2	G	144	LEU	4.4
1	D	1117	PHE	4.3
2	H	112	ILE	4.3
2	G	112	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	1087	THR	4.2
1	B	1110	TYR	4.1
1	B	587	SER	4.1
1	D	791	VAL	3.9
2	G	60	GLY	3.8
1	A	700	GLN	3.8
1	A	794	GLY	3.7
1	B	593	VAL	3.7
1	B	789	PHE	3.7
1	C	1121	PHE	3.7
2	F	143	PHE	3.6
2	F	6	LEU	3.6
1	A	783	LEU	3.6
2	G	65	THR	3.6
1	D	796	GLU	3.6
1	B	632	THR	3.5
1	D	1120	ILE	3.5
1	A	818	ILE	3.5
1	B	874	VAL	3.5
1	D	1110	TYR	3.4
1	A	1110	TYR	3.3
2	E	118	CYS	3.3
2	F	142	ALA	3.3
1	C	895	ASN	3.2
1	A	911	VAL	3.2
2	G	66	ALA	3.2
1	D	885	PRO	3.2
1	B	783	LEU	3.2
2	G	145	GLU	3.2
2	E	6	LEU	3.1
1	B	556	MET	3.1
2	F	113	LEU	3.1
1	D	874	VAL	3.1
2	G	119	ASP	3.1
1	B	1133	LEU	3.1
2	F	144	LEU	3.1
2	G	113	LEU	3.1
2	H	158	PHE	3.1
2	E	47	ASP	3.1
2	G	138	TRP	3.0
2	H	125	VAL	3.0
1	D	909	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	652	CYS	3.0
2	G	6	LEU	3.0
1	D	653	PHE	3.0
1	A	633	VAL	2.9
2	G	34	PRO	2.9
1	C	1092	GLU	2.9
2	H	131	GLY	2.9
1	D	1137	MET	2.9
1	C	802	GLU	2.9
1	A	789	PHE	2.8
1	D	872	TYR	2.8
2	F	53	LEU	2.8
1	D	1144	PHE	2.8
2	H	78	PHE	2.8
2	G	110	PRO	2.8
1	D	1116	TYR	2.8
1	D	596	ILE	2.8
2	E	112	ILE	2.8
1	A	632	THR	2.8
1	B	557	SER	2.7
2	G	62	GLU	2.7
1	A	557	SER	2.7
2	H	126	VAL	2.7
2	G	47	ASP	2.7
2	F	107	ASP	2.7
2	G	77	GLY	2.7
2	G	159	TYR	2.6
2	G	35	THR	2.6
2	G	115	GLY	2.6
1	D	863	VAL	2.6
2	H	47	ASP	2.6
1	D	864	THR	2.6
2	G	61	THR	2.6
1	D	840	GLU	2.6
2	H	109	VAL	2.6
2	H	157	ILE	2.6
1	B	594	GLY	2.6
1	B	984	ILE	2.6
2	G	141	CYS	2.5
1	B	869	LEU	2.5
2	G	120	LEU	2.5
2	G	165	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	619	VAL	2.5
1	D	1088	PHE	2.5
2	E	60	GLY	2.5
1	A	1113	MET	2.5
1	C	966	LEU	2.5
1	A	1124	LEU	2.5
1	B	649	PHE	2.5
1	D	896	SER	2.5
1	C	1117	PHE	2.4
1	D	959	LEU	2.4
1	B	1005	ASN	2.4
1	B	850	LEU	2.4
1	A	612	GLU	2.4
1	D	1138	HIS	2.4
1	C	959	LEU	2.4
1	C	1078	THR	2.4
2	F	35	THR	2.4
2	H	66	ALA	2.4
2	F	158	PHE	2.4
1	B	653	PHE	2.4
2	E	51	CYS	2.4
2	F	51	CYS	2.4
2	H	61	THR	2.4
2	H	160	ASP	2.4
1	C	885	PRO	2.3
2	F	46	VAL	2.3
1	A	909	HIS	2.3
1	D	1092	GLU	2.3
1	D	984	ILE	2.3
2	H	107	ASP	2.3
1	D	839	ILE	2.3
1	B	561	ASN	2.3
1	C	1088	PHE	2.3
2	F	82	TYR	2.3
2	H	62	GLU	2.3
1	C	984	ILE	2.3
1	A	1063	TYR	2.3
1	B	555	GLN	2.3
1	D	875	GLY	2.3
2	F	139	ASN	2.3
2	H	65	THR	2.3
2	F	130	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	63	GLN	2.2
1	D	850	LEU	2.2
2	H	140	ASN	2.2
2	E	82	TYR	2.2
1	B	839	ILE	2.2
1	B	713	THR	2.2
2	E	46	VAL	2.2
1	D	841	TYR	2.2
1	D	861	GLY	2.2
2	F	65	THR	2.2
1	A	801	LEU	2.2
2	H	44	VAL	2.2
1	D	845	GLY	2.2
2	G	143	PHE	2.1
1	A	841	TYR	2.1
1	C	1132	ASN	2.1
1	D	818	ILE	2.1
2	G	10	GLY	2.1
1	B	1070	TYR	2.1
1	D	967	ALA	2.1
1	B	795	GLU	2.1
2	G	166	ASN	2.1
2	E	63	GLN	2.1
1	D	1100	PHE	2.1
1	C	803	VAL	2.1
1	C	801	LEU	2.1
2	G	111	MET	2.1
2	H	143	PHE	2.1
1	C	897	VAL	2.1
1	C	876	ASP	2.1
1	D	803	VAL	2.1
1	B	596	ILE	2.1
2	F	112	ILE	2.1
2	G	114	VAL	2.0
1	B	677	LEU	2.0
2	E	142	ALA	2.0
2	E	159	TYR	2.0
1	C	1133	LEU	2.0
2	F	120	LEU	2.0
1	D	1113	MET	2.0
1	C	785	LEU	2.0
1	C	883	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	611	PRO	2.0
1	B	782	PRO	2.0
2	H	111	MET	2.0
2	F	97	ARG	2.0
2	H	130	GLN	2.0
1	D	643	LEU	2.0
2	G	68	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)

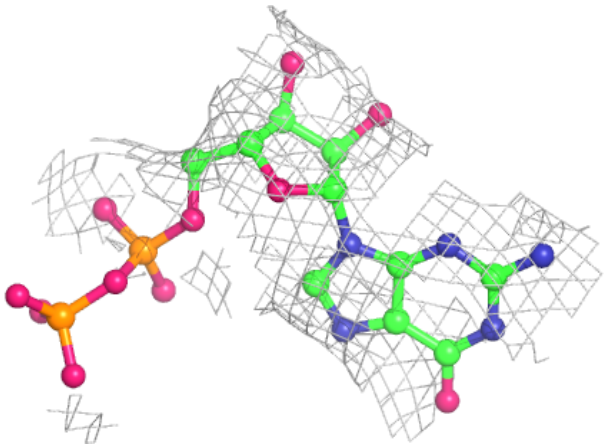
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

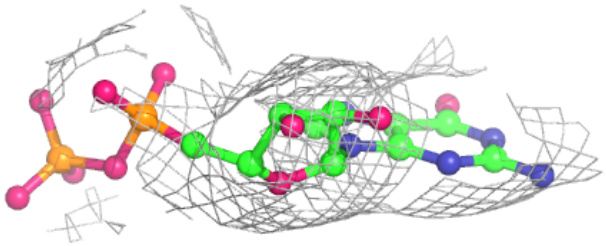
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GDP	G	201	28/28	0.86	0.21	107,139,151,162	0
3	MG	H	200	1/1	0.89	0.29	113,113,113,113	0
4	GDP	E	201	28/28	0.89	0.23	91,127,141,183	0
3	MG	E	200	1/1	0.89	0.22	88,88,88,88	0
4	GDP	F	201	28/28	0.91	0.24	97,120,134,138	0
4	GDP	H	201	28/28	0.91	0.25	123,139,162,166	0
3	MG	G	200	1/1	0.93	0.24	108,108,108,108	0
3	MG	F	200	1/1	0.97	0.28	88,88,88,88	0
5	AF3	E	202	4/4	0.98	0.42	89,128,128,129	0
5	AF3	G	202	4/4	0.98	0.39	87,91,97,125	0
5	AF3	H	202	4/4	0.98	0.35	115,121,159,159	0
5	AF3	F	202	4/4	0.99	0.33	91,103,128,169	0

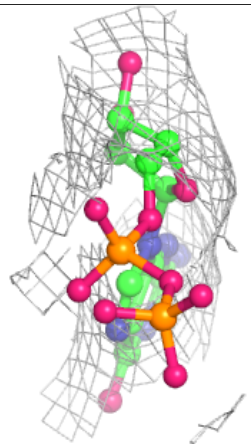
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP G 201:

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

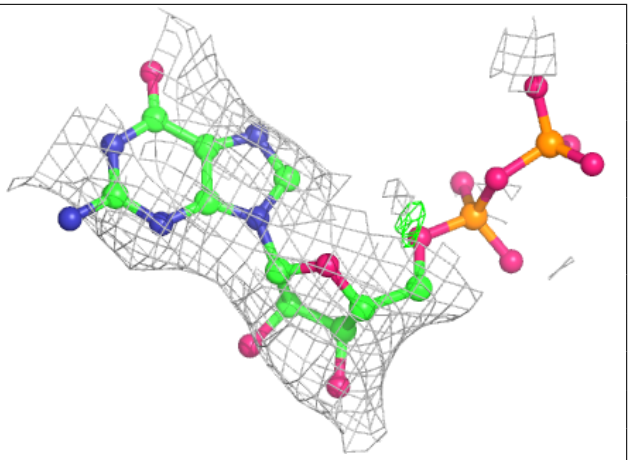


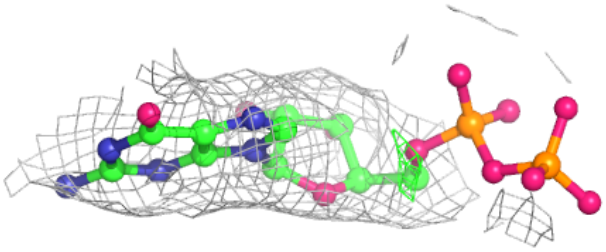


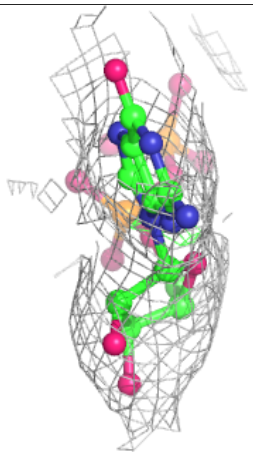


Electron density around GDP E 201:

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

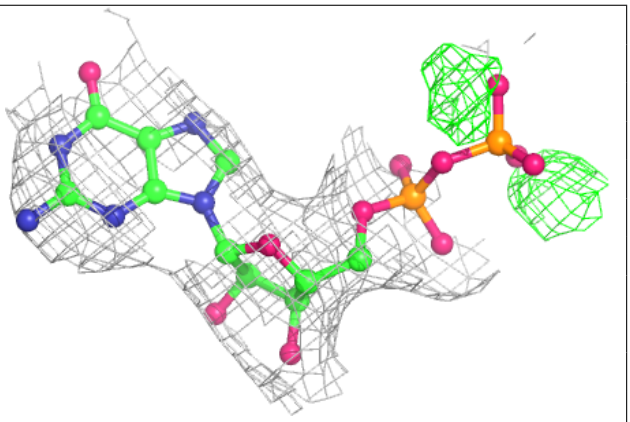


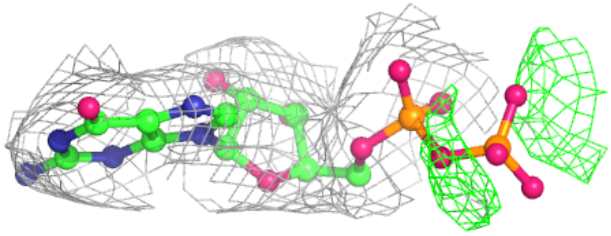


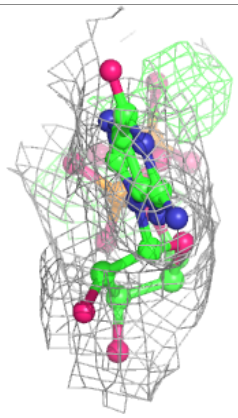


Electron density around GDP F 201:

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

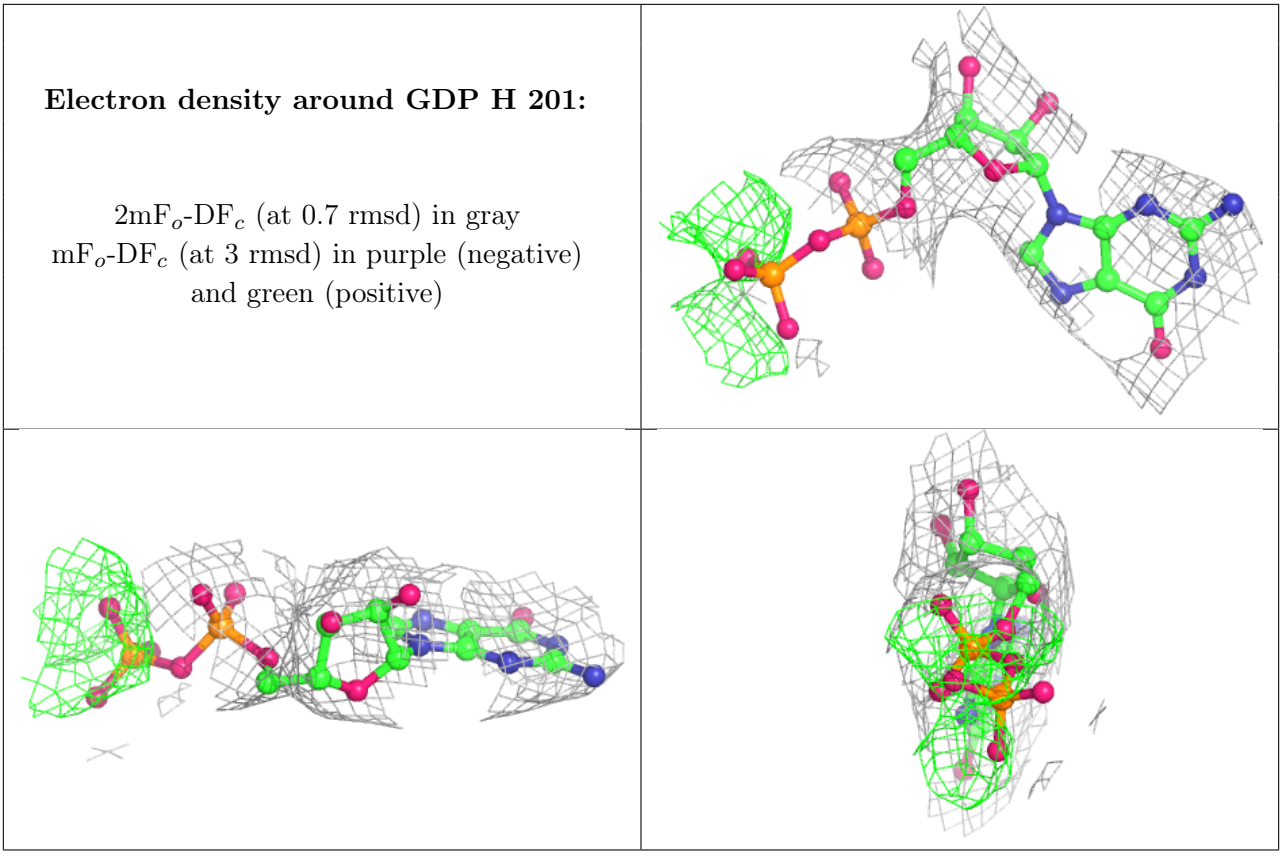






Electron density around GDP H 201:

$2mF_o$-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.