Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 03:57 PM EST

PDB ID	:	4FMC
Title	:	EspG-Rab1 complex
Authors	:	Shao, F.; Zhu, Y.
Deposited on	:	2012-06-16
Resolution	:	2.80 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:

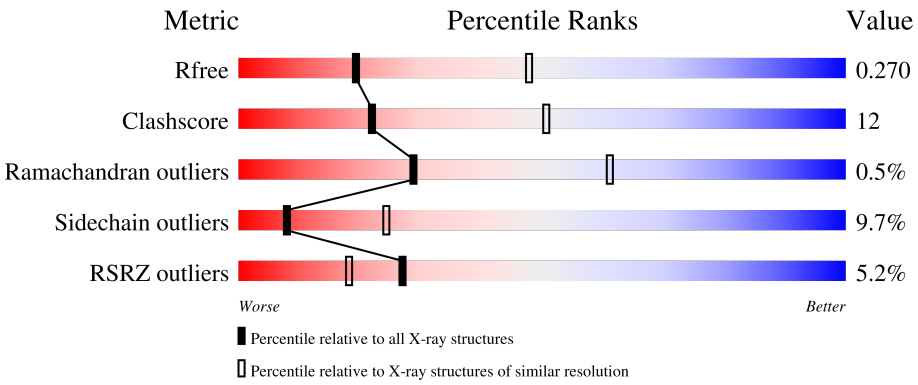
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	351	% 73% 22% 5% •
1	C	351	2% 72% 26% •
1	E	351	8% 70% 26% • •
2	B	171	81% 16% •
2	D	171	2% 70% 25% 5%

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Mol	Chain	Length	Quality of chain
3	F	117	31% 44% 16% • 38%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11470 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 ROrf2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2722	1684	478	544	16	0	0	0
1	C	350	2713	1679	477	541	16	0	0	0
1	E	348	2698	1670	474	538	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ASN	ASP	SEE REMARK 999	UNP O52121
A	244	THR	SER	SEE REMARK 999	UNP O52121
A	269	LYS	ASN	SEE REMARK 999	UNP O52121
A	376	ILE	THR	SEE REMARK 999	UNP O52121
C	123	ASN	ASP	SEE REMARK 999	UNP O52121
C	244	THR	SER	SEE REMARK 999	UNP O52121
C	269	LYS	ASN	SEE REMARK 999	UNP O52121
C	376	ILE	THR	SEE REMARK 999	UNP O52121
E	123	ASN	ASP	SEE REMARK 999	UNP O52121
E	244	THR	SER	SEE REMARK 999	UNP O52121
E	269	LYS	ASN	SEE REMARK 999	UNP O52121
E	376	ILE	THR	SEE REMARK 999	UNP O52121

- Molecule 2 is a protein called Ras-related protein Rab-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	171	1369	873	223	268	5	0	0	0
2	D	171	1369	873	223	268	5	0	0	0

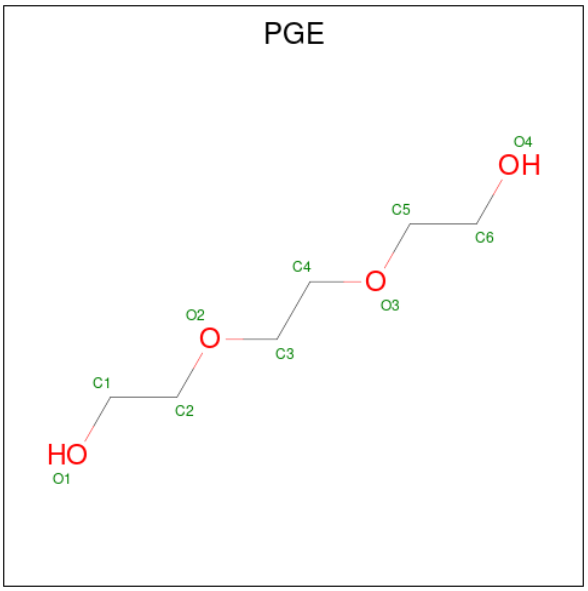
- Molecule 3 is a protein called Ras-related protein Rab-1A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	73	504	307	89	108	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

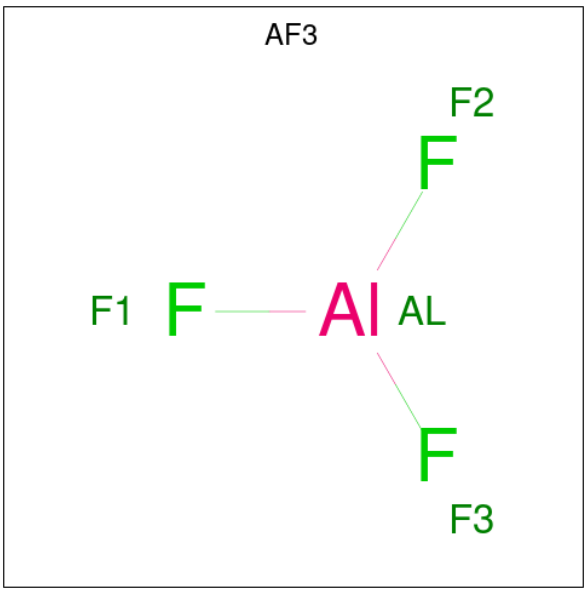
Chain	Residue	Modelled	Actual	Comment	Reference
F	116	ASN	-	expression tag	UNP P62820
F	117	VAL	-	expression tag	UNP P62820
F	118	ASN	-	expression tag	UNP P62820
F	119	LYS	-	expression tag	UNP P62820
F	120	LEU	-	expression tag	UNP P62820
F	121	LEU	-	expression tag	UNP P62820
F	122	VAL	-	expression tag	UNP P62820
F	123	GLY	-	expression tag	UNP P62820
F	124	ASN	-	expression tag	UNP P62820
F	125	LYS	-	expression tag	UNP P62820
F	126	CYS	-	expression tag	UNP P62820
F	127	ASP	-	expression tag	UNP P62820
F	128	LEU	-	expression tag	UNP P62820
F	129	THR	-	expression tag	UNP P62820
F	130	THR	-	expression tag	UNP P62820

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



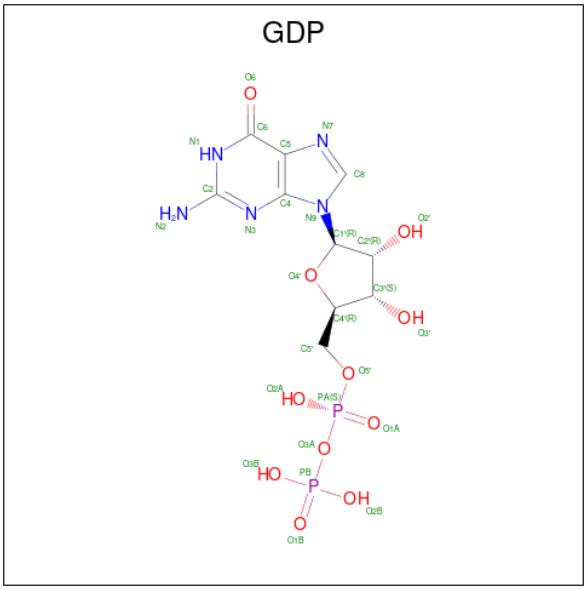
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
5	B	1	4	1	3	0	0
5	D	1	4	1	3	0	0
5	F	1	3	1	2	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P 28 10 5 11 2	0	0
6	D	1	Total C N O P 28 10 5 11 2	0	0
6	F	1	Total C O P 10 1 7 2	0	0

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

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

- Molecule 8 is water.

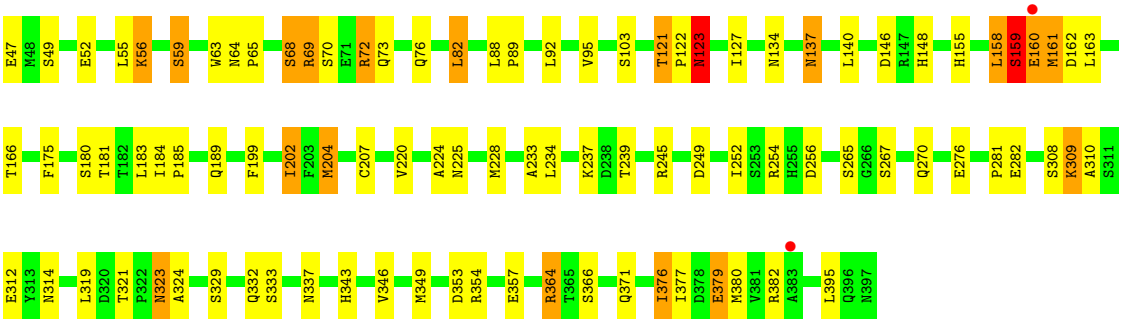
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	B	2	Total O 2 2	0	0
8	C	1	Total O 1 1	0	0
8	D	1	Total O 1 1	0	0

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.

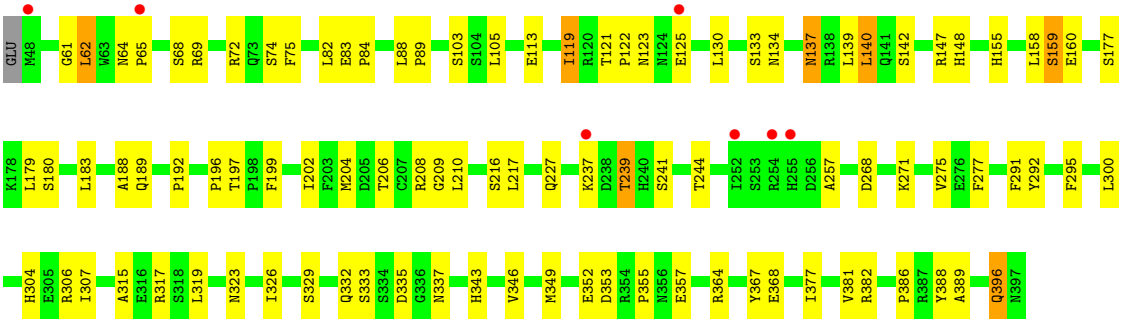
- Molecule 1: ROrf2

Chain A:



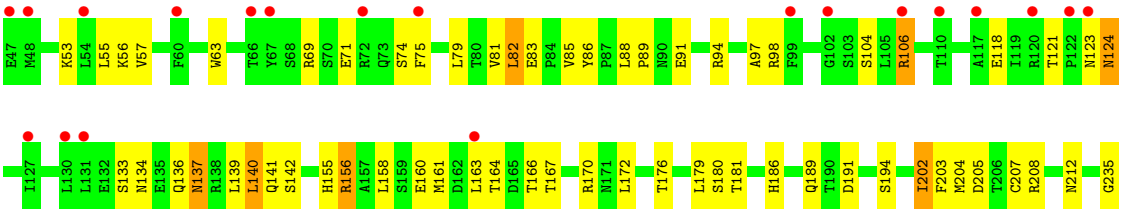
- Molecule 1: ROrf2

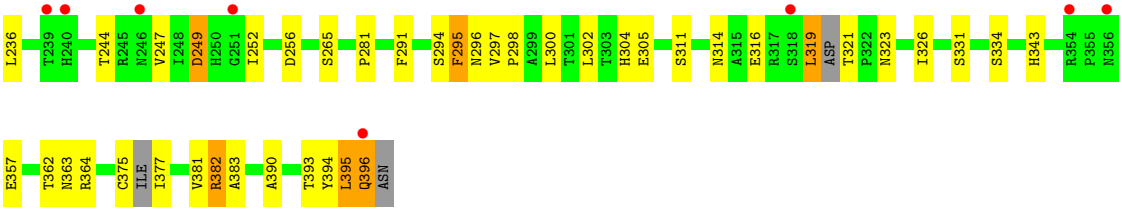
Chain C:



- Molecule 1: ROrf2

Chain E:



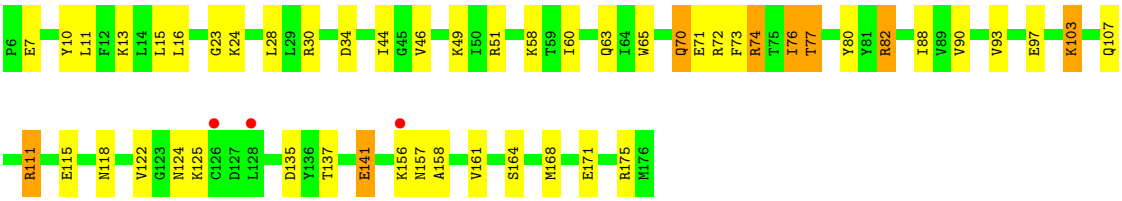


• Molecule 2: Ras-related protein Rab-1A

Chain B:

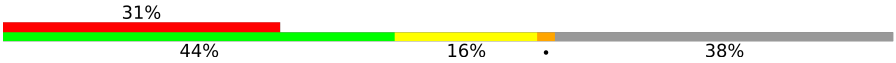
• Molecule 2: Ras-related protein Rab-1A

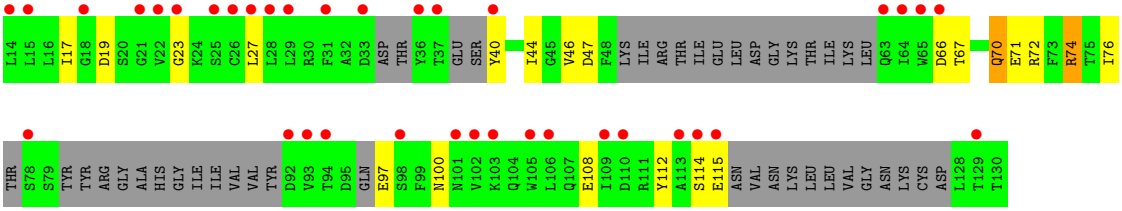
Chain D:



• Molecule 3: Ras-related protein Rab-1A

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.57Å 152.71Å 226.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.67 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 97.2 (49.67-2.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.277 0.223 , 0.270	Depositor DCC
R_{free} test set	2391 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	74.3	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11470	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, PGE, 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	0.64	0/2770	0.74	2/3761 (0.1%)
1	C	0.49	0/2761	0.69	1/3749 (0.0%)
1	E	0.45	0/2744	0.64	3/3722 (0.1%)
2	B	0.62	0/1392	0.73	0/1879
2	D	0.51	0/1392	0.65	0/1879
3	F	0.42	0/501	0.75	1/671 (0.1%)
All	All	0.54	0/11560	0.69	7/15661 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	364	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	302	LEU	CA-CB-CG	5.68	128.36	115.30
3	F	112	TYR	N-CA-C	5.63	126.19	111.00
1	E	383	ALA	N-CA-CB	-5.57	102.30	110.10
1	A	364	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	159	SER	N-CA-C	5.45	125.72	111.00
1	E	136	GLN	CB-CA-C	-5.09	100.21	110.40

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	2722	0	2686	76	0
1	C	2713	0	2680	63	0
1	E	2698	0	2663	69	0
2	B	1369	0	1364	21	0
2	D	1369	0	1364	38	0
3	F	504	0	417	13	0
4	A	10	0	14	1	0
5	B	4	0	0	0	0
5	D	4	0	0	0	0
5	F	3	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	6	0
6	F	10	0	0	1	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
All	All	11470	0	11212	267	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 12.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TRP:CD1	1:A:158:LEU:HD21	1.57	1.39
1:A:202:ILE:HD11	1:A:377:ILE:HG12	1.33	1.10
1:C:62:LEU:O	1:C:62:LEU:HD12	1.51	1.09
1:A:63:TRP:CD1	1:A:158:LEU:CD2	2.34	1.09
1:A:158:LEU:O	1:A:159:SER:HB2	1.52	1.08
1:C:396:GLN:HE21	1:C:396:GLN:HA	1.16	1.05
1:A:202:ILE:HD13	1:A:380:MET:HE1	1.47	0.96
1:A:63:TRP:NE1	1:A:158:LEU:HD21	1.81	0.96
2:D:73:PHE:O	2:D:77:THR:HB	1.68	0.91
1:E:123:ASN:O	1:E:124:ASN:HB2	1.70	0.90
1:A:137:ASN:HD22	1:A:137:ASN:H	1.16	0.90
3:F:114:SER:O	3:F:115:GLU:HG3	1.74	0.88
1:A:160:GLU:O	1:A:160:GLU:HG3	1.71	0.88
2:B:71:GLU:OE1	2:B:72:ARG:HD2	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ARG:HH21	1:E:382:ARG:HG3	1.40	0.85
1:E:314:ASN:HD22	1:E:321:THR:HG21	1.42	0.84
1:A:323:ASN:HD21	2:B:44:ILE:H	1.25	0.84
1:C:61:GLY:CA	1:C:137:ASN:HA	2.07	0.84
1:A:202:ILE:HD13	1:A:380:MET:CE	2.07	0.83
1:C:396:GLN:HA	1:C:396:GLN:NE2	1.96	0.81
1:E:88:LEU:HB3	1:E:89:PRO:HD2	1.62	0.80
1:A:134:ASN:H	1:A:137:ASN:HD21	1.26	0.79
1:C:62:LEU:HD12	1:C:62:LEU:C	2.00	0.79
1:C:61:GLY:HA2	1:C:137:ASN:HA	1.66	0.78
1:E:395:LEU:O	1:E:396:GLN:HB2	1.82	0.78
1:A:63:TRP:HD1	1:A:158:LEU:CD2	1.92	0.78
1:C:61:GLY:O	1:C:64:ASN:HB2	1.83	0.78
1:A:158:LEU:O	1:A:159:SER:CB	2.32	0.77
1:C:134:ASN:H	1:C:137:ASN:HD21	1.30	0.77
1:A:161:MET:O	1:A:395:LEU:HD22	1.86	0.76
1:A:121:THR:HB	1:A:123:ASN:ND2	2.02	0.75
1:A:121:THR:CB	1:A:123:ASN:HD21	2.02	0.73
1:A:376:ILE:HG12	1:A:379:GLU:HB2	1.72	0.72
1:C:179:LEU:O	1:C:364:ARG:NH2	2.23	0.71
1:E:377:ILE:O	1:E:381:VAL:HG23	1.90	0.71
1:A:343:HIS:CD2	1:A:364:ARG:HG3	2.25	0.70
1:A:314:ASN:HD22	1:A:321:THR:HG21	1.55	0.70
2:B:15:LEU:HD12	2:B:65:TRP:HB2	1.73	0.69
1:C:306:ARG:NH1	1:C:349:MET:O	2.26	0.68
1:A:160:GLU:O	1:A:160:GLU:CG	2.41	0.68
1:C:323:ASN:HD21	2:D:44:ILE:H	1.42	0.68
2:D:15:LEU:HD12	2:D:65:TRP:HB2	1.77	0.67
1:E:191:ASP:HB3	1:E:194:SER:HB2	1.77	0.66
1:C:61:GLY:HA3	1:C:137:ASN:HA	1.78	0.64
1:A:254:ARG:NH2	1:A:276:GLU:OE2	2.30	0.64
1:E:323:ASN:HD21	3:F:44:ILE:H	1.44	0.64
1:A:137:ASN:H	1:A:137:ASN:ND2	1.92	0.64
1:E:314:ASN:ND2	1:E:321:THR:HG21	2.14	0.63
1:A:121:THR:HB	1:A:123:ASN:HD21	1.62	0.62
2:B:70:GLN:NE2	2:B:72:ARG:H	1.97	0.62
1:C:72:ARG:HA	1:C:75:PHE:CD2	2.34	0.62
1:C:367:TYR:HB3	1:C:386:PRO:HA	1.81	0.62
1:A:82:LEU:HG	1:A:95:VAL:HG11	1.82	0.61
1:A:88:LEU:HB3	1:A:89:PRO:CD	2.30	0.61
1:A:204:MET:SD	1:A:239:THR:HB	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HG13	1:A:265:SER:O	2.01	0.60
1:E:204:MET:O	1:E:208:ARG:HD3	2.01	0.60
1:E:294:SER:O	1:E:297:VAL:HG23	2.02	0.60
1:E:166:THR:HG22	1:E:170:ARG:HD2	1.83	0.60
1:E:133:SER:HB3	1:E:140:LEU:HD22	1.84	0.60
1:E:235:GLY:HA3	1:E:244:THR:HG23	1.83	0.60
1:A:121:THR:CB	1:A:123:ASN:ND2	2.64	0.60
1:A:92:LEU:HD11	1:A:146:ASP:O	2.01	0.59
1:E:63:TRP:CZ3	1:E:142:SER:HB3	2.37	0.59
2:B:70:GLN:HE22	2:B:72:ARG:HG2	1.66	0.59
1:A:332:GLN:HA	1:A:337:ASN:O	2.02	0.59
1:A:69:ARG:HA	1:A:72:ARG:HG3	1.86	0.58
1:C:61:GLY:HA2	1:C:137:ASN:CA	2.32	0.58
1:C:343:HIS:CD2	1:C:364:ARG:HG3	2.38	0.58
1:A:82:LEU:HG	1:A:95:VAL:CG1	2.34	0.58
2:D:82:ARG:HD2	2:D:82:ARG:O	2.04	0.58
1:A:137:ASN:HD22	1:A:137:ASN:N	1.86	0.57
1:C:62:LEU:C	1:C:62:LEU:CD1	2.71	0.57
1:E:88:LEU:HB3	1:E:89:PRO:CD	2.34	0.57
1:C:62:LEU:O	1:C:62:LEU:CD1	2.40	0.57
3:F:70:GLN:OE1	3:F:71:GLU:N	2.37	0.57
1:C:377:ILE:O	1:C:381:VAL:HG23	2.05	0.57
1:E:186:HIS:CE1	1:E:191:ASP:OD1	2.58	0.57
1:C:61:GLY:O	1:C:64:ASN:CB	2.51	0.57
1:E:208:ARG:HB3	3:F:40:TYR:O	2.05	0.57
2:D:15:LEU:CD1	2:D:65:TRP:HB2	2.35	0.57
1:E:133:SER:CB	1:E:140:LEU:HD22	2.35	0.56
1:A:181:THR:HG23	1:A:364:ARG:NH2	2.19	0.56
1:C:343:HIS:NE2	1:C:364:ARG:NH1	2.52	0.56
2:D:156:LYS:HB2	6:D:202:GDP:N1	2.21	0.56
1:E:244:THR:OG1	1:E:247:VAL:HG23	2.05	0.56
2:D:103:LYS:HE3	2:D:103:LYS:HA	1.88	0.56
1:A:233:ALA:HB1	1:A:252:ILE:HG23	1.87	0.55
1:A:312:GLU:OE2	2:B:65:TRP:HH2	1.88	0.55
1:E:106:ARG:HG3	1:E:118:GLU:HB3	1.87	0.55
1:E:382:ARG:HH21	1:E:382:ARG:CG	2.15	0.55
1:A:343:HIS:NE2	1:A:364:ARG:HG3	2.22	0.55
1:C:353:ASP:O	1:C:355:PRO:HD3	2.07	0.55
1:C:209:GLY:HA3	1:C:291:PHE:CE1	2.42	0.54
1:E:170:ARG:NH2	1:E:212:ASN:O	2.40	0.54
1:A:123:ASN:N	1:A:123:ASN:HD22	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:HIS:CD2	1:E:364:ARG:HG3	2.42	0.54
2:B:73:PHE:O	2:B:77:THR:HB	2.07	0.54
1:E:294:SER:O	1:E:296:ASN:N	2.41	0.54
1:C:134:ASN:H	1:C:137:ASN:ND2	2.01	0.54
1:E:163:LEU:HD21	1:E:172:LEU:HD22	1.89	0.54
1:E:294:SER:C	1:E:296:ASN:N	2.59	0.54
2:D:71:GLU:HA	2:D:74:ARG:HD3	1.90	0.54
2:D:125:LYS:HG2	6:D:202:GDP:C6	2.43	0.54
1:A:68:SER:O	1:A:69:ARG:HB3	2.08	0.53
1:E:294:SER:C	1:E:296:ASN:H	2.11	0.53
1:E:382:ARG:HG3	1:E:382:ARG:NH2	2.14	0.53
3:F:23:GLY:O	3:F:27:LEU:HB2	2.08	0.53
1:A:63:TRP:HD1	1:A:158:LEU:HD23	1.73	0.53
2:B:28:LEU:HD21	2:B:49:LYS:HB2	1.91	0.53
1:A:70:SER:O	1:A:73:GLN:HB2	2.08	0.53
2:D:74:ARG:HH11	2:D:74:ARG:HG2	1.74	0.53
1:A:234:LEU:HD23	1:A:252:ILE:HD11	1.90	0.53
1:E:137:ASN:H	1:E:137:ASN:HD22	1.56	0.53
1:E:304:HIS:CG	1:E:305:GLU:N	2.77	0.53
1:A:333:SER:OG	1:A:337:ASN:HB2	2.08	0.52
1:A:324:ALA:HB3	2:B:41:ILE:HD11	1.92	0.52
2:D:70:GLN:NE2	2:D:72:ARG:H	2.07	0.52
1:E:88:LEU:CB	1:E:89:PRO:HD2	2.38	0.52
2:B:15:LEU:CD1	2:B:65:TRP:HB2	2.37	0.51
2:D:70:GLN:HE22	2:D:72:ARG:HG2	1.75	0.51
2:D:125:LYS:HG2	6:D:202:GDP:C5	2.46	0.51
1:C:103:SER:HB3	1:C:122:PRO:HD3	1.92	0.51
1:E:134:ASN:H	1:E:137:ASN:HD21	1.59	0.51
2:D:88:ILE:HG13	2:D:168:MET:HE3	1.92	0.50
1:C:257:ALA:HB1	1:C:275:VAL:HA	1.94	0.50
1:C:317:ARG:O	1:C:319:LEU:HD12	2.11	0.50
3:F:71:GLU:HA	3:F:74:ARG:CD	2.42	0.50
2:D:30:ARG:O	2:D:34:ASP:HA	2.11	0.49
1:C:268:ASP:HA	1:C:271:LYS:HB2	1.94	0.49
1:C:68:SER:O	1:C:69:ARG:CB	2.59	0.49
1:C:155:HIS:HE1	1:C:180:SER:O	1.96	0.49
1:E:88:LEU:HB2	1:E:91:GLU:HG3	1.94	0.49
1:C:199:PHE:O	1:C:202:ILE:HG12	2.12	0.49
1:C:315:ALA:C	1:C:317:ARG:H	2.16	0.49
2:D:161:VAL:O	2:D:164:SER:HB2	2.13	0.49
2:B:70:GLN:HE22	2:B:72:ARG:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:O	1:A:202:ILE:HG12	2.12	0.49
1:A:207:CYS:CB	1:A:239:THR:HG22	2.43	0.49
1:C:304:HIS:HD2	2:D:80:TYR:OH	1.95	0.49
1:E:55:LEU:HD23	1:E:56:LYS:HE3	1.95	0.49
3:F:114:SER:O	3:F:115:GLU:CG	2.54	0.49
1:A:207:CYS:HB3	1:A:239:THR:HG22	1.94	0.49
1:A:281:PRO:HD2	1:A:282:GLU:OE2	2.13	0.48
1:C:133:SER:CB	1:C:140:LEU:HD22	2.43	0.48
1:C:333:SER:OG	1:C:337:ASN:HB2	2.13	0.48
1:E:85:VAL:HG12	1:E:331:SER:CB	2.43	0.48
1:E:156:ARG:HA	1:E:394:TYR:O	2.13	0.48
1:A:162:ASP:OD2	1:A:163:LEU:N	2.46	0.48
1:A:202:ILE:HG21	1:A:380:MET:HE1	1.95	0.48
1:E:82:LEU:HD12	1:E:97:ALA:HB2	1.94	0.48
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.96	0.48
1:E:194:SER:O	3:F:72:ARG:HD3	2.14	0.48
1:E:297:VAL:HB	1:E:298:PRO:HD3	1.94	0.48
1:C:204:MET:O	1:C:208:ARG:HD3	2.13	0.48
1:E:382:ARG:CG	1:E:382:ARG:NH2	2.74	0.48
2:B:82:ARG:NH2	2:B:114:SER:HB2	2.29	0.48
1:C:304:HIS:HA	1:C:307:ILE:HD12	1.96	0.47
1:E:98:ARG:HG2	1:E:104:SER:HB2	1.96	0.47
1:A:160:GLU:O	1:A:162:ASP:N	2.48	0.47
1:C:206:THR:HG23	1:C:291:PHE:CD2	2.50	0.47
1:A:312:GLU:OE2	2:B:65:TRP:CH2	2.67	0.47
1:A:148:HIS:HB3	1:C:148:HIS:CE1	2.50	0.47
2:D:10:TYR:HB2	2:D:60:ILE:HG23	1.97	0.47
1:C:61:GLY:HA2	1:C:137:ASN:O	2.15	0.47
2:D:28:LEU:HD21	2:D:49:LYS:HB2	1.97	0.47
1:E:53:LYS:O	1:E:57:VAL:HG23	2.15	0.47
1:A:55:LEU:O	1:A:59:SER:HB2	2.14	0.46
1:A:202:ILE:HD11	1:A:377:ILE:CG1	2.23	0.46
1:A:56:LYS:HD3	1:A:56:LYS:HA	1.64	0.46
1:C:113:GLU:OE1	1:C:147:ARG:NH2	2.48	0.46
1:C:396:GLN:HE21	1:C:396:GLN:CA	2.06	0.46
2:D:93:VAL:HG22	2:D:124:ASN:O	2.14	0.46
2:B:46:VAL:HG21	2:B:80:TYR:CE2	2.51	0.46
1:C:88:LEU:HB3	1:C:89:PRO:HD2	1.96	0.46
1:E:294:SER:O	1:E:295:PHE:C	2.53	0.46
1:A:353:ASP:OD2	1:A:354:ARG:HG3	2.15	0.46
1:C:105:LEU:HD13	1:C:119:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:GLN:O	2:D:111:ARG:HB2	2.15	0.46
2:D:13:LYS:HE2	2:D:63:GLN:HE22	1.81	0.46
2:D:74:ARG:HG2	2:D:74:ARG:NH1	2.31	0.46
1:C:323:ASN:ND2	2:D:44:ILE:H	2.13	0.46
1:E:155:HIS:HB2	1:E:393:THR:HG23	1.97	0.46
2:D:71:GLU:OE1	2:D:72:ARG:HD2	2.15	0.45
1:E:123:ASN:O	1:E:124:ASN:CB	2.50	0.45
1:A:155:HIS:HE1	1:A:180:SER:O	2.00	0.45
4:A:401:PGE:H4	1:C:304:HIS:HE1	1.82	0.45
1:C:69:ARG:HA	1:C:72:ARG:CG	2.46	0.45
1:E:155:HIS:HE1	1:E:180:SER:O	1.99	0.45
2:D:90:VAL:HA	2:D:122:VAL:O	2.17	0.45
1:E:181:THR:HG23	1:E:364:ARG:NH2	2.32	0.45
2:B:157:ASN:O	2:B:158:ALA:HB3	2.16	0.45
1:A:158:LEU:HD12	1:A:175:PHE:CZ	2.52	0.45
1:E:319:LEU:C	1:E:321:THR:HG22	2.38	0.45
3:F:23:GLY:H	6:F:202:GDP:PA	2.40	0.44
1:C:177:SER:HB2	1:C:343:HIS:CD2	2.51	0.44
1:E:81:VAL:O	1:E:83:GLU:HG2	2.18	0.44
1:E:204:MET:HB3	1:E:208:ARG:NH1	2.32	0.44
3:F:71:GLU:HA	3:F:74:ARG:HD3	1.99	0.44
2:D:157:ASN:O	2:D:158:ALA:HB3	2.18	0.44
1:A:49:SER:HB3	1:A:52:GLU:OE1	2.17	0.44
1:A:72:ARG:O	1:A:76:GLN:HG2	2.17	0.44
1:C:192:PRO:HG2	1:C:388:TYR:CZ	2.53	0.44
1:E:296:ASN:HA	1:E:363:ASN:ND2	2.33	0.44
1:E:252:ILE:HG22	1:E:256:ASP:HB2	2.00	0.44
2:B:82:ARG:HA	2:B:82:ARG:HD2	1.79	0.44
1:E:86:TYR:O	1:E:94:ARG:HD2	2.17	0.44
1:C:210:LEU:HB3	1:C:227:GLN:HB3	1.99	0.44
2:D:24:LYS:NZ	6:D:202:GDP:O2B	2.44	0.44
1:A:308:SER:OG	2:B:80:TYR:OH	2.26	0.44
1:C:188:ALA:O	2:D:72:ARG:NH2	2.51	0.43
1:A:148:HIS:CE1	1:A:183:LEU:HD13	2.53	0.43
1:A:158:LEU:CD1	1:A:175:PHE:CZ	3.00	0.43
2:D:46:VAL:HG21	2:D:80:TYR:CE2	2.54	0.43
2:D:23:GLY:HA2	6:D:202:GDP:PA	2.58	0.43
1:A:245:ARG:HH21	1:A:249:ASP:CG	2.21	0.43
1:E:158:LEU:O	1:E:161:MET:HE3	2.18	0.43
1:E:85:VAL:HG12	1:E:331:SER:HB3	1.99	0.43
1:C:69:ARG:HA	1:C:72:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:O	1:A:202:ILE:CG1	2.67	0.43
2:B:161:VAL:O	2:B:164:SER:HB2	2.19	0.43
2:D:30:ARG:HG2	2:D:161:VAL:HG21	2.01	0.43
2:D:70:GLN:HE22	2:D:72:ARG:H	1.67	0.43
1:E:75:PHE:O	1:E:79:LEU:N	2.42	0.43
2:B:125:LYS:HG2	6:B:202:GDP:C5	2.54	0.42
1:C:64:ASN:HA	1:C:65:PRO:HD3	1.87	0.42
1:E:249:ASP:O	1:E:281:PRO:HG3	2.19	0.42
1:E:141:GLN:HA	1:E:180:SER:OG	2.20	0.42
1:A:224:ALA:O	1:A:228:MET:HG2	2.20	0.42
1:A:184:ILE:HG22	1:A:185:PRO:O	2.19	0.42
3:F:46:VAL:HG22	3:F:67:THR:HG22	2.01	0.42
1:C:183:LEU:HD23	1:C:389:ALA:HB2	2.02	0.42
2:D:137:THR:O	2:D:141:GLU:HB2	2.20	0.42
1:E:202:ILE:HD12	1:E:203:PHE:CE1	2.55	0.42
1:E:205:ASP:HB3	1:E:291:PHE:O	2.20	0.42
1:A:252:ILE:HG22	1:A:256:ASP:HB2	2.01	0.42
1:A:309:LYS:HD2	1:A:309:LYS:HA	1.84	0.42
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.95	0.42
2:D:88:ILE:HG13	2:D:168:MET:CE	2.49	0.42
1:E:176:THR:HA	1:E:179:LEU:HD12	2.02	0.42
1:A:267:SER:OG	1:A:270:GLN:HG3	2.19	0.41
1:A:310:ALA:HB2	1:A:349:MET:HG2	2.01	0.41
1:C:61:GLY:O	1:C:64:ASN:N	2.54	0.41
1:A:123:ASN:ND2	1:A:123:ASN:N	2.68	0.41
2:D:76:ILE:HG21	2:D:76:ILE:HD13	1.64	0.41
1:C:137:ASN:HD22	1:C:137:ASN:H	1.69	0.41
1:C:332:GLN:HA	1:C:337:ASN:O	2.20	0.41
1:E:208:ARG:O	1:E:212:ASN:ND2	2.52	0.41
1:E:362:THR:O	1:E:390:ALA:HA	2.20	0.41
2:B:82:ARG:NH2	2:B:82:ARG:O	2.52	0.41
2:B:76:ILE:HG21	2:B:76:ILE:HD13	1.68	0.41
1:C:121:THR:OG1	1:C:125:GLU:HB3	2.20	0.41
1:C:292:TYR:HD2	1:C:295:PHE:CE1	2.39	0.41
1:C:196:PRO:HB2	1:C:197:THR:HG23	2.03	0.41
2:D:118:ASN:OD1	2:D:175:ARG:NH1	2.54	0.41
2:D:125:LYS:HE2	6:D:202:GDP:C8	2.56	0.41
1:E:134:ASN:N	1:E:137:ASN:HD21	2.19	0.40
3:F:47:ASP:O	3:F:66:ASP:N	2.48	0.40
1:A:64:ASN:HA	1:A:65:PRO:HD3	1.90	0.40
1:C:83:GLU:HA	1:C:84:PRO:HD2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LEU:HD22	1:C:277:PHE:HE2	1.86	0.40
3:F:97:GLU:HA	3:F:100:ASN:ND2	2.36	0.40
1:A:103:SER:HB3	1:A:122:PRO:HD3	2.02	0.40
1:E:71:GLU:O	1:E:74:SER:HB2	2.22	0.40
1:E:79:LEU:C	1:E:81:VAL:H	2.25	0.40
1:E:202:ILE:HA	1:E:205:ASP:HB2	2.04	0.40
1:E:291:PHE:CD1	1:E:326:ILE:HD13	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	349/351 (99%)	331 (95%)	15 (4%)	3 (1%)	17	46
1	C	348/351 (99%)	316 (91%)	30 (9%)	2 (1%)	25	56
1	E	342/351 (97%)	313 (92%)	27 (8%)	2 (1%)	25	56
2	B	169/171 (99%)	159 (94%)	10 (6%)	0	100	100
2	D	169/171 (99%)	157 (93%)	12 (7%)	0	100	100
3	F	57/117 (49%)	55 (96%)	2 (4%)	0	100	100
All	All	1434/1512 (95%)	1331 (93%)	96 (7%)	7 (0%)	29	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	A	161	MET
1	E	124	ASN
1	C	352	GLU
1	E	295	PHE

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Mol	Chain	Res	Type
1	C	239	THR
1	A	123	ASN

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	312/312 (100%)	280 (90%)	32 (10%)	7 21
1	C	311/312 (100%)	284 (91%)	27 (9%)	10 30
1	E	309/312 (99%)	282 (91%)	27 (9%)	10 30
2	B	151/151 (100%)	136 (90%)	15 (10%)	8 23
2	D	151/151 (100%)	134 (89%)	17 (11%)	6 18
3	F	45/104 (43%)	39 (87%)	6 (13%)	4 12
All	All	1279/1342 (95%)	1155 (90%)	124 (10%)	8 24

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	56	LYS
1	A	59	SER
1	A	68	SER
1	A	69	ARG
1	A	72	ARG
1	A	82	LEU
1	A	121	THR
1	A	123	ASN
1	A	127	ILE
1	A	137	ASN
1	A	140	LEU
1	A	158	LEU
1	A	159	SER
1	A	160	GLU
1	A	166	THR

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Mol	Chain	Res	Type
1	A	189	GLN
1	A	202	ILE
1	A	204	MET
1	A	225	ASN
1	A	237	LYS
1	A	309	LYS
1	A	319	LEU
1	A	323	ASN
1	A	329	SER
1	A	346	VAL
1	A	357	GLU
1	A	366	SER
1	A	371	GLN
1	A	376	ILE
1	A	379	GLU
1	A	382	ARG
2	B	11	LEU
2	B	16	LEU
2	B	51	ARG
2	B	56	ASP
2	B	58	LYS
2	B	70	GLN
2	B	74	ARG
2	B	76	ILE
2	B	77	THR
2	B	103	LYS
2	B	114	SER
2	B	115	GLU
2	B	130	THR
2	B	138	THR
2	B	141	GLU
1	C	62	LEU
1	C	74	SER
1	C	82	LEU
1	C	119	ILE
1	C	123	ASN
1	C	130	LEU
1	C	137	ASN
1	C	139	LEU
1	C	140	LEU
1	C	142	SER
1	C	159	SER

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Mol	Chain	Res	Type
1	C	160	GLU
1	C	189	GLN
1	C	216	SER
1	C	237	LYS
1	C	239	THR
1	C	241	SER
1	C	244	THR
1	C	300	LEU
1	C	326	ILE
1	C	329	SER
1	C	335	ASP
1	C	346	VAL
1	C	357	GLU
1	C	368	GLU
1	C	382	ARG
1	C	396	GLN
2	D	7	GLU
2	D	11	LEU
2	D	16	LEU
2	D	51	ARG
2	D	58	LYS
2	D	70	GLN
2	D	74	ARG
2	D	76	ILE
2	D	77	THR
2	D	82	ARG
2	D	97	GLU
2	D	103	LYS
2	D	111	ARG
2	D	115	GLU
2	D	135	ASP
2	D	141	GLU
2	D	171	GLU
1	E	69	ARG
1	E	82	LEU
1	E	106	ARG
1	E	121	THR
1	E	137	ASN
1	E	139	LEU
1	E	140	LEU
1	E	156	ARG
1	E	160	GLU

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Mol	Chain	Res	Type
1	E	164	THR
1	E	167	THR
1	E	189	GLN
1	E	202	ILE
1	E	207	CYS
1	E	236	LEU
1	E	249	ASP
1	E	265	SER
1	E	300	LEU
1	E	311	SER
1	E	316	GLU
1	E	319	LEU
1	E	334	SER
1	E	357	GLU
1	E	375	CYS
1	E	382	ARG
1	E	395	LEU
1	E	396	GLN
3	F	17	ILE
3	F	19	ASP
3	F	70	GLN
3	F	74	ARG
3	F	76	ILE
3	F	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	123	ASN
1	A	137	ASN
1	A	155	HIS
1	A	304	HIS
1	A	314	ASN
1	A	323	ASN
1	A	397	ASN
2	B	70	GLN
1	C	111	ASN
1	C	123	ASN
1	C	137	ASN
1	C	155	HIS
1	C	171	ASN

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Mol	Chain	Res	Type
1	C	270	GLN
1	C	304	HIS
1	C	323	ASN
1	C	332	GLN
1	C	396	GLN
2	D	63	GLN
2	D	70	GLN
1	E	137	ASN
1	E	155	HIS
1	E	250	HIS
1	E	270	GLN
1	E	314	ASN
1	E	323	ASN
1	E	363	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	PGE	A	401	-	9,9,9	1.39	2 (22%)	8,8,8	0.96	1 (12%)
6	GDP	F	202	5,7	7,9,30	2.03	2 (28%)	12,14,47	1.76	4 (33%)
5	AF3	B	201	6,8	0,3,3	-	-	-		
6	GDP	D	202	5,7	24,30,30	1.86	3 (12%)	30,47,47	1.58	7 (23%)
5	AF3	D	201	6,8	0,3,3	-	-	-		
6	GDP	B	202	5,7	24,30,30	1.72	3 (12%)	30,47,47	1.71	6 (20%)
5	AF3	F	201	6	0,2,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	D	202	5,7	-	5/12/32/32	0/3/3/3
6	GDP	B	202	5,7	-	3/12/32/32	0/3/3/3
4	PGE	A	401	-	-	4/7/7/7	-
6	GDP	F	202	5,7	-	1/9/9/32	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	202	GDP	O6-C6	6.90	1.37	1.23
6	B	202	GDP	O6-C6	6.01	1.35	1.23
6	D	202	GDP	PB-O1B	3.41	1.61	1.50
6	F	202	GDP	PB-O1B	3.22	1.60	1.50
6	F	202	GDP	PA-O1A	3.00	1.61	1.50
6	B	202	GDP	PA-O1A	2.89	1.61	1.50
6	D	202	GDP	O4'-C1'	2.64	1.44	1.41
4	A	401	PGE	O3-C5	2.31	1.52	1.42
4	A	401	PGE	O2-C2	2.08	1.51	1.42
6	B	202	GDP	O4'-C1'	2.06	1.44	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	202	GDP	PA-O3A-PB	-5.50	113.95	132.83
6	B	202	GDP	PA-O3A-PB	-5.36	114.43	132.83
6	B	202	GDP	C3'-C2'-C1'	4.02	107.03	100.98
6	F	202	GDP	PA-O3A-PB	-3.21	121.81	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	202	GDP	O2B-PB-O3A	2.93	114.46	104.64
6	B	202	GDP	C5-C6-N1	2.89	119.06	113.95
6	B	202	GDP	C2-N1-C6	-2.74	120.05	125.10
6	F	202	GDP	O3B-PB-O3A	2.54	113.15	104.64
6	D	202	GDP	C3'-C2'-C1'	2.45	104.67	100.98
6	B	202	GDP	O3B-PB-O3A	2.40	112.69	104.64
6	D	202	GDP	C8-N7-C5	2.39	107.55	102.99
6	B	202	GDP	C8-N7-C5	2.33	107.43	102.99
6	F	202	GDP	O3A-PA-O5'	2.25	109.60	102.58
4	A	401	PGE	O3-C5-C6	2.22	119.84	110.07
6	D	202	GDP	C2-N1-C6	-2.19	121.06	125.10
6	D	202	GDP	N2-C2-N1	2.15	121.29	116.71
6	D	202	GDP	C5-C6-N1	2.15	117.74	113.95
6	D	202	GDP	PA-O5'-C5'	-2.02	109.82	121.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	202	GDP	PA-O3A-PB-O3B
6	D	202	GDP	C5'-O5'-PA-O1A
6	D	202	GDP	C5'-O5'-PA-O2A
6	D	202	GDP	O4'-C4'-C5'-O5'
6	D	202	GDP	C3'-C4'-C5'-O5'
4	A	401	PGE	O1-C1-C2-O2
4	A	401	PGE	O3-C5-C6-O4
6	B	202	GDP	PA-O3A-PB-O2B
4	A	401	PGE	C3-C4-O3-C5
4	A	401	PGE	O2-C3-C4-O3
6	F	202	GDP	C5'-O5'-PA-O1A
6	D	202	GDP	C5'-O5'-PA-O3A
6	B	202	GDP	PA-O3A-PB-O1B

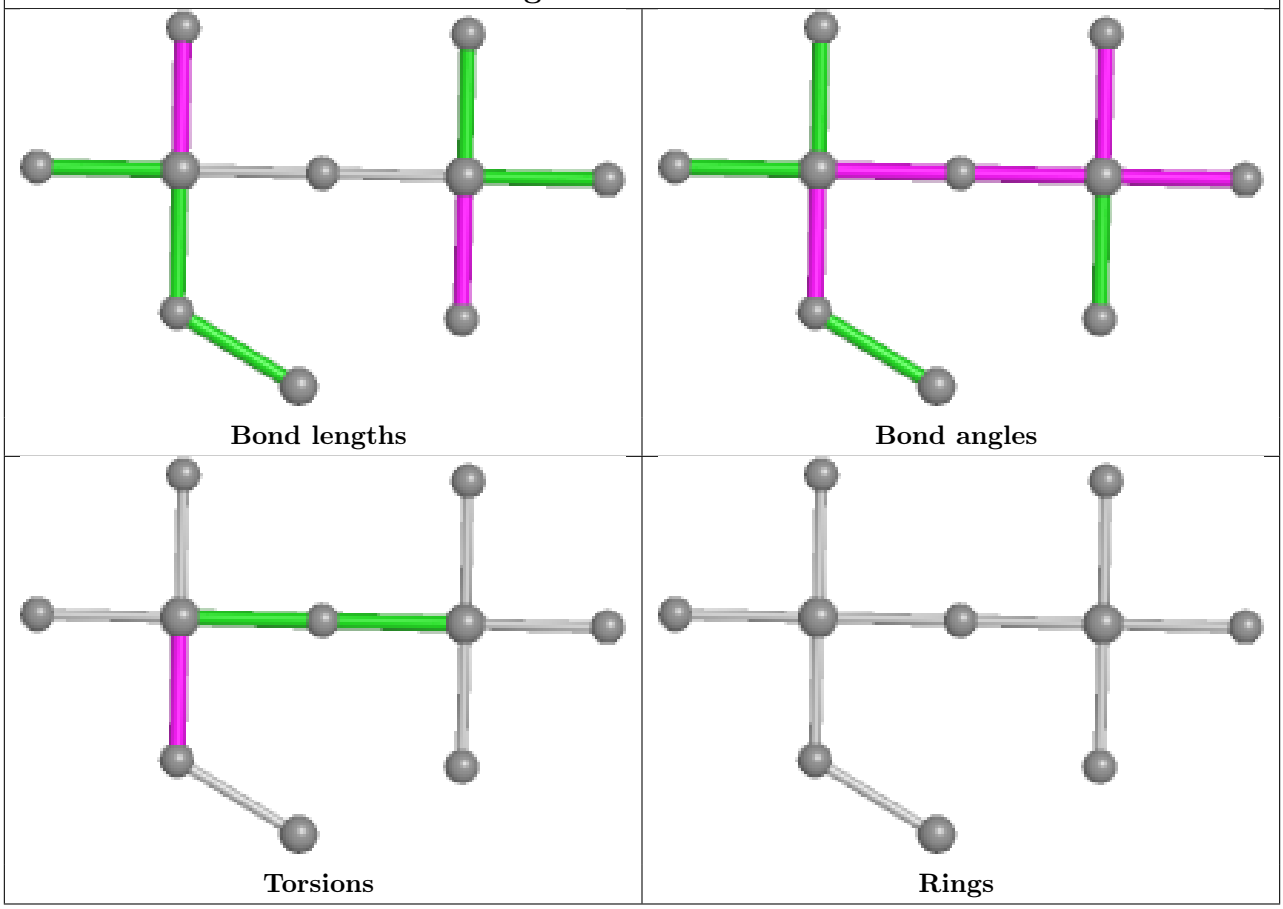
There are no ring outliers.

4 monomers are involved in 9 short contacts:

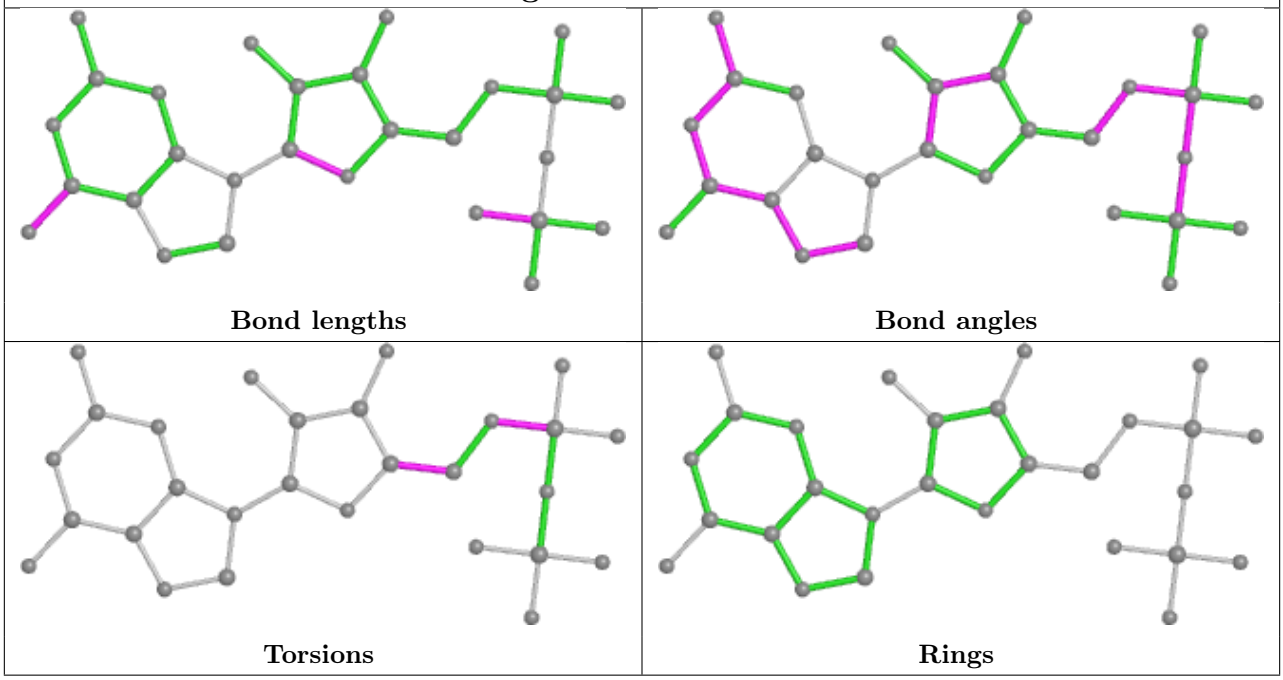
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	PGE	1	0
6	F	202	GDP	1	0
6	D	202	GDP	6	0
6	B	202	GDP	1	0

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

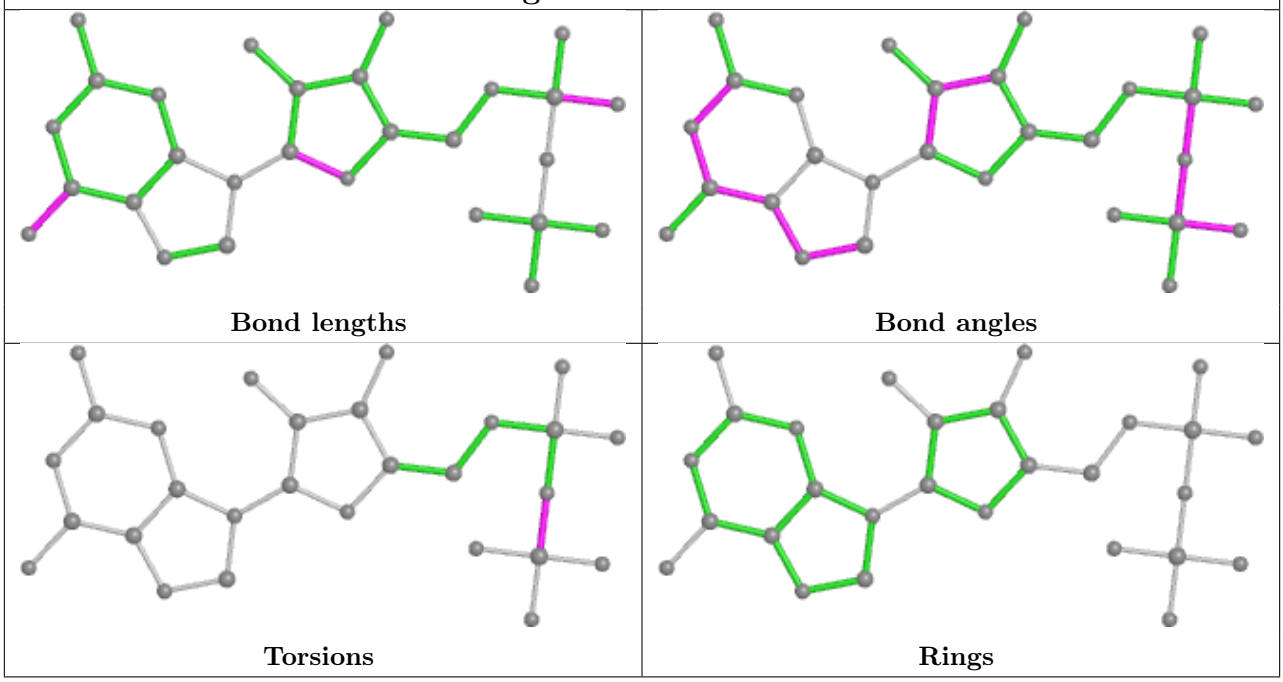
Ligand GDP F 202



Ligand GDP D 202



Ligand GDP B 202



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	351/351 (100%)	-0.03	2 (0%) 89 86	44, 70, 104, 118	0
1	C	350/351 (99%)	0.11	7 (2%) 65 56	49, 100, 158, 174	0
1	E	348/351 (99%)	0.46	28 (8%) 12 6	61, 126, 222, 273	0
2	B	171/171 (100%)	-0.23	0 100 100	47, 66, 89, 114	0
2	D	171/171 (100%)	0.11	3 (1%) 68 61	57, 98, 135, 165	0
3	F	73/117 (62%)	2.28	36 (49%) 0 0	181, 242, 269, 306	0
All	All	1464/1512 (96%)	0.23	76 (5%) 27 18	44, 91, 218, 306	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	64	ILE	9.2
3	F	109	ILE	7.5
3	F	40	TYR	6.6
3	F	102	VAL	5.5
3	F	22	VAL	5.5
3	F	63	GLN	5.5
3	F	101	ASN	4.8
3	F	94	THR	4.7
3	F	113	ALA	4.5
3	F	92	ASP	4.2
3	F	93	VAL	4.2
1	E	131	LEU	4.2
3	F	37	THR	4.2
3	F	29	LEU	4.0
3	F	114	SER	4.0
3	F	33	ASP	3.8
3	F	14	LEU	3.7
1	E	240	HIS	3.7
3	F	115	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
3	F	26	CYS	3.6
1	C	65	PRO	3.6
3	F	105	TRP	3.5
1	E	48	MET	3.5
1	E	239	THR	3.4
1	E	356	ASN	3.4
3	F	18	GLY	3.2
2	D	126	CYS	3.1
1	A	160	GLU	3.1
1	E	75	PHE	3.1
1	E	127	ILE	3.1
1	E	246	ASN	3.0
3	F	129	THR	3.0
1	E	117	ALA	2.9
1	C	252	ILE	2.9
1	E	120	ARG	2.9
3	F	15	LEU	2.9
3	F	66	ASP	2.8
1	E	66	THR	2.8
3	F	27	LEU	2.7
3	F	106	LEU	2.7
3	F	25	SER	2.7
1	C	125	GLU	2.6
1	E	106	ARG	2.6
1	E	396	GLN	2.6
1	E	122	PRO	2.6
1	E	72	ARG	2.6
3	F	65	TRP	2.6
1	C	254	ARG	2.5
1	E	318	SER	2.5
1	C	48	MET	2.5
1	C	255	HIS	2.5
1	E	123	ASN	2.4
2	D	156	LYS	2.4
1	E	163	LEU	2.4
1	E	354	ARG	2.4
1	E	130	LEU	2.3
2	D	128	LEU	2.3
3	F	21	GLY	2.3
3	F	31	PHE	2.3
3	F	36	TYR	2.3
1	E	251	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	78	SER	2.3
3	F	28	LEU	2.2
1	E	60	PHE	2.2
1	E	102	GLY	2.2
1	E	110	THR	2.2
1	E	47	GLU	2.2
1	E	54	LEU	2.1
3	F	110	ASP	2.1
1	A	383	ALA	2.1
1	E	67	TYR	2.1
1	C	237	LYS	2.1
3	F	103	LYS	2.0
3	F	98	SER	2.0
3	F	23	GLY	2.0
1	E	99	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
5	AF3	F	201	3/4	0.65	0.24	34,34,34,34	0
6	GDP	F	202	10/28	0.70	0.26	197,202,204,204	0
7	MG	F	203	1/1	0.75	0.17	192,192,192,192	0
4	PGE	A	401	10/10	0.80	0.38	61,68,73,74	0
5	AF3	D	201	4/4	0.92	0.17	37,38,38,38	0
7	MG	B	203	1/1	0.93	0.12	52,52,52,52	0
6	GDP	D	202	28/28	0.95	0.17	69,98,113,120	0
5	AF3	B	201	4/4	0.98	0.06	36,38,38,39	0

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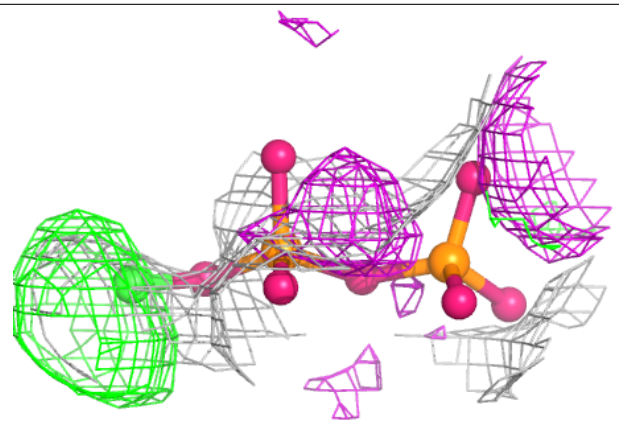
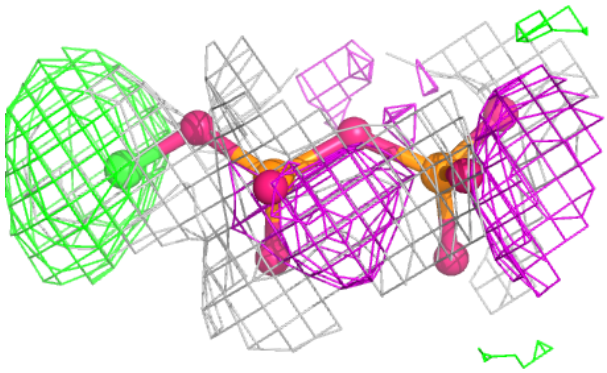
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	D	203	1/1	0.99	0.12	78,78,78,78	0
6	GDP	B	202	28/28	0.99	0.16	45,58,64,68	0

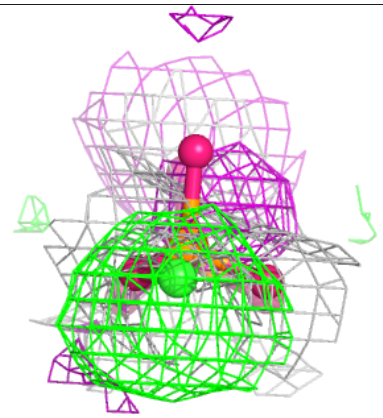
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP F 202:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

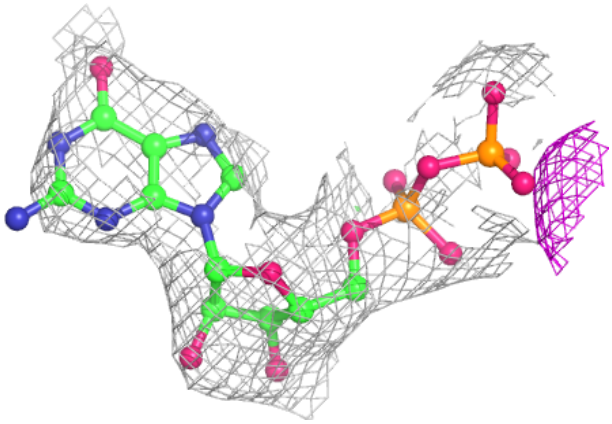


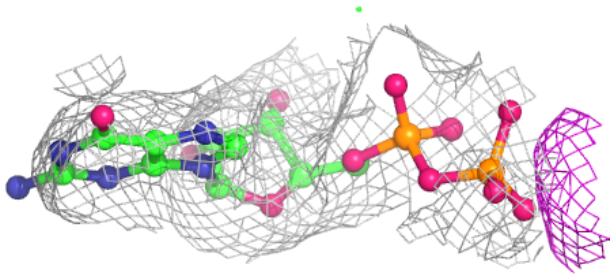


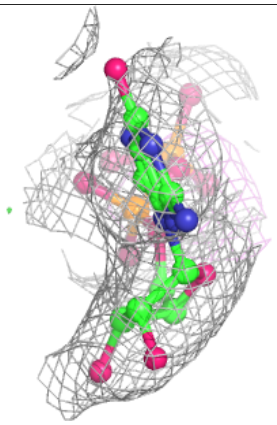


Electron density around GDP D 202:

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

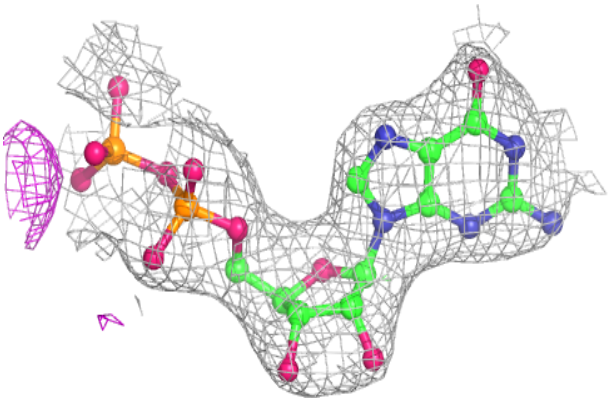


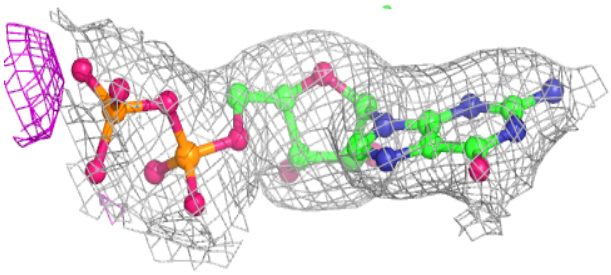


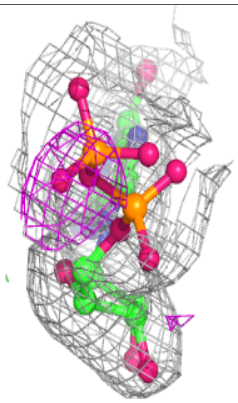


Electron density around GDP B 202:

$2mF_o$-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.