Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 11:03 PM EDT

PDB ID	:	4FMD / pdb_00004fmd
Title	:	EspG-Rab1 complex structure at 3.05 A
Authors	:	Shao, F.; Zhu, Y.
Deposited on	:	2012-06-16
Resolution	:	3.05 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:

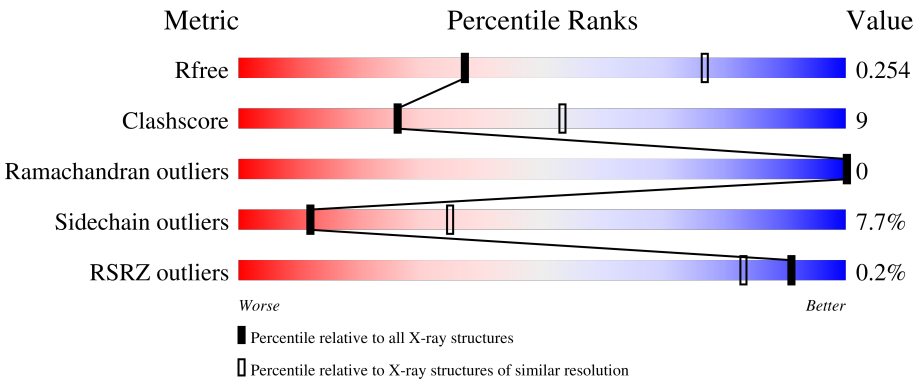
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	77% 20% •
1	C	351	70% 26% •
1	E	351	% 76% 21% •
2	B	171	85% 12% •
2	D	171	81% 18% •

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Mol	Chain	Length	Quality of chain
3	F	164	68% 21% • 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12146 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 EspG protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2721	1682	478	545	16	0	0	0
1	C	351	2721	1682	478	545	16	0	0	0
1	E	350	2713	1678	476	543	16	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ASN	ASP	SEE REMARK 999	UNP Q5WMC0
A	244	THR	SER	SEE REMARK 999	UNP Q5WMC0
A	269	LYS	ASN	SEE REMARK 999	UNP Q5WMC0
C	123	ASN	ASP	SEE REMARK 999	UNP Q5WMC0
C	244	THR	SER	SEE REMARK 999	UNP Q5WMC0
C	269	LYS	ASN	SEE REMARK 999	UNP Q5WMC0
E	123	ASN	ASP	SEE REMARK 999	UNP Q5WMC0
E	244	THR	SER	SEE REMARK 999	UNP Q5WMC0
E	269	LYS	ASN	SEE REMARK 999	UNP Q5WMC0

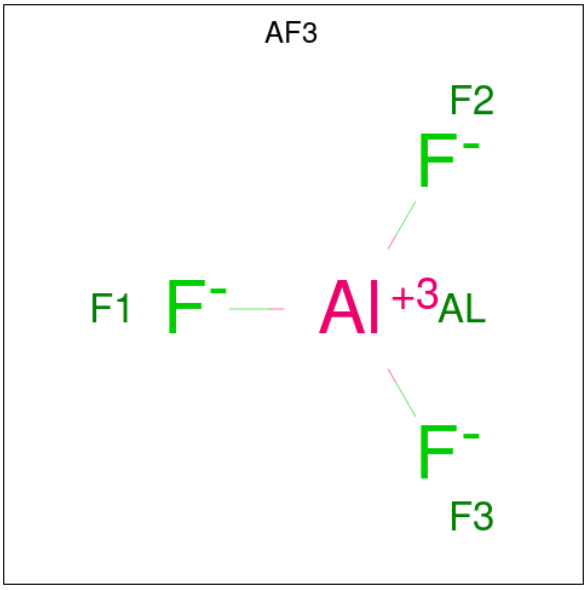
- Molecule 2 is a protein called Ras-related protein Rab-1A.

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.

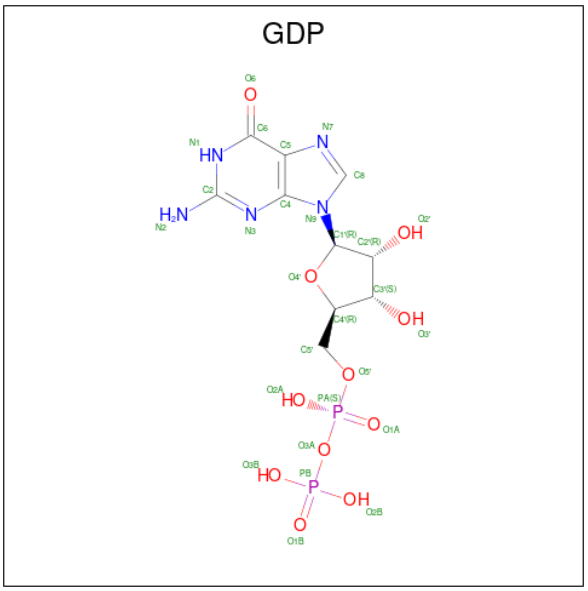
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	149	1131	712	187	228	4	0	0	0

- Molecule 4 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

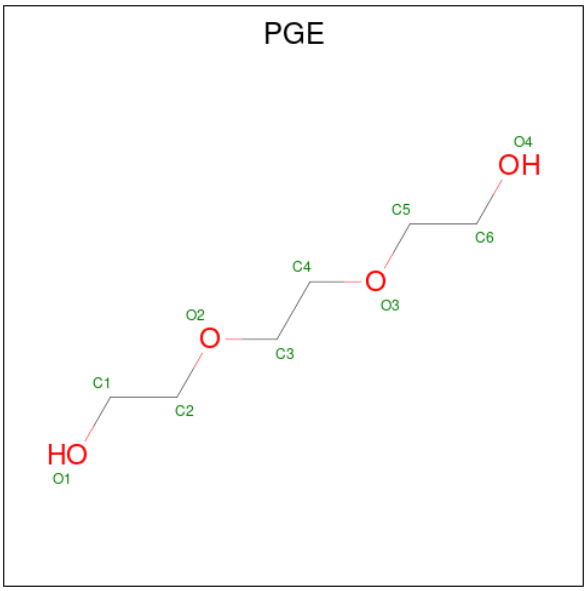


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
5	D	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
5	F	1	28	10	5	11	2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

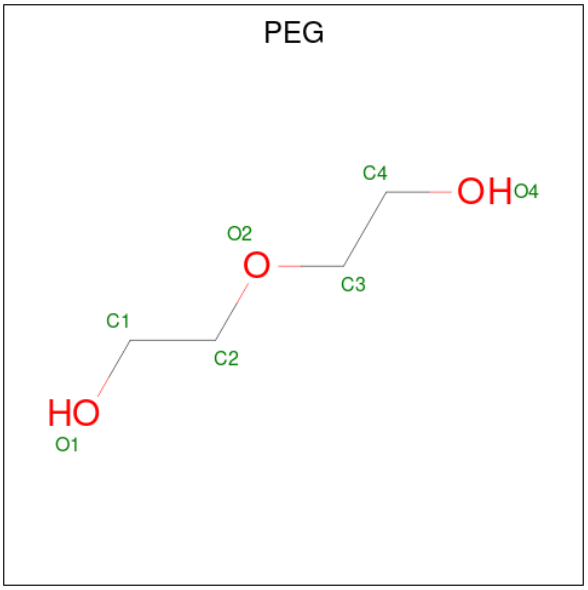
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	B	1	1	1	0	0
			Total	Mg		
6	D	1	1	1	0	0
			Total	Mg		
6	F	1	1	1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 5 3 2	0	0

- Molecule 9 is water.

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

3 Residue-property plots (i)

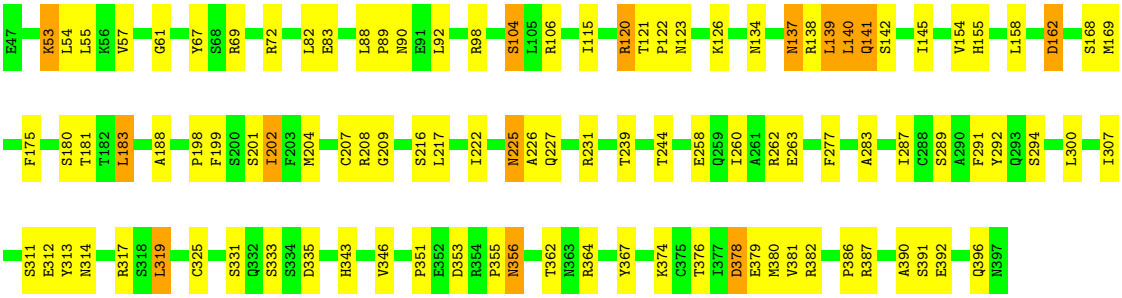
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: EspG protein

Chain A:

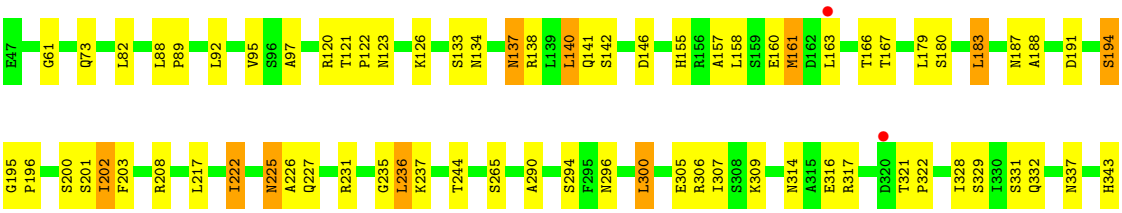
- Molecule 1: EspG protein

Chain C:



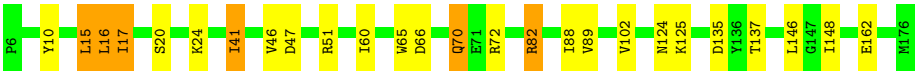
- Molecule 1: EspG protein

Chain E:



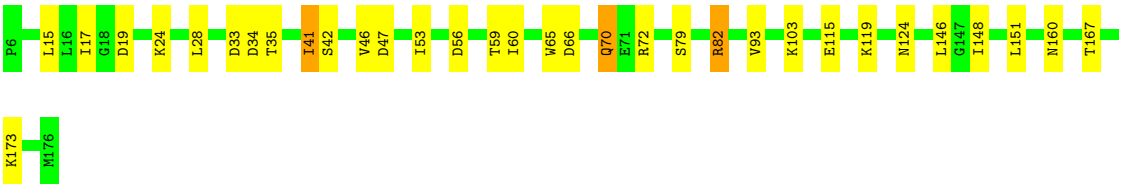
• Molecule 2: Ras-related protein Rab-1A

Chain B:



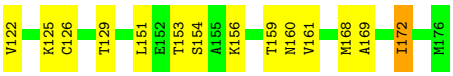
• Molecule 2: Ras-related protein Rab-1A

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	106.57Å 153.22Å 230.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.05 50.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.05) 98.9 (50.00-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.266 0.205 , 0.254	Depositor DCC
R_{free} test set	1811 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	79.6	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12146	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: PGE, GDP, AF3, MG, PEG

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	0/2769	0.91	1/3760 (0.0%)
1	C	0.55	0/2769	0.89	1/3760 (0.0%)
1	E	0.52	0/2761	0.92	7/3749 (0.2%)
2	B	0.58	0/1392	0.86	0/1879
2	D	0.52	0/1392	0.84	0/1879
3	F	0.53	0/1145	0.81	0/1549
All	All	0.56	0/12228	0.88	9/16576 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	201	SER	N-CA-CB	-9.19	95.81	110.98
1	A	124	ASN	N-CA-C	7.41	121.66	112.47
1	E	163	LEU	CB-CA-C	-7.36	101.27	111.95
1	E	163	LEU	N-CA-C	7.19	122.85	107.67
1	E	195	GLY	CA-C-N	6.26	126.00	119.05
1	E	195	GLY	C-N-CA	6.26	126.00	119.05
1	C	201	SER	N-CA-CB	-6.10	99.45	111.60
1	E	201	SER	N-CA-C	5.69	120.97	112.94
1	E	200	SER	CB-CA-C	5.69	122.20	110.31

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	2721	0	2682	56	0
1	C	2721	0	2682	68	0
1	E	2713	0	2676	53	0
2	B	1369	0	1365	17	0
2	D	1369	0	1366	19	0
3	F	1131	0	1083	24	0
4	B	4	0	0	0	0
4	D	4	0	0	0	0
4	F	4	0	0	0	0
5	B	28	0	12	0	0
5	D	28	0	12	1	0
5	F	28	0	12	1	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	C	10	0	14	1	0
8	E	5	0	5	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
All	All	12146	0	11909	226	0

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

All (226) 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:E:134:ASN:H	1:E:137:ASN:HD21	1.14	0.95
1:C:54:LEU:HD21	1:C:82:LEU:HD11	1.50	0.93
1:C:134:ASN:H	1:C:137:ASN:HD21	1.08	0.92
1:C:225:ASN:HD22	1:C:225:ASN:H	1.15	0.89
1:A:134:ASN:H	1:A:137:ASN:HD21	1.15	0.89
3:F:15:LEU:HD12	3:F:65:TRP:HB2	1.53	0.87
1:A:283:ALA:O	1:A:287:ILE:HG12	1.75	0.87
1:A:351:PRO:HG2	1:C:188:ALA:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:LEU:HD12	2:D:65:TRP:HB2	1.62	0.81
1:C:356:ASN:ND2	1:C:356:ASN:O	2.13	0.80
1:E:134:ASN:N	1:E:137:ASN:HD21	1.81	0.79
2:B:15:LEU:HD12	2:B:65:TRP:HB2	1.66	0.77
1:A:199:PHE:O	1:A:202:ILE:HG13	1.86	0.76
1:C:162:ASP:O	1:C:168:SER:HB3	1.86	0.75
1:A:202:ILE:HG12	1:A:380:MET:HE1	1.69	0.74
1:E:377:ILE:O	1:E:381:VAL:HG23	1.88	0.73
1:E:88:LEU:HB3	1:E:89:PRO:CD	2.18	0.73
1:C:225:ASN:HD22	1:C:225:ASN:N	1.88	0.70
1:E:222:ILE:HG22	1:E:227:GLN:HG3	1.72	0.70
2:D:41:ILE:HD13	2:D:41:ILE:H	1.56	0.70
1:C:134:ASN:H	1:C:137:ASN:ND2	1.85	0.70
1:E:179:LEU:O	1:E:364:ARG:NH2	2.26	0.69
1:A:202:ILE:HD11	1:A:377:ILE:HG12	1.74	0.69
1:C:353:ASP:O	1:C:355:PRO:HD3	1.93	0.68
2:B:47:ASP:HB3	2:B:66:ASP:HB3	1.75	0.67
1:A:155:HIS:HB2	1:A:393:THR:HG23	1.75	0.67
1:C:54:LEU:HD21	1:C:82:LEU:CD1	2.24	0.66
1:A:181:THR:HG23	1:A:364:ARG:NH2	2.10	0.65
2:B:16:LEU:HD12	2:B:88:ILE:HB	1.79	0.65
1:E:158:LEU:HB2	1:E:161:MET:HE2	1.78	0.65
1:C:202:ILE:HG12	1:C:380:MET:HE1	1.79	0.64
1:C:225:ASN:H	1:C:225:ASN:ND2	1.93	0.64
1:E:294:SER:OG	3:F:70:GLN:HG2	1.99	0.63
1:C:88:LEU:HB3	1:C:89:PRO:CD	2.29	0.62
3:F:30:ARG:HB3	3:F:161:VAL:HG11	1.81	0.62
1:A:82:LEU:HD12	1:A:97:ALA:HB2	1.83	0.61
1:C:137:ASN:HD22	1:C:138:ARG:N	1.98	0.60
1:E:82:LEU:HD12	1:E:97:ALA:HB2	1.84	0.60
3:F:70:GLN:HE21	3:F:72:ARG:HG2	1.67	0.60
1:A:137:ASN:HD22	1:A:137:ASN:H	1.49	0.60
1:E:82:LEU:HG	1:E:95:VAL:HG11	1.82	0.60
1:A:294:SER:OG	2:B:70:GLN:HG2	2.01	0.59
1:E:157:ALA:HB1	1:E:161:MET:HG3	1.84	0.59
1:A:192:PRO:HG2	1:A:388:TYR:CZ	2.36	0.59
2:B:41:ILE:N	2:B:41:ILE:HD13	2.16	0.59
3:F:47:ASP:HB3	3:F:66:ASP:HB3	1.83	0.59
1:E:88:LEU:HB3	1:E:89:PRO:HD2	1.85	0.59
1:A:163:LEU:HD22	1:A:395:LEU:HD11	1.85	0.59
1:C:61:GLY:O	1:C:67:TYR:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:HD23	2:D:160:ASN:HD22	1.68	0.58
1:A:222:ILE:HG22	1:A:227:GLN:HG3	1.85	0.58
1:A:192:PRO:HG2	1:A:388:TYR:CE1	2.37	0.58
1:E:155:HIS:HE1	1:E:180:SER:O	1.87	0.58
1:C:137:ASN:HD22	1:C:138:ARG:H	1.51	0.57
3:F:120:LEU:HB3	3:F:168:MET:HE2	1.84	0.57
2:B:82:ARG:HH21	2:B:82:ARG:HG3	1.69	0.57
1:C:181:THR:HG22	1:C:391:SER:HB3	1.86	0.57
1:E:306:ARG:NH1	1:E:349:MET:O	2.37	0.57
1:E:217:LEU:HG	1:E:222:ILE:HD13	1.86	0.56
1:A:88:LEU:HB3	1:A:89:PRO:CD	2.35	0.56
1:A:137:ASN:HD22	1:A:138:ARG:H	1.53	0.56
1:C:300:LEU:HD22	1:C:307:ILE:CD1	2.35	0.56
1:A:134:ASN:N	1:A:137:ASN:HD21	1.96	0.55
1:C:356:ASN:C	1:C:356:ASN:HD22	2.14	0.55
1:C:53:LYS:O	1:C:57:VAL:HG23	2.06	0.55
1:E:146:ASP:HB3	1:E:183:LEU:HD12	1.87	0.55
1:E:222:ILE:HG23	1:E:226:ALA:HB3	1.88	0.55
1:A:155:HIS:HE1	1:A:180:SER:O	1.90	0.54
2:B:41:ILE:H	2:B:41:ILE:CD1	2.20	0.54
1:A:300:LEU:HD22	1:A:307:ILE:CD1	2.37	0.54
1:C:376:THR:O	1:C:380:MET:HG3	2.07	0.54
1:A:217:LEU:HG	1:A:222:ILE:HD13	1.90	0.54
1:A:312:GLU:OE2	2:B:65:TRP:HH2	1.91	0.54
1:A:376:THR:O	1:A:380:MET:HG3	2.09	0.53
1:A:91:GLU:OE2	1:A:94:ARG:NH2	2.40	0.53
1:A:82:LEU:HG	1:A:95:VAL:CG1	2.39	0.53
3:F:126:CYS:SG	3:F:154:SER:HB2	2.48	0.53
1:E:133:SER:CB	1:E:140:LEU:HD22	2.39	0.53
1:A:82:LEU:HG	1:A:95:VAL:HG11	1.91	0.52
1:E:61:GLY:HA3	1:E:137:ASN:HA	1.91	0.52
1:C:120:ARG:NH2	1:C:126:LYS:HD3	2.25	0.52
1:C:155:HIS:HE1	1:C:180:SER:O	1.93	0.52
1:E:343:HIS:CD2	1:E:364:ARG:HG3	2.45	0.52
3:F:15:LEU:HB3	3:F:87:ILE:HG12	1.92	0.52
2:B:70:GLN:NE2	2:B:72:ARG:HG2	2.24	0.52
1:C:198:PRO:HB2	1:C:381:VAL:HG22	1.91	0.52
2:D:119:LYS:HD2	2:D:148:ILE:HD11	1.91	0.52
1:E:187:ASN:O	1:E:191:ASP:HB2	2.10	0.52
1:E:367:TYR:HB3	1:E:386:PRO:HA	1.92	0.51
1:A:106:ARG:C	1:A:106:ARG:HD2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HD22	1:A:137:ASN:N	2.08	0.51
1:C:208:ARG:HD3	5:D:202:GDP:H5"	1.91	0.51
1:A:157:ALA:HB3	1:A:395:LEU:HA	1.92	0.51
1:C:209:GLY:HA3	1:C:291:PHE:CE1	2.46	0.51
1:A:183:LEU:HD21	1:A:387:ARG:HG3	1.92	0.51
1:E:376:THR:O	1:E:380:MET:HG3	2.11	0.51
3:F:82:ARG:HD3	3:F:82:ARG:H	1.75	0.51
1:A:310:ALA:HB2	1:A:349:MET:HG2	1.92	0.51
2:B:41:ILE:N	2:B:41:ILE:CD1	2.73	0.51
1:E:137:ASN:HD22	1:E:137:ASN:N	2.08	0.50
3:F:22:VAL:O	3:F:125:LYS:HE3	2.11	0.50
1:A:377:ILE:O	1:A:381:VAL:HG23	2.12	0.50
3:F:106:LEU:HA	3:F:109:ILE:HD12	1.94	0.50
2:D:47:ASP:HB3	2:D:66:ASP:HB3	1.94	0.50
1:C:137:ASN:ND2	1:C:138:ARG:N	2.60	0.50
1:C:283:ALA:O	1:C:287:ILE:HG12	2.11	0.50
1:E:137:ASN:HD22	1:E:137:ASN:H	1.59	0.49
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.92	0.49
1:C:222:ILE:HG22	1:C:227:GLN:HG3	1.95	0.49
2:D:146:LEU:HB3	2:D:148:ILE:HD13	1.95	0.49
1:E:305:GLU:O	1:E:309:LYS:HG2	2.12	0.49
1:A:181:THR:HG23	1:A:364:ARG:HH21	1.77	0.49
1:A:137:ASN:H	1:A:137:ASN:ND2	2.09	0.48
3:F:82:ARG:HB3	3:F:112:TYR:O	2.13	0.48
1:A:188:ALA:HB3	1:C:351:PRO:HG2	1.94	0.48
3:F:151:LEU:HD23	3:F:160:ASN:HD22	1.79	0.48
1:E:120:ARG:NE	1:E:126:LYS:HG2	2.29	0.48
3:F:99:PHE:O	3:F:102:VAL:HB	2.14	0.48
1:C:98:ARG:HG2	1:C:104:SER:HB2	1.95	0.48
1:C:121:THR:HB	1:C:122:PRO:HD2	1.96	0.48
1:C:199:PHE:O	1:C:202:ILE:HG13	2.15	0.47
1:E:208:ARG:HD3	5:F:202:GDP:H5'	1.95	0.47
1:C:226:ALA:HB1	1:C:260:ILE:HG23	1.96	0.47
2:B:10:TYR:HB2	2:B:60:ILE:HG12	1.96	0.47
3:F:28:LEU:HD22	3:F:66:ASP:HB2	1.97	0.47
1:A:317:ARG:HB2	1:A:319:LEU:HG	1.97	0.47
1:E:191:ASP:HB3	1:E:194:SER:HB2	1.97	0.47
1:E:158:LEU:O	1:E:161:MET:HG2	2.15	0.47
1:A:305:GLU:OE2	7:C:401:PGE:H2	2.15	0.47
1:E:73:GLN:HE21	1:E:160:GLU:HG3	1.79	0.47
1:C:356:ASN:ND2	1:C:356:ASN:C	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:PHE:HB3	1:E:236:LEU:HD11	1.96	0.46
2:B:89:VAL:HG11	2:B:102:VAL:HG13	1.97	0.46
1:E:235:GLY:HA3	1:E:244:THR:HG23	1.98	0.46
1:C:202:ILE:HG21	1:C:289:SER:HA	1.97	0.46
1:E:231:ARG:NH1	1:E:237:LYS:O	2.48	0.46
1:A:343:HIS:NE2	1:A:364:ARG:HG3	2.30	0.46
2:D:93:VAL:HG22	2:D:124:ASN:O	2.16	0.46
1:A:146:ASP:HB3	1:A:183:LEU:HD12	1.96	0.46
2:D:19:ASP:O	2:D:24:LYS:NZ	2.49	0.46
1:A:63:TRP:CD1	1:A:158:LEU:HD13	2.52	0.45
1:A:343:HIS:CD2	1:A:364:ARG:HG3	2.51	0.45
1:C:169:MET:HG2	1:C:325:CYS:SG	2.56	0.45
1:C:367:TYR:HB3	1:C:386:PRO:HA	1.98	0.45
1:A:106:ARG:HD2	1:A:106:ARG:O	2.17	0.45
1:C:258:GLU:O	1:C:262:ARG:HB2	2.17	0.45
1:E:314:ASN:HD22	1:E:321:THR:HG21	1.81	0.45
1:A:377:ILE:HA	1:A:380:MET:HE2	1.99	0.44
1:E:166:THR:HG23	1:E:322:PRO:HG3	1.99	0.44
1:E:300:LEU:HD22	1:E:307:ILE:HD13	1.99	0.44
1:C:209:GLY:HA2	2:D:41:ILE:HG22	2.00	0.44
1:C:225:ASN:N	1:C:225:ASN:ND2	2.58	0.44
1:C:294:SER:OG	2:D:70:GLN:HG2	2.16	0.44
2:D:119:LYS:HB2	2:D:148:ILE:HG13	2.00	0.44
1:A:137:ASN:HD22	1:A:138:ARG:N	2.15	0.44
1:C:154:VAL:HA	1:C:392:GLU:O	2.17	0.44
1:C:333:SER:C	1:C:335:ASP:H	2.25	0.44
1:C:378:ASP:O	1:C:382:ARG:HG2	2.18	0.44
1:E:188:ALA:O	3:F:72:ARG:NH2	2.50	0.44
1:C:314:ASN:HD22	1:C:319:LEU:HB2	1.83	0.44
1:C:115:ILE:HD13	1:C:139:LEU:HD13	1.99	0.44
1:E:137:ASN:ND2	1:E:138:ARG:H	2.15	0.44
1:A:175:PHE:CE2	1:A:179:LEU:HD11	2.53	0.43
1:C:88:LEU:HB3	1:C:89:PRO:HD2	1.99	0.43
3:F:30:ARG:NH2	3:F:156:LYS:O	2.51	0.43
2:D:17:ILE:HD13	2:D:17:ILE:HA	1.86	0.43
2:B:17:ILE:HD13	2:B:17:ILE:HA	1.80	0.43
1:A:333:SER:C	1:A:335:ASP:H	2.26	0.43
1:E:82:LEU:HG	1:E:95:VAL:CG1	2.47	0.43
2:B:124:ASN:CG	2:B:125:LYS:H	2.26	0.43
1:C:217:LEU:HD22	1:C:277:PHE:CE2	2.54	0.43
1:C:343:HIS:CD2	1:C:364:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ALA:HB1	1:E:328:ILE:HD13	2.00	0.43
1:A:79:LEU:O	1:A:82:LEU:HB2	2.19	0.43
1:C:106:ARG:C	1:C:106:ARG:HD2	2.43	0.43
2:B:146:LEU:HB2	2:B:148:ILE:HD12	2.00	0.43
1:C:313:TYR:CE2	1:C:317:ARG:NH2	2.87	0.43
3:F:120:LEU:HD11	3:F:151:LEU:HD13	2.01	0.43
1:E:332:GLN:HA	1:E:337:ASN:O	2.19	0.43
2:D:72:ARG:HA	2:D:72:ARG:HD2	1.81	0.43
1:A:254:ARG:NH2	1:A:276:GLU:OE2	2.52	0.42
1:E:137:ASN:HD22	1:E:138:ARG:H	1.67	0.42
1:E:379:GLU:HG3	1:E:382:ARG:HH22	1.83	0.42
3:F:169:ALA:O	3:F:172:ILE:HG22	2.19	0.42
1:E:141:GLN:HA	1:E:180:SER:HB3	2.02	0.42
1:E:196:PRO:HD2	3:F:71:GLU:CD	2.45	0.42
1:C:141:GLN:HA	1:C:180:SER:HB3	2.02	0.42
1:C:199:PHE:HA	1:C:292:TYR:CE1	2.54	0.42
1:C:355:PRO:O	1:C:356:ASN:HB3	2.19	0.42
1:E:317:ARG:HG2	1:E:317:ARG:HH11	1.85	0.42
1:A:353:ASP:C	1:A:353:ASP:OD2	2.62	0.42
1:C:217:LEU:HD22	1:C:277:PHE:HE2	1.83	0.42
1:A:160:GLU:CD	1:A:160:GLU:H	2.26	0.42
2:D:41:ILE:H	2:D:41:ILE:CD1	2.25	0.42
2:B:24:LYS:HE2	2:B:24:LYS:HB2	1.88	0.42
1:E:225:ASN:HD22	1:E:225:ASN:HA	1.66	0.42
1:C:140:LEU:HD12	1:C:145:ILE:HD11	2.01	0.42
1:A:152:ILE:HA	1:A:182:THR:HB	2.02	0.41
1:C:158:LEU:HD23	1:C:175:PHE:CZ	2.55	0.41
1:A:179:LEU:O	1:A:364:ARG:NH2	2.42	0.41
2:D:59:THR:C	2:D:60:ILE:HG13	2.45	0.41
1:E:294:SER:C	1:E:296:ASN:N	2.74	0.41
2:D:28:LEU:HD12	2:D:28:LEU:HA	1.77	0.41
1:E:121:THR:HB	1:E:122:PRO:HD2	2.02	0.41
1:A:183:LEU:HD21	1:A:387:ARG:CG	2.50	0.41
1:C:134:ASN:N	1:C:137:ASN:HD21	1.93	0.41
3:F:79:SER:HA	3:F:82:ARG:HE	1.86	0.41
1:C:277:PHE:O	1:C:283:ALA:HB2	2.21	0.41
1:C:312:GLU:OE2	2:D:65:TRP:HH2	2.03	0.41
2:D:56:ASP:HB2	2:D:173:LYS:HE3	2.03	0.41
1:A:163:LEU:CD2	1:A:395:LEU:HD11	2.51	0.41
1:C:183:LEU:HD11	1:C:387:ARG:HD2	2.03	0.41
1:C:374:LYS:HB2	1:C:379:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:SER:HB3	3:F:159:THR:HB	2.01	0.41
2:B:72:ARG:HA	2:B:72:ARG:HD2	1.64	0.40
1:C:207:CYS:HB3	1:C:231:ARG:HH11	1.86	0.40
1:C:343:HIS:NE2	1:C:364:ARG:NH1	2.68	0.40
2:D:79:SER:HA	2:D:82:ARG:HE	1.86	0.40
3:F:122:VAL:HG13	3:F:153:THR:CG2	2.51	0.40
1:C:69:ARG:HG3	1:C:72:ARG:HD3	2.03	0.40
1:C:204:MET:HB3	1:C:208:ARG:HH11	1.85	0.40
1:E:202:ILE:HG12	1:E:380:MET:HE1	2.03	0.40
1:A:306:ARG:HD2	1:A:349:MET:O	2.20	0.40
1:C:362:THR:O	1:C:390:ALA:HA	2.21	0.40
1:E:202:ILE:H	1:E:202:ILE:HG13	1.68	0.40
1:E:194:SER:HB3	3:F:72:ARG:NH2	2.37	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%)	329 (94%)	20 (6%)	0	100	100
1	C	349/351 (99%)	318 (91%)	31 (9%)	0	100	100
1	E	348/351 (99%)	324 (93%)	24 (7%)	0	100	100
2	B	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
2	D	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
3	F	143/164 (87%)	133 (93%)	10 (7%)	0	100	100
All	All	1527/1559 (98%)	1429 (94%)	98 (6%)	0	100	100

There are no Ramachandran outliers to report.

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%)	286 (92%)	26 (8%)	10	32
1	C	312/312 (100%)	284 (91%)	28 (9%)	9	29
1	E	311/312 (100%)	292 (94%)	19 (6%)	17	42
2	B	151/151 (100%)	139 (92%)	12 (8%)	11	34
2	D	151/151 (100%)	139 (92%)	12 (8%)	11	34
3	F	119/144 (83%)	111 (93%)	8 (7%)	15	39
All	All	1356/1382 (98%)	1251 (92%)	105 (8%)	12	35

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	55	LEU
1	A	82	LEU
1	A	92	LEU
1	A	120	ARG
1	A	123	ASN
1	A	137	ASN
1	A	140	LEU
1	A	158	LEU
1	A	160	GLU
1	A	163	LEU
1	A	167	THR
1	A	177	SER
1	A	183	LEU
1	A	202	ILE
1	A	237	LYS
1	A	241	SER
1	A	317	ARG
1	A	321	THR
1	A	323	ASN
1	A	329	SER
1	A	346	VAL

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Mol	Chain	Res	Type
1	A	362	THR
1	A	382	ARG
1	A	393	THR
1	A	396	GLN
2	B	15	LEU
2	B	16	LEU
2	B	17	ILE
2	B	20	SER
2	B	41	ILE
2	B	46	VAL
2	B	51	ARG
2	B	70	GLN
2	B	82	ARG
2	B	135	ASP
2	B	137	THR
2	B	162	GLU
1	C	53	LYS
1	C	55	LEU
1	C	83	GLU
1	C	90	ASN
1	C	92	LEU
1	C	104	SER
1	C	120	ARG
1	C	123	ASN
1	C	137	ASN
1	C	139	LEU
1	C	140	LEU
1	C	141	GLN
1	C	142	SER
1	C	162	ASP
1	C	183	LEU
1	C	202	ILE
1	C	216	SER
1	C	225	ASN
1	C	239	THR
1	C	244	THR
1	C	263	GLU
1	C	311	SER
1	C	319	LEU
1	C	331	SER
1	C	346	VAL
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	378	ASP
1	C	396	GLN
2	D	33	ASP
2	D	34	ASP
2	D	35	THR
2	D	41	ILE
2	D	42	SER
2	D	46	VAL
2	D	53	ILE
2	D	70	GLN
2	D	82	ARG
2	D	103	LYS
2	D	115	GLU
2	D	167	THR
1	E	92	LEU
1	E	123	ASN
1	E	137	ASN
1	E	140	LEU
1	E	142	SER
1	E	161	MET
1	E	167	THR
1	E	183	LEU
1	E	194	SER
1	E	202	ILE
1	E	222	ILE
1	E	225	ASN
1	E	236	LEU
1	E	265	SER
1	E	300	LEU
1	E	316	GLU
1	E	329	SER
1	E	331	SER
1	E	396	GLN
3	F	27	LEU
3	F	37	THR
3	F	41	ILE
3	F	82	ARG
3	F	102	VAL
3	F	116	ASN
3	F	129	THR
3	F	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	137	ASN
1	A	155	HIS
1	A	212	ASN
1	A	246	ASN
1	A	356	ASN
2	B	96	GLN
2	B	163	GLN
1	C	90	ASN
1	C	111	ASN
1	C	136	GLN
1	C	137	ASN
1	C	153	GLN
1	C	155	HIS
1	C	189	GLN
1	C	225	ASN
1	C	240	HIS
1	C	246	ASN
1	C	314	ASN
2	D	63	GLN
2	D	70	GLN
2	D	96	GLN
1	E	73	GLN
1	E	123	ASN
1	E	124	ASN
1	E	136	GLN
1	E	137	ASN
1	E	155	HIS
1	E	225	ASN
1	E	332	GLN
1	E	363	ASN
3	F	70	GLN
3	F	118	ASN
3	F	160	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
8	PEG	E	401	-	4,4,6	0.58	0	3,3,5	0.49	0
5	GDP	D	202	6,4	29,30,30	1.84	3 (10%)	45,47,47	1.73	9 (20%)
7	PGE	C	401	-	9,9,9	1.02	0	8,8,8	0.80	0
5	GDP	B	202	6,4	29,30,30	1.88	5 (17%)	45,47,47	1.80	8 (17%)
4	AF3	F	201	9,5	0,3,3	-	-	-		
5	GDP	F	202	6,4	29,30,30	1.71	2 (6%)	45,47,47	1.78	9 (20%)
4	AF3	D	201	9,5	0,3,3	-	-	-		
4	AF3	B	201	9,5	0,3,3	-	-	-		

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
8	PEG	E	401	-	-	1/2/2/4	-
7	PGE	C	401	-	-	5/7/7/7	-
5	GDP	D	202	6,4	-	0/16/32/32	0/3/3/3
5	GDP	B	202	6,4	-	2/16/32/32	0/3/3/3
5	GDP	F	202	6,4	-	4/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	202	GDP	O6-C6	7.31	1.37	1.23
5	B	202	GDP	O6-C6	7.02	1.36	1.23
5	F	202	GDP	O6-C6	6.77	1.36	1.23
5	D	202	GDP	PB-O1B	3.42	1.61	1.50
5	F	202	GDP	PA-O3A	3.20	1.63	1.59
5	B	202	GDP	PB-O1B	3.13	1.60	1.50
5	B	202	GDP	PA-O3A	3.00	1.62	1.59
5	B	202	GDP	PA-O1A	2.81	1.60	1.50
5	D	202	GDP	PA-O3A	2.68	1.62	1.59
5	B	202	GDP	C5-N7	-2.05	1.35	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	202	GDP	C5-C4-N3	-6.05	118.75	128.39
5	B	202	GDP	C5-C4-N3	-5.81	119.14	128.39
5	B	202	GDP	C2-N3-C4	5.69	122.11	112.30
5	F	202	GDP	C2-N3-C4	5.67	122.07	112.30
5	D	202	GDP	C2-N3-C4	5.66	122.05	112.30
5	D	202	GDP	C5-C4-N3	-5.17	120.16	128.39
5	B	202	GDP	N9-C4-N3	3.98	133.90	125.95
5	F	202	GDP	N9-C4-N3	3.84	133.62	125.95
5	D	202	GDP	C6-C5-N7	2.68	135.16	130.29
5	B	202	GDP	C3'-C2'-C1'	2.67	106.51	101.46
5	D	202	GDP	N9-C4-N3	2.66	131.28	125.95
5	F	202	GDP	C2-N1-C6	-2.46	120.65	125.11
5	B	202	GDP	O6-C6-C5	-2.41	120.17	126.53
5	B	202	GDP	PA-O5'-C5'	-2.35	107.91	121.35
5	D	202	GDP	C2-N1-C6	-2.32	120.91	125.11
5	D	202	GDP	C4-C5-N7	-2.30	107.02	110.67
5	D	202	GDP	N9-C8-N7	-2.28	109.18	113.40
5	B	202	GDP	C2-N1-C6	-2.24	121.05	125.11
5	D	202	GDP	N2-C2-N1	2.24	121.49	116.76
5	F	202	GDP	PA-O5'-C5'	-2.20	108.74	121.35
5	D	202	GDP	C3'-C2'-C1'	2.12	105.46	101.46
5	F	202	GDP	C5-C6-N1	2.07	118.52	113.25
5	F	202	GDP	O6-C6-C5	-2.04	121.15	126.53
5	F	202	GDP	C6-C5-N7	2.04	134.00	130.29
5	F	202	GDP	N9-C8-N7	-2.02	109.66	113.40
5	B	202	GDP	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	202	GDP	PA-O3A-PB-O3B
5	F	202	GDP	O4'-C4'-C5'-O5'
5	F	202	GDP	C3'-C4'-C5'-O5'
8	E	401	PEG	O1-C1-C2-O2
7	C	401	PGE	O1-C1-C2-O2
7	C	401	PGE	O2-C3-C4-O3
7	C	401	PGE	C4-C3-O2-C2
7	C	401	PGE	O3-C5-C6-O4
7	C	401	PGE	C1-C2-O2-C3
5	F	202	GDP	PB-O3A-PA-O2A
5	B	202	GDP	PA-O3A-PB-O1B
5	F	202	GDP	PB-O3A-PA-O1A

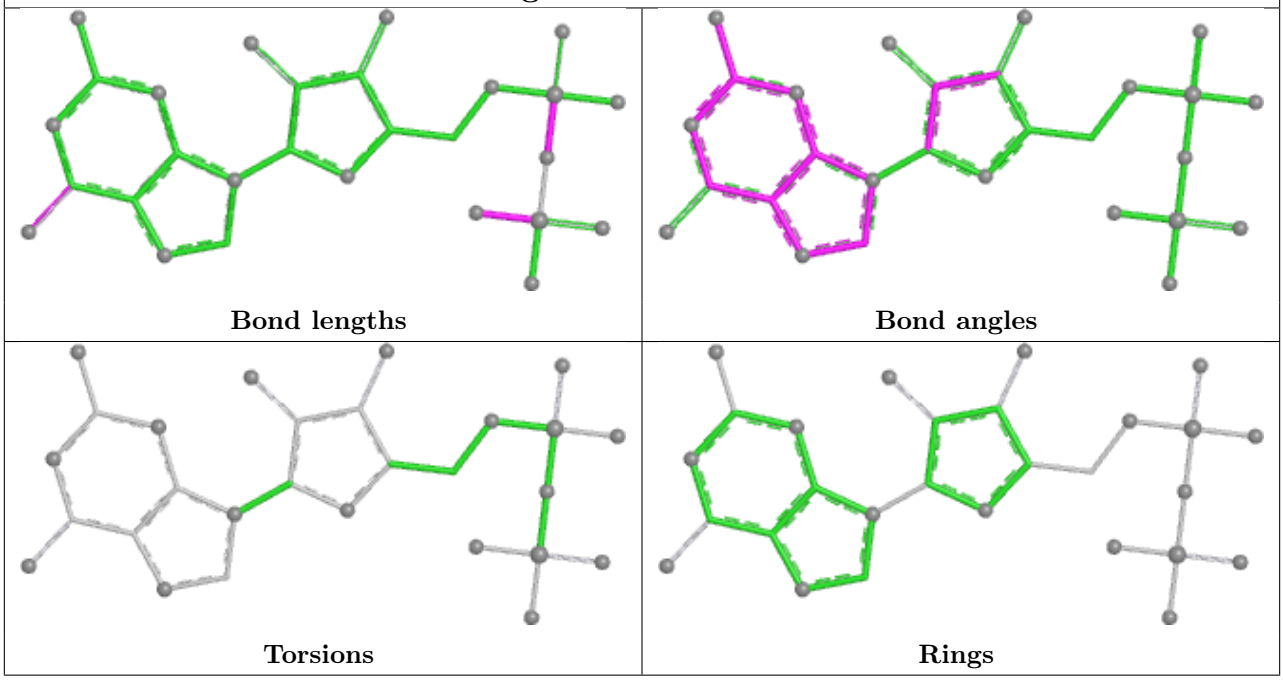
There are no ring outliers.

3 monomers are involved in 3 short contacts:

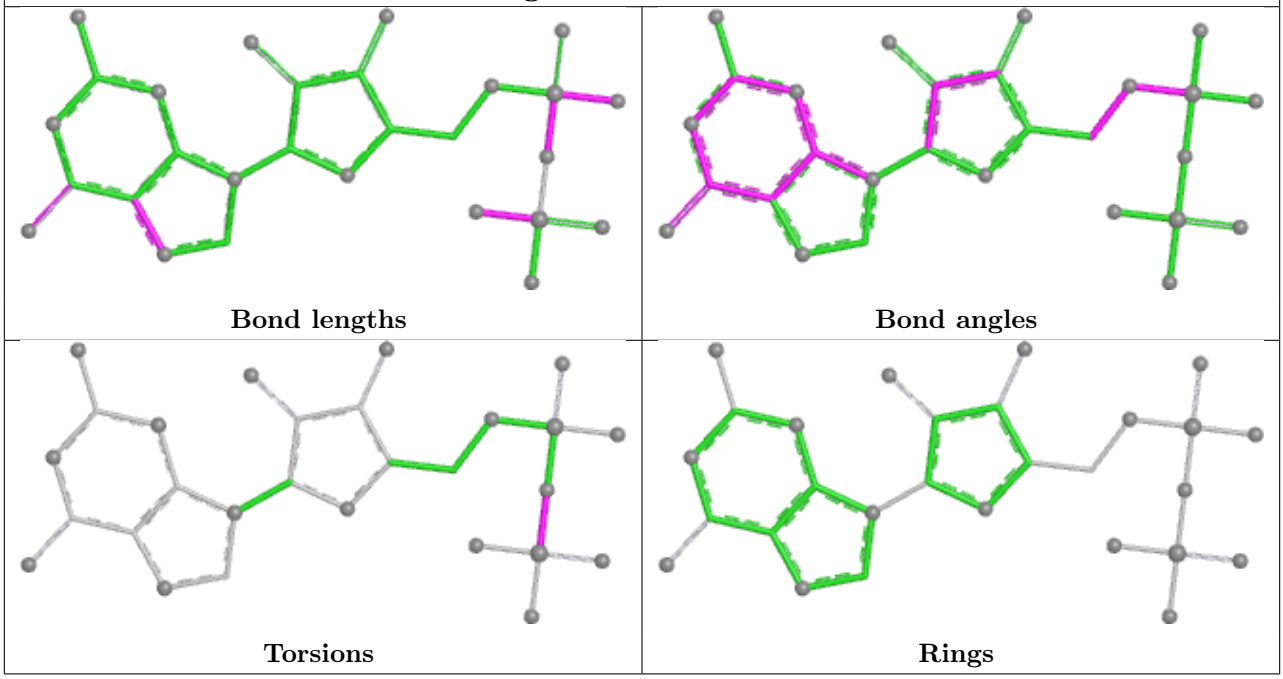
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	202	GDP	1	0
7	C	401	PGE	1	0
5	F	202	GDP	1	0

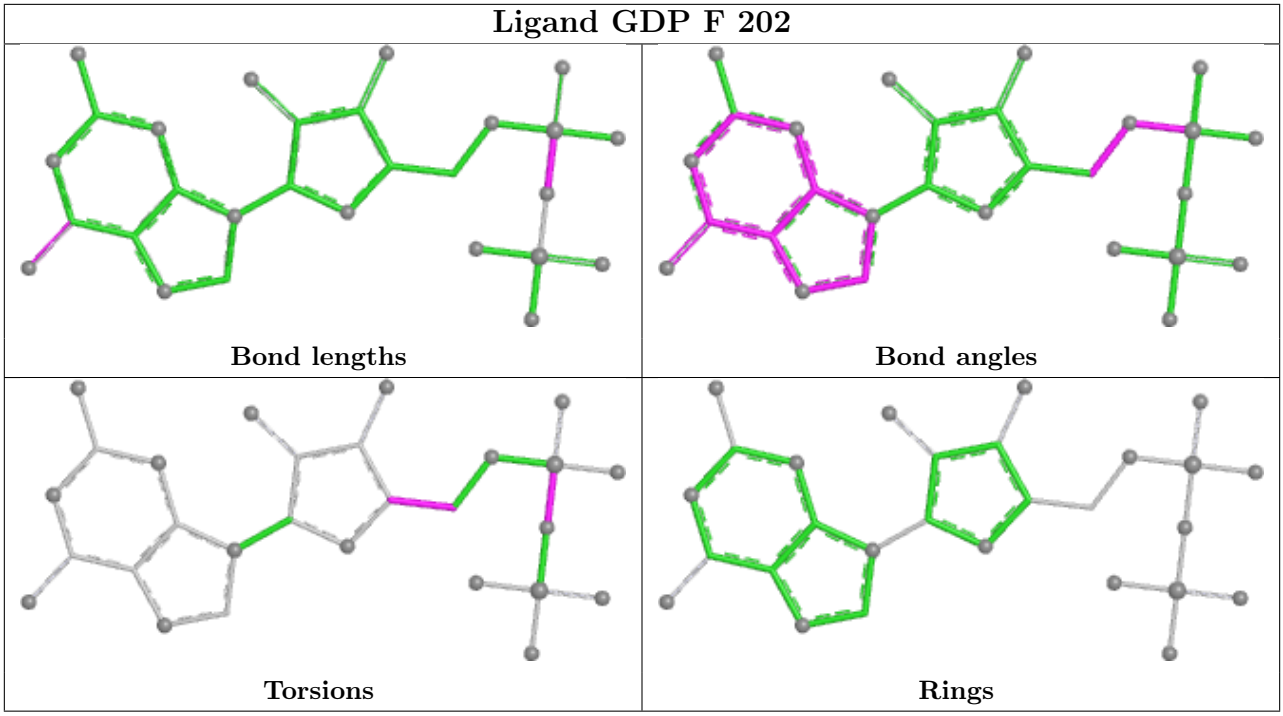
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 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%)	-0.45	1 (0%)	90	80	52, 76, 110, 126	0
1	C	351/351 (100%)	-0.34	0	100	100	57, 96, 146, 162	0
1	E	350/351 (99%)	-0.35	2 (0%)	85	69	68, 108, 154, 175	0
2	B	171/171 (100%)	-0.42	0	100	100	61, 81, 104, 126	0
2	D	171/171 (100%)	-0.45	0	100	100	62, 107, 146, 165	0
3	F	149/164 (90%)	-0.24	0	100	100	99, 155, 203, 243	0
All	All	1543/1559 (98%)	-0.38	3 (0%)	91	83	52, 95, 160, 243	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ASN	2.6
1	E	320	ASP	2.5
1	E	163	LEU	2.4

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

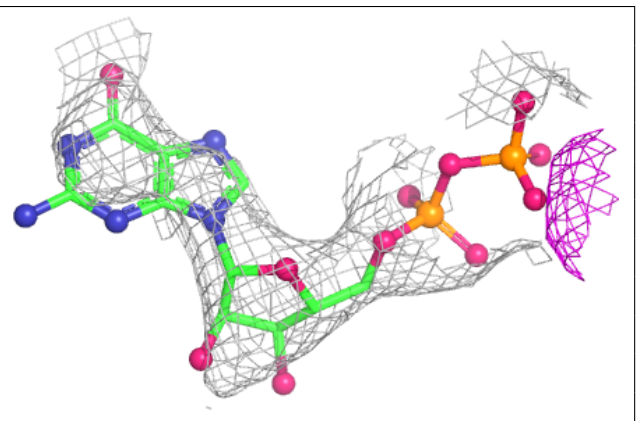
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

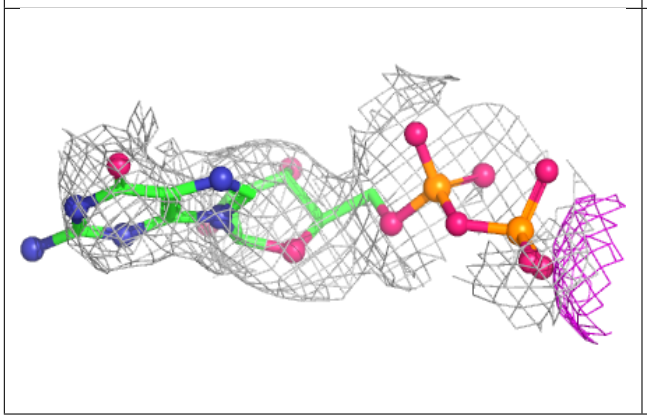
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PGE	C	401	10/10	0.75	0.29	64,69,73,74	0
8	PEG	E	401	5/7	0.77	0.34	94,94,95,96	0
4	AF3	F	201	4/4	0.90	0.17	62,62,62,62	0
4	AF3	D	201	4/4	0.93	0.17	50,50,51,51	0
5	GDP	F	202	28/28	0.95	0.06	117,128,141,143	0
6	MG	F	203	1/1	0.97	0.04	91,91,91,91	0
5	GDP	D	202	28/28	0.97	0.05	78,98,111,115	0
5	GDP	B	202	28/28	0.97	0.06	57,70,75,77	0
6	MG	D	203	1/1	0.98	0.03	69,69,69,69	0
4	AF3	B	201	4/4	0.98	0.14	48,49,49,50	0
6	MG	B	203	1/1	0.99	0.03	53,53,53,53	0

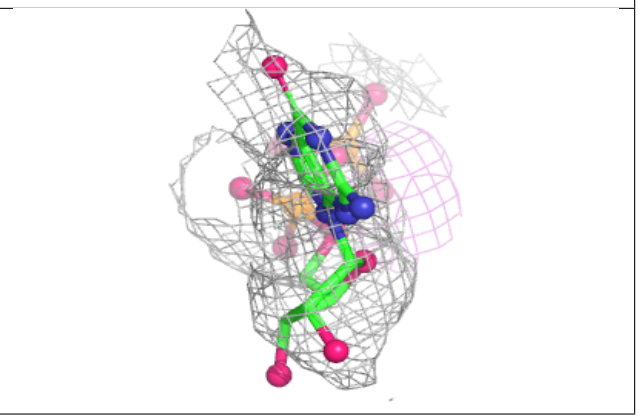
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

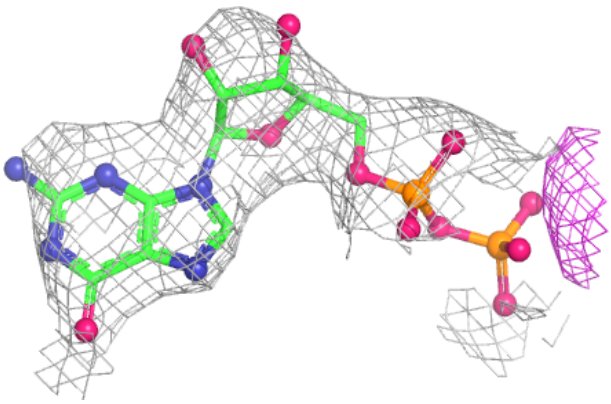


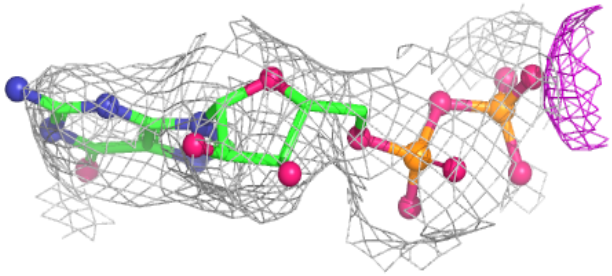


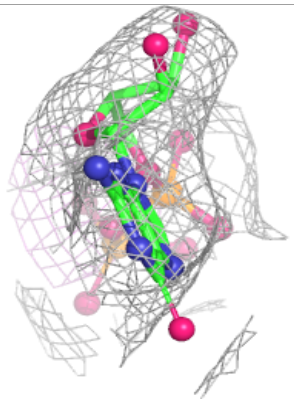


Electron density around GDP D 202:

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

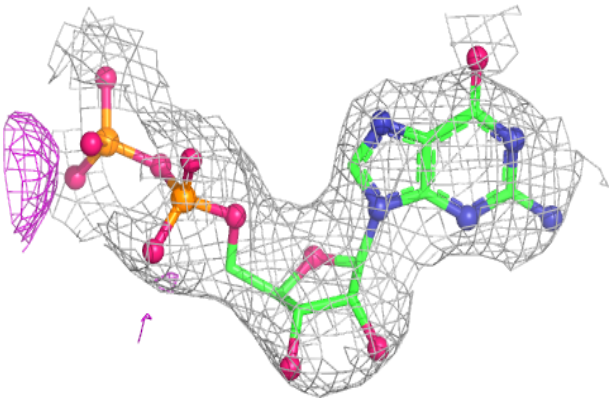


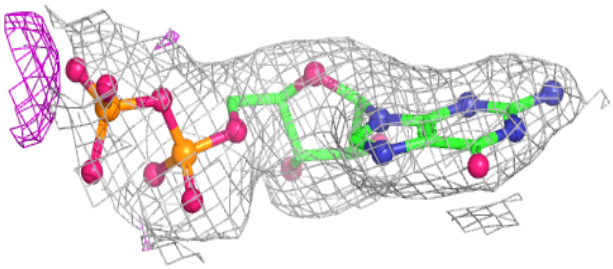


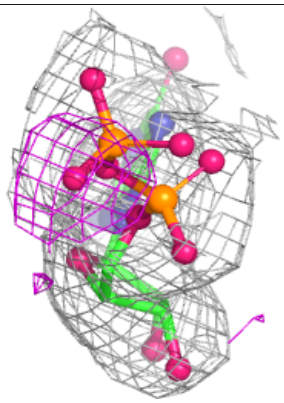


Electron density around GDP B 202:

$2mF_o$-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.