



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:57 PM UTC

PDB ID : 4HLQ / pdb_00004hlq
Title : Crystal structure of human rab1b bound to GDP and BEF3 in complex with the GAP domain of TBC1D20 from homo sapiens
Authors : Gazdag, E.M.; Gavriljuk, K.; Itzen, A.; Koetting, C.; Gerwert, K.; Goody, R.S.
Deposited on : 2012-10-17
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

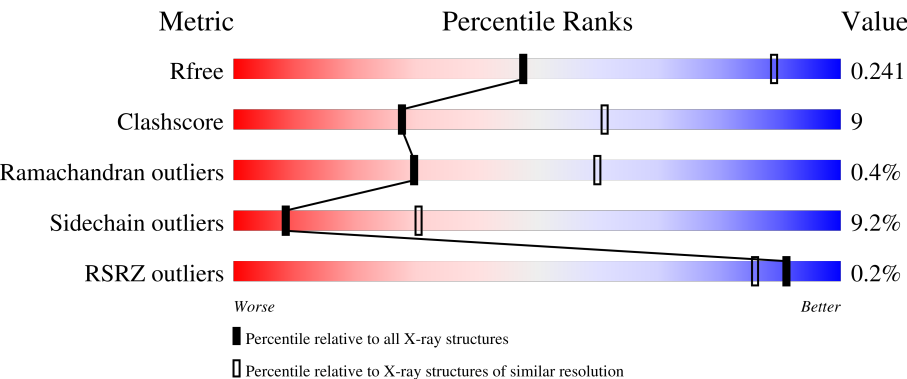
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	305	71%19%• 8%
1	C	305	69%21%• 8%
1	E	305	70%20%• 8%
1	G	305	% 70%18%• 8%

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Mol	Chain	Length	Quality of chain
1	I	305	69%20%8%
2	B	175	78%18%
2	D	175	70%23%
2	F	175	77%16%5%
2	H	175	82%13%
2	J	175	82%15%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17765 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 TBC1 domain family member 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	4	0	0
			2242	1442	391	397	12			
1	C	281	Total	C	N	O	S	0	0	0
			2240	1439	388	401	12			
1	E	281	Total	C	N	O	S	0	0	0
			2246	1442	389	403	12			
1	G	281	Total	C	N	O	S	0	0	0
			2118	1361	365	382	10			
1	I	281	Total	C	N	O	S	0	0	0
			2237	1439	387	399	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1332	845	218	265	4			
2	D	170	Total	C	N	O	S	0	0	0
			1327	845	217	261	4			
2	F	172	Total	C	N	O	S	0	0	0
			1321	839	219	260	3			
2	H	170	Total	C	N	O	S	4	0	0
			1202	752	203	245	2			
2	J	171	Total	C	N	O	S	0	0	0
			1259	799	205	251	4			

There are 15 discrepancies between the modelled and reference sequences:

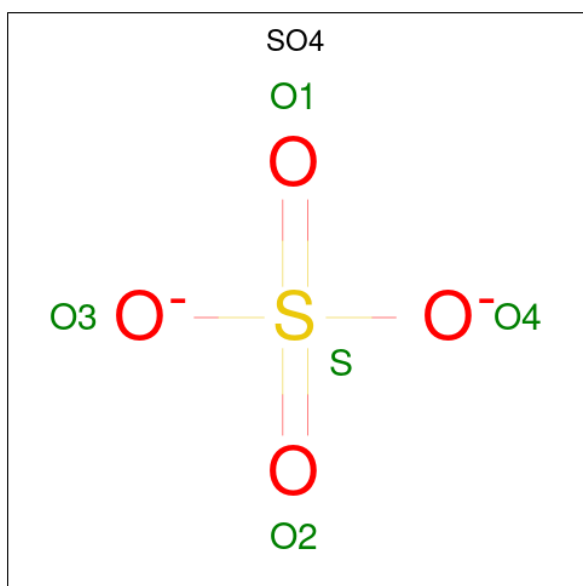
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q9H0U4
B	1	HIS	-	expression tag	UNP Q9H0U4
B	2	MET	-	expression tag	UNP Q9H0U4
D	0	GLY	-	expression tag	UNP Q9H0U4
D	1	HIS	-	expression tag	UNP Q9H0U4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	MET	-	expression tag	UNP Q9H0U4
F	0	GLY	-	expression tag	UNP Q9H0U4
F	1	HIS	-	expression tag	UNP Q9H0U4
F	2	MET	-	expression tag	UNP Q9H0U4
H	0	GLY	-	expression tag	UNP Q9H0U4
H	1	HIS	-	expression tag	UNP Q9H0U4
H	2	MET	-	expression tag	UNP Q9H0U4
J	0	GLY	-	expression tag	UNP Q9H0U4
J	1	HIS	-	expression tag	UNP Q9H0U4
J	2	MET	-	expression tag	UNP Q9H0U4

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

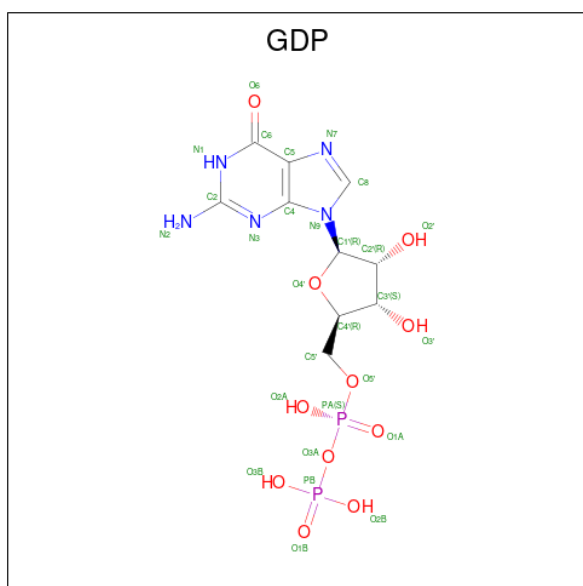


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

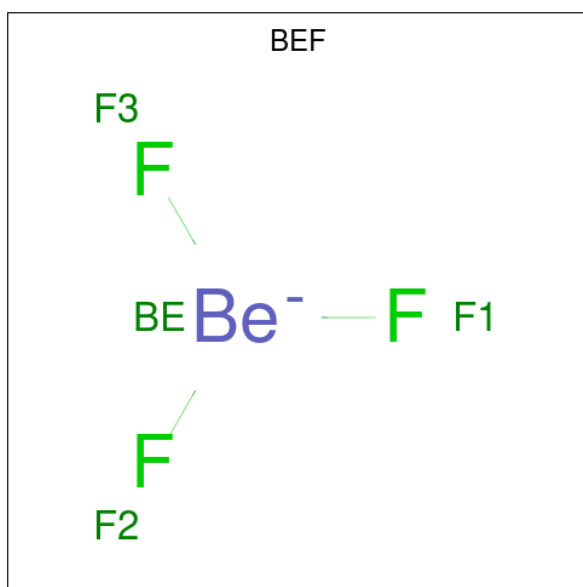
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0

- 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
5	B	1	Total C N O P 28 10 5 11 2	0	0
5	D	1	Total C N O P 28 10 5 11 2	0	0
5	F	1	Total C N O P 28 10 5 11 2	0	0
5	H	1	Total C N O P 28 10 5 11 2	0	0
5	J	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Be	F	0	0
			4	1	3		
6	D	1	Total	Be	F	0	0
			4	1	3		
6	F	1	Total	Be	F	0	0
			4	1	3		
6	H	1	Total	Be	F	0	0
			4	1	3		
6	J	1	Total	Be	F	0	0
			4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	4	Total	O	0	0
			4	4		
7	C	7	Total	O	0	0
			7	7		
7	D	4	Total	O	0	0
			4	4		
7	E	8	Total	O	0	0
			8	8		
7	F	4	Total	O	0	0
			4	4		
7	G	4	Total	O	0	0
			4	4		

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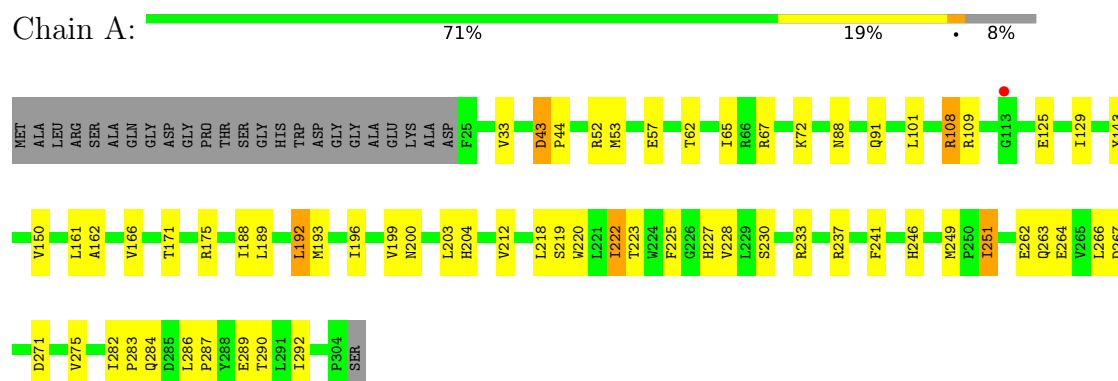
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	2	Total 2	O 2	0	0
7	I	7	Total 7	O 7	0	0
7	J	2	Total 2	O 2	0	0

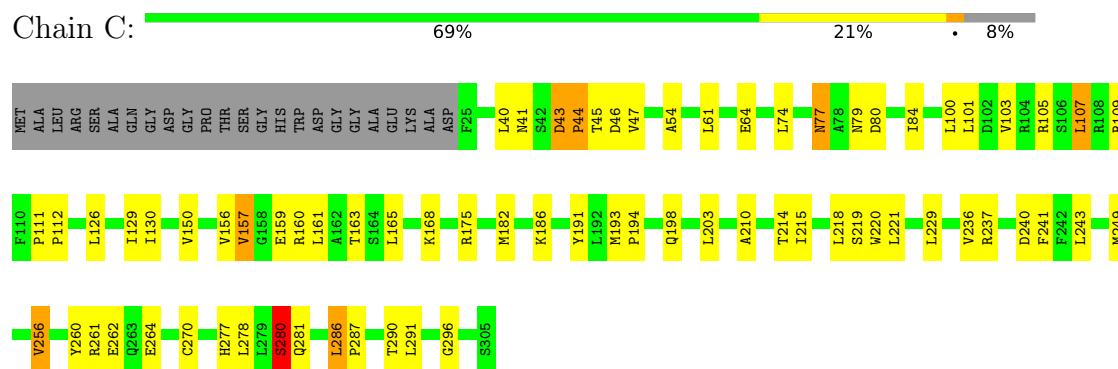
3 Residue-property plots

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.

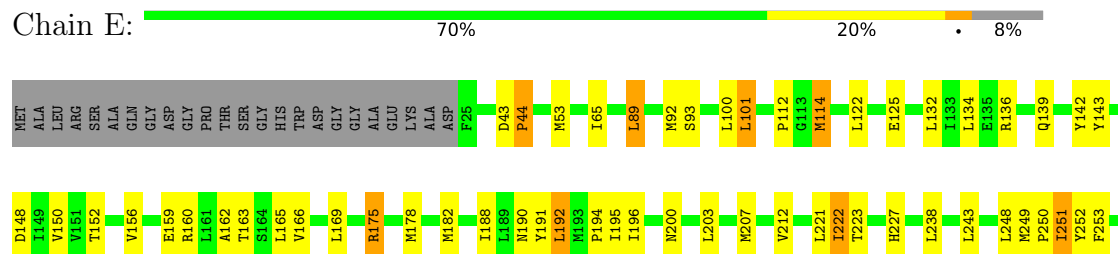
- Molecule 1: TBC1 domain family member 20



- Molecule 1: TBC1 domain family member 20

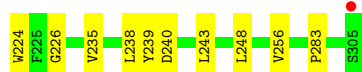
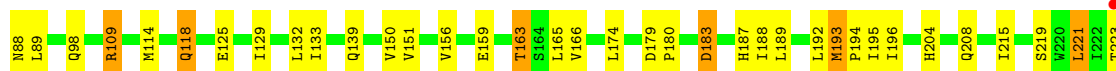


- Molecule 1: TBC1 domain family member 20

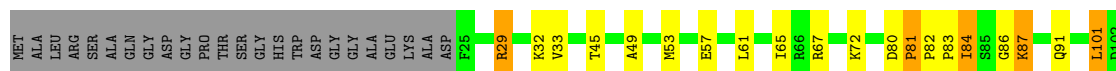




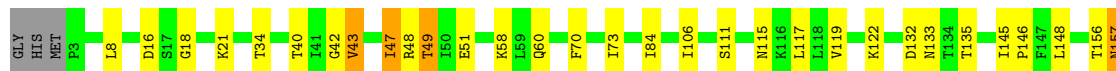
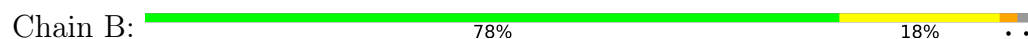
- Molecule 1: TBC1 domain family member 20



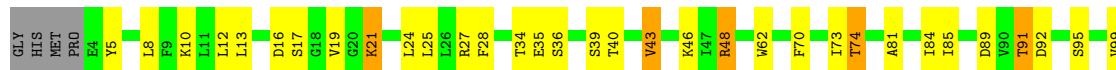
- Molecule 1: TBC1 domain family member 20



- Molecule 2: Ras-related protein Rab-1B



- Molecule 2: Ras-related protein Rab-1B





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

Chain F: 77% 16% 5% .



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

Chain H: 82% 13% . .



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

Chain J: 82% 15% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.17Å 118.64Å 290.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 3.30 49.22 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-3.30) 99.9 (49.22-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.206 , 0.274 (Not available) , 0.241	Depositor DCC
R_{free} test set	2334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17765	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, BEF, SO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/2298	0.91	2/3130 (0.1%)
1	C	0.49	0/2296	0.91	2/3129 (0.1%)
1	E	0.45	0/2302	0.85	2/3137 (0.1%)
1	G	0.49	0/2172	0.92	1/2975 (0.0%)
1	I	0.45	0/2293	0.91	4/3125 (0.1%)
2	B	0.45	0/1353	0.81	0/1832
2	D	0.46	0/1348	0.82	1/1825 (0.1%)
2	F	0.45	0/1342	0.79	0/1818
2	H	0.83	1/1221 (0.1%)	0.90	2/1667 (0.1%)
2	J	0.48	0/1280	0.80	0/1744
All	All	0.50	1/17905 (0.0%)	0.87	14/24382 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	79	ARG	CD-NE	-23.58	1.13	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	79	ARG	CG-CD-NE	10.60	135.32	112.00
1	C	280	SER	N-CA-C	9.46	124.83	112.72
1	G	87	LYS	N-CA-C	6.11	117.94	109.15
2	H	79	ARG	CD-NE-CZ	-5.88	116.16	124.40
2	D	156	THR	N-CA-C	5.77	118.96	110.30
1	A	246	HIS	CA-C-N	5.51	125.86	119.47
1	A	246	HIS	C-N-CA	5.51	125.86	119.47
1	C	61	LEU	N-CA-C	5.49	117.69	111.11
1	E	114	MET	CA-C-N	5.34	125.34	119.90
1	E	114	MET	C-N-CA	5.34	125.34	119.90
1	I	86	GLY	N-CA-C	5.29	118.64	112.50
1	I	81	PRO	CA-C-N	5.11	123.34	119.66
1	I	81	PRO	C-N-CA	5.11	123.34	119.66
1	I	84	ILE	N-CA-C	5.11	115.33	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ARG	Sidechain
1	A	43	ASP	Peptide
1	C	280	SER	Peptide
1	C	43	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2242	0	2195	45	0
1	C	2240	0	2190	46	0
1	E	2246	0	2195	45	0
1	G	2118	0	1943	36	0
1	I	2237	0	2189	50	0
2	B	1332	0	1278	21	0
2	D	1327	0	1300	26	0
2	F	1321	0	1268	20	0
2	H	1202	0	1014	19	0
2	J	1259	0	1123	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	I	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	0	0
5	F	28	0	12	1	0
5	H	28	0	12	7	0
5	J	28	0	12	3	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
6	F	4	0	0	0	0
6	H	4	0	0	1	0
6	J	4	0	0	1	0
7	A	9	0	0	1	0
7	B	4	0	0	0	0
7	C	7	0	0	0	0
7	D	4	0	0	0	0
7	E	8	0	0	0	0
7	F	4	0	0	0	0
7	G	4	0	0	1	0
7	H	2	0	0	0	0
7	I	7	0	0	0	0
7	J	2	0	0	0	0
All	All	17765	0	16755	311	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 (311) 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:114:MET:HE1	1:E:122:LEU:HD12	1.38	1.03
1:G:79:ASN:H	1:G:79:ASN:HD22	1.06	0.96
1:E:175:ARG:O	1:E:175:ARG:HD3	1.77	0.83
1:G:98:GLN:HG2	2:H:67:GLN:HE21	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:177:PHE:HZ	1:I:221:LEU:HD22	1.47	0.80
1:E:175:ARG:HD3	1:E:175:ARG:C	2.08	0.79
1:A:241:PHE:HZ	1:A:249:MET:HE3	1.49	0.77
2:H:45:PHE:HB3	2:H:62:TRP:CD1	2.19	0.77
1:G:109:ARG:HG2	1:G:151:VAL:HG11	1.65	0.77
2:B:49:THR:HG22	2:B:58:LYS:HD3	1.67	0.76
1:I:87:LYS:H	1:I:87:LYS:HD2	1.51	0.76
1:E:143:TYR:CE1	1:E:222:ILE:HG23	2.22	0.75
2:H:20:GLY:HA2	5:H:202:GDP:H5''	1.70	0.74
1:E:101:LEU:HD21	2:F:18:GLY:HA3	1.70	0.72
1:I:193:MET:HE1	1:I:207:MET:HE2	1.71	0.72
1:G:79:ASN:H	1:G:79:ASN:ND2	1.86	0.71
1:A:228:VAL:CG1	1:A:282:ILE:HG21	2.20	0.71
1:C:241:PHE:CZ	1:C:249:MET:HE3	2.25	0.71
2:H:20:GLY:HA2	5:H:202:GDP:C5'	2.22	0.70
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.56	0.70
1:I:80:ASP:HB2	1:I:81:PRO:HD2	1.75	0.69
1:I:177:PHE:CZ	1:I:221:LEU:HD22	2.27	0.68
1:E:175:ARG:HG3	1:E:175:ARG:HH11	1.57	0.68
1:A:62:THR:OG1	1:A:65:ILE:HD13	1.93	0.68
2:H:14:ILE:HG21	2:H:78:TYR:OH	1.94	0.68
2:D:5:TYR:OH	2:D:8:LEU:HD12	1.94	0.67
1:A:143:TYR:CE1	1:A:222:ILE:HG23	2.29	0.67
1:I:143:TYR:CE1	1:I:222:ILE:HG23	2.30	0.67
1:I:241:PHE:HZ	1:I:249:MET:HE2	1.60	0.67
1:I:179:ASP:O	2:J:69:ARG:NH2	2.28	0.67
1:G:159:GLU:O	1:G:163:THR:HG22	1.95	0.66
1:A:203:LEU:HD12	1:A:262:GLU:HG3	1.77	0.66
1:G:79:ASN:HD22	1:G:79:ASN:N	1.83	0.66
1:I:246:HIS:HE1	1:I:248:LEU:HD12	1.60	0.66
2:H:6:ASP:HB2	2:H:56:THR:O	1.96	0.65
1:G:125:GLU:O	1:G:129:ILE:HG12	1.97	0.65
1:A:241:PHE:CZ	1:A:249:MET:HE3	2.32	0.64
1:A:241:PHE:HZ	1:A:249:MET:CE	2.09	0.64
1:A:230:SER:H	1:A:284:GLN:HE22	1.47	0.62
2:J:115:ASN:HB3	2:J:165:MET:HE2	1.80	0.62
1:C:241:PHE:HZ	1:C:249:MET:HE3	1.62	0.62
2:D:151:SER:HB3	2:D:156:THR:HG23	1.82	0.62
5:H:202:GDP:H5'	5:H:202:GDP:C8	2.35	0.61
1:C:74:LEU:O	1:C:168:LYS:HD3	2.00	0.61
1:I:224:TRP:HZ3	1:I:243:LEU:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:202:GDP:H5'	5:H:202:GDP:H8	1.66	0.61
1:A:125:GLU:O	1:A:129:ILE:HD12	2.00	0.61
1:I:29:ARG:HD2	1:I:61:LEU:HD22	1.82	0.61
1:C:107:LEU:C	1:C:109:ARG:H	2.08	0.61
1:A:67:ARG:NH1	3:A:401:SO4:O2	2.33	0.61
2:B:21:LYS:N	5:B:202:GDP:O3B	2.33	0.61
2:B:132:ASP:HB3	2:B:135:THR:OG1	2.01	0.60
2:D:70:PHE:O	2:D:73:ILE:HG22	2.01	0.60
1:C:43:ASP:HB3	1:C:44:PRO:HD3	1.84	0.60
2:B:48:ARG:NH2	2:B:159:GLU:OE1	2.35	0.60
1:E:143:TYR:HE1	1:E:222:ILE:HG23	1.63	0.60
2:H:45:PHE:HB3	2:H:62:TRP:HD1	1.63	0.60
1:A:241:PHE:CZ	1:A:249:MET:CE	2.85	0.60
1:A:150:VAL:HG22	1:A:166:VAL:HG11	1.84	0.59
1:E:238:LEU:HD21	1:E:253:PHE:CE2	2.37	0.59
1:G:150:VAL:HG22	1:G:166:VAL:HG11	1.83	0.59
1:A:57:GLU:HG3	1:A:289:GLU:HG2	1.83	0.58
1:A:192:LEU:O	1:A:196:ILE:HG12	2.02	0.58
1:E:125:GLU:HG2	1:E:159:GLU:HG3	1.85	0.58
1:A:188:ILE:O	1:A:251:ILE:HD13	2.04	0.58
2:F:27:ARG:HB3	2:F:158:VAL:HG11	1.86	0.57
1:E:150:VAL:HG22	1:E:166:VAL:HG11	1.85	0.57
1:C:77:ASN:C	1:C:77:ASN:HD22	2.13	0.57
2:F:89:ASP:OD1	2:F:91:THR:HG22	2.04	0.57
2:B:115:ASN:HD21	2:B:172:ARG:HD3	1.70	0.57
1:C:249:MET:HE1	1:C:296:GLY:HA2	1.87	0.57
1:E:162:ALA:O	1:E:166:VAL:HG23	2.04	0.56
1:C:129:ILE:HD11	1:C:159:GLU:HG3	1.86	0.56
1:C:157:VAL:HG13	1:C:161:LEU:CB	2.35	0.56
1:I:111:PRO:HG2	1:I:114:MET:HB2	1.88	0.56
1:C:54:ALA:O	1:C:237:ARG:NH1	2.39	0.56
2:J:121:ASN:HA	2:J:150:THR:O	2.06	0.56
2:D:43:VAL:HG13	2:D:62:TRP:HD1	1.70	0.55
1:E:112:PRO:HB2	1:I:302:PHE:HZ	1.71	0.55
1:I:45:THR:HG21	1:I:72:LYS:HD2	1.89	0.55
1:A:143:TYR:HE1	1:A:222:ILE:HG23	1.70	0.55
1:C:77:ASN:HD22	1:C:79:ASN:H	1.53	0.55
2:H:14:ILE:HD11	2:H:106:ILE:HD11	1.87	0.55
1:A:287:PRO:HB2	1:A:290:THR:HB	1.89	0.55
1:E:182:MET:HE2	2:F:70:PHE:HA	1.88	0.55
1:C:157:VAL:CG1	1:C:161:LEU:HB3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ASP:HA	1:G:66:ARG:HG3	1.87	0.54
1:A:52:ARG:HA	1:E:92:MET:HE1	1.90	0.54
1:E:175:ARG:HH11	1:E:175:ARG:CG	2.20	0.54
1:G:235:VAL:HA	1:G:238:LEU:HD23	1.88	0.54
2:F:125:LEU:HD11	5:F:202:GDP:N2	2.22	0.54
1:E:53:MET:HE2	1:E:53:MET:HA	1.88	0.54
2:J:85:ILE:HG12	2:J:117:LEU:HD23	1.90	0.54
1:I:171:THR:HG23	1:I:172:HIS:ND1	2.23	0.54
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.73	0.54
1:E:188:ILE:O	1:E:191:TYR:HB2	2.08	0.54
1:C:157:VAL:HG13	1:C:161:LEU:HB3	1.91	0.53
1:C:229:LEU:HD21	1:C:286:LEU:HD12	1.91	0.53
1:G:129:ILE:HG23	1:G:163:THR:HB	1.91	0.53
1:G:239:TYR:O	1:G:243:LEU:HB2	2.08	0.53
1:E:249:MET:HE2	1:E:295:ALA:HB1	1.91	0.53
1:G:183:ASP:O	1:G:187:HIS:ND1	2.42	0.53
1:C:156:VAL:CG2	1:C:236:VAL:HG11	2.39	0.52
1:A:189:LEU:HA	1:A:251:ILE:HD11	1.92	0.52
2:D:132:ASP:HB2	2:D:135:THR:HG23	1.90	0.52
1:C:256:VAL:CG1	1:C:291:LEU:HD22	2.40	0.52
1:E:175:ARG:C	1:E:175:ARG:CD	2.82	0.52
1:I:193:MET:HB3	1:I:194:PRO:CD	2.40	0.52
1:I:241:PHE:CZ	1:I:249:MET:HE2	2.42	0.52
2:B:156:THR:HG22	2:B:157:ASN:HB2	1.92	0.52
1:C:193:MET:CE	1:C:214:THR:HG22	2.39	0.52
1:G:139:GLN:NE2	7:G:404:HOH:O	2.43	0.52
1:I:188:ILE:HG23	1:I:248:LEU:HD23	1.92	0.52
1:A:218:LEU:HD23	2:B:42:GLY:HA2	1.92	0.51
1:A:262:GLU:HG2	1:A:266:LEU:CD1	2.39	0.51
1:A:188:ILE:O	1:A:251:ILE:CD1	2.58	0.51
1:C:237:ARG:HD2	1:C:237:ARG:O	2.10	0.51
1:A:228:VAL:HG12	1:A:282:ILE:HG21	1.93	0.51
1:I:249:MET:CE	1:I:295:ALA:HB1	2.41	0.51
1:I:32:LYS:HE3	1:I:61:LEU:HD11	1.93	0.51
1:E:223:THR:HG21	1:E:227:HIS:HB2	1.93	0.51
2:B:117:LEU:HD23	2:B:119:VAL:HG23	1.93	0.51
2:D:70:PHE:O	2:D:74:THR:HG23	2.10	0.51
1:I:87:LYS:HD2	1:I:87:LYS:N	2.25	0.51
1:E:248:LEU:O	1:E:251:ILE:HG13	2.10	0.51
2:J:139:PHE:O	2:J:142:SER:HB3	2.10	0.51
1:I:83:PRO:HB3	1:I:136:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:20:GLY:HA3	2:J:121:ASN:HD22	1.76	0.50
2:D:159:GLU:O	2:D:163:MET:HG2	2.11	0.50
1:E:192:LEU:HD23	1:E:196:ILE:HD11	1.94	0.50
5:H:202:GDP:C5'	5:H:202:GDP:H8	2.24	0.50
1:A:286:LEU:HD12	1:A:286:LEU:H	1.77	0.50
1:C:77:ASN:HB3	1:C:80:ASP:OD2	2.12	0.50
1:E:277:HIS:HB2	2:F:45:PHE:CE1	2.47	0.50
1:C:191:TYR:O	1:C:194:PRO:HD2	2.12	0.50
2:B:84:ILE:HD12	2:B:106:ILE:HG23	1.93	0.50
1:C:286:LEU:HD23	1:C:287:PRO:HD2	1.93	0.50
1:G:192:LEU:O	1:G:196:ILE:HG12	2.12	0.50
1:A:53:MET:HE2	1:A:53:MET:HA	1.93	0.49
2:D:19:VAL:HG23	2:D:21:LYS:HG3	1.93	0.49
2:B:117:LEU:CD2	2:B:119:VAL:HG23	2.42	0.49
2:F:148:LEU:HD23	2:F:157:ASN:HB3	1.95	0.49
1:I:231:ASP:O	1:I:235:VAL:HG23	2.11	0.49
2:H:17:SER:HA	6:H:203:BEF:F3	2.02	0.49
1:I:184:ASN:O	1:I:188:ILE:HG12	2.12	0.49
1:A:189:LEU:HD11	1:A:218:LEU:HD13	1.93	0.49
1:A:230:SER:HB3	1:A:284:GLN:NE2	2.28	0.49
1:E:132:LEU:O	1:E:136:ARG:HG3	2.13	0.49
2:F:113:ASN:HB3	2:F:172:ARG:HE	1.78	0.49
1:C:156:VAL:HG12	1:C:157:VAL:HG23	1.94	0.49
1:A:200:ASN:C	1:A:200:ASN:HD22	2.20	0.49
1:C:256:VAL:HG13	1:C:291:LEU:HD22	1.95	0.49
2:D:21:LYS:HB2	2:D:21:LYS:NZ	2.27	0.49
1:G:193:MET:HA	1:G:193:MET:HE3	1.95	0.49
2:B:47:ILE:HG12	2:B:58:LYS:HD2	1.93	0.48
2:H:70:PHE:O	2:H:74:THR:HG22	2.13	0.48
2:D:24:LEU:HD23	2:D:152:ALA:HB2	1.96	0.48
1:G:66:ARG:NH1	1:G:240:ASP:OD2	2.47	0.48
1:I:189:LEU:HB3	1:I:214:THR:HB	1.95	0.48
1:C:182:MET:HE1	1:C:218:LEU:HD11	1.94	0.48
1:I:101:LEU:HD11	2:J:18:GLY:HA3	1.95	0.48
2:D:43:VAL:HG13	2:D:62:TRP:CD1	2.49	0.48
2:F:47:ILE:HG21	2:F:58:LYS:HE2	1.96	0.48
2:F:104:GLN:HB3	2:F:108:ARG:NH1	2.29	0.48
1:I:61:LEU:H	1:I:61:LEU:HD12	1.78	0.48
1:I:32:LYS:HE2	1:I:57:GLU:O	2.14	0.47
2:J:20:GLY:HA2	5:J:202:GDP:O1A	2.14	0.47
1:E:207:MET:HE1	1:E:258:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:MET:HE3	1:C:214:THR:HG22	1.95	0.47
1:G:193:MET:HB3	1:G:194:PRO:HD3	1.95	0.47
1:I:223:THR:HG21	1:I:227:HIS:HB2	1.97	0.47
1:A:237:ARG:NH2	1:A:292:ILE:HD13	2.29	0.47
2:D:24:LEU:HD21	2:D:121:ASN:HD21	1.79	0.47
2:B:70:PHE:O	2:B:73:ILE:HG22	2.14	0.47
1:E:89:LEU:O	1:E:93:SER:HB2	2.15	0.47
1:E:148:ASP:OD2	1:E:227:HIS:CD2	2.68	0.47
1:E:192:LEU:CD2	1:E:196:ILE:HD11	2.44	0.47
1:C:277:HIS:O	1:C:281:GLN:CB	2.63	0.46
2:B:117:LEU:HD12	2:B:146:PRO:HB2	1.97	0.46
1:C:237:ARG:O	1:C:240:ASP:HB2	2.15	0.46
1:E:160:ARG:O	1:E:163:THR:HG22	2.15	0.46
1:G:84:ILE:HD13	1:G:84:ILE:H	1.79	0.46
1:G:204:HIS:CE1	1:G:208:GLN:HE21	2.33	0.46
1:G:98:GLN:HG2	2:H:67:GLN:NE2	2.20	0.46
1:I:188:ILE:HG23	1:I:248:LEU:CD2	2.46	0.46
1:A:62:THR:HG1	1:A:65:ILE:HD13	1.80	0.46
1:A:228:VAL:HG13	1:A:282:ILE:HG21	1.96	0.46
1:I:29:ARG:O	1:I:33:VAL:HG23	2.15	0.46
1:A:263:GLN:O	1:A:267:ASP:HB3	2.15	0.46
1:G:223:THR:H	1:G:224:TRP:HA	1.80	0.46
1:G:43:ASP:CB	1:G:44:PRO:HD3	2.45	0.46
2:H:89:ASP:OD2	2:H:91:THR:HG22	2.15	0.46
1:C:44:PRO:O	1:C:45:THR:C	2.59	0.46
1:A:43:ASP:CB	1:A:44:PRO:HD3	2.46	0.46
2:F:11:LEU:HD12	2:F:61:ILE:HG12	1.97	0.46
1:C:77:ASN:ND2	1:C:79:ASN:H	2.13	0.46
1:I:220:TRP:CD1	1:I:228:VAL:HG21	2.51	0.46
1:I:193:MET:HE3	1:I:193:MET:HA	1.98	0.45
1:C:43:ASP:HB3	1:C:44:PRO:CD	2.47	0.45
1:I:169:LEU:HD11	1:I:224:TRP:CH2	2.51	0.45
2:J:20:GLY:CA	5:J:202:GDP:O1A	2.64	0.45
1:E:305:SER:HA	2:H:92:ASP:CG	2.42	0.45
1:I:81:PRO:HA	1:I:82:PRO:HD3	1.84	0.45
1:C:157:VAL:CG1	1:C:161:LEU:CB	2.95	0.45
1:E:143:TYR:CE2	1:E:178:MET:HG2	2.51	0.45
2:F:115:ASN:ND2	2:F:172:ARG:NH2	2.64	0.45
2:F:43:VAL:HG13	2:F:62:TRP:CD1	2.51	0.45
5:H:202:GDP:C5'	5:H:202:GDP:C8	3.00	0.45
2:D:122:LYS:HB3	2:D:125:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:VAL:HG13	2:F:62:TRP:HD1	1.81	0.45
2:F:27:ARG:HG3	2:F:152:ALA:HA	1.99	0.45
1:A:241:PHE:CZ	1:A:249:MET:HE2	2.52	0.45
2:H:77:TYR:CD1	2:H:77:TYR:N	2.85	0.45
2:J:12:LEU:HD23	2:J:84:ILE:HG12	1.99	0.45
2:J:28:PHE:CE2	2:J:48:ARG:HG2	2.52	0.45
1:E:261:ARG:NH1	1:E:264:GLU:OE1	2.50	0.44
1:E:43:ASP:CB	1:E:44:PRO:HD3	2.48	0.44
2:F:49:THR:HG22	2:F:58:LYS:HG3	1.99	0.44
1:E:207:MET:HE1	1:E:258:VAL:HG13	2.00	0.44
2:B:115:ASN:ND2	2:B:172:ARG:HH21	2.15	0.44
2:D:19:VAL:HA	2:D:89:ASP:HB2	1.99	0.44
2:D:12:LEU:HB3	2:D:84:ILE:HG12	1.99	0.44
2:D:13:LEU:HD23	2:D:85:ILE:HB	1.99	0.44
1:I:246:HIS:CE1	1:I:248:LEU:HD12	2.47	0.44
1:C:210:ALA:HB2	1:C:270:CYS:SG	2.58	0.44
1:I:49:ALA:O	1:I:53:MET:HG2	2.18	0.44
1:A:88:ASN:HB3	1:A:91:GLN:HB3	2.00	0.44
1:C:220:TRP:N	1:C:220:TRP:CD1	2.86	0.44
1:E:203:LEU:HD22	1:E:207:MET:HE3	2.00	0.44
1:G:189:LEU:HG	1:G:221:LEU:HD12	2.00	0.44
2:J:111:SER:HB3	2:J:114:VAL:HB	1.99	0.44
1:C:280:SER:H	1:C:281:GLN:CB	2.31	0.43
2:D:92:ASP:HB3	2:D:95:SER:OG	2.17	0.43
1:G:87:LYS:HA	1:G:88:ASN:HA	1.51	0.43
2:H:77:TYR:N	2:H:77:TYR:HD1	2.16	0.43
2:D:132:ASP:HB2	2:D:135:THR:CG2	2.48	0.43
1:C:160:ARG:O	1:C:163:THR:HG22	2.18	0.43
2:F:25:LEU:HD12	2:F:63:ASP:HB2	2.01	0.43
1:G:179:ASP:HB3	1:G:180:PRO:HD2	2.01	0.43
1:I:122:LEU:O	1:I:125:GLU:HB2	2.18	0.43
1:I:193:MET:HE1	1:I:207:MET:CE	2.44	0.43
1:C:229:LEU:HD21	1:C:286:LEU:CD1	2.47	0.43
1:E:249:MET:HE3	1:E:252:TYR:HB2	1.99	0.43
2:H:103:LEU:HD21	2:H:143:LEU:HD11	2.00	0.43
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.26	0.43
2:B:122:LYS:HG2	5:B:202:GDP:C6	2.53	0.43
1:E:249:MET:N	1:E:250:PRO:CD	2.82	0.43
1:E:305:SER:HA	2:H:92:ASP:HB2	2.00	0.43
1:G:226:GLY:HA2	1:G:235:VAL:HG21	1.99	0.43
1:C:130:ILE:HG12	1:C:150:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:THR:O	1:E:156:VAL:HG23	2.18	0.43
1:C:261:ARG:NH2	1:C:278:LEU:O	2.52	0.43
2:D:10:LYS:HG2	2:D:81:ALA:HA	2.01	0.43
1:C:161:LEU:O	1:C:165:LEU:HG	2.19	0.42
2:F:27:ARG:HD2	2:F:155:ALA:HB2	2.01	0.42
1:I:222:ILE:HD13	1:I:222:ILE:HA	1.89	0.42
1:I:150:VAL:HG22	1:I:166:VAL:HG11	2.01	0.42
1:C:105:ARG:CZ	2:D:39:SER:HB3	2.49	0.42
2:F:89:ASP:HB3	2:F:92:ASP:HB3	2.01	0.42
2:J:11:LEU:HD21	2:J:59:LEU:HD23	2.00	0.42
1:G:47:VAL:HA	1:G:50:LEU:HD12	2.02	0.42
1:G:223:THR:N	1:G:224:TRP:HA	2.34	0.42
1:I:224:TRP:CZ3	1:I:243:LEU:HD22	2.48	0.42
2:D:89:ASP:CG	2:D:91:THR:HG22	2.44	0.42
1:A:193:MET:HE3	1:A:204:HIS:CD2	2.54	0.42
2:B:8:LEU:HD12	2:B:58:LYS:HG2	2.01	0.42
1:G:114:MET:HG3	1:G:118:GLN:HG2	2.02	0.42
2:B:60:GLN:O	2:B:60:GLN:HG3	2.20	0.42
1:C:156:VAL:HG21	1:C:236:VAL:CG1	2.49	0.42
1:C:157:VAL:HG13	1:C:161:LEU:HB2	2.02	0.42
2:D:48:ARG:NH2	2:D:159:GLU:OE1	2.53	0.42
2:D:110:ALA:HB1	2:D:114:VAL:HG11	2.02	0.42
1:A:101:LEU:HD21	2:B:18:GLY:HA3	2.02	0.41
1:C:103:VAL:HG13	1:C:126:LEU:HD23	2.01	0.41
2:D:28:PHE:CE2	2:D:48:ARG:HG2	2.55	0.41
1:G:215:ILE:H	1:G:215:ILE:HD12	1.85	0.41
1:C:111:PRO:HA	1:C:112:PRO:HD3	1.90	0.41
2:D:16:ASP:O	2:D:19:VAL:HG22	2.20	0.41
1:C:220:TRP:CD1	1:C:220:TRP:H	2.38	0.41
1:I:103:VAL:HG13	1:I:126:LEU:HD23	2.01	0.41
1:I:152:THR:HG23	1:I:232:PHE:CE1	2.55	0.41
1:I:221:LEU:HD23	1:I:250:PRO:HB2	2.02	0.41
1:G:66:ARG:O	1:G:70:TRP:HB2	2.20	0.41
1:I:249:MET:N	1:I:250:PRO:CD	2.83	0.41
1:E:148:ASP:OD2	1:E:227:HIS:HD2	2.04	0.41
1:G:65:ILE:HG22	1:G:66:ARG:N	2.35	0.41
2:H:23:CYS:HB2	5:H:202:GDP:O5'	2.19	0.41
1:A:72:LYS:NZ	7:A:501:HOH:O	2.54	0.41
2:B:159:GLU:O	2:B:163:MET:HG2	2.20	0.41
1:E:165:LEU:O	1:E:169:LEU:HD12	2.20	0.41
1:I:220:TRP:HD1	1:I:228:VAL:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:GLN:O	1:I:127:ILE:HG13	2.21	0.41
5:J:202:GDP:O3B	6:J:203:BEF:F2	2.28	0.41
1:A:220:TRP:HB3	1:A:225:PHE:CE2	2.56	0.41
1:A:223:THR:HG21	1:A:227:HIS:HB2	2.02	0.41
1:E:134:LEU:HD11	1:E:142:TYR:HB2	2.03	0.41
1:E:191:TYR:O	1:E:195:ILE:HG13	2.21	0.41
1:G:188:ILE:HG23	1:G:248:LEU:HD22	2.03	0.41
2:B:42:GLY:O	2:B:43:VAL:HG23	2.21	0.41
1:C:107:LEU:HD22	2:D:36:SER:HB2	2.02	0.41
1:A:162:ALA:O	1:A:166:VAL:HG23	2.21	0.40
1:A:282:ILE:HG13	1:A:283:PRO:HD2	2.03	0.40
1:E:190:ASN:O	1:E:194:PRO:HD2	2.22	0.40
1:I:249:MET:HE1	1:I:295:ALA:C	2.46	0.40
1:G:73:LEU:HD23	1:G:73:LEU:HA	1.97	0.40
2:B:51:GLU:CD	2:B:51:GLU:H	2.29	0.40
1:E:139:GLN:H	1:E:139:GLN:CD	2.30	0.40
2:H:169:ILE:HD13	2:H:169:ILE:HA	2.00	0.40
2:F:86:VAL:HG11	2:F:99:VAL:HG13	2.04	0.40
1:G:235:VAL:O	1:G:238:LEU:HB2	2.21	0.40
1:I:182:MET:HG3	2:J:69:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/305 (91%)	264 (95%)	14 (5%)	0	100	100
1	C	279/305 (92%)	266 (95%)	11 (4%)	2 (1%)	18	49
1	E	279/305 (92%)	267 (96%)	11 (4%)	1 (0%)	30	60
1	G	279/305 (92%)	266 (95%)	9 (3%)	4 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	279/305 (92%)	276 (99%)	3 (1%)	0	100	100
2	B	170/175 (97%)	161 (95%)	9 (5%)	0	100	100
2	D	168/175 (96%)	163 (97%)	5 (3%)	0	100	100
2	F	170/175 (97%)	159 (94%)	10 (6%)	1 (1%)	21	52
2	H	168/175 (96%)	156 (93%)	11 (6%)	1 (1%)	21	52
2	J	169/175 (97%)	161 (95%)	7 (4%)	1 (1%)	21	52
All	All	2239/2400 (93%)	2139 (96%)	90 (4%)	10 (0%)	30	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	56	SER
2	H	155	ALA
2	F	114	VAL
1	E	44	PRO
1	G	46	ASP
1	G	283	PRO
2	J	122	LYS
1	G	44	PRO
1	C	44	PRO
1	C	47	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/271 (88%)	225 (94%)	14 (6%)	18	46
1	C	241/271 (89%)	217 (90%)	24 (10%)	7	27
1	E	242/271 (89%)	224 (93%)	18 (7%)	13	38
1	G	206/271 (76%)	182 (88%)	24 (12%)	5	20
1	I	240/271 (89%)	220 (92%)	20 (8%)	10	34
2	B	138/151 (91%)	126 (91%)	12 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	141/151 (93%)	124 (88%)	17 (12%)	5	20
2	F	135/151 (89%)	119 (88%)	16 (12%)	5	20
2	H	103/151 (68%)	93 (90%)	10 (10%)	8	28
2	J	117/151 (78%)	107 (92%)	10 (8%)	10	33
All	All	1802/2110 (85%)	1637 (91%)	165 (9%)	8	30

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	108	ARG
1	A	161	LEU
1	A	171	THR
1	A	175	ARG
1	A	192	LEU
1	A	199	VAL
1	A	212	VAL
1	A	219	SER
1	A	222	ILE
1	A	251	ILE
1	A	264	GLU
1	A	271	ASP
1	A	275	VAL
2	B	16	ASP
2	B	34	THR
2	B	40	THR
2	B	43	VAL
2	B	47	ILE
2	B	49	THR
2	B	111	SER
2	B	133	ASN
2	B	145	ILE
2	B	148	LEU
2	B	157	ASN
2	B	165	MET
1	C	40	LEU
1	C	41	ASN
1	C	46	ASP
1	C	64	GLU
1	C	77	ASN
1	C	84	ILE

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Mol	Chain	Res	Type
1	C	100	LEU
1	C	101	LEU
1	C	107	LEU
1	C	157	VAL
1	C	175	ARG
1	C	186	LYS
1	C	198	GLN
1	C	203	LEU
1	C	215	ILE
1	C	219	SER
1	C	221	LEU
1	C	243	LEU
1	C	256	VAL
1	C	260	TYR
1	C	262	GLU
1	C	264	GLU
1	C	286	LEU
1	C	290	THR
2	D	17	SER
2	D	21	LYS
2	D	25	LEU
2	D	27	ARG
2	D	34	THR
2	D	35	GLU
2	D	40	THR
2	D	43	VAL
2	D	46	LYS
2	D	48	ARG
2	D	74	THR
2	D	91	THR
2	D	99	VAL
2	D	118	LEU
2	D	135	THR
2	D	143	LEU
2	D	156	THR
1	E	65	ILE
1	E	89	LEU
1	E	100	LEU
1	E	101	LEU
1	E	175	ARG
1	E	192	LEU
1	E	200	ASN

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Mol	Chain	Res	Type
1	E	212	VAL
1	E	221	LEU
1	E	222	ILE
1	E	243	LEU
1	E	251	ILE
1	E	257	ILE
1	E	266	LEU
1	E	272	MET
1	E	280	SER
1	E	284	GLN
1	E	293	SER
2	F	8	LEU
2	F	12	LEU
2	F	25	LEU
2	F	27	ARG
2	F	34	THR
2	F	43	VAL
2	F	47	ILE
2	F	49	THR
2	F	62	TRP
2	F	100	LYS
2	F	108	ARG
2	F	118	LEU
2	F	145	ILE
2	F	148	LEU
2	F	165	MET
2	F	172	ARG
1	G	30	LYS
1	G	36	ILE
1	G	53	MET
1	G	57	GLU
1	G	62	THR
1	G	65	ILE
1	G	75	ASN
1	G	79	ASN
1	G	84	ILE
1	G	89	LEU
1	G	109	ARG
1	G	118	GLN
1	G	132	LEU
1	G	133	ILE
1	G	156	VAL

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Mol	Chain	Res	Type
1	G	163	THR
1	G	165	LEU
1	G	174	LEU
1	G	183	ASP
1	G	193	MET
1	G	195	ILE
1	G	219	SER
1	G	221	LEU
1	G	256	VAL
2	H	17	SER
2	H	27	ARG
2	H	34	THR
2	H	48	ARG
2	H	77	TYR
2	H	91	THR
2	H	103	LEU
2	H	112	GLU
2	H	143	LEU
2	H	154	ASN
1	I	29	ARG
1	I	65	ILE
1	I	67	ARG
1	I	84	ILE
1	I	87	LYS
1	I	91	GLN
1	I	101	LEU
1	I	139	GLN
1	I	203	LEU
1	I	221	LEU
1	I	222	ILE
1	I	228	VAL
1	I	238	LEU
1	I	243	LEU
1	I	248	LEU
1	I	251	ILE
1	I	266	LEU
1	I	269	ASP
1	I	281	GLN
1	I	298	LEU
2	J	11	LEU
2	J	13	LEU
2	J	27	ARG

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Mol	Chain	Res	Type
2	J	34	THR
2	J	40	THR
2	J	47	ILE
2	J	86	VAL
2	J	104	GLN
2	J	127	THR
2	J	165	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	79	ASN
1	A	91	GLN
1	A	144	GLN
1	A	184	ASN
1	A	200	ASN
1	A	204	HIS
1	A	284	GLN
2	B	113	ASN
2	B	115	ASN
2	B	121	ASN
1	C	37	HIS
1	C	38	GLN
1	C	77	ASN
1	C	88	ASN
1	C	91	GLN
1	C	98	GLN
1	C	141	HIS
1	C	144	GLN
1	C	198	GLN
1	C	227	HIS
1	C	263	GLN
1	C	277	HIS
2	D	101	GLN
2	D	121	ASN
1	E	88	ASN
1	E	91	GLN
1	E	118	GLN
1	E	144	GLN
1	E	200	ASN
1	E	227	HIS

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Mol	Chain	Res	Type
1	E	281	GLN
2	F	115	ASN
2	F	133	ASN
2	F	154	ASN
1	G	26	ASN
1	G	75	ASN
1	G	79	ASN
1	G	88	ASN
1	G	91	GLN
1	G	98	GLN
1	G	123	GLN
1	G	139	GLN
1	G	144	GLN
1	G	190	ASN
1	G	200	ASN
1	G	208	GLN
1	G	277	HIS
1	I	41	ASN
1	I	75	ASN
1	I	77	ASN
1	I	98	GLN
1	I	118	GLN
1	I	137	ASN
1	I	198	GLN
1	I	200	ASN
1	I	284	GLN
2	J	104	GLN
2	J	115	ASN
2	J	121	ASN
2	J	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	GDP	D	202	6	29,30,30	1.35	3 (10%)	45,47,47	1.63	8 (17%)
3	SO4	E	402	-	4,4,4	0.25	0	6,6,6	0.12	0
5	GDP	H	202	4,6	29,30,30	1.27	3 (10%)	45,47,47	1.72	9 (20%)
6	BEF	D	203	5	0,3,3	-	-	-	-	-
3	SO4	E	401	-	4,4,4	0.26	0	6,6,6	0.09	0
6	BEF	B	203	5	0,3,3	-	-	-	-	-
6	BEF	F	203	5	0,3,3	-	-	-	-	-
6	BEF	H	203	5	0,3,3	-	-	-	-	-
6	BEF	J	203	5	0,3,3	-	-	-	-	-
5	GDP	B	202	4,6	29,30,30	1.34	4 (13%)	45,47,47	1.63	9 (20%)
3	SO4	I	401	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	C	401	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	A	401	-	4,4,4	0.22	0	6,6,6	0.21	0
5	GDP	J	202	4,6	29,30,30	1.29	3 (10%)	45,47,47	1.77	10 (22%)
5	GDP	F	202	4,6	29,30,30	1.29	4 (13%)	45,47,47	1.65	8 (17%)

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
5	GDP	D	202	6	-	1/16/32/32	0/3/3/3
5	GDP	H	202	4,6	-	6/16/32/32	0/3/3/3
5	GDP	B	202	4,6	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	J	202	4,6	-	2/16/32/32	0/3/3/3
5	GDP	F	202	4,6	-	2/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	202	GDP	C5-N7	-3.02	1.33	1.39
5	D	202	GDP	C5-C6	-3.00	1.33	1.44
5	D	202	GDP	C5-N7	-2.94	1.33	1.39
5	B	202	GDP	C5-C6	-2.89	1.33	1.44
5	H	202	GDP	C5-C6	-2.74	1.34	1.44
5	J	202	GDP	C5-C6	-2.74	1.34	1.44
5	F	202	GDP	C5-N7	-2.71	1.33	1.39
5	J	202	GDP	C5-N7	-2.66	1.33	1.39
5	F	202	GDP	C5-C6	-2.64	1.34	1.44
5	H	202	GDP	C5-N7	-2.64	1.33	1.39
5	B	202	GDP	PB-O3B	-2.44	1.45	1.54
5	D	202	GDP	PA-O3A	2.34	1.62	1.59
5	F	202	GDP	PA-O3A	2.28	1.62	1.59
5	J	202	GDP	O4'-C1'	2.23	1.47	1.42
5	B	202	GDP	O4'-C1'	2.18	1.47	1.42
5	H	202	GDP	O4'-C1'	2.09	1.46	1.42
5	F	202	GDP	PB-O3B	-2.05	1.47	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	202	GDP	C2-N3-C4	5.28	121.39	112.30
5	F	202	GDP	C2-N3-C4	5.05	121.00	112.30
5	H	202	GDP	C2-N3-C4	4.93	120.79	112.30
5	J	202	GDP	C5-C4-N3	-4.87	120.63	128.39
5	D	202	GDP	C2-N3-C4	4.70	120.39	112.30
5	B	202	GDP	C2-N3-C4	4.59	120.20	112.30
5	H	202	GDP	C5-C4-N3	-4.51	121.21	128.39
5	F	202	GDP	C5-C4-N3	-4.46	121.30	128.39
5	D	202	GDP	C5-C4-N3	-4.43	121.35	128.39
5	B	202	GDP	C5-C4-N3	-4.31	121.53	128.39
5	D	202	GDP	C2-N1-C6	-3.89	118.05	125.11
5	B	202	GDP	C2-N1-C6	-3.71	118.39	125.11
5	H	202	GDP	C2-N1-C6	-3.70	118.40	125.11
5	J	202	GDP	C2-N1-C6	-3.69	118.41	125.11
5	F	202	GDP	C2-N1-C6	-3.61	118.57	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	202	GDP	O4'-C1'-N9	3.10	115.37	108.36
5	F	202	GDP	N9-C8-N7	-2.82	108.17	113.40
5	D	202	GDP	N9-C8-N7	-2.76	108.28	113.40
5	D	202	GDP	N9-C4-N3	2.71	131.38	125.95
5	J	202	GDP	N9-C4-N3	2.65	131.25	125.95
5	J	202	GDP	N9-C8-N7	-2.62	108.53	113.40
5	D	202	GDP	C5-C6-N1	2.61	119.89	113.25
5	B	202	GDP	C5'-C4'-C3'	-2.57	105.97	115.21
5	J	202	GDP	C5-C6-N1	2.55	119.74	113.25
5	B	202	GDP	N9-C8-N7	-2.55	108.68	113.40
5	D	202	GDP	O6-C6-C5	-2.45	120.06	126.53
5	B	202	GDP	N9-C4-N3	2.44	130.84	125.95
5	H	202	GDP	C5-C6-N1	2.44	119.46	113.25
5	H	202	GDP	N9-C8-N7	-2.42	108.91	113.40
5	H	202	GDP	N9-C4-N3	2.41	130.77	125.95
5	J	202	GDP	N1-C2-N3	-2.36	119.00	123.32
5	F	202	GDP	N9-C4-N3	2.35	130.65	125.95
5	F	202	GDP	C5-C6-N1	2.35	119.22	113.25
5	F	202	GDP	N1-C2-N3	-2.25	119.21	123.32
5	H	202	GDP	N1-C2-N3	-2.23	119.23	123.32
5	J	202	GDP	C8-N7-C5	2.22	108.22	104.26
5	B	202	GDP	C5-C6-N1	2.21	118.88	113.25
5	F	202	GDP	C8-N7-C5	2.20	108.17	104.26
5	B	202	GDP	O6-C6-C5	-2.18	120.79	126.53
5	J	202	GDP	C5'-C4'-C3'	-2.17	107.39	115.21
5	H	202	GDP	O6-C6-C5	-2.13	120.91	126.53
5	B	202	GDP	O3B-PB-O2B	2.08	115.61	107.80
5	D	202	GDP	N1-C2-N3	-2.08	119.51	123.32
5	J	202	GDP	O6-C6-C5	-2.02	121.20	126.53

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	202	GDP	C5'-O5'-PA-O3A
5	F	202	GDP	O4'-C4'-C5'-O5'
5	H	202	GDP	C5'-O5'-PA-O3A
5	H	202	GDP	C5'-O5'-PA-O1A
5	H	202	GDP	C5'-O5'-PA-O2A
5	H	202	GDP	C4'-C5'-O5'-PA
5	B	202	GDP	O4'-C4'-C5'-O5'
5	B	202	GDP	C3'-C4'-C5'-O5'

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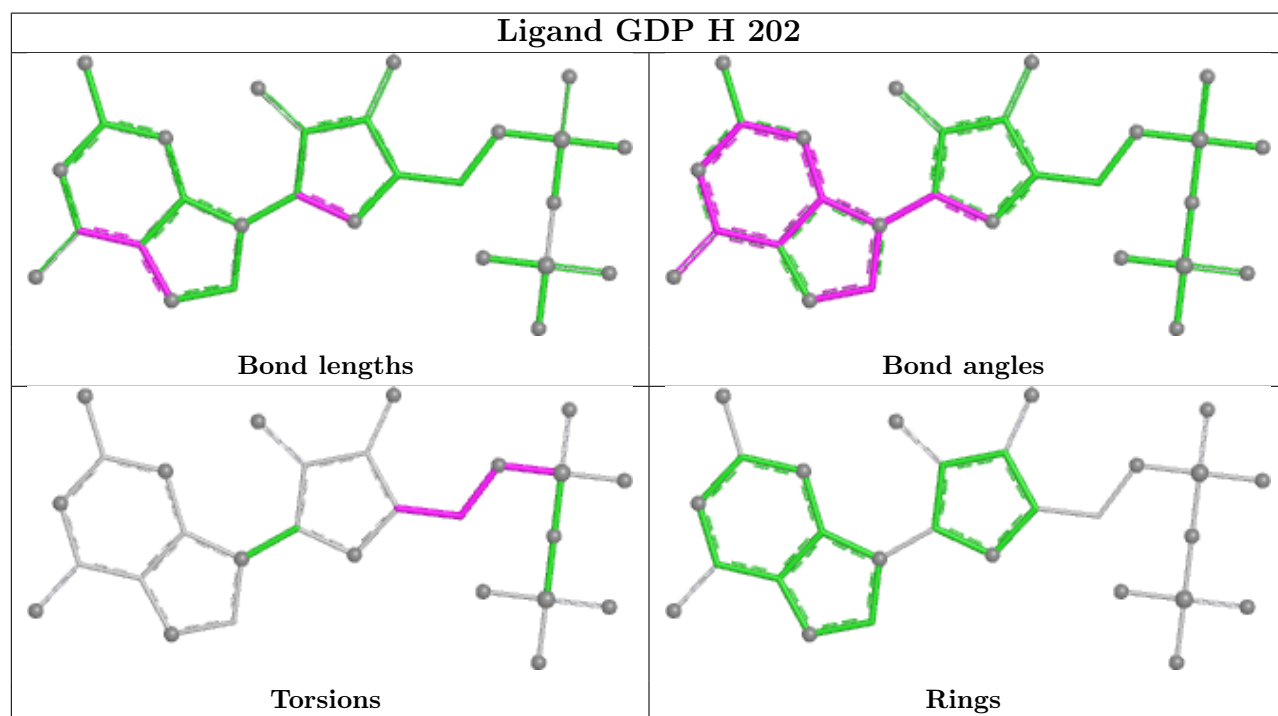
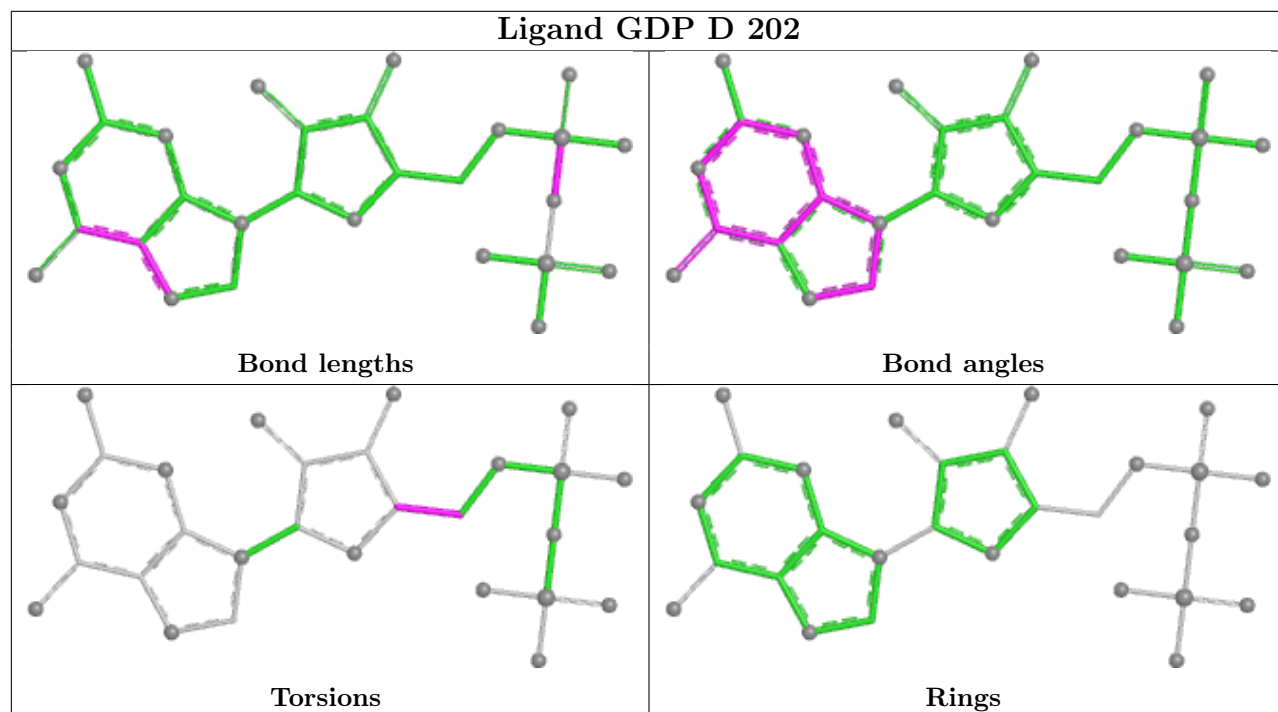
Mol	Chain	Res	Type	Atoms
5	J	202	GDP	O4'-C4'-C5'-O5'
5	J	202	GDP	C3'-C4'-C5'-O5'
5	F	202	GDP	C3'-C4'-C5'-O5'
5	D	202	GDP	O4'-C4'-C5'-O5'
5	B	202	GDP	C5'-O5'-PA-O1A
5	H	202	GDP	O4'-C4'-C5'-O5'
5	H	202	GDP	C3'-C4'-C5'-O5'

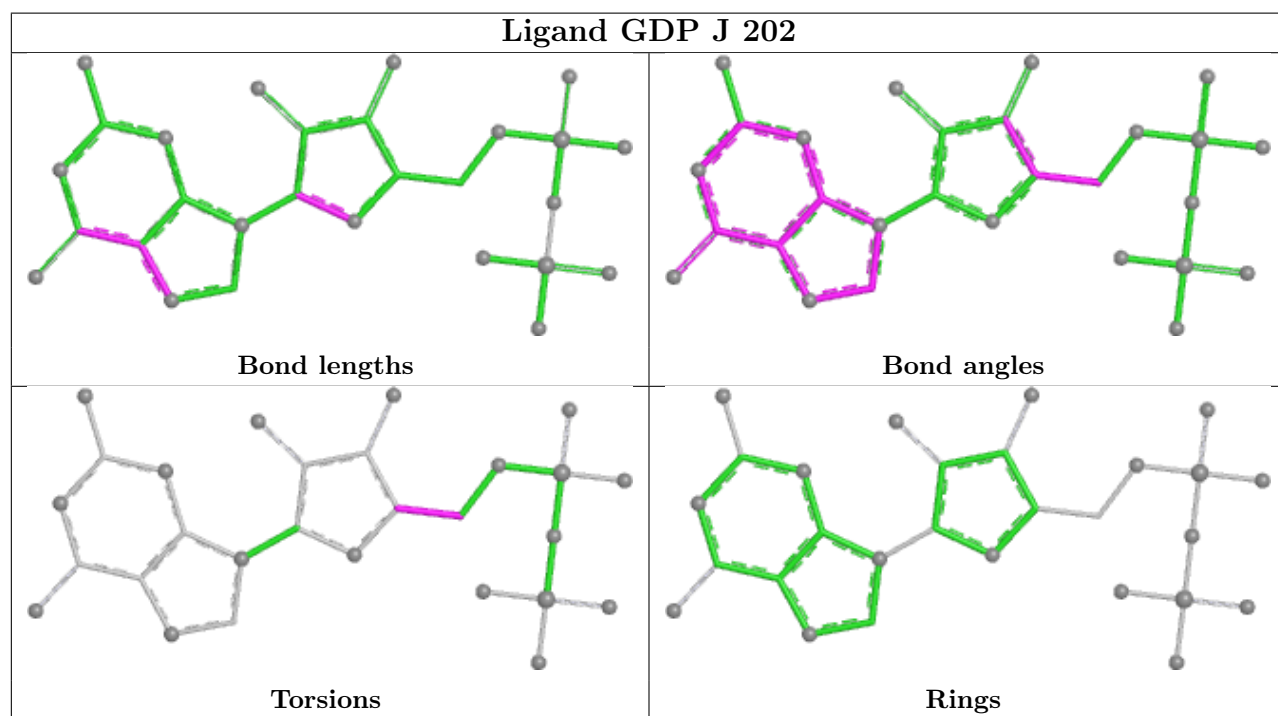
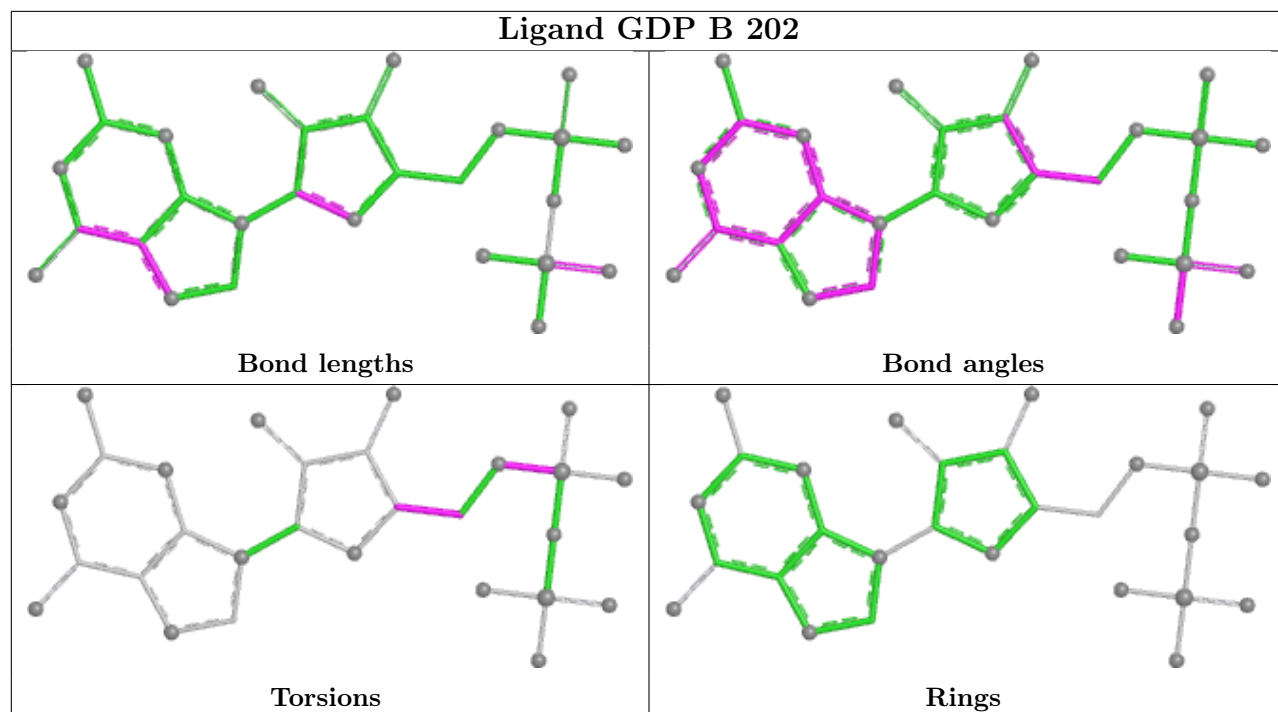
There are no ring outliers.

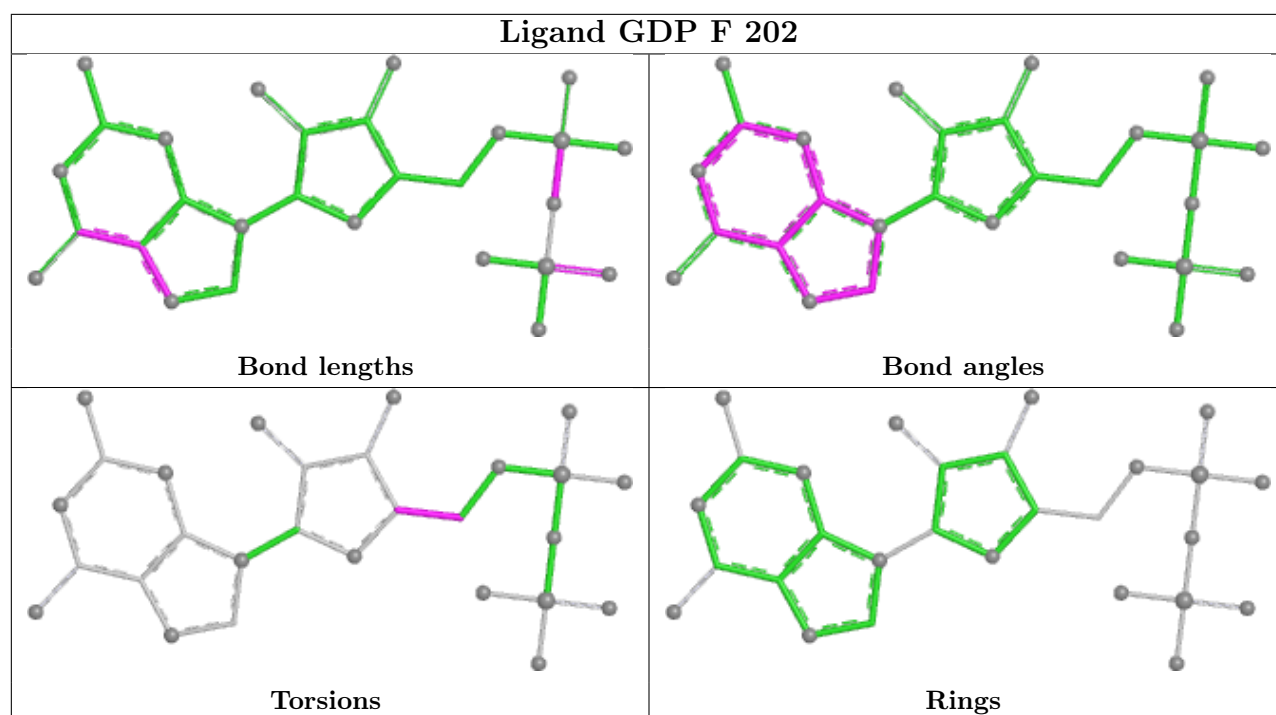
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	202	GDP	7	0
6	H	203	BEF	1	0
6	J	203	BEF	1	0
5	B	202	GDP	2	0
3	A	401	SO4	1	0
5	J	202	GDP	3	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	280/305 (91%)	-0.45	1 (0%) 88 79	43, 62, 90, 109	1 (0%)
1	C	281/305 (92%)	-0.45	0 100 100	51, 66, 86, 110	0
1	E	281/305 (92%)	-0.38	0 100 100	51, 71, 100, 118	0
1	G	281/305 (92%)	0.04	2 (0%) 84 70	74, 96, 128, 157	0
1	I	281/305 (92%)	-0.32	1 (0%) 88 79	57, 74, 104, 117	0
2	B	172/175 (98%)	-0.31	0 100 100	51, 68, 97, 118	0
2	D	170/175 (97%)	-0.31	0 100 100	59, 76, 101, 116	0
2	F	172/175 (98%)	-0.30	0 100 100	57, 72, 100, 120	0
2	H	170/175 (97%)	0.18	0 100 100	74, 101, 141, 163	1 (0%)
2	J	171/175 (97%)	-0.06	0 100 100	71, 90, 118, 131	0
All	All	2259/2400 (94%)	-0.25	4 (0%) 91 86	43, 75, 114, 163	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	305	SER	2.5
1	G	305	SER	2.4
1	A	113	GLY	2.4
1	G	223	THR	2.1

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 ⓘ

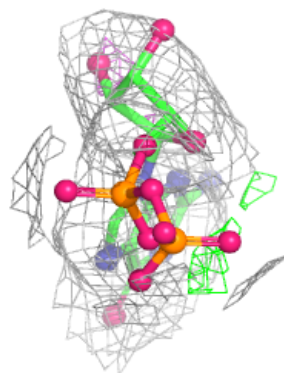
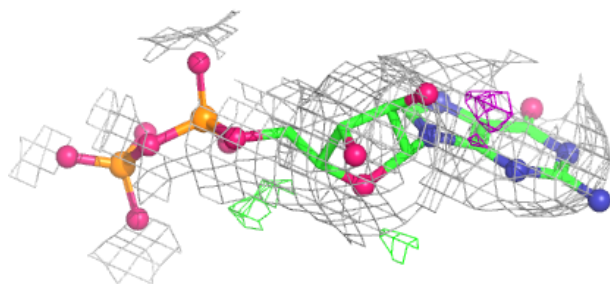
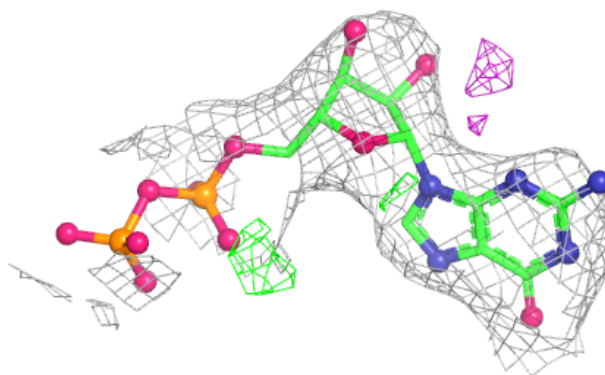
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	401	5/5	0.78	0.10	101,101,102,102	0
3	SO4	C	401	5/5	0.78	0.17	124,124,124,124	0
3	SO4	E	401	5/5	0.84	0.08	106,106,107,107	0
6	BEF	H	203	4/4	0.84	0.10	103,104,104,104	0
4	MG	F	201	1/1	0.89	0.08	61,61,61,61	0
5	GDP	J	202	28/28	0.91	0.09	84,90,92,93	0
6	BEF	D	203	4/4	0.92	0.09	75,75,76,76	0
5	GDP	H	202	28/28	0.92	0.07	64,70,80,80	0
4	MG	D	201	1/1	0.93	0.12	55,55,55,55	0
3	SO4	I	401	5/5	0.93	0.08	107,107,107,107	0
6	BEF	J	203	4/4	0.93	0.09	95,96,96,96	0
6	BEF	F	203	4/4	0.94	0.06	70,70,70,71	0
3	SO4	E	402	5/5	0.95	0.06	105,105,105,105	0
5	GDP	B	202	28/28	0.95	0.07	51,56,57,58	0
5	GDP	F	202	28/28	0.95	0.07	54,59,64,64	0
5	GDP	D	202	28/28	0.96	0.07	63,64,67,68	0
4	MG	B	201	1/1	0.96	0.07	65,65,65,65	0
4	MG	H	201	1/1	0.97	0.04	61,61,61,61	0
6	BEF	B	203	4/4	0.97	0.06	64,64,64,64	0
4	MG	J	201	1/1	0.97	0.07	61,61,61,61	0

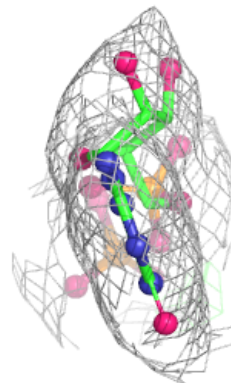
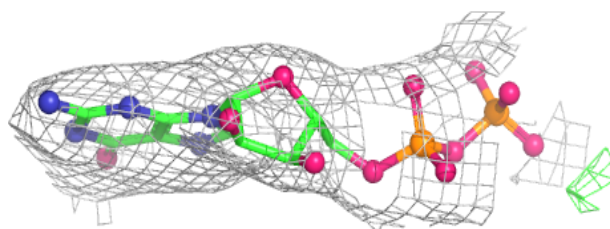
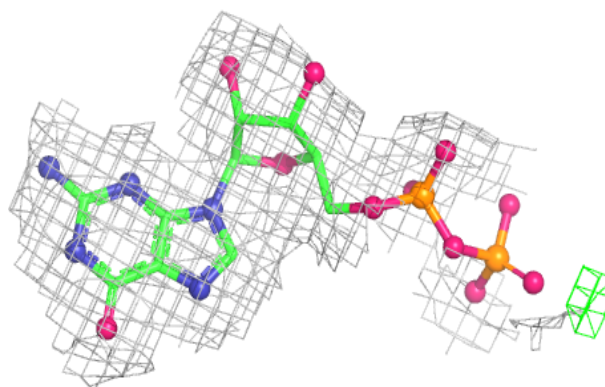
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP J 202:

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

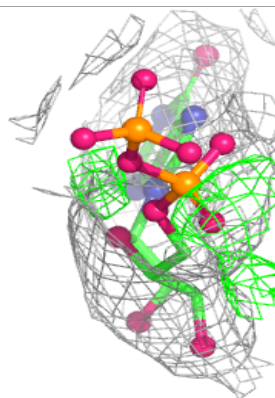
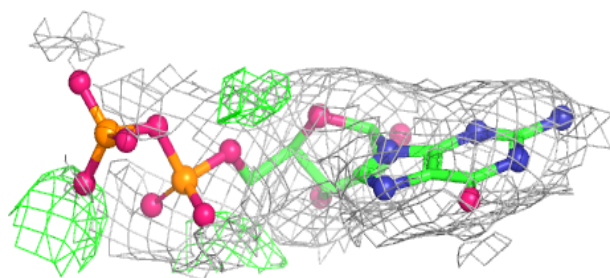
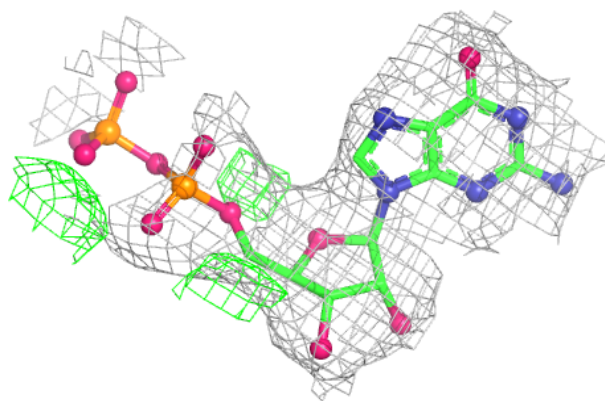
**Electron density around GDP H 202:**

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

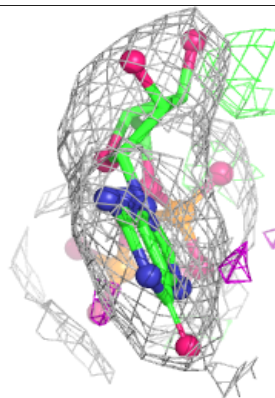
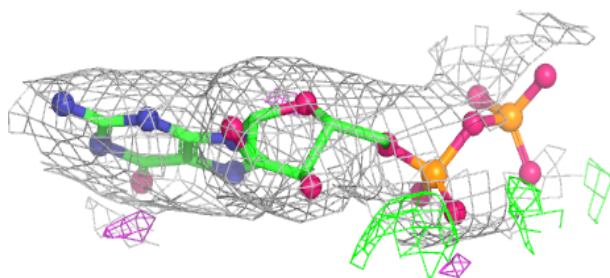
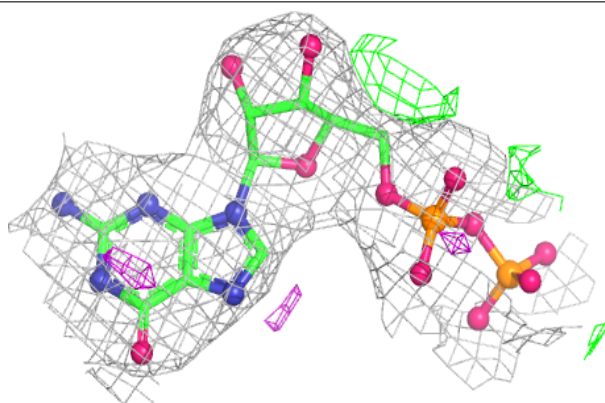


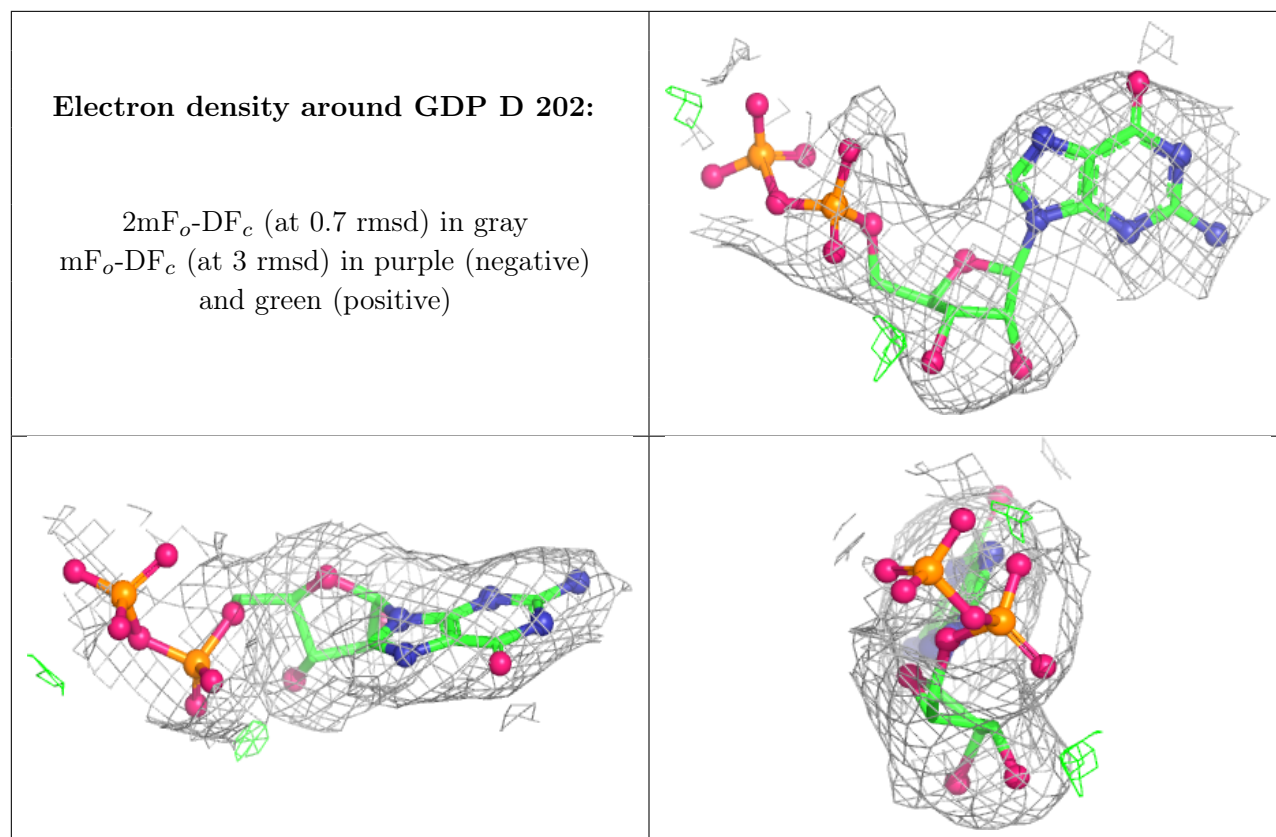
Electron density around GDP B 202:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.