



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 09:24 pm BST

PDB ID : 5OXF
Title : An oligomerised bacterial dynamin pair provides a mechanism for the long range sensing and tethering of membranes
Authors : Liu, J.W.; Noel, J.K.; Low, H.H.
Deposited on : 2017-09-06
Resolution : 3.94 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

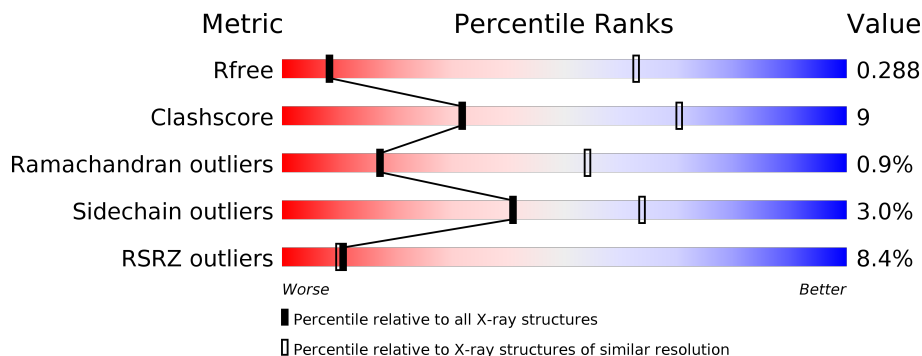
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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 on 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	732	 11% 81% 14% . .
1	B	732	 10% 67% 12% . 19%
2	C	614	 5% 75% 20% . .
2	D	614	 4% 72% 21% . . .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 19587 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 GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	703	Total	C	N	O	S	0	0	0
			5050	3197	863	976	14			
1	B	591	Total	C	N	O	S	0	0	0
			4465	2846	744	861	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	729	LYS	-	expression tag	UNP A0A1D9BJX7
A	730	LEU	-	expression tag	UNP A0A1D9BJX7
A	731	HIS	-	expression tag	UNP A0A1D9BJX7
A	732	HIS	-	expression tag	UNP A0A1D9BJX7
B	729	LYS	-	expression tag	UNP A0A1D9BJX7
B	730	LEU	-	expression tag	UNP A0A1D9BJX7
B	731	HIS	-	expression tag	UNP A0A1D9BJX7
B	732	HIS	-	expression tag	UNP A0A1D9BJX7

- Molecule 2 is a protein called GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	601	Total	C	N	O	S	0	0	0
			4980	3221	802	946	11			
2	D	601	Total	C	N	O	S	0	0	0
			4980	3221	802	946	11			

There are 10 discrepancies between the modelled and reference sequences:

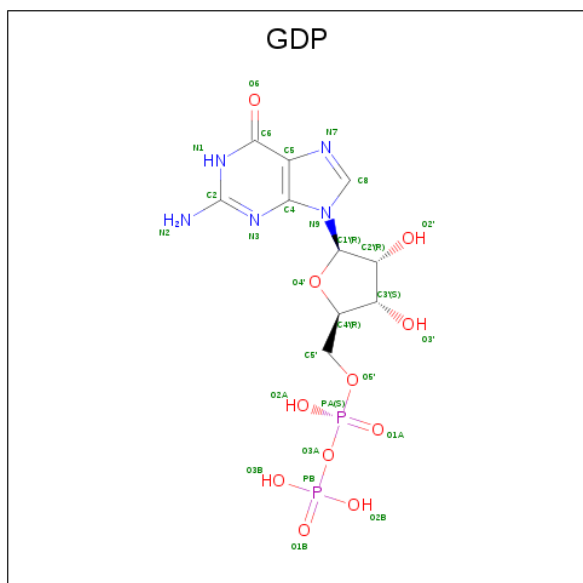
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A1D9BKH6
C	-1	SER	-	expression tag	UNP A0A1D9BKH6
C	0	HIS	-	expression tag	UNP A0A1D9BKH6
C	610	HIS	-	expression tag	UNP A0A1D9BKH6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	611	HIS	-	expression tag	UNP A0A1D9BKH6
D	-2	GLY	-	expression tag	UNP A0A1D9BKH6
D	-1	SER	-	expression tag	UNP A0A1D9BKH6
D	0	HIS	-	expression tag	UNP A0A1D9BKH6
D	610	HIS	-	expression tag	UNP A0A1D9BKH6
D	611	HIS	-	expression tag	UNP A0A1D9BKH6

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

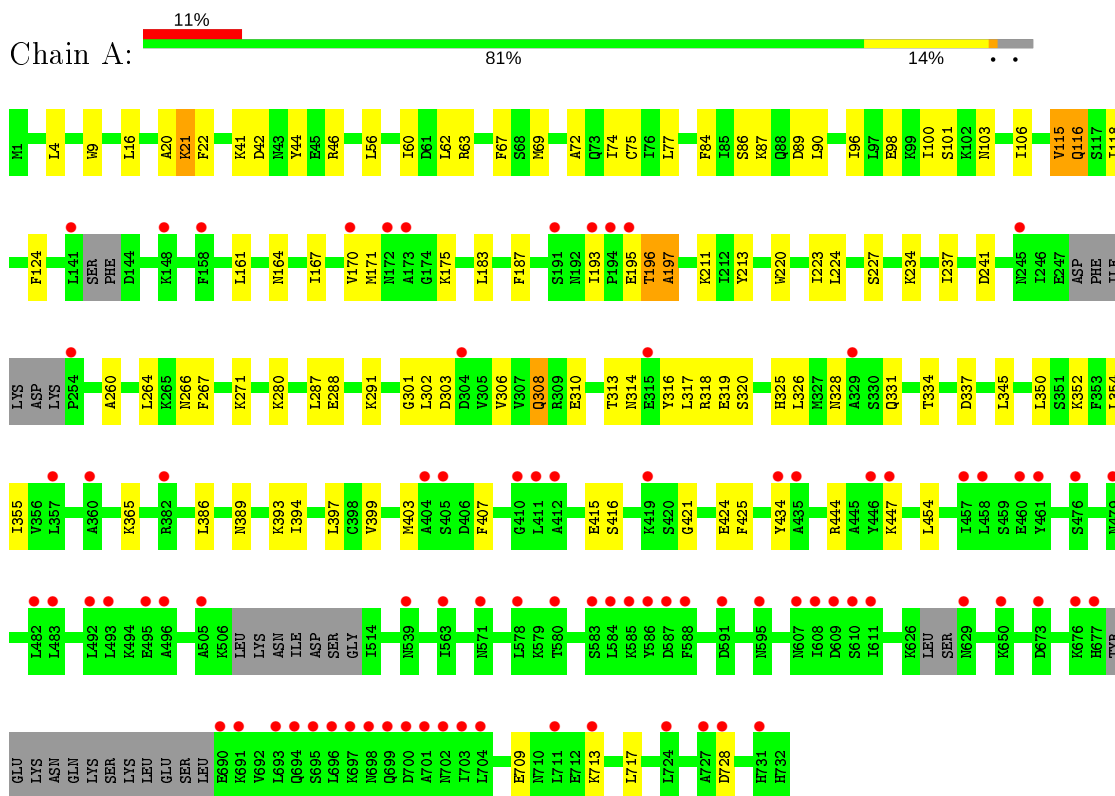


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

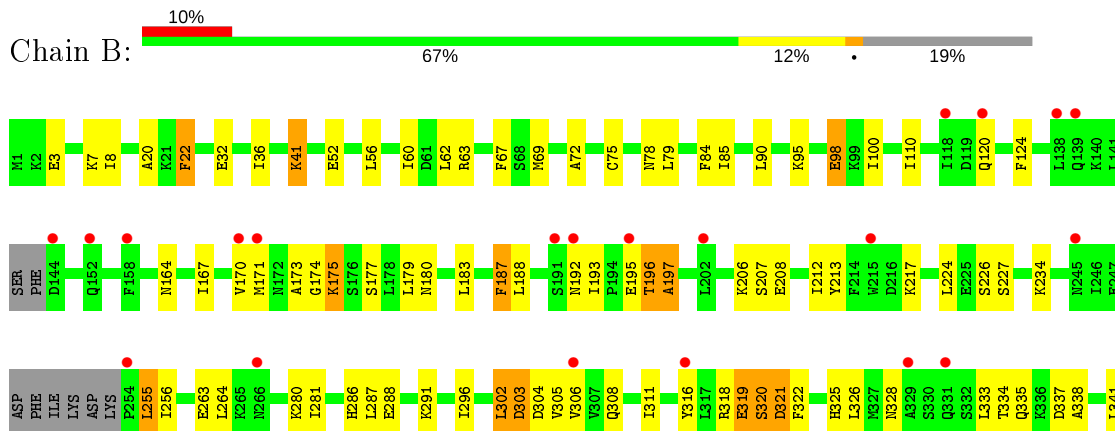
3 Residue-property plots [i](#)

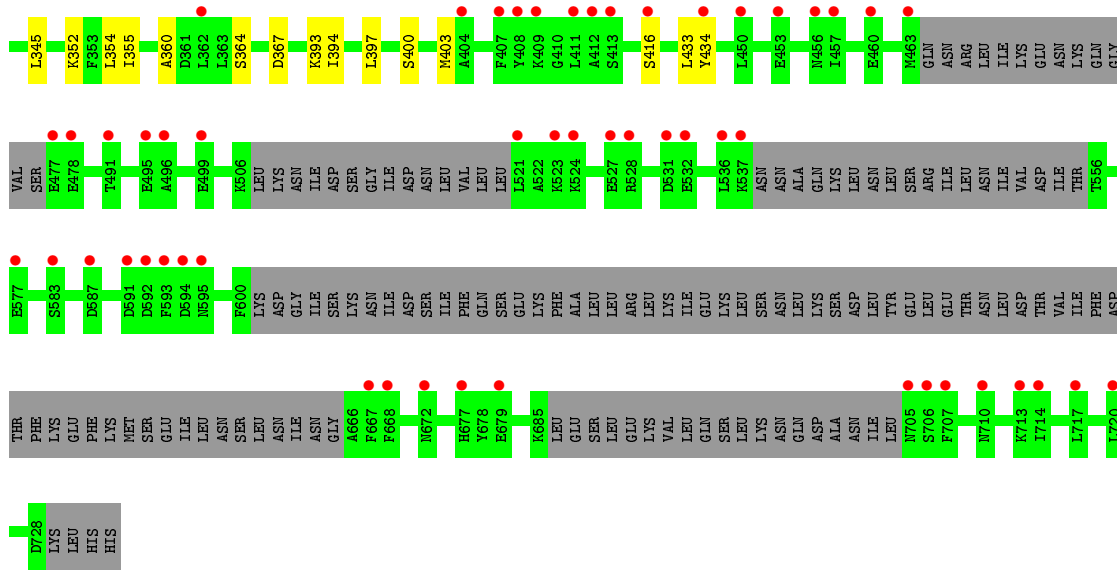
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

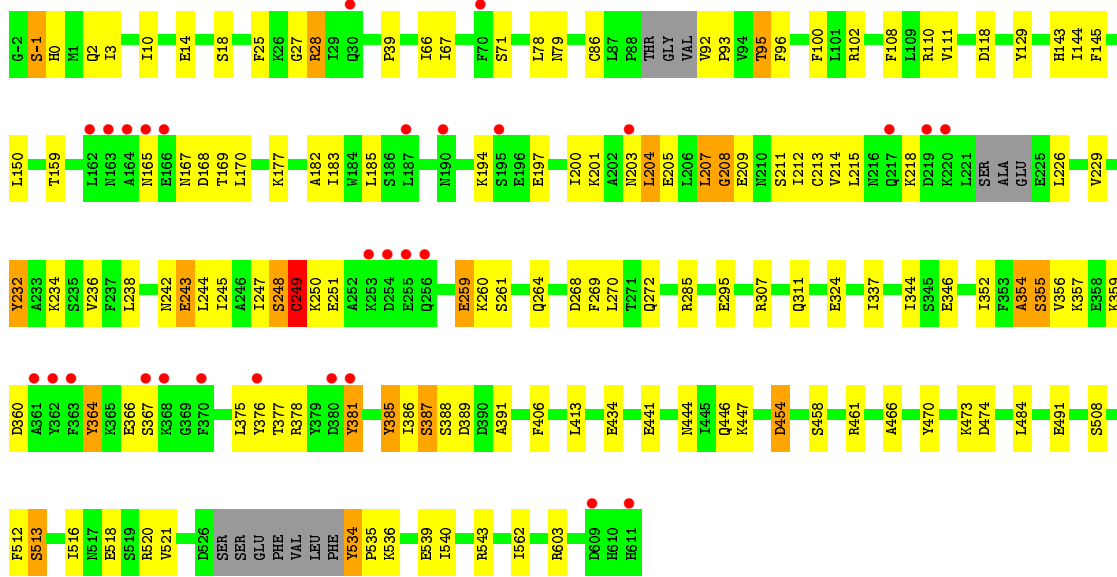
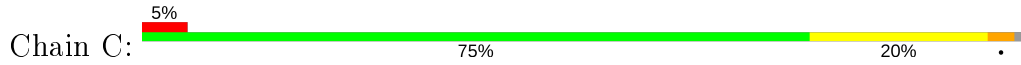


- Molecule 1: GTP-binding protein

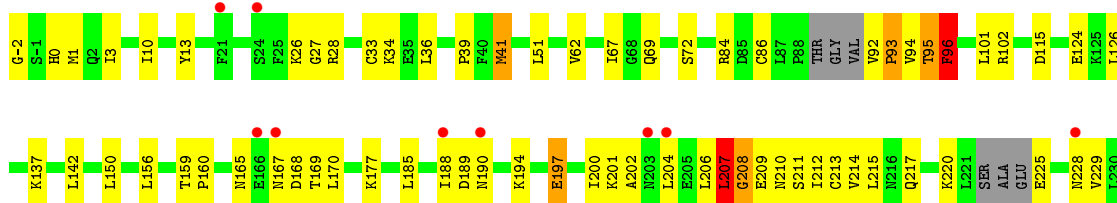


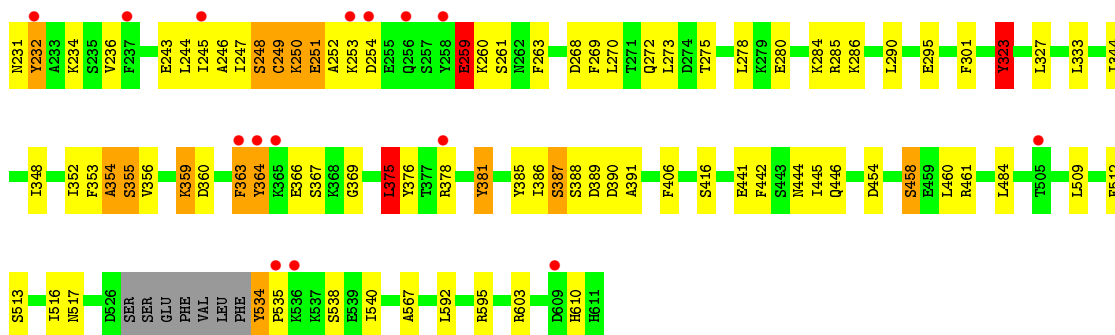


• Molecule 2: GTP-binding protein



• Molecule 2: GTP-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.72Å 228.68Å 318.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.98 – 3.94 58.98 – 3.94	Depositor EDS
% Data completeness (in resolution range)	95.5 (58.98-3.94) 95.6 (58.98-3.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.88Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.259 , 0.288 0.260 , 0.288	Depositor DCC
R_{free} test set	3499 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	154.3	Xtrriage
Anisotropy	0.637	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 204.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19587	wwPDB-VP
Average B, all atoms (Å ²)	232.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/5100	0.47	0/6891
1	B	0.27	0/4511	0.51	1/6069 (0.0%)
2	C	0.33	0/5067	0.61	2/6805 (0.0%)
2	D	0.32	1/5067 (0.0%)	0.65	8/6805 (0.1%)
All	All	0.30	1/19745 (0.0%)	0.56	11/26570 (0.0%)

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	B	0	7
2	C	0	12
2	D	0	15
All	All	0	36

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	323	TYR	CD2-CE2	5.06	1.47	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	375	LEU	CB-CG-CD2	-9.03	95.65	111.00
2	D	375	LEU	CB-CG-CD1	8.91	126.15	111.00
2	D	323	TYR	CB-CG-CD2	8.11	125.86	121.00
2	D	207	LEU	CA-CB-CG	7.99	133.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	323	TYR	CB-CG-CD1	-7.17	116.70	121.00
2	C	207	LEU	CA-CB-CG	6.92	131.22	115.30
2	D	96	PHE	N-CA-C	6.91	129.66	111.00
2	C	364	TYR	CA-CB-CG	5.88	124.57	113.40
2	D	207	LEU	CB-CG-CD2	5.73	120.74	111.00
1	B	255	LEU	CA-CB-CG	5.49	127.92	115.30
2	D	208	GLY	N-CA-C	5.26	126.24	113.10

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	LEU	Peptide
1	A	196	THR	Peptide
1	B	196	THR	Peptide
1	B	255	LEU	Peptide
1	B	302	LEU	Peptide
1	B	319	GLU	Peptide
1	B	320	SER	Peptide
1	B	433	LEU	Peptide
1	B	84	PHE	Peptide
2	C	177	LYS	Peptide
2	C	208	GLY	Peptide
2	C	248	SER	Peptide
2	C	249	CYS	Peptide
2	C	259	GLU	Peptide
2	C	354	ALA	Peptide
2	C	359	LYS	Peptide
2	C	360	ASP	Peptide
2	C	381	TYR	Peptide
2	C	387	SER	Peptide
2	C	92	VAL	Peptide
2	C	95	THR	Peptide
2	D	177	LYS	Peptide
2	D	208	GLY	Peptide
2	D	244	LEU	Peptide
2	D	248	SER	Peptide
2	D	259	GLU	Peptide
2	D	354	ALA	Peptide
2	D	359	LYS	Peptide
2	D	360	ASP	Peptide
2	D	381	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	D	387	SER	Peptide
2	D	41	MET	Peptide
2	D	92	VAL	Peptide
2	D	93	PRO	Peptide
2	D	94	VAL	Peptide
2	D	95	THR	Peptide

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	5050	0	4539	68	0
1	B	4465	0	4249	75	0
2	C	4980	0	5023	94	0
2	D	4980	0	5023	115	0
3	A	28	0	12	1	0
3	B	28	0	12	3	0
3	C	28	0	12	0	0
3	D	28	0	12	4	0
All	All	19587	0	18882	341	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 (341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:375:LEU:HD12	2:D:376:TYR:H	1.06	1.16
1:A:171:MET:CE	1:A:196:THR:HG21	1.77	1.13
1:A:171:MET:HE3	1:A:196:THR:HG21	1.29	1.05
2:D:367:SER:N	2:D:375:LEU:HD13	1.74	1.01
2:D:375:LEU:CD1	2:D:376:TYR:H	1.74	1.01
2:C:364:TYR:HB3	2:C:378:ARG:HA	1.52	0.91
2:D:367:SER:H	2:D:375:LEU:HD13	1.30	0.88
2:D:375:LEU:HD12	2:D:376:TYR:N	1.90	0.85
1:A:100:ILE:HD11	2:D:10:ILE:HA	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:518:GLU:O	2:C:521:VAL:HG12	1.84	0.77
1:A:16:LEU:HD13	1:A:74:ILE:HD11	1.65	0.77
2:C:364:TYR:CB	2:C:378:ARG:HA	2.17	0.75
1:B:164:ASN:ND2	1:B:320:SER:OG	2.20	0.74
2:C:170:LEU:HD23	2:C:170:LEU:H	1.53	0.73
2:C:209:GLU:O	2:C:243:GLU:HB2	1.89	0.72
1:A:63:ARG:NH1	2:C:446:GLN:O	2.23	0.71
1:B:20:ALA:HB2	1:B:78:ASN:HB2	1.73	0.71
1:B:403:MET:HB3	1:B:416:SER:HB2	1.71	0.71
2:D:366:GLU:HA	2:D:375:LEU:CD1	2.21	0.71
1:A:352:LYS:HA	1:A:393:LYS:HG2	1.72	0.70
2:C:366:GLU:H	2:C:376:TYR:HD1	1.40	0.70
2:D:364:TYR:CB	2:D:378:ARG:HA	2.22	0.69
2:C:212:ILE:HD11	2:C:269:PHE:CG	2.27	0.69
1:B:196:THR:HG23	1:B:303:ASP:HB3	1.74	0.69
2:C:386:ILE:HG21	2:C:513:SER:HA	1.76	0.68
2:D:366:GLU:HA	2:D:375:LEU:HD11	1.77	0.67
2:D:367:SER:N	2:D:375:LEU:CD1	2.55	0.67
2:D:364:TYR:HB3	2:D:378:ARG:HA	1.77	0.67
1:B:217:LYS:HD3	1:B:256:ILE:HG23	1.77	0.67
1:B:183:LEU:HD22	1:B:287:LEU:HD13	1.77	0.67
1:B:167:ILE:HD11	1:B:326:LEU:HD11	1.75	0.67
1:A:223:ILE:HA	1:A:306:VAL:HG21	1.77	0.66
1:A:709:GLU:O	1:A:713:LYS:HG2	1.95	0.66
1:B:303:ASP:OD2	1:B:304:ASP:N	2.28	0.66
2:C:251:GLU:O	2:C:261:SER:OG	2.11	0.65
2:C:182:ALA:HB3	2:C:207:LEU:HD22	1.78	0.65
2:C:215:LEU:O	2:C:248:SER:HA	1.96	0.65
2:D:115:ASP:OD2	2:D:137:LYS:NZ	2.28	0.65
2:D:212:ILE:HD11	2:D:269:PHE:CG	2.32	0.65
2:D:210:ASN:HA	2:D:243:GLU:HG3	1.79	0.65
1:A:334:THR:O	1:A:337:ASP:N	2.30	0.64
2:D:150:LEU:HD11	2:D:270:LEU:HB3	1.79	0.64
2:C:0:HIS:HA	2:C:3:ILE:HD12	1.80	0.62
1:B:318:ARG:O	1:B:320:SER:N	2.32	0.62
1:B:333:LEU:HD21	1:B:338:ALA:HB2	1.81	0.61
2:D:217:GLN:HB3	3:D:1000:GDP:O6	2.00	0.61
1:A:288:GLU:HA	1:A:291:LYS:HB3	1.82	0.61
2:D:84:ARG:NH2	2:D:124:GLU:OE2	2.29	0.61
2:C:182:ALA:O	2:C:211:SER:OG	2.18	0.61
2:C:484:LEU:HD12	2:D:484:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:165:ASN:HB3	2:C:168:ASP:HB2	1.83	0.61
2:D:211:SER:H	2:D:243:GLU:HB2	1.66	0.60
1:A:167:ILE:HD11	1:A:326:LEU:HD11	1.82	0.60
1:B:352:LYS:HG2	1:B:393:LYS:O	2.01	0.60
2:D:209:GLU:O	2:D:243:GLU:HG2	2.01	0.60
1:B:62:LEU:HD21	1:B:72:ALA:HB2	1.83	0.60
2:D:86:CYS:HB3	2:D:126:LEU:HD23	1.83	0.60
2:D:0:HIS:HA	2:D:3:ILE:HD12	1.82	0.60
2:D:367:SER:H	2:D:375:LEU:CD1	2.10	0.60
1:A:183:LEU:HD22	1:A:287:LEU:HD13	1.83	0.60
2:C:167:ASN:HA	2:C:170:LEU:HD21	1.83	0.59
2:C:367:SER:HB2	2:C:375:LEU:HD12	1.82	0.59
2:D:386:ILE:HG21	2:D:513:SER:HA	1.84	0.59
1:B:334:THR:O	1:B:337:ASP:N	2.34	0.59
2:D:259:GLU:CD	2:D:260:LYS:H	2.05	0.59
2:D:375:LEU:CD1	2:D:376:TYR:N	2.56	0.59
1:A:220:TRP:CH2	1:A:237:ILE:HD11	2.38	0.59
1:B:100:ILE:HD11	2:C:10:ILE:HA	1.83	0.59
2:C:209:GLU:OE1	2:C:209:GLU:N	2.36	0.59
2:C:212:ILE:CD1	2:C:269:PHE:CD2	2.85	0.58
1:B:217:LYS:HB2	1:B:256:ILE:HA	1.84	0.58
2:C:212:ILE:HD11	2:C:269:PHE:CD2	2.37	0.58
2:D:301:PHE:CE1	2:D:460:LEU:HD22	2.39	0.58
2:D:169:THR:OG1	2:D:201:LYS:HA	2.04	0.58
2:C:364:TYR:O	2:D:364:TYR:OH	2.20	0.58
1:A:86:SER:HB3	1:A:90:LEU:HB2	1.84	0.58
1:B:197:ALA:HB3	1:B:308:GLN:NE2	2.19	0.58
2:D:26:LYS:HZ2	2:D:280:GLU:HG2	1.69	0.57
1:A:352:LYS:HG2	1:A:393:LYS:O	2.05	0.57
2:D:249:CYS:HB2	2:D:261:SER:O	2.04	0.57
2:C:387:SER:OG	2:C:391:ALA:N	2.35	0.57
1:A:115:VAL:O	1:A:116:GLN:HB2	2.04	0.57
1:A:197:ALA:HB3	1:A:308:GLN:OE1	2.04	0.57
2:D:301:PHE:HE1	2:D:460:LEU:HD22	1.70	0.57
2:D:210:ASN:HA	2:D:243:GLU:CG	2.34	0.57
2:D:364:TYR:HB2	2:D:378:ARG:HA	1.87	0.56
2:C:375:LEU:HD23	2:C:375:LEU:H	1.71	0.56
1:A:171:MET:SD	1:A:196:THR:HG21	2.46	0.56
2:C:150:LEU:HD11	2:C:270:LEU:HB3	1.86	0.56
2:C:352:ILE:O	2:C:355:SER:HB2	2.06	0.55
2:D:228:ASN:HA	2:D:231:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:HB3	1:A:416:SER:HB2	1.87	0.55
2:C:229:VAL:HA	2:C:232:TYR:CD2	2.41	0.55
2:C:169:THR:OG1	2:C:201:LYS:HG2	2.05	0.55
2:D:250:LYS:HE3	2:D:251:GLU:HB2	1.87	0.55
2:C:234:LYS:O	2:C:238:LEU:HB2	2.07	0.55
2:C:66:ILE:HD13	2:C:183:ILE:HB	1.89	0.55
2:D:229:VAL:HA	2:D:232:TYR:CD2	2.42	0.55
2:D:333:LEU:HD11	2:D:416:SER:HB3	1.89	0.55
2:C:534:TYR:HB2	2:C:535:PRO:HD3	1.89	0.55
2:D:210:ASN:HB2	2:D:278:LEU:HD21	1.88	0.55
2:D:348:ILE:O	2:D:352:ILE:HG12	2.06	0.55
1:A:310:GLU:OE2	1:A:314:ASN:ND2	2.41	0.54
2:D:363:PHE:HB3	2:D:381:TYR:CE1	2.43	0.54
2:C:208:GLY:O	2:C:209:GLU:OE1	2.25	0.54
2:C:387:SER:O	2:C:389:ASP:N	2.40	0.54
1:A:224:LEU:O	1:A:227:SER:OG	2.23	0.54
2:C:110:ARG:HB3	2:C:143:HIS:HB2	1.89	0.54
2:D:165:ASN:HB3	2:D:168:ASP:HB2	1.90	0.54
2:C:311:GLN:NE2	2:C:434:GLU:HB3	2.23	0.54
2:D:215:LEU:O	2:D:248:SER:HA	2.08	0.54
2:C:447:LYS:NZ	2:C:454:ASP:OD1	2.37	0.53
1:B:227:SER:O	1:B:234:LYS:HB2	2.09	0.53
1:B:303:ASP:CG	1:B:308:GLN:HE21	2.11	0.53
1:B:171:MET:SD	1:B:196:THR:HG21	2.49	0.53
1:A:345:LEU:HD21	1:A:394:ILE:HD11	1.90	0.53
2:D:534:TYR:HB2	2:D:535:PRO:HD3	1.91	0.53
1:A:84:PHE:CE2	1:A:118:ILE:HG23	2.43	0.53
2:C:226:LEU:H	2:C:226:LEU:HD23	1.74	0.52
1:B:345:LEU:HD21	1:B:394:ILE:HD11	1.91	0.52
2:C:249:CYS:O	2:C:250:LYS:HB2	2.09	0.52
2:D:62:VAL:HG21	2:D:275:THR:HB	1.92	0.52
1:A:334:THR:HB	1:A:337:ASP:HB2	1.92	0.52
2:D:250:LYS:HG2	3:D:1000:GDP:O6	2.10	0.52
2:C:232:TYR:O	2:C:236:VAL:HG23	2.10	0.52
2:D:352:ILE:O	2:D:355:SER:HB2	2.10	0.52
2:D:387:SER:O	2:D:389:ASP:N	2.43	0.51
1:B:226:SER:CB	1:B:306:VAL:HG21	2.39	0.51
2:D:202:ALA:HB2	2:D:206:LEU:HB3	1.93	0.51
1:B:288:GLU:HA	1:B:291:LYS:HB3	1.93	0.51
2:C:79:ASN:OD1	2:C:86:CYS:N	2.41	0.51
2:D:212:ILE:HD11	2:D:269:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLN:HB3	1:B:434:TYR:HD2	1.74	0.51
1:B:79:LEU:HD23	1:B:85:ILE:HG22	1.93	0.51
2:C:295:GLU:OE1	2:C:603:ARG:NH1	2.44	0.51
2:D:167:ASN:HB3	2:D:170:LEU:HD21	1.92	0.51
1:A:77:LEU:HD21	1:A:106:ILE:HD11	1.93	0.51
2:D:167:ASN:O	2:D:170:LEU:HD23	2.12	0.50
2:D:387:SER:HB2	2:D:391:ALA:HB2	1.92	0.50
1:B:72:ALA:HA	1:B:75:CYS:SG	2.52	0.50
2:C:197:GLU:O	2:C:200:ILE:HG13	2.12	0.50
2:C:264:GLN:O	2:C:268:ASP:HB2	2.11	0.50
1:A:713:LYS:O	1:A:717:LEU:HG	2.11	0.50
2:D:-2:GLY:O	2:D:1:MET:HG2	2.12	0.50
2:C:66:ILE:HG13	2:C:78:LEU:HD21	1.94	0.50
1:A:84:PHE:HE2	1:A:118:ILE:HG23	1.75	0.50
1:B:197:ALA:HB3	1:B:308:GLN:HE22	1.77	0.50
2:D:69:GLN:HB2	2:D:72:SER:HB3	1.94	0.50
2:C:169:THR:HG21	2:C:201:LYS:HA	1.94	0.50
1:A:318:ARG:O	1:A:320:SER:N	2.45	0.49
2:D:253:LYS:O	2:D:254:ASP:HB2	2.12	0.49
1:A:313:THR:O	1:A:317:LEU:HB3	2.13	0.49
1:B:333:LEU:CD2	1:B:338:ALA:HB2	2.43	0.49
2:C:218:LYS:NZ	2:C:260:LYS:HD2	2.27	0.49
2:C:108:PHE:HB2	2:C:145:PHE:HB2	1.94	0.49
2:D:28:ARG:HD2	2:D:28:ARG:N	2.27	0.49
1:A:196:THR:HG23	1:A:197:ALA:HB2	1.94	0.49
1:B:321:ASP:O	1:B:322:PHE:HB2	2.13	0.49
1:A:170:VAL:HG22	1:A:171:MET:H	1.78	0.49
2:C:27:GLY:C	2:C:28:ARG:HD2	2.33	0.49
2:D:286:LYS:O	2:D:290:LEU:HG	2.12	0.49
2:D:354:ALA:C	2:D:356:VAL:H	2.15	0.49
1:A:227:SER:O	1:A:234:LYS:HB2	2.12	0.49
2:C:218:LYS:HZ2	2:C:260:LYS:HD2	1.78	0.49
1:B:226:SER:HB2	1:B:306:VAL:HG21	1.95	0.49
1:B:263:GLU:HG3	1:B:264:LEU:N	2.28	0.49
2:C:466:ALA:HB3	2:C:470:TYR:HE2	1.78	0.48
2:D:212:ILE:CD1	2:D:269:PHE:CD2	2.96	0.48
2:D:366:GLU:H	2:D:376:TYR:HD1	1.61	0.48
1:B:288:GLU:HA	1:B:291:LYS:CB	2.43	0.48
2:C:250:LYS:O	2:C:251:GLU:HG3	2.13	0.48
2:D:444:ASN:O	2:D:446:GLN:HG2	2.12	0.48
1:A:62:LEU:HD21	1:A:72:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD21	1:B:355:ILE:HD11	1.95	0.48
2:C:185:LEU:HD12	2:C:214:VAL:HB	1.95	0.48
2:C:244:LEU:HD23	2:C:245:ILE:H	1.78	0.48
1:A:4:LEU:HD21	1:A:106:ILE:HD12	1.96	0.48
2:D:214:VAL:HA	2:D:247:ILE:O	2.13	0.48
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.76	0.48
2:D:295:GLU:OE1	2:D:603:ARG:NH1	2.46	0.48
2:D:95:THR:OG1	2:D:96:PHE:HB2	2.13	0.48
1:B:303:ASP:CG	1:B:304:ASP:H	2.12	0.48
2:D:34:LYS:HG3	2:D:51:LEU:HB3	1.95	0.48
1:B:90:LEU:HD23	1:B:110:ILE:HD12	1.96	0.48
1:B:173:ALA:HA	1:B:328:ASN:HB2	1.94	0.47
2:C:204:LEU:O	2:C:285:ARG:NH1	2.47	0.47
2:C:100:PHE:O	2:C:144:ILE:N	2.45	0.47
2:C:354:ALA:C	2:C:356:VAL:H	2.17	0.47
1:A:196:THR:HG22	1:A:303:ASP:OD1	2.13	0.47
2:C:508:SER:HB3	2:C:543:ARG:HG3	1.96	0.47
2:D:260:LYS:HD2	2:D:260:LYS:HA	1.31	0.47
2:C:307:ARG:NH1	2:C:441:GLU:OE1	2.46	0.47
1:B:320:SER:C	1:B:322:PHE:H	2.19	0.47
2:C:357:LYS:HB2	2:C:385:TYR:CD2	2.50	0.47
1:A:454:LEU:HD11	1:A:717:LEU:HB3	1.96	0.47
1:A:171:MET:HE3	1:A:196:THR:CG2	2.21	0.47
2:C:-1:SER:O	2:C:2:GLN:HB2	2.15	0.47
2:D:354:ALA:O	2:D:356:VAL:N	2.35	0.47
1:B:124:PHE:HB2	1:B:434:TYR:CD1	2.50	0.46
2:C:28:ARG:HD2	2:C:28:ARG:N	2.30	0.46
1:B:177:SER:HB3	3:B:1000:GDP:O2A	2.15	0.46
2:C:95:THR:HG23	2:C:96:PHE:H	1.80	0.46
2:D:352:ILE:HD12	2:D:509:LEU:HD13	1.97	0.46
2:C:512:PHE:CE2	2:C:540:ILE:HA	2.50	0.46
2:D:251:GLU:HG2	2:D:251:GLU:O	2.15	0.46
2:D:442:PHE:HA	2:D:445:ILE:HG12	1.96	0.46
1:A:87:LYS:HB2	1:A:89:ASP:CG	2.36	0.46
2:D:96:PHE:CE1	2:D:160:PRO:HG3	2.51	0.46
2:D:170:LEU:HD23	2:D:170:LEU:H	1.79	0.46
2:D:512:PHE:CE2	2:D:540:ILE:HA	2.51	0.46
1:B:207:SER:OG	1:B:208:GLU:N	2.49	0.46
1:B:325:HIS:HB3	1:B:355:ILE:HD13	1.98	0.46
1:B:170:VAL:HG22	1:B:171:MET:H	1.81	0.46
1:B:352:LYS:HE3	2:C:-1:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:ALA:HB1	2:D:207:LEU:H	1.80	0.46
1:A:20:ALA:HA	1:A:75:CYS:HA	1.98	0.46
1:B:213:TYR:HB2	1:B:280:LYS:HB2	1.97	0.46
2:C:212:ILE:HD12	2:C:269:PHE:CD2	2.50	0.46
1:B:164:ASN:ND2	1:B:320:SER:HG	2.13	0.45
2:D:27:GLY:C	2:D:28:ARG:HD2	2.37	0.45
2:D:204:LEU:O	2:D:285:ARG:NH1	2.49	0.45
1:A:193:ILE:HG23	1:A:195:GLU:O	2.17	0.45
1:B:3:GLU:O	1:B:7:LYS:HG3	2.17	0.45
2:C:203:ASN:C	2:C:205:GLU:H	2.20	0.45
1:A:301:GLY:C	1:A:302:LEU:HD12	2.36	0.45
2:D:150:LEU:HD21	2:D:270:LEU:HD22	1.99	0.45
1:B:180:ASN:OD1	1:B:187:PHE:N	2.44	0.45
2:C:118:ASP:OD1	2:D:102:ARG:NH1	2.50	0.45
1:A:328:ASN:HB3	1:A:331:GLN:HG2	1.99	0.45
1:B:120:GLN:HB3	1:B:434:TYR:CD2	2.51	0.45
1:B:22:PHE:CD2	1:B:75:CYS:HB2	2.52	0.45
2:C:444:ASN:O	2:C:446:GLN:HG2	2.16	0.45
1:B:56:LEU:O	1:B:60:ILE:HG13	2.17	0.45
2:D:220:LYS:HE2	3:D:1000:GDP:HN21	1.82	0.45
2:D:458:SER:HA	2:D:461:ARG:HD3	1.98	0.44
2:D:261:SER:O	2:D:263:PHE:N	2.50	0.44
1:A:98:GLU:HA	1:A:101:SER:O	2.17	0.44
1:A:288:GLU:HA	1:A:291:LYS:CB	2.46	0.44
1:A:124:PHE:HB2	1:A:434:TYR:CD1	2.52	0.44
2:C:208:GLY:C	2:C:209:GLU:OE1	2.55	0.44
1:A:264:LEU:HD12	1:A:266:ASN:N	2.33	0.44
1:A:164:ASN:HB3	1:A:320:SER:HA	1.99	0.44
1:B:193:ILE:HG23	1:B:195:GLU:O	2.18	0.44
2:C:473:LYS:HG3	2:C:474:ASP:N	2.31	0.44
2:D:101:LEU:HB2	2:D:156:LEU:HB2	2.00	0.44
2:D:269:PHE:CZ	2:D:273:LEU:HD21	2.52	0.44
1:A:56:LEU:O	1:A:60:ILE:HG13	2.16	0.44
2:C:458:SER:HA	2:C:461:ARG:HD3	2.00	0.44
2:C:242:ASN:OD1	2:C:242:ASN:N	2.50	0.44
1:A:67:PHE:CD2	2:C:441:GLU:HA	2.53	0.44
2:C:344:ILE:HG12	2:C:406:PHE:CD1	2.53	0.43
2:D:592:LEU:HD23	2:D:595:ARG:NH1	2.33	0.43
2:C:387:SER:HB3	2:C:391:ALA:HB2	2.00	0.43
2:D:213:CYS:HB3	2:D:246:ALA:HB2	2.00	0.43
1:A:100:ILE:HG23	2:D:13:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ILE:O	1:B:41:LYS:HB3	2.18	0.43
2:C:67:ILE:HD12	2:C:207:LEU:HD21	1.99	0.43
1:A:407:PHE:CE1	1:A:415:GLU:HA	2.53	0.43
1:B:302:LEU:O	1:B:305:VAL:HG22	2.19	0.43
1:A:62:LEU:HD13	1:A:69:MET:HE1	2.01	0.43
2:C:167:ASN:HA	2:C:170:LEU:CD2	2.46	0.43
1:B:360:ALA:HB3	1:B:400:SER:HB2	2.00	0.43
2:D:458:SER:HA	2:D:461:ARG:HH11	1.83	0.43
1:B:196:THR:HG23	1:B:197:ALA:HB2	2.00	0.43
2:C:337:ILE:HG12	2:C:413:LEU:HD13	2.00	0.43
2:C:367:SER:OG	2:C:377:THR:HG23	2.19	0.43
2:C:67:ILE:HA	2:C:159:THR:OG1	2.18	0.43
2:D:231:ASN:OD1	2:D:232:TYR:N	2.52	0.43
2:D:232:TYR:O	2:D:236:VAL:HG23	2.19	0.43
1:A:96:ILE:HG23	1:A:389:ASN:ND2	2.33	0.43
1:B:175:LYS:HG2	3:B:1000:GDP:O3B	2.19	0.43
2:D:41:MET:HG3	2:D:595:ARG:HG2	2.00	0.43
1:B:20:ALA:HA	1:B:75:CYS:HB3	2.01	0.43
1:B:212:ILE:HD13	1:B:281:ILE:HG12	2.01	0.43
1:A:115:VAL:HG12	1:A:116:GLN:N	2.34	0.42
1:A:21:LYS:N	1:A:75:CYS:SG	2.90	0.42
1:B:32:GLU:O	1:B:36:ILE:HG12	2.18	0.42
2:C:213:CYS:HB2	2:C:242:ASN:ND2	2.34	0.42
2:C:512:PHE:O	2:C:516:ILE:HG12	2.18	0.42
2:D:189:ASP:C	2:D:190:ASN:HD22	2.23	0.42
2:C:521:VAL:HG22	2:C:521:VAL:O	2.19	0.42
2:D:352:ILE:HB	2:D:540:ILE:HG21	2.01	0.42
2:D:323:TYR:OH	2:D:567:ALA:O	2.30	0.42
2:C:354:ALA:O	2:C:356:VAL:N	2.35	0.42
1:B:174:GLY:HA2	3:B:1000:GDP:O3A	2.19	0.42
1:B:280:LYS:HB3	1:B:280:LYS:HE2	1.84	0.42
2:C:268:ASP:O	2:C:272:GLN:HG2	2.20	0.42
2:C:375:LEU:CD2	2:C:375:LEU:H	2.32	0.42
1:A:399:VAL:HG21	1:A:425:PHE:HB2	2.00	0.42
1:B:63:ARG:NH1	2:D:446:GLN:O	2.52	0.42
2:D:327:LEU:HA	2:D:327:LEU:HD12	1.90	0.42
2:D:261:SER:C	2:D:263:PHE:N	2.73	0.42
2:D:355:SER:O	2:D:386:ILE:HD12	2.19	0.42
2:D:67:ILE:HA	2:D:159:THR:OG1	2.20	0.42
1:A:421:GLY:HA2	1:A:424:GLU:OE1	2.20	0.42
2:C:167:ASN:CA	2:C:170:LEU:HD21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:ASN:HA	2:D:234:LYS:HE3	2.01	0.42
2:D:512:PHE:O	2:D:516:ILE:HG12	2.20	0.42
1:B:364:SER:O	1:B:367:ASP:HB2	2.20	0.42
2:C:536:LYS:HD2	2:C:539:GLU:CD	2.40	0.42
1:A:354:LEU:HD11	1:A:397:LEU:HG	2.02	0.41
1:B:354:LEU:HD11	1:B:397:LEU:HG	2.02	0.41
2:C:562:ILE:HD13	2:C:562:ILE:HA	1.90	0.41
1:A:325:HIS:HB3	1:A:355:ILE:HD13	2.02	0.41
2:D:126:LEU:HD11	2:D:142:LEU:HD13	2.02	0.41
2:D:69:GLN:NE2	2:D:194:LYS:HD2	2.35	0.41
1:A:9:TRP:HA	1:A:41:LYS:HB3	2.03	0.41
2:C:183:ILE:HD11	2:C:270:LEU:HD21	2.03	0.41
2:D:344:ILE:HG12	2:D:406:PHE:CD1	2.56	0.41
2:D:513:SER:O	2:D:517:ASN:ND2	2.45	0.41
2:D:284:LYS:HE2	2:D:610:HIS:HB2	2.03	0.41
1:B:67:PHE:CD2	2:D:441:GLU:HA	2.55	0.41
2:C:111:VAL:HG21	2:C:129:TYR:CD2	2.56	0.41
1:A:271:LYS:HE2	1:A:271:LYS:HB3	1.80	0.41
1:A:447:LYS:HD2	1:A:728:ASP:HB2	2.03	0.41
1:B:217:LYS:O	1:B:217:LYS:HG2	2.21	0.41
2:D:250:LYS:HD3	3:D:1000:GDP:C6	2.56	0.41
2:D:268:ASP:O	2:D:272:GLN:HG2	2.20	0.41
2:D:386:ILE:HG12	2:D:513:SER:HB2	2.02	0.41
1:A:264:LEU:HD12	1:A:266:ASN:H	1.84	0.41
1:A:175:LYS:HG2	3:A:1000:GDP:O3B	2.21	0.41
1:B:179:LEU:HD11	1:B:296:ILE:HG21	2.03	0.41
1:B:224:LEU:O	1:B:227:SER:OG	2.25	0.41
2:D:188:ILE:HA	2:D:215:LEU:HD11	2.03	0.41
1:B:52:GLU:OE1	1:B:52:GLU:N	2.49	0.40
2:D:197:GLU:O	2:D:200:ILE:HG13	2.21	0.40
1:B:206:LYS:HA	1:B:286:HIS:NE2	2.36	0.40
1:B:303:ASP:OD1	1:B:308:GLN:NE2	2.40	0.40
1:B:311:ILE:HD13	1:B:311:ILE:HA	1.90	0.40
1:B:62:LEU:HD13	1:B:69:MET:HE1	2.02	0.40
2:C:366:GLU:N	2:C:376:TYR:HD1	2.13	0.40
1:A:211:LYS:HE2	1:A:260:ALA:HB1	2.03	0.40
1:A:264:LEU:HD13	1:A:267:PHE:HD1	1.87	0.40
1:B:226:SER:HB3	1:B:306:VAL:HG21	2.03	0.40
1:B:95:LYS:O	1:B:98:GLU:HB2	2.21	0.40
2:C:247:ILE:HG13	2:C:248:SER:N	2.36	0.40
2:D:202:ALA:HB1	2:D:207:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:CYS:O	2:D:36:LEU:HB2	2.21	0.40
1:A:213:TYR:HB2	1:A:280:LYS:HB3	2.03	0.40
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.90	0.40
2:D:363:PHE:HB3	2:D:381:TYR:CD1	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	691/732 (94%)	635 (92%)	52 (8%)	4 (1%)	25	62
1	B	575/732 (79%)	520 (90%)	49 (8%)	6 (1%)	15	52
2	C	593/614 (97%)	531 (90%)	57 (10%)	5 (1%)	19	57
2	D	593/614 (97%)	535 (90%)	50 (8%)	8 (1%)	12	47
All	All	2452/2692 (91%)	2221 (91%)	208 (8%)	23 (1%)	17	54

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	ALA
1	B	321	ASP
2	C	355	SER
2	C	388	SER
2	D	355	SER
2	D	388	SER
1	A	197	ALA
1	A	319	GLU
1	B	303	ASP
1	B	319	GLU
1	B	335	GLN

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Mol	Chain	Res	Type
2	C	249	CYS
2	D	249	CYS
1	A	116	GLN
2	C	39	PRO
2	D	39	PRO
2	D	252	ALA
1	B	192	ASN
2	C	93	PRO
2	D	245	ILE
2	D	369	GLY
2	D	93	PRO
1	A	115	VAL

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	452/683 (66%)	439 (97%)	13 (3%)	42	64
1	B	444/683 (65%)	438 (99%)	6 (1%)	67	80
2	C	558/569 (98%)	537 (96%)	21 (4%)	33	58
2	D	558/569 (98%)	537 (96%)	21 (4%)	33	58
All	All	2012/2504 (80%)	1951 (97%)	61 (3%)	41	64

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	22	PHE
1	A	42	ASP
1	A	44	TYR
1	A	46	ARG
1	A	103	ASN
1	A	187	PHE
1	A	241	ASP
1	A	308	GLN

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Mol	Chain	Res	Type
1	A	316	TYR
1	A	350	LEU
1	A	365	LYS
1	A	444	ARG
1	B	22	PHE
1	B	41	LYS
1	B	98	GLU
1	B	175	LYS
1	B	187	PHE
1	B	316	TYR
2	C	-1	SER
2	C	14	GLU
2	C	18	SER
2	C	25	PHE
2	C	28	ARG
2	C	71	SER
2	C	102	ARG
2	C	194	LYS
2	C	204	LEU
2	C	232	TYR
2	C	243	GLU
2	C	259	GLU
2	C	324	GLU
2	C	346	GLU
2	C	381	TYR
2	C	385	TYR
2	C	454	ASP
2	C	491	GLU
2	C	513	SER
2	C	520	ARG
2	C	534	TYR
2	D	96	PHE
2	D	185	LEU
2	D	197	GLU
2	D	207	LEU
2	D	225	GLU
2	D	232	TYR
2	D	250	LYS
2	D	251	GLU
2	D	259	GLU
2	D	323	TYR
2	D	353	PHE

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Mol	Chain	Res	Type
2	D	359	LYS
2	D	363	PHE
2	D	364	TYR
2	D	375	LEU
2	D	385	TYR
2	D	390	ASP
2	D	454	ASP
2	D	458	SER
2	D	534	TYR
2	D	538	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	B	164	ASN
1	B	308	GLN
2	C	311	GLN
2	D	30	GLN
2	D	610	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
3	GDP	D	1000	-	24,30,30	1.02	1 (4%)	31,47,47	1.99	7 (22%)
3	GDP	A	1000	-	24,30,30	1.15	2 (8%)	31,47,47	1.91	8 (25%)
3	GDP	C	1000	-	24,30,30	1.10	2 (8%)	31,47,47	1.95	8 (25%)
3	GDP	B	1000	-	24,30,30	1.22	2 (8%)	31,47,47	1.89	7 (22%)

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
3	GDP	D	1000	-	-	0/12/32/32	0/3/3/3
3	GDP	A	1000	-	-	1/12/32/32	0/3/3/3
3	GDP	C	1000	-	-	2/12/32/32	0/3/3/3
3	GDP	B	1000	-	-	2/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	GDP	C6-C5	4.36	1.48	1.41
3	A	1000	GDP	C6-C5	4.01	1.48	1.41
3	C	1000	GDP	C6-C5	3.87	1.48	1.41
3	D	1000	GDP	C6-C5	3.41	1.47	1.41
3	B	1000	GDP	C5-C4	2.50	1.47	1.40
3	A	1000	GDP	C5-C4	2.39	1.47	1.40
3	C	1000	GDP	C5-C4	2.28	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1000	GDP	C6-C5-C4	-5.56	115.49	120.80
3	D	1000	GDP	C2-N3-C4	5.14	121.23	115.36
3	B	1000	GDP	C2-N3-C4	5.02	121.09	115.36
3	A	1000	GDP	C2-N3-C4	4.93	120.99	115.36
3	C	1000	GDP	C2-N3-C4	4.83	120.87	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1000	GDP	C6-C5-C4	-4.23	116.76	120.80
3	B	1000	GDP	C6-N1-C2	4.04	122.34	115.93
3	C	1000	GDP	C6-N1-C2	3.99	122.27	115.93
3	B	1000	GDP	C5-C6-N1	-3.96	118.01	123.43
3	A	1000	GDP	C6-N1-C2	3.92	122.15	115.93
3	A	1000	GDP	C5-C6-N1	-3.80	118.23	123.43
3	B	1000	GDP	C6-C5-C4	-3.78	117.19	120.80
3	D	1000	GDP	N3-C2-N1	-3.78	122.18	127.22
3	A	1000	GDP	C6-C5-C4	-3.72	117.24	120.80
3	C	1000	GDP	C5-C6-N1	-3.72	118.34	123.43
3	A	1000	GDP	PA-O3A-PB	-3.70	120.13	132.83
3	C	1000	GDP	N3-C2-N1	-3.53	122.51	127.22
3	D	1000	GDP	C6-N1-C2	3.38	121.30	115.93
3	D	1000	GDP	PA-O3A-PB	-3.37	121.27	132.83
3	B	1000	GDP	N3-C2-N1	-3.30	122.82	127.22
3	A	1000	GDP	N3-C2-N1	-3.26	122.88	127.22
3	B	1000	GDP	PA-O3A-PB	-3.11	122.17	132.83
3	B	1000	GDP	C4-C5-N7	-2.93	106.34	109.40
3	C	1000	GDP	C3'-C2'-C1'	2.86	105.29	100.98
3	D	1000	GDP	C1'-N9-C4	-2.74	121.82	126.64
3	C	1000	GDP	PA-O3A-PB	-2.73	123.45	132.83
3	A	1000	GDP	C4-C5-N7	-2.48	106.81	109.40
3	D	1000	GDP	C5-C6-N1	-2.45	120.08	123.43
3	C	1000	GDP	C4-C5-N7	-2.21	107.10	109.40
3	A	1000	GDP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1000	GDP	O4'-C4'-C5'-O5'
3	C	1000	GDP	C3'-C4'-C5'-O5'
3	A	1000	GDP	PB-O3A-PA-O1A
3	B	1000	GDP	PB-O3A-PA-O1A
3	B	1000	GDP	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 8 short contacts:

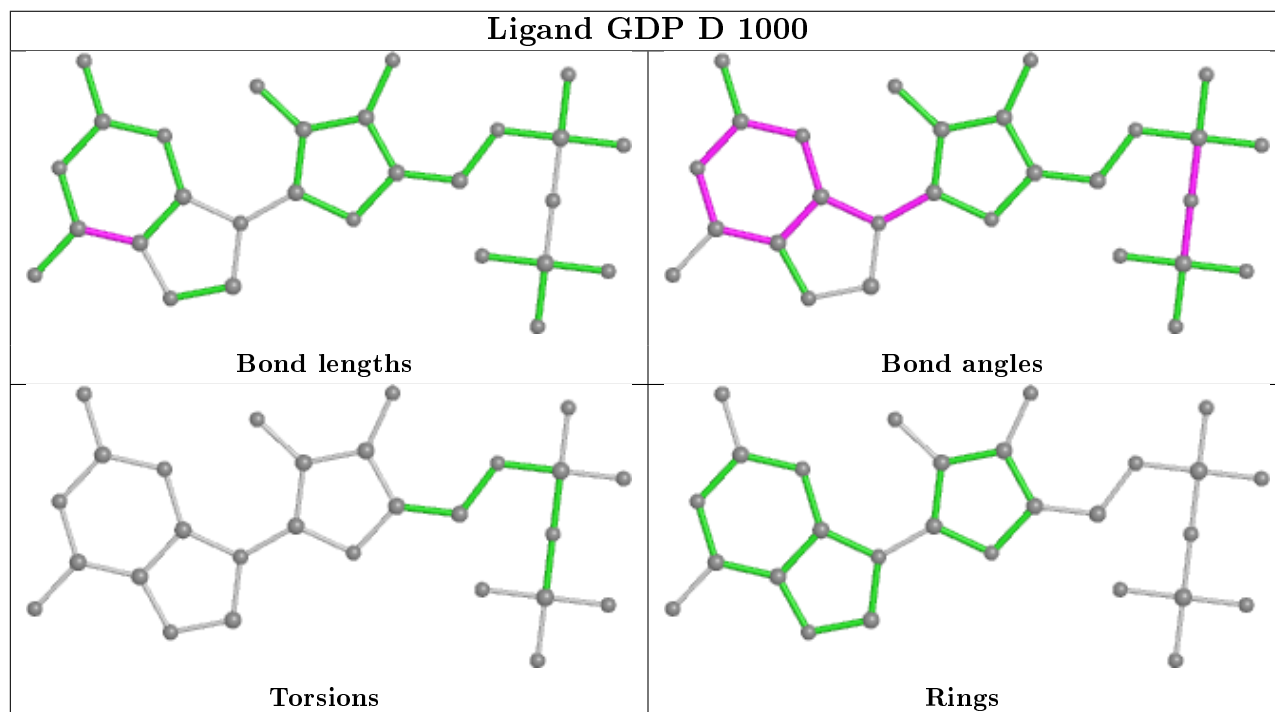
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1000	GDP	4	0

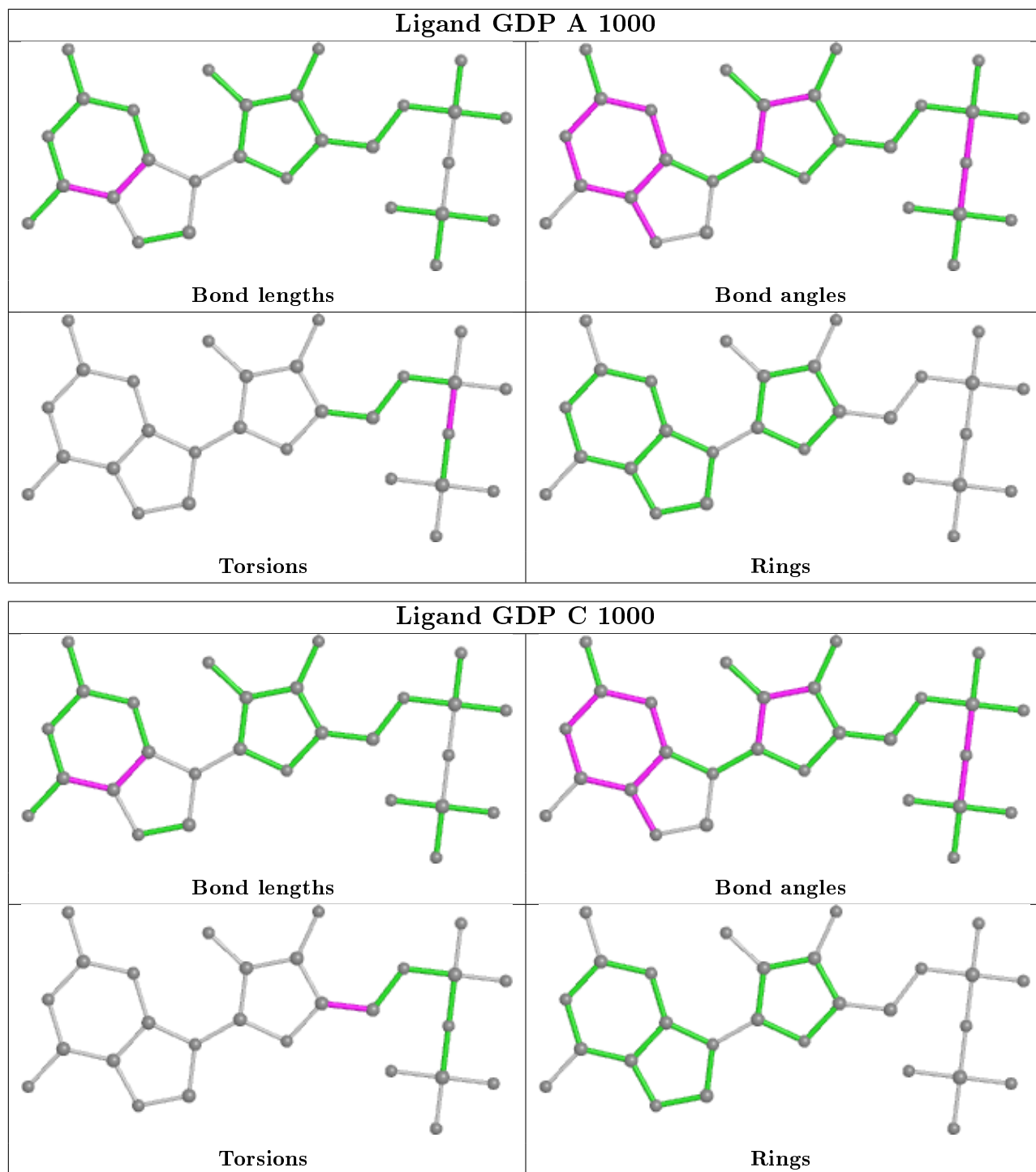
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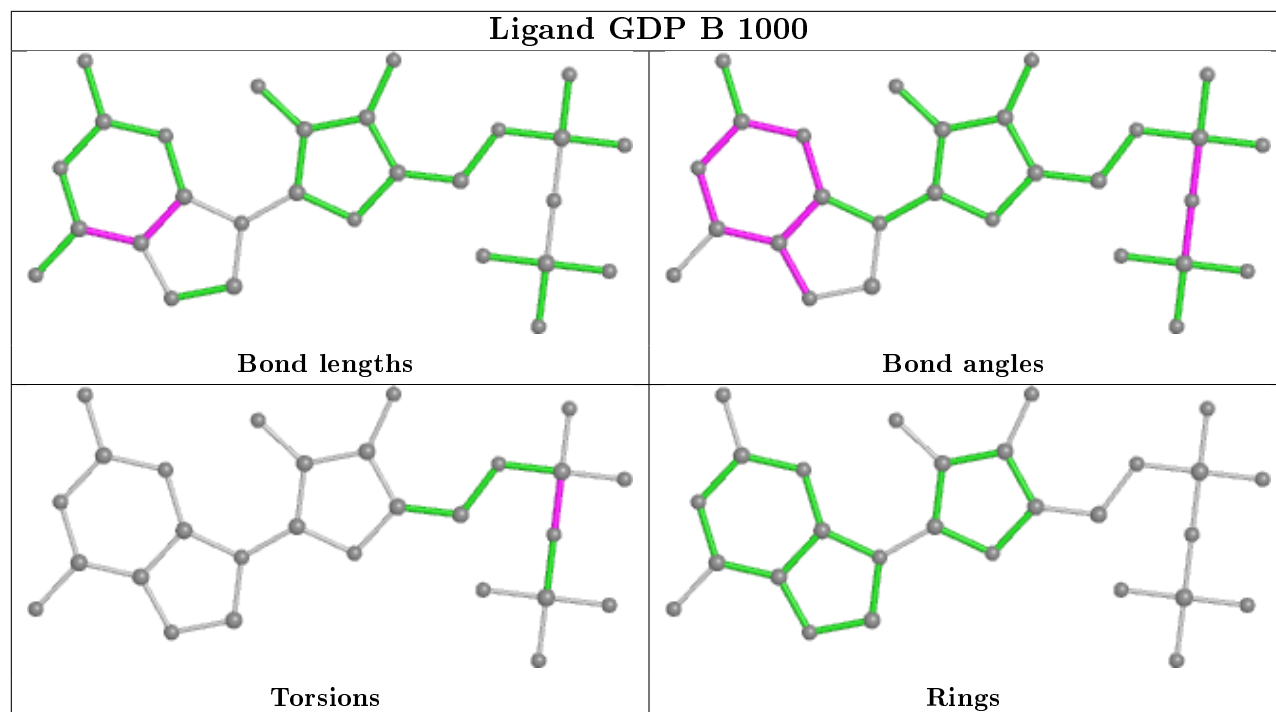
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	GDP	1	0
3	B	1000	GDP	3	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	703/732 (96%)	0.54	84 (11%) 4 5	105, 265, 557, 679	0
1	B	591/732 (80%)	0.56	73 (12%) 4 5	97, 241, 507, 596	0
2	C	601/614 (97%)	0.27	29 (4%) 30 26	97, 172, 336, 480	0
2	D	601/614 (97%)	0.22	24 (3%) 38 31	105, 177, 331, 507	0
All	All	2496/2692 (92%)	0.40	210 (8%) 11 10	97, 205, 490, 679	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	584	LEU	8.6
1	A	610	SER	8.3
1	A	690	GLU	8.2
1	B	717	LEU	6.8
1	A	587	ASP	6.1
1	A	591	ASP	5.9
1	A	194	PRO	5.9
1	A	724	LEU	5.9
1	B	592	ASP	5.8
1	A	700	ASP	5.7
1	B	705	ASN	5.7
1	A	607	ASN	5.6
2	C	370	PHE	5.6
1	A	496	ALA	5.5
1	A	691	LYS	5.3
1	A	609	ASP	5.3
2	C	254	ASP	5.2
1	B	495	GLU	5.2
1	A	586	TYR	5.0
1	B	138	LEU	5.0
1	A	141	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	434	TYR	4.9
1	A	195	GLU	4.9
1	B	537	LYS	4.7
2	C	163	ASN	4.7
1	A	698	ASN	4.7
1	A	676	LYS	4.7
1	B	192	ASN	4.6
1	A	482	LEU	4.4
1	A	434	TYR	4.4
1	B	594	ASP	4.4
1	A	173	ALA	4.4
2	C	164	ALA	4.2
1	B	713	LYS	4.2
1	A	492	LEU	4.1
2	C	190	ASN	4.1
1	A	578	LEU	4.0
1	B	191	SER	4.0
2	C	253	LYS	4.0
2	C	380	ASP	4.0
2	C	368	LYS	4.0
1	A	699	GLN	4.0
1	B	413	SER	4.0
1	A	694	GLN	4.0
1	B	408	TYR	3.9
1	B	477	GLU	3.9
1	A	588	PHE	3.9
2	D	203	ASN	3.9
2	D	256	GLN	3.8
1	A	727	ALA	3.8
1	B	710	ASN	3.8
1	A	701	ALA	3.8
1	A	172	ASN	3.7
1	A	608	ILE	3.7
1	A	677	HIS	3.7
2	D	254	ASP	3.7
2	D	253	LYS	3.6
1	A	583	SER	3.6
1	A	585	LYS	3.6
1	A	495	GLU	3.5
2	D	204	LEU	3.4
1	A	493	LEU	3.4
1	A	571	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	404	ALA	3.3
2	C	611	HIS	3.3
1	B	409	LYS	3.3
1	B	158	PHE	3.3
1	A	460	GLU	3.3
1	A	731	HIS	3.3
1	A	170	VAL	3.3
1	A	695	SER	3.2
1	A	702	ASN	3.2
1	B	527	GLU	3.2
1	B	591	ASP	3.2
1	A	693	LEU	3.2
2	D	363	PHE	3.2
2	D	364	TYR	3.2
1	B	587	ASP	3.2
1	A	703	ILE	3.1
1	B	411	LEU	3.1
2	D	505	THR	3.1
2	C	30	GLN	3.1
1	A	254	PRO	3.1
1	B	706	SER	3.1
2	C	220	LYS	3.0
2	D	21	PHE	3.0
1	B	139	GLN	3.0
1	A	713	LYS	3.0
1	B	362	LEU	3.0
2	D	535	PRO	3.0
1	B	170	VAL	3.0
1	B	524	LYS	3.0
1	A	696	LEU	3.0
1	B	171	MET	2.9
1	A	704	LEU	2.9
2	C	162	LEU	2.9
1	A	304	ASP	2.9
1	A	411	LEU	2.9
2	C	367	SER	2.9
2	C	165	ASN	2.9
2	C	217	GLN	2.9
2	C	362	TYR	2.9
1	B	450	LEU	2.9
1	B	463	MET	2.9
2	D	365	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	593	PHE	2.9
1	A	479	ASN	2.9
1	B	460	GLU	2.9
1	A	595	ASN	2.9
1	B	668	PHE	2.8
1	B	499	GLU	2.8
1	B	245	ASN	2.8
1	B	595	ASN	2.8
1	B	120	GLN	2.8
1	B	577	GLU	2.8
1	B	536	LEU	2.8
2	C	187	LEU	2.8
2	D	228	ASN	2.8
2	D	609	ASP	2.8
2	C	166	GLU	2.8
1	B	456	ASN	2.7
1	B	407	PHE	2.7
1	B	457	ILE	2.7
1	B	532	GLU	2.7
1	B	679	GLU	2.7
1	A	435	ALA	2.7
1	A	563	ILE	2.7
1	A	360	ALA	2.7
1	B	254	PRO	2.6
2	C	255	GLU	2.6
2	C	219	ASP	2.6
1	A	711	LEU	2.6
1	A	419	LYS	2.6
1	A	457	ILE	2.6
1	A	245	ASN	2.6
1	A	191	SER	2.6
1	A	697	LYS	2.6
2	C	70	PHE	2.5
1	A	611	ILE	2.5
2	C	361	ALA	2.5
1	B	195	GLU	2.5
1	B	266	ASN	2.5
1	B	215	TRP	2.5
1	A	357	LEU	2.5
2	D	190	ASN	2.5
2	D	258	TYR	2.5
1	B	331	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	329	ALA	2.5
1	B	453	GLU	2.4
1	B	491	THR	2.4
2	D	536	LYS	2.4
1	A	461	TYR	2.4
1	A	315	GLU	2.4
1	B	528	ARG	2.4
1	B	412	ALA	2.4
1	A	458	LEU	2.4
1	A	673	ASP	2.3
1	B	583	SER	2.3
2	C	195	SER	2.3
2	D	166	GLU	2.3
1	A	728	ASP	2.3
1	B	118	ILE	2.3
1	B	714	ILE	2.3
2	C	256	GLN	2.3
2	C	363	PHE	2.3
2	D	237	PHE	2.3
1	B	531	ASP	2.3
1	B	404	ALA	2.3
1	A	405	SER	2.3
1	B	523	LYS	2.3
1	B	672	ASN	2.3
2	D	232	TYR	2.3
2	D	188	ILE	2.3
1	B	306	VAL	2.3
1	B	329	ALA	2.2
2	D	245	ILE	2.2
1	A	158	PHE	2.2
1	B	720	LEU	2.2
1	A	476	SER	2.2
2	C	203	ASN	2.2
2	C	381	TYR	2.2
2	C	609	ASP	2.2
1	A	447	LYS	2.2
1	B	478	GLU	2.2
1	A	446	TYR	2.2
1	B	496	ALA	2.2
1	A	148	LYS	2.2
1	A	629	ASN	2.2
1	A	650	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	539	ASN	2.1
1	B	677	HIS	2.1
1	A	483	LEU	2.1
1	B	202	LEU	2.1
1	B	521	LEU	2.1
1	A	382	ARG	2.1
1	A	193	ILE	2.1
2	D	167	ASN	2.1
1	A	410	GLY	2.1
2	C	376	TYR	2.1
1	B	707	PHE	2.1
1	B	667	PHE	2.1
2	D	24	SER	2.1
1	A	412	ALA	2.1
1	B	416	SER	2.0
1	A	505	ALA	2.0
1	B	144	ASP	2.0
2	D	378	ARG	2.0
1	B	316	TYR	2.0
1	A	580	THR	2.0
1	B	152	GLN	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 carbohydrates 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.

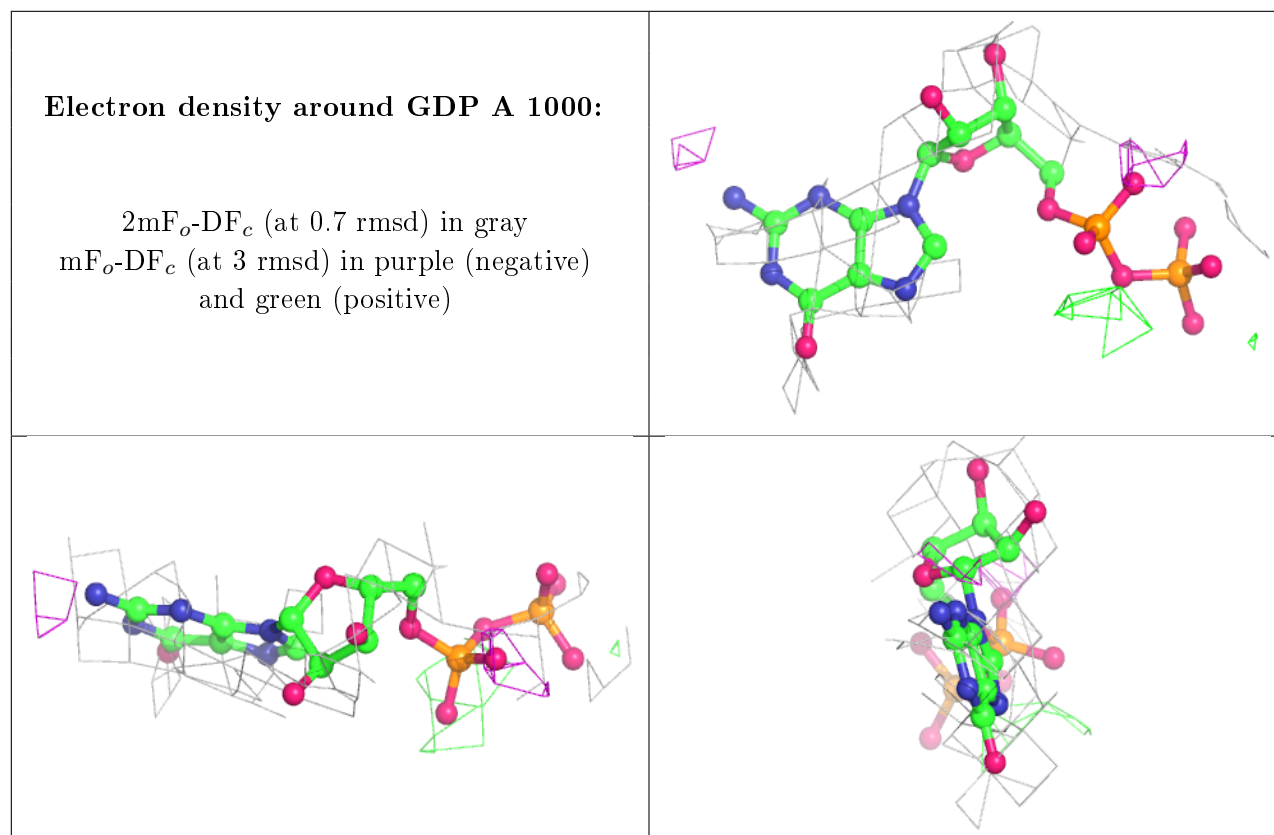
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GDP	A	1000	28/28	0.84	0.29	180,260,315,330	0
3	GDP	B	1000	28/28	0.87	0.28	159,248,280,299	0

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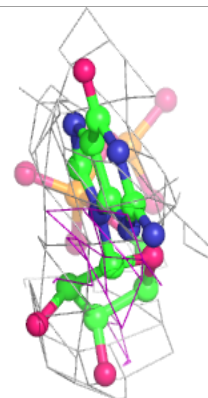
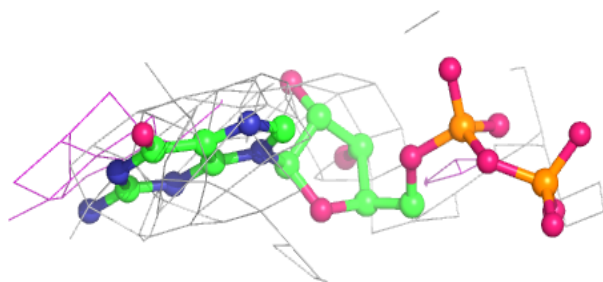
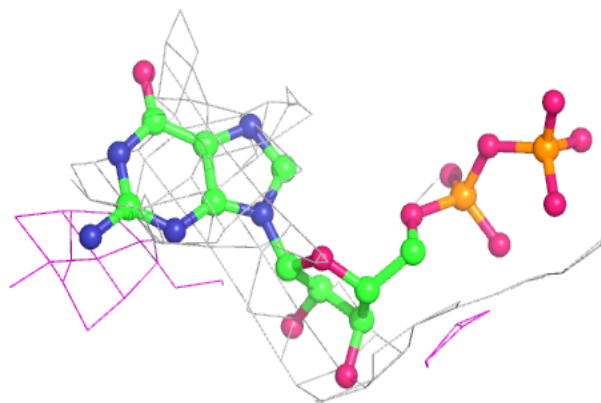
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GDP	C	1000	28/28	0.89	0.28	172,205,272,311	0
3	GDP	D	1000	28/28	0.92	0.23	183,210,303,332	0

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.

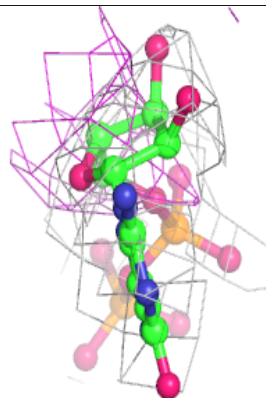
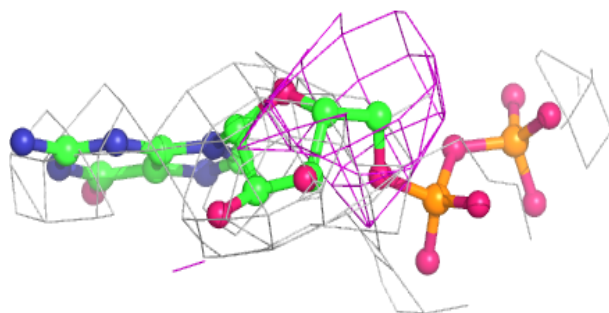
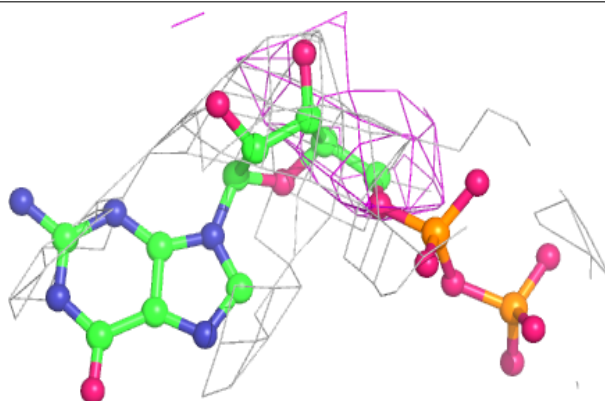


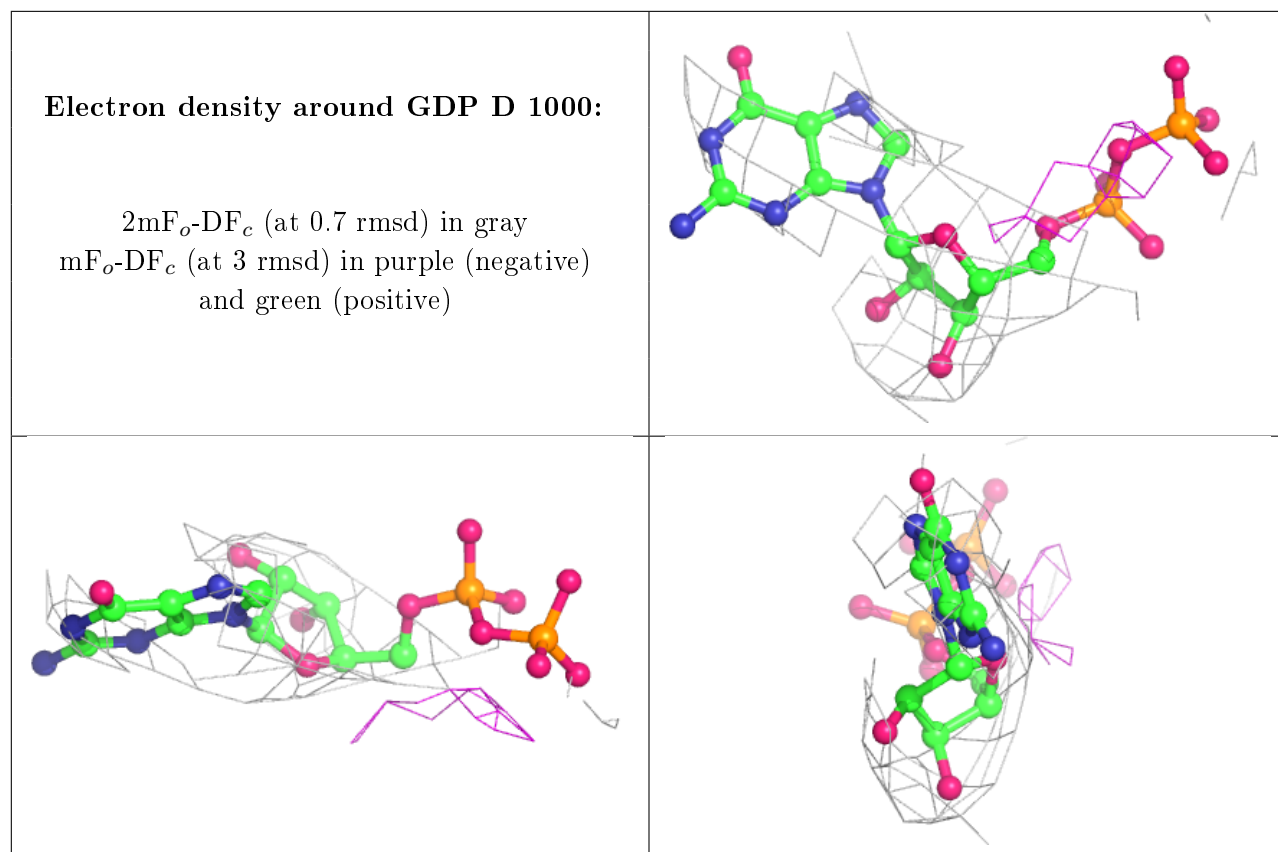
Electron density around GDP B 1000:

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

**Electron density around GDP C 1000:**

$2mF_o-DF_c$ (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.