



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:40 pm BST

PDB ID : 1FQJ
Title : CRYSTAL STRUCTURE OF THE HETEROTRIMERIC COMPLEX OF THE RGS DOMAIN OF RGS9, THE GAMMA SUBUNIT OF PHOSPHODIESTERASE AND THE GT/I1 CHIMERA ALPHA SUBUNIT [(RGS9)-(PDEGAMMA)-(GT/I1ALPHA)-(GDP)-(ALF4)-(MG2+)]
Authors : Slep, K.C.; Kercher, M.A.; He, W.; Cowan, C.W.; Wensel, T.G.; Sigler, P.B.
Deposited on : 2000-09-05
Resolution : 2.02 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

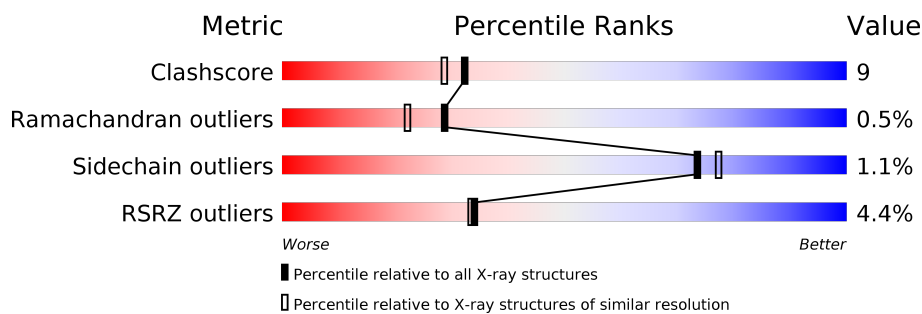
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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))
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	325	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	D	325	<div> <div>9%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	B	147	<div> <div>3%</div> <div>76%</div> <div>14%</div> <div>.</div> <div>10%</div> </div>
2	E	147	<div> <div>%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
3	C	42	<div> <div>2%</div> <div>69%</div> <div>17%</div> <div>5%</div> <div>10%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8107 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 Guanine nucleotide-binding protein G(t) subunit alpha-1, Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(t) subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2555	1620	423	493	19			
1	D	315	Total	C	N	O	S	0	0	0
			2539	1610	420	490	19			

- Molecule 2 is a protein called Regulator of G-protein signaling 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1111	718	194	193	6			
2	E	141	Total	C	N	O	S	0	0	0
			1181	766	205	204	6			

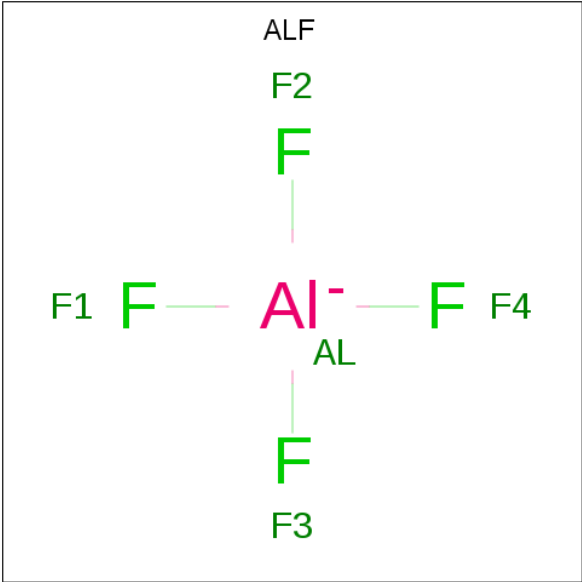
- Molecule 3 is a protein called Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	38	Total	C	N	O	S	0	0	0
			297	192	45	58	2			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

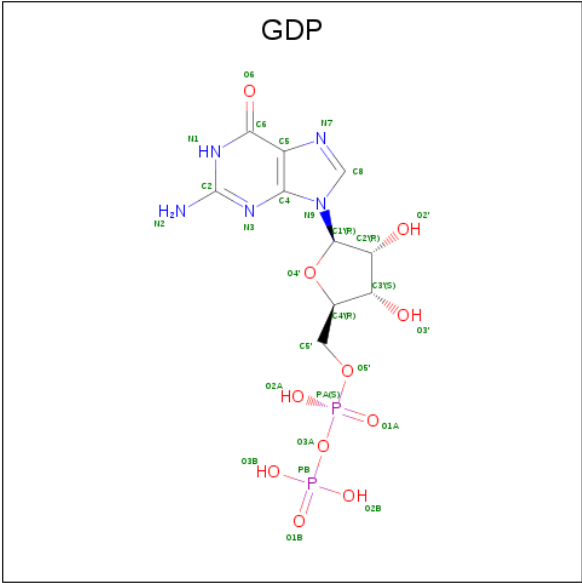
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

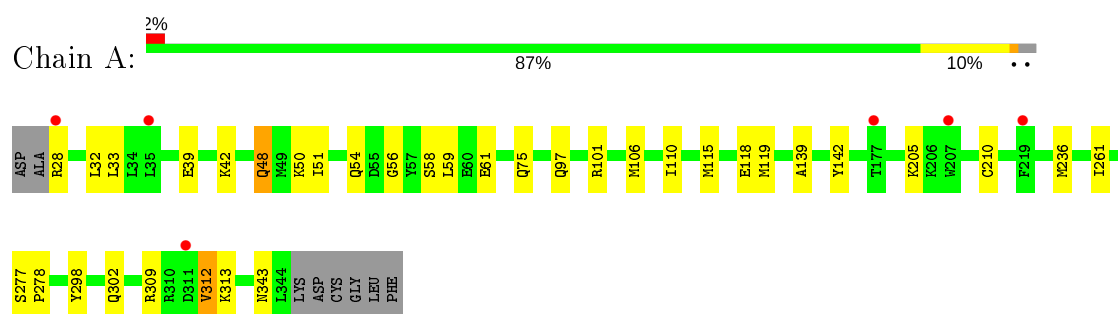
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	169	Total	O	0	0
			169	169		
7	B	40	Total	O	0	0
			40	40		
7	C	16	Total	O	0	0
			16	16		
7	D	88	Total	O	0	0
			88	88		
7	E	43	Total	O	0	0
			43	43		

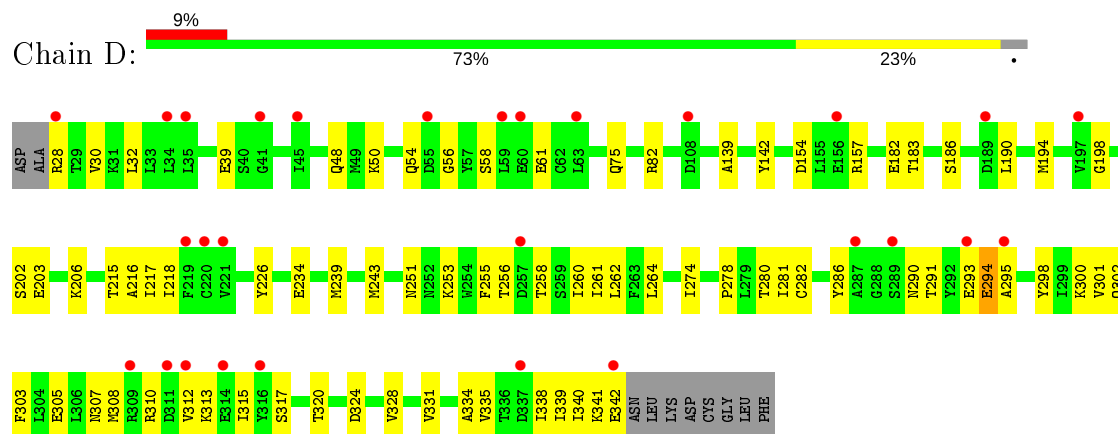
3 Residue-property plots [i](#)

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.

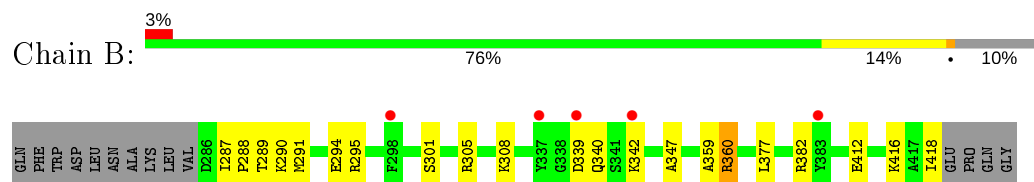
- Molecule 1: Guanine nucleotide-binding protein G(t) subunit alpha-1, Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(t) subunit alpha-1



- Molecule 1: Guanine nucleotide-binding protein G(t) subunit alpha-1, Guanine nucleotide-binding protein G(i) subunit alpha-1, Guanine nucleotide-binding protein G(t) subunit alpha-1

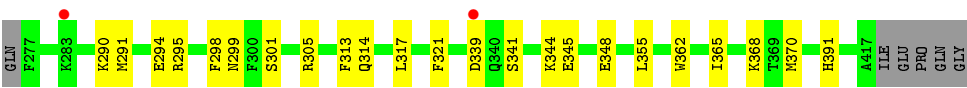


- Molecule 2: Regulator of G-protein signaling 9

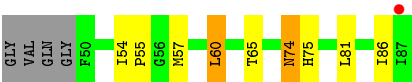


- Molecule 2: Regulator of G-protein signaling 9





● Molecule 3: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.61Å 115.94Å 134.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.02 37.14 – 2.02	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-2.02) 96.7 (37.14-2.02)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.265 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	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	0.95	EDS
Total number of atoms	8107	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, ALF, 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	0.36	0/2598	0.59	0/3500
1	D	0.34	0/2582	0.56	0/3478
2	B	0.35	0/1139	0.52	0/1526
2	E	0.36	0/1212	0.54	0/1626
3	C	0.37	0/305	0.56	0/414
All	All	0.35	0/7836	0.56	0/10544

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2555	0	2537	29	0
1	D	2539	0	2520	67	0
2	B	1111	0	1120	21	0
2	E	1181	0	1187	20	0
3	C	297	0	275	6	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	5	0	0	0	0
6	A	28	0	12	1	0
6	D	28	0	12	2	0
7	A	169	0	0	3	0
7	B	40	0	0	0	0
7	C	16	0	0	0	0
7	D	88	0	0	7	0
7	E	43	0	0	2	0
All	All	8107	0	7663	135	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 (135) 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:B:360:ARG:HH11	2:B:360:ARG:HB3	1.46	0.81
1:D:291:THR:HG22	1:D:293:GLU:H	1.46	0.79
1:D:278:PRO:HB2	1:D:280:THR:HG22	1.66	0.78
1:D:298:TYR:O	1:D:302:GLN:HG2	1.86	0.76
1:D:198:GLY:HA3	1:D:203:GLU:HG2	1.66	0.75
1:A:309:ARG:NH1	1:A:313:LYS:HG2	2.02	0.73
1:D:48:GLN:HG3	1:D:328:VAL:HG21	1.69	0.73
1:A:309:ARG:HH11	1:A:313:LYS:HG2	1.55	0.72
2:B:295:ARG:HH11	2:E:295:ARG:HG3	1.58	0.69
1:D:253:LYS:HA	1:D:256:THR:HG23	1.75	0.68
1:A:205:LYS:HE2	7:A:428:HOH:O	1.93	0.68
1:A:106:MET:HE1	1:A:118:GLU:HG3	1.75	0.67
1:D:48:GLN:HA	1:D:48:GLN:HE21	1.60	0.65
1:D:203:GLU:HG3	7:D:405:HOH:O	1.96	0.64
1:A:205:LYS:HE3	2:B:359:ALA:O	1.97	0.64
2:E:290:LYS:O	2:E:294:GLU:HG3	1.98	0.64
1:D:50:LYS:HE2	1:D:56:GLY:O	1.98	0.63
1:D:334:ALA:O	1:D:338:ILE:HG13	1.98	0.63
1:A:115:MET:SD	1:A:119:MET:HE2	2.40	0.62
1:A:110:ILE:HD12	1:A:110:ILE:O	1.99	0.62
2:B:295:ARG:NH1	2:E:295:ARG:HG3	2.15	0.61
2:E:301:SER:O	2:E:305:ARG:HG3	2.01	0.60
2:B:340:GLN:HG3	2:B:382:ARG:HH12	1.64	0.60
2:B:360:ARG:NH1	2:B:360:ARG:HB3	2.14	0.58
1:D:291:THR:HB	1:D:294:GLU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:HA	1:A:48:GLN:HE21	1.70	0.57
1:D:307:ASN:O	1:D:310:ARG:HB2	2.04	0.56
1:D:261:ILE:HD12	1:D:261:ILE:N	2.20	0.56
1:D:39:GLU:N	6:D:361:GDP:O3B	2.40	0.55
1:D:320:THR:HG22	1:D:331:VAL:HG21	1.89	0.55
1:A:261:ILE:N	1:A:261:ILE:HD12	2.22	0.54
3:C:74:ASN:HD22	3:C:75:HIS:N	2.06	0.54
1:D:186:SER:HA	1:D:190:LEU:O	2.08	0.54
1:D:262:LEU:O	1:D:317:SER:HA	2.08	0.54
1:D:217:ILE:HD11	1:D:255:PHE:CE1	2.43	0.54
2:E:365:ILE:HD11	2:E:370:MET:CE	2.38	0.53
1:D:308:MET:C	1:D:310:ARG:H	2.12	0.53
2:B:290:LYS:HG2	2:B:294:GLU:OE2	2.09	0.53
1:D:291:THR:HG22	1:D:293:GLU:N	2.19	0.53
2:E:344:LYS:O	2:E:348:GLU:HG2	2.08	0.53
7:D:393:HOH:O	2:E:368:LYS:HG3	2.09	0.52
1:D:48:GLN:HA	1:D:48:GLN:NE2	2.24	0.52
3:C:60:LEU:HD13	3:C:65:THR:HG23	1.90	0.51
1:D:58:SER:OG	1:D:61:GLU:HG3	2.09	0.51
1:D:261:ILE:HG21	1:D:335:VAL:HG22	1.94	0.50
1:A:32:LEU:HD23	1:A:33:LEU:N	2.27	0.50
2:B:288:PRO:HG2	2:B:308:LYS:HG2	1.95	0.49
2:B:288:PRO:CG	2:B:308:LYS:HG2	2.42	0.49
1:A:106:MET:O	1:A:110:ILE:HG13	2.12	0.49
2:B:418:ILE:HD13	2:E:305:ARG:NE	2.28	0.49
1:D:154:ASP:OD2	1:D:157:ARG:NE	2.46	0.49
1:D:28:ARG:HG3	1:D:190:LEU:HD22	1.95	0.48
1:D:139:ALA:HA	1:D:142:TYR:CE1	2.48	0.48
1:D:50:LYS:HG3	1:D:54:GLN:HE21	1.78	0.48
2:B:301:SER:O	2:B:305:ARG:HG2	2.13	0.48
1:D:75:GLN:HG2	7:D:391:HOH:O	2.12	0.48
1:D:301:VAL:O	1:D:305:GLU:HG2	2.13	0.48
1:D:182:GLU:HG2	1:D:183:THR:N	2.28	0.48
1:D:215:THR:O	1:D:258:THR:HG23	2.14	0.48
1:A:32:LEU:HD23	1:A:32:LEU:C	2.33	0.48
2:B:295:ARG:HG3	2:E:291:MET:SD	2.53	0.48
1:D:32:LEU:HD11	1:D:218:ILE:HG13	1.96	0.48
2:B:416:LYS:N	2:B:416:LYS:HD2	2.29	0.47
2:E:298:PHE:O	2:E:299:ASN:HB3	2.14	0.47
2:E:365:ILE:HD11	2:E:370:MET:HE2	1.97	0.47
1:D:243:MET:HA	1:D:303:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:GLU:HG3	7:E:456:HOH:O	2.13	0.47
1:D:203:GLU:OE1	1:D:206:LYS:NZ	2.34	0.47
1:A:50:LYS:HA	1:A:54:GLN:HB2	1.97	0.47
1:D:183:THR:CG2	1:D:194:MET:HB3	2.45	0.47
1:D:264:LEU:CD1	1:D:300:LYS:HB2	2.45	0.46
1:D:274:ILE:HG13	1:D:290:ASN:HB3	1.96	0.46
2:B:339:ASP:OD2	2:B:342:LYS:HE3	2.15	0.46
2:E:291:MET:O	2:E:295:ARG:HG2	2.16	0.46
2:E:339:ASP:OD1	2:E:341:SER:OG	2.29	0.46
1:D:340:ILE:C	1:D:342:GLU:H	2.19	0.46
2:B:340:GLN:HG3	2:B:382:ARG:NH1	2.30	0.46
3:C:81:LEU:HA	3:C:86:ILE:HD12	1.98	0.46
1:D:324:ASP:O	1:D:328:VAL:HG23	2.16	0.46
1:D:243:MET:HG2	1:D:303:PHE:CE1	2.51	0.46
1:A:97:GLN:O	1:A:101:ARG:HG2	2.16	0.46
1:D:226:TYR:HA	1:D:239:MET:HB2	1.98	0.46
1:D:39:GLU:HA	6:D:361:GDP:O3B	2.15	0.46
1:D:206:LYS:HD3	2:E:321:PHE:O	2.16	0.45
1:A:115:MET:HA	1:A:119:MET:HE2	1.99	0.45
1:A:210:CYS:HA	7:A:395:HOH:O	2.16	0.45
1:A:298:TYR:O	1:A:302:GLN:HG2	2.16	0.45
1:D:260:ILE:HB	1:D:315:ILE:HD12	1.97	0.45
1:D:339:ILE:HG23	7:D:446:HOH:O	2.17	0.45
1:D:32:LEU:HD13	1:D:216:ALA:HB3	1.99	0.45
1:A:39:GLU:HA	6:A:360:GDP:O3B	2.16	0.45
2:B:289:THR:HA	2:B:418:ILE:CG2	2.47	0.45
1:A:115:MET:HA	1:A:119:MET:CE	2.46	0.45
1:A:277:SER:HA	1:A:278:PRO:HD3	1.81	0.45
3:C:54:ILE:HA	3:C:55:PRO:HD3	1.85	0.45
1:D:324:ASP:HA	7:D:447:HOH:O	2.17	0.44
1:D:215:THR:C	1:D:258:THR:HG23	2.38	0.44
2:B:291:MET:SD	2:E:295:ARG:HD2	2.58	0.44
1:D:202:SER:HA	2:E:362:TRP:CE3	2.53	0.44
1:D:28:ARG:CG	1:D:190:LEU:HD22	2.47	0.44
1:D:75:GLN:CD	7:D:401:HOH:O	2.55	0.44
1:D:278:PRO:HG2	1:D:281:ILE:HG13	2.00	0.43
2:E:365:ILE:HG22	2:E:391:HIS:CD2	2.53	0.43
1:A:110:ILE:HD12	1:A:110:ILE:C	2.38	0.43
1:D:82:ARG:NH2	7:D:376:HOH:O	2.51	0.43
1:D:183:THR:HG23	1:D:194:MET:HB3	1.99	0.43
1:D:32:LEU:HD12	1:D:216:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:THR:O	1:D:313:LYS:NZ	2.43	0.43
1:A:139:ALA:HA	1:A:142:TYR:CE1	2.53	0.42
3:C:55:PRO:O	3:C:57:MET:HE2	2.19	0.42
1:D:335:VAL:HA	1:D:338:ILE:HD12	2.01	0.42
2:E:313:PHE:CZ	2:E:317:LEU:HD11	2.54	0.42
2:E:344:LYS:HB3	7:E:456:HOH:O	2.19	0.42
2:B:412:GLU:HG3	2:B:416:LYS:NZ	2.34	0.42
1:A:309:ARG:NH2	1:A:312:VAL:HG11	2.35	0.42
1:A:51:ILE:HA	1:A:56:GLY:HA2	2.02	0.42
1:D:30:VAL:HG23	1:D:215:THR:HB	2.02	0.42
1:A:115:MET:SD	1:A:119:MET:CE	3.08	0.41
1:D:217:ILE:HD11	1:D:255:PHE:CZ	2.55	0.41
2:B:418:ILE:O	2:B:418:ILE:HG23	2.21	0.41
1:A:106:MET:CE	1:A:118:GLU:HG3	2.46	0.41
1:A:58:SER:OG	1:A:61:GLU:HG3	2.19	0.41
3:C:60:LEU:O	3:C:60:LEU:HD12	2.21	0.41
2:B:287:ILE:HG23	2:B:287:ILE:O	2.21	0.41
2:B:347:ALA:HB1	2:B:377:LEU:CD2	2.51	0.41
1:D:294:GLU:HG3	1:D:295:ALA:N	2.36	0.41
1:D:251:ASN:CG	1:D:308:MET:HG2	2.41	0.41
1:A:28:ARG:NH1	1:A:343:ASN:HB3	2.35	0.41
1:D:226:TYR:O	1:D:282:CYS:HB2	2.21	0.41
1:D:286:TYR:OH	1:D:294:GLU:HG3	2.21	0.41
1:D:264:LEU:HD11	1:D:300:LYS:HB2	2.03	0.40
1:D:48:GLN:CA	1:D:48:GLN:HE21	2.24	0.40
1:A:75:GLN:HG3	7:A:397:HOH:O	2.22	0.40
1:D:291:THR:HB	1:D:294:GLU:CB	2.49	0.40
1:D:243:MET:HG2	1:D:303:PHE:CZ	2.57	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	315/325 (97%)	308 (98%)	6 (2%)	1 (0%)	41	36
1	D	313/325 (96%)	296 (95%)	13 (4%)	4 (1%)	12	5
2	B	131/147 (89%)	125 (95%)	6 (5%)	0	100	100
2	E	139/147 (95%)	133 (96%)	6 (4%)	0	100	100
3	C	36/42 (86%)	36 (100%)	0	0	100	100
All	All	934/986 (95%)	898 (96%)	31 (3%)	5 (0%)	29	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	VAL
1	D	294	GLU
1	D	234	GLU
1	D	341	LYS
1	D	312	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	284/290 (98%)	280 (99%)	4 (1%)	67	70
1	D	282/290 (97%)	282 (100%)	0	100	100
2	B	116/128 (91%)	115 (99%)	1 (1%)	78	82
2	E	123/128 (96%)	121 (98%)	2 (2%)	62	66
3	C	31/33 (94%)	29 (94%)	2 (6%)	17	11
All	All	836/869 (96%)	827 (99%)	9 (1%)	73	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	48	GLN
1	A	59	LEU

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Mol	Chain	Res	Type
1	A	236	MET
2	B	360	ARG
3	C	60	LEU
3	C	74	ASN
2	E	314	GLN
2	E	355	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	HIS
1	A	90	GLN
1	A	97	GLN
1	A	184	GLN
1	A	290	ASN
1	A	343	ASN
2	B	315	HIS
3	C	74	ASN
1	D	48	GLN
1	D	54	GLN
1	D	184	GLN
1	D	290	ASN
2	E	311	GLN
2	E	314	GLN
2	E	340	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ALF	A	362	1,4,7,6	0,4,4	0.00	-	-		
6	GDP	A	360	5,4	24,30,30	2.84	7 (29%)	31,47,47	3.45	10 (32%)
5	ALF	D	363	4,7,6	0,4,4	0.00	-	-		
6	GDP	D	361	5,4	24,30,30	2.83	6 (25%)	31,47,47	3.41	9 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	A	360	5,4	-	2/12/32/32	0/3/3/3
6	GDP	D	361	5,4	-	3/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	360	GDP	C2-N1	8.51	1.50	1.35
6	D	361	GDP	C2-N1	8.34	1.50	1.35
6	A	360	GDP	O4'-C1'	6.93	1.50	1.41
6	D	361	GDP	O4'-C1'	6.53	1.50	1.41
6	A	360	GDP	O6-C6	4.31	1.35	1.24
6	D	361	GDP	PB-O2B	-4.13	1.38	1.54
6	D	361	GDP	O6-C6	3.91	1.34	1.24
6	D	361	GDP	C8-N7	3.73	1.41	1.34
6	A	360	GDP	PB-O2B	-3.35	1.41	1.54
6	A	360	GDP	C8-N7	3.27	1.40	1.34
6	D	361	GDP	O4'-C4'	2.86	1.51	1.45
6	A	360	GDP	O3'-C3'	2.76	1.49	1.43
6	A	360	GDP	O4'-C4'	2.66	1.50	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	361	GDP	C6-C5-C4	-11.65	109.68	120.80
6	A	360	GDP	C6-C5-C4	-11.40	109.92	120.80
6	A	360	GDP	N2-C2-N3	8.61	131.82	117.79
6	D	361	GDP	N2-C2-N3	8.41	131.49	117.79
6	A	360	GDP	N2-C2-N1	-5.74	108.32	117.25
6	D	361	GDP	N2-C2-N1	-5.65	108.46	117.25
6	A	360	GDP	N3-C2-N1	-5.52	119.86	127.22
6	D	361	GDP	N3-C2-N1	-5.38	120.05	127.22
6	D	361	GDP	C4-C5-N7	-4.94	104.25	109.40
6	A	360	GDP	C4-C5-N7	-4.79	104.41	109.40
6	D	361	GDP	C2-N3-C4	4.10	120.04	115.36
6	A	360	GDP	O3B-PB-O3A	-4.01	91.17	104.64
6	A	360	GDP	C2-N3-C4	3.73	119.61	115.36
6	D	361	GDP	O3B-PB-O2B	3.11	119.51	107.64
6	D	361	GDP	C2'-C3'-C4'	2.85	108.18	102.64
6	A	360	GDP	C2'-C3'-C4'	2.75	107.99	102.64
6	A	360	GDP	O2B-PB-O1B	2.55	120.65	110.68
6	D	361	GDP	O2'-C2'-C3'	2.45	119.76	111.82
6	A	360	GDP	O2'-C2'-C3'	2.32	119.33	111.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	360	GDP	PA-O3A-PB-O2B
6	D	361	GDP	PA-O3A-PB-O2B
6	A	360	GDP	PA-O3A-PB-O1B
6	D	361	GDP	PA-O3A-PB-O1B
6	D	361	GDP	PA-O3A-PB-O3B

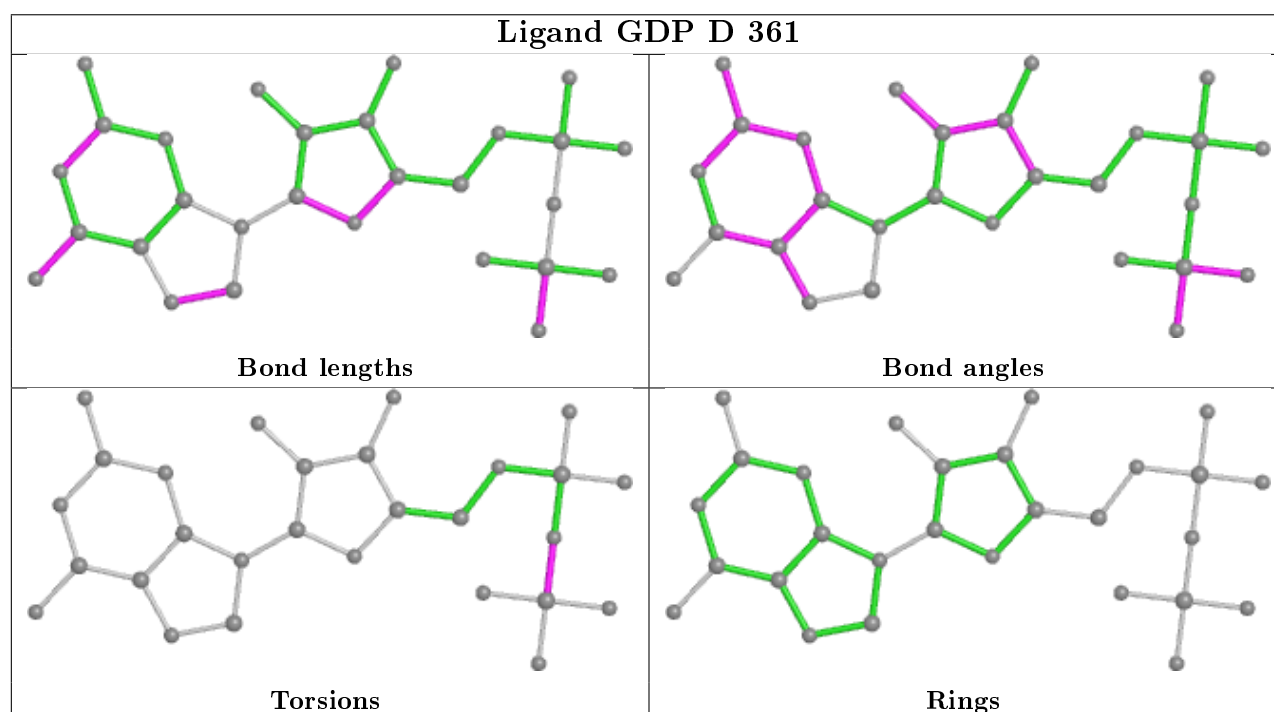
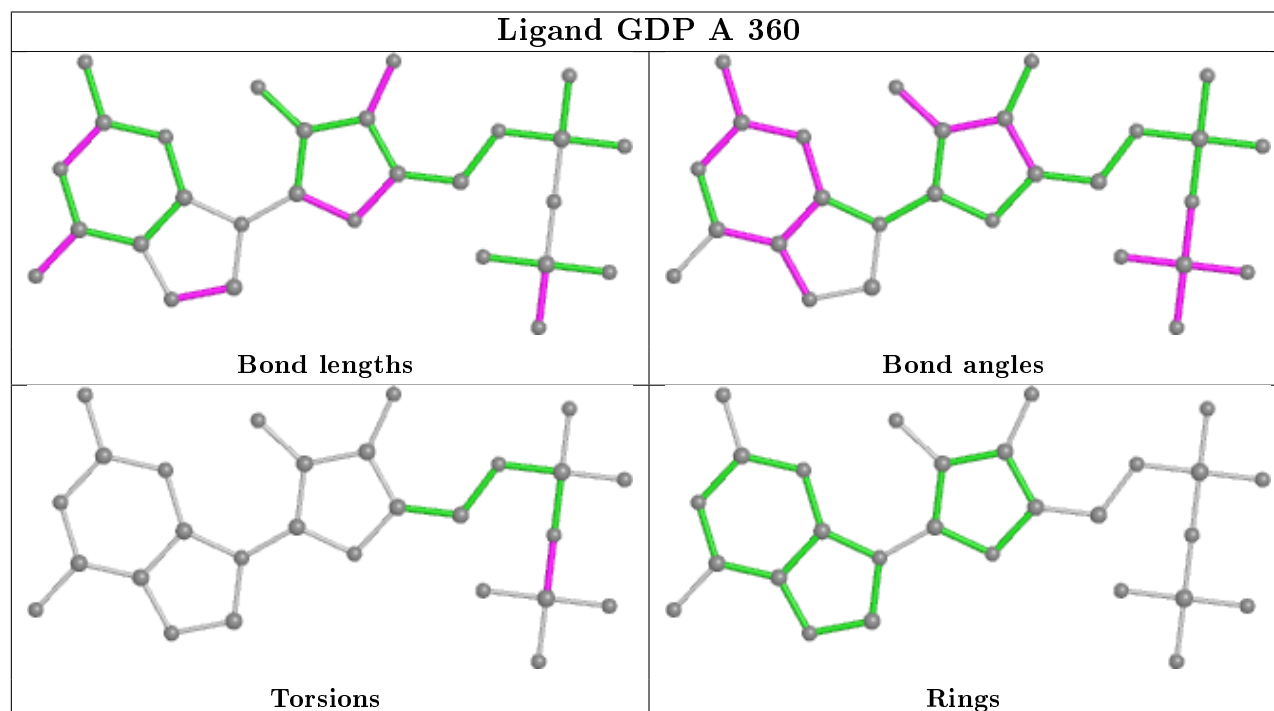
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	360	GDP	1	0
6	D	361	GDP	2	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	317/325 (97%)	0.11	6 (1%) 66 66	13, 24, 50, 74	0
1	D	315/325 (96%)	0.51	28 (8%) 9 9	14, 37, 65, 89	0
2	B	133/147 (90%)	0.20	5 (3%) 40 40	16, 32, 56, 68	0
2	E	141/147 (95%)	0.03	2 (1%) 75 74	14, 32, 56, 63	0
3	C	38/42 (90%)	0.07	1 (2%) 56 55	17, 33, 58, 65	0
All	All	944/986 (95%)	0.24	42 (4%) 34 33	13, 31, 58, 89	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	311	ASP	4.9
1	D	220	CYS	3.9
1	D	293	GLU	3.8
1	D	59	LEU	3.8
1	D	309	ARG	3.2
1	D	257	ASP	3.1
2	E	283	LYS	3.1
2	B	339	ASP	3.1
1	D	45	ILE	3.1
1	A	311	ASP	2.9
3	C	87	ILE	2.9
1	D	41	GLY	2.8
1	D	287	ALA	2.8
1	D	60	GLU	2.7
2	B	342	LYS	2.7
1	D	197	VAL	2.7
1	D	342	GLU	2.7
2	B	383	TYR	2.6
1	D	289	SER	2.6
1	D	189	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	316	TYR	2.6
1	A	219	PHE	2.5
1	D	55	ASP	2.5
2	E	339	ASP	2.5
1	A	28	ARG	2.4
1	D	314	GLU	2.4
1	D	156	GLU	2.4
1	D	312	VAL	2.3
1	D	219	PHE	2.3
2	B	337	TYR	2.2
1	D	34	LEU	2.2
1	D	28	ARG	2.2
1	D	35	LEU	2.1
1	A	35	LEU	2.1
1	D	295	ALA	2.1
2	B	298	PHE	2.1
1	D	108	ASP	2.1
1	A	207	TRP	2.1
1	D	63	LEU	2.0
1	D	221	VAL	2.0
1	D	337	ASP	2.0
1	A	177	THR	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.

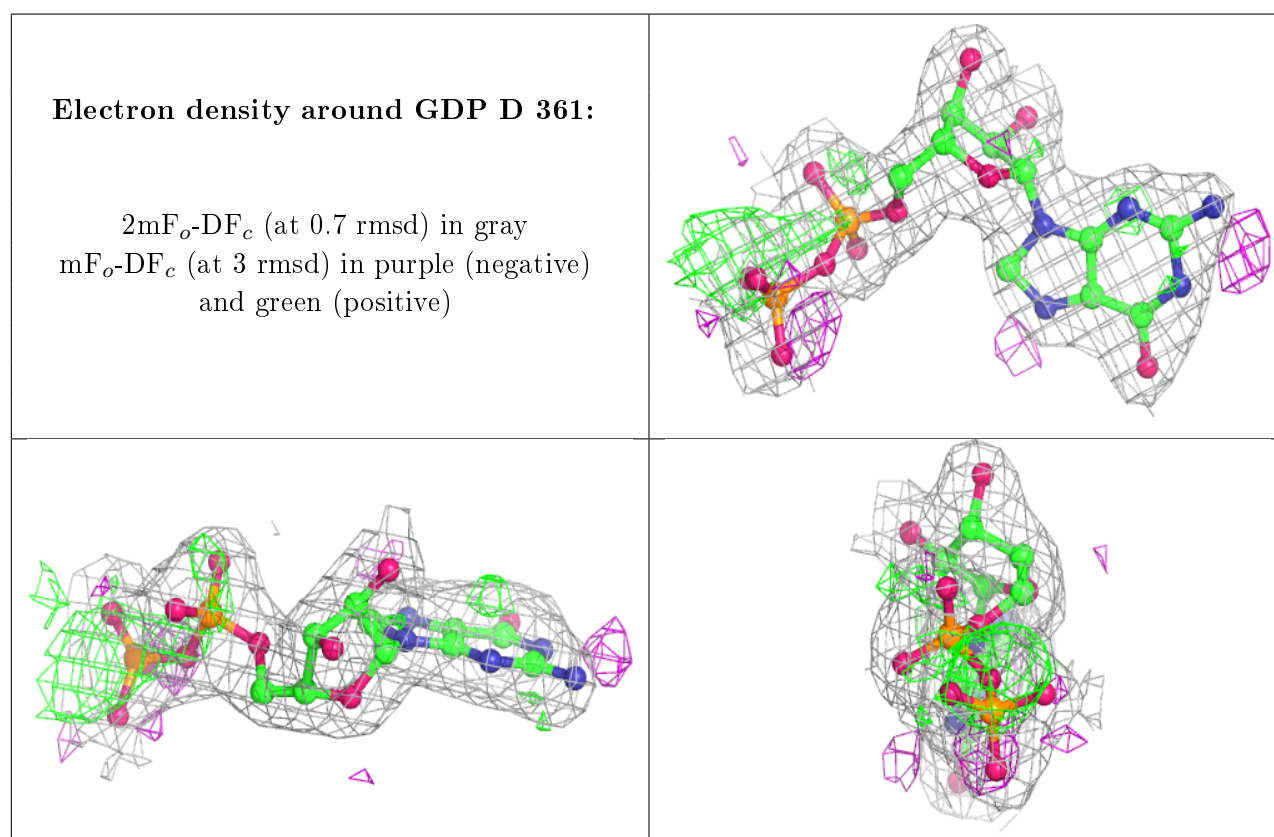
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	352	1/1	0.93	0.33	22,22,22,22	0

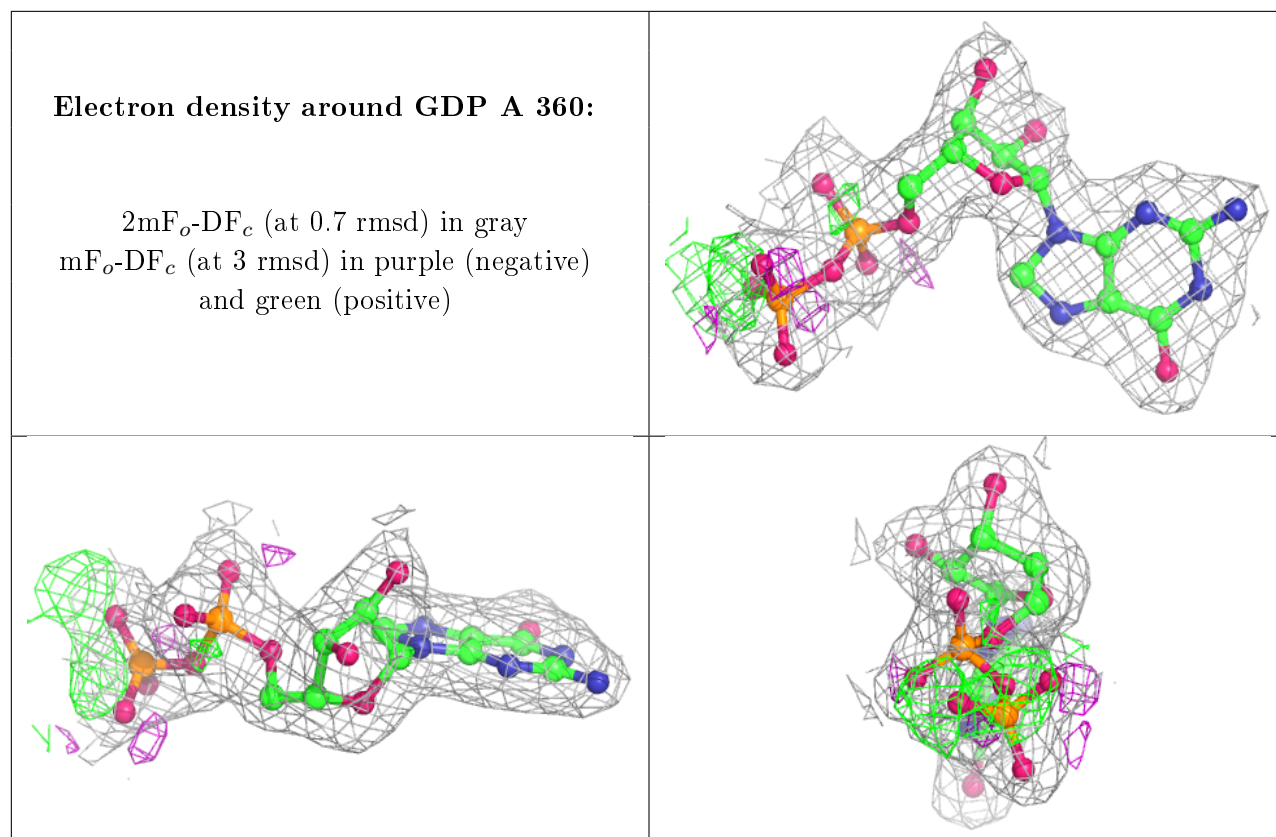
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	352	1/1	0.94	0.30	17,17,17,17	0
5	ALF	A	362	5/5	0.94	0.28	16,17,22,25	0
6	GDP	D	361	28/28	0.94	0.21	10,19,26,29	0
6	GDP	A	360	28/28	0.96	0.21	7,14,21,21	0
5	ALF	D	363	5/5	0.98	0.24	13,14,18,20	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.