Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:33 AM EDT

PDB ID	:	3AB3 / pdb_00003ab3
Title	:	Crystal structure of p115RhoGEF RGS domain in complex with G alpha 13
Authors	:	Kukimoto-Niino, M.; Mishima, C.; Shirouzu, M.; Kozasa, T.; Yokoyama, S.
Deposited on	:	2009-11-30
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

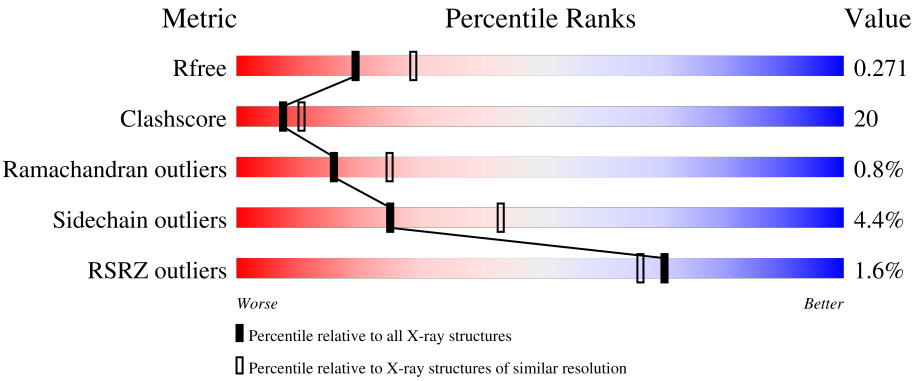
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	362	56% 30% 11%
1	C	362	54% 30% 12%
2	B	246	42% 30% 26%
2	D	246	37% 27% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ALF	C	602	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8246 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(k) subunit alpha, Guanine nucleotide-binding protein subunit alpha-13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2660	1694	472	484	10			
1	C	318	Total	C	N	O	S	0	0	0
			2627	1674	466	477	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ARG	-	linker	UNP Q9DC51
A	45	SER	-	linker	UNP Q9DC51
A	46	ALA	-	linker	UNP Q9DC51
C	44	ARG	-	linker	UNP Q9DC51
C	45	SER	-	linker	UNP Q9DC51
C	46	ALA	-	linker	UNP Q9DC51

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1475	931	267	268	9			
2	D	165	Total	C	N	O	S	0	0	0
			1329	841	237	242	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP Q92888
B	-11	ALA	-	expression tag	UNP Q92888
B	-10	MET	-	expression tag	UNP Q92888
B	-9	GLY	-	expression tag	UNP Q92888
B	-8	ILE	-	expression tag	UNP Q92888

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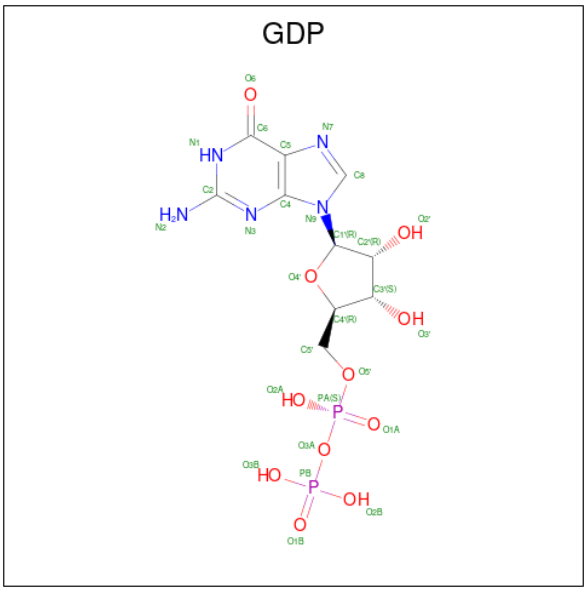
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP Q92888
B	-6	CYS	-	expression tag	UNP Q92888
B	-5	GLY	-	expression tag	UNP Q92888
B	-4	GLY	-	expression tag	UNP Q92888
B	-3	ILE	-	expression tag	UNP Q92888
B	-2	LEU	-	expression tag	UNP Q92888
B	-1	VAL	-	expression tag	UNP Q92888
B	0	PRO	-	expression tag	UNP Q92888
D	-12	GLY	-	expression tag	UNP Q92888
D	-11	ALA	-	expression tag	UNP Q92888
D	-10	MET	-	expression tag	UNP Q92888
D	-9	GLY	-	expression tag	UNP Q92888
D	-8	ILE	-	expression tag	UNP Q92888
D	-7	GLN	-	expression tag	UNP Q92888
D	-6	CYS	-	expression tag	UNP Q92888
D	-5	GLY	-	expression tag	UNP Q92888
D	-4	GLY	-	expression tag	UNP Q92888
D	-3	ILE	-	expression tag	UNP Q92888
D	-2	LEU	-	expression tag	UNP Q92888
D	-1	VAL	-	expression tag	UNP Q92888
D	0	PRO	-	expression tag	UNP Q92888

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

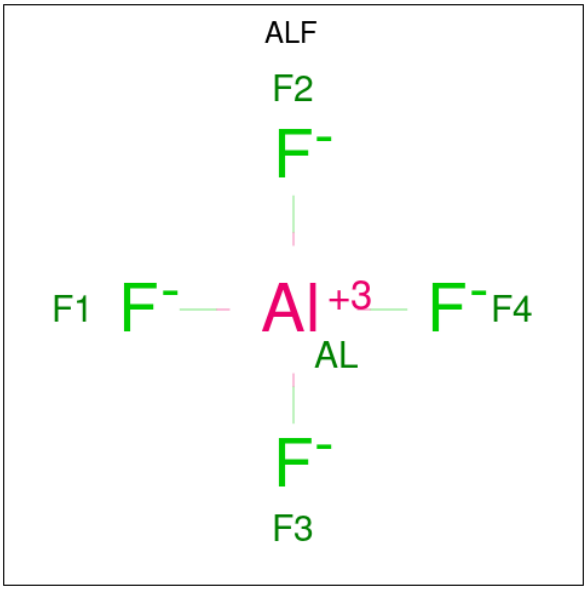
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



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

- Molecule 6 is water.

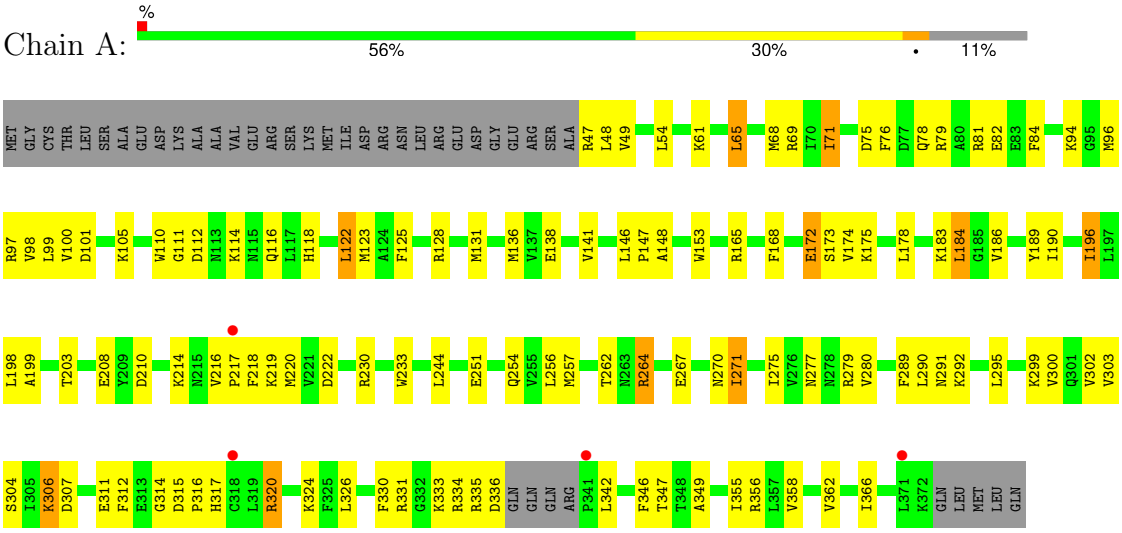
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	41	Total O 41 41	0	0
6	B	12	Total O 12 12	0	0
6	C	30	Total O 30 30	0	0
6	D	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

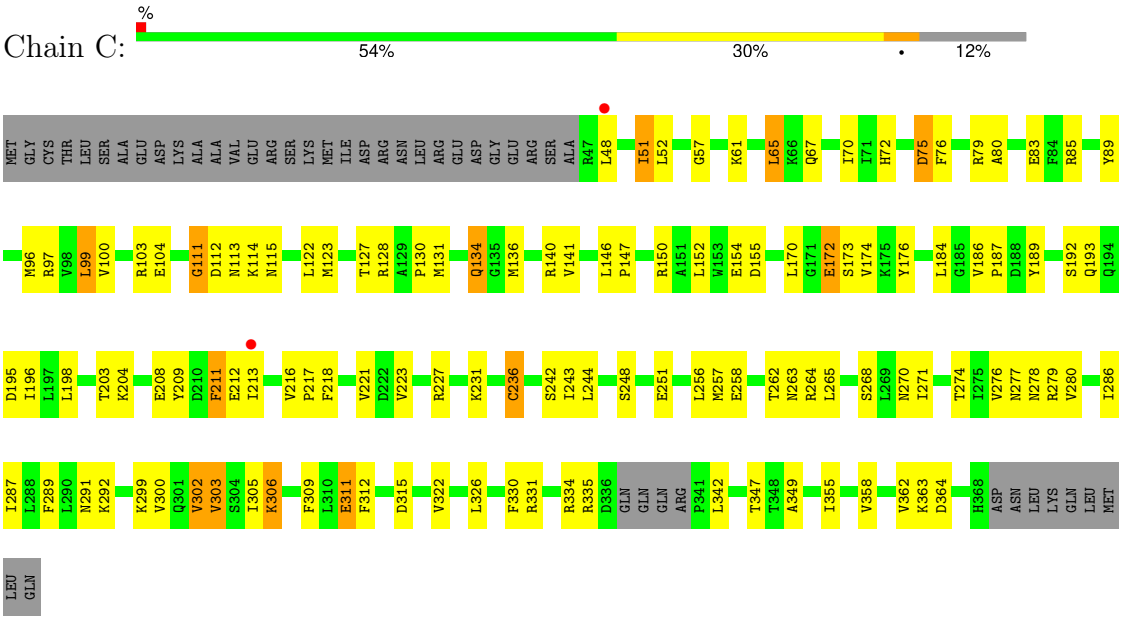
• Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha, Guanine nucleotide-binding protein subunit alpha-13

Chain A:



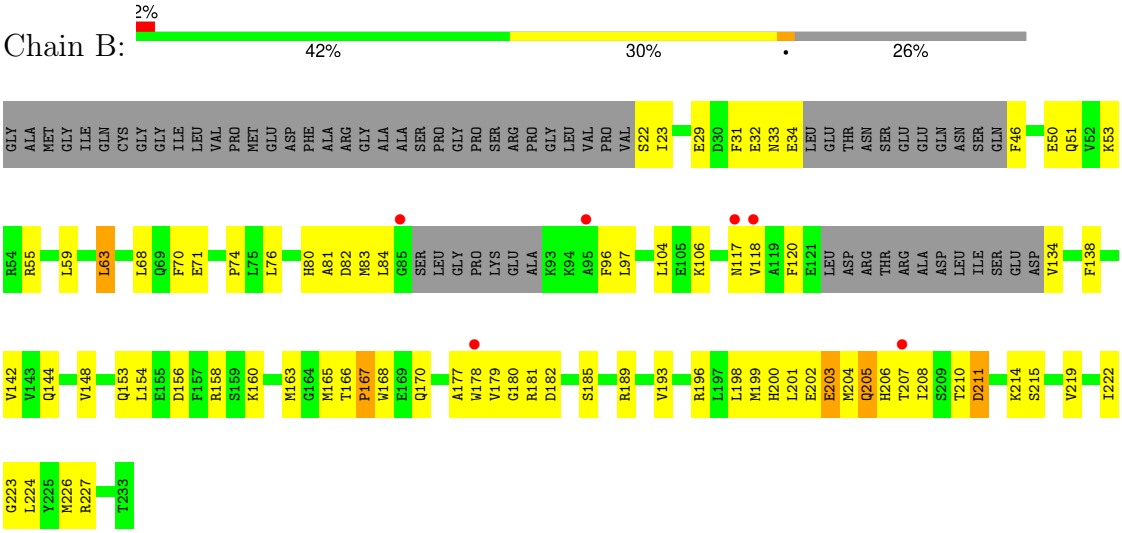
• Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha, Guanine nucleotide-binding protein subunit alpha-13

Chain C:



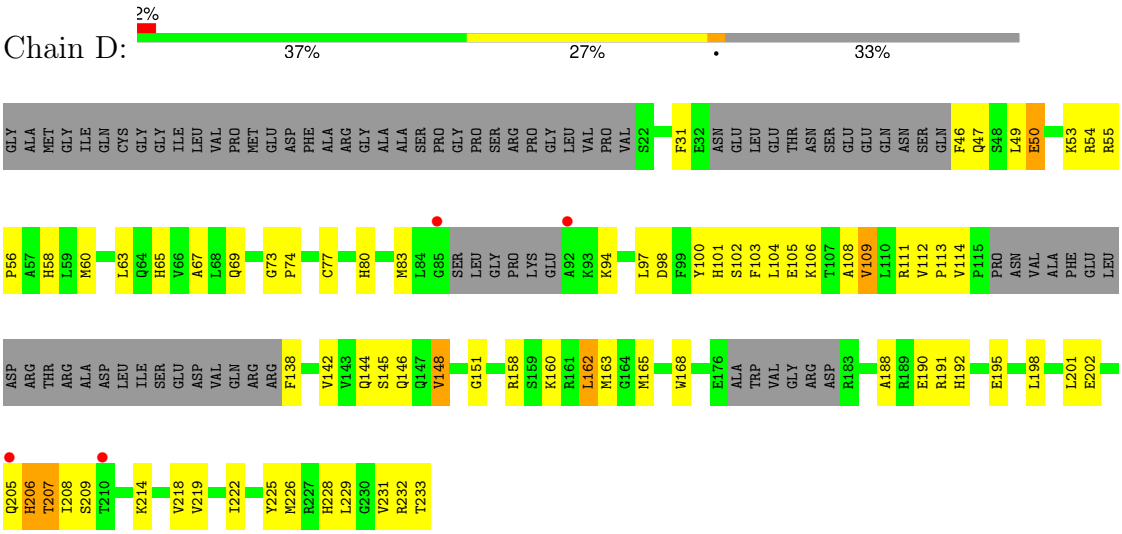
• Molecule 2: Rho guanine nucleotide exchange factor 1

Chain B:



• Molecule 2: Rho guanine nucleotide exchange factor 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.48Å 70.64Å 88.08Å 77.77° 84.45° 80.11°	Depositor
Resolution (Å)	48.88 – 2.40 48.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	81.7 (48.88-2.40) 81.7 (48.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.280 0.200 , 0.271	Depositor DCC
R_{free} test set	3734 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8246	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.58	0/2712	0.97	9/3651 (0.2%)
1	C	0.56	0/2679	0.97	11/3607 (0.3%)
2	B	0.54	0/1502	0.97	6/2022 (0.3%)
2	D	0.45	0/1351	0.92	3/1815 (0.2%)
All	All	0.55	0/8244	0.97	29/11095 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	GLY	N-CA-C	-8.31	101.40	113.86
1	A	299	LYS	N-CA-C	7.30	119.24	111.28
1	C	111	GLY	N-CA-C	-6.87	103.98	112.77
1	A	141	VAL	N-CA-C	-6.09	104.36	111.00
1	C	315	ASP	CA-C-N	5.99	126.41	119.47
1	C	315	ASP	C-N-CA	5.99	126.41	119.47
1	A	315	ASP	CA-C-N	5.96	125.66	119.82
1	A	315	ASP	C-N-CA	5.96	125.66	119.82
1	A	71	ILE	N-CA-C	5.95	116.12	110.53
1	C	186	VAL	CA-C-N	5.94	125.64	119.05
1	C	186	VAL	C-N-CA	5.94	125.64	119.05
1	C	51	ILE	N-CA-C	5.88	116.34	107.75
1	C	264	ARG	N-CA-C	5.86	117.67	111.28
2	B	104	LEU	N-CA-C	5.85	118.79	111.24
2	B	167	PRO	N-CA-C	5.83	120.35	111.19
2	D	73	GLY	CA-C-N	5.82	125.30	119.24
2	D	73	GLY	C-N-CA	5.82	125.30	119.24
2	B	97	LEU	N-CA-C	-5.79	104.57	111.69
1	C	347	THR	N-CA-C	5.79	118.99	109.85
1	A	271	ILE	N-CA-C	-5.71	105.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	113	ASN	N-CA-C	5.55	118.09	111.71
2	B	96	PHE	N-CA-C	-5.34	107.77	114.56
1	C	134	GLN	N-CA-C	-5.29	106.80	113.20
1	C	299	LYS	N-CA-C	5.18	117.00	111.36
1	A	264	ARG	N-CA-C	5.12	116.86	111.28
2	D	168	TRP	N-CA-C	5.11	118.25	111.30
2	B	168	TRP	N-CA-C	5.08	118.59	111.74
2	B	181	ARG	N-CA-C	-5.03	106.06	113.61
1	A	184	LEU	N-CA-C	-5.03	106.99	113.23

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	2660	0	2662	98	0
1	C	2627	0	2628	114	0
2	B	1475	0	1457	71	0
2	D	1329	0	1320	67	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	12	1	0
4	C	28	0	12	1	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	41	0	0	2	0
6	B	12	0	0	1	0
6	C	30	0	0	4	0
6	D	4	0	0	0	0
All	All	8246	0	8091	327	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 20.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HE	1:A:324:LYS:HE3	1.20	0.99
1:C:123:MET:HE2	1:C:123:MET:HA	1.42	0.97
1:C:213:ILE:HD12	6:C:378:HOH:O	1.65	0.96
2:B:193:VAL:HA	2:B:196:ARG:NH1	1.85	0.92
2:B:211:ASP:HB3	2:B:214:LYS:HB3	1.55	0.86
2:D:226:MET:HB3	2:D:231:VAL:HB	1.55	0.86
1:C:311:GLU:CD	1:C:311:GLU:H	1.81	0.86
1:A:320:ARG:HE	1:A:324:LYS:CE	1.89	0.85
2:B:29:GLU:HA	2:B:32:GLU:HG3	1.58	0.85
2:B:193:VAL:HA	2:B:196:ARG:HH11	1.40	0.85
2:D:226:MET:HA	2:D:226:MET:HE2	1.58	0.85
1:A:270:ASN:HB3	2:B:163:MET:HE1	1.59	0.82
2:D:114:VAL:HG12	2:D:142:VAL:HG13	1.60	0.82
1:C:270:ASN:HB3	2:D:163:MET:HE1	1.60	0.82
1:A:320:ARG:NE	1:A:324:LYS:HE3	1.95	0.82
1:A:302:VAL:HG23	1:A:303:VAL:HG23	1.64	0.80
1:C:280:VAL:HG22	2:D:207:THR:HG21	1.65	0.79
2:B:205:GLN:C	2:B:205:GLN:CD	2.51	0.78
2:D:50:GLU:HG2	2:D:53:LYS:HE2	1.67	0.77
2:D:60:MET:HE2	2:D:198:LEU:HA	1.69	0.75
1:C:331:ARG:HG3	1:C:342:LEU:HD23	1.70	0.74
2:D:160:LYS:HD3	2:D:163:MET:HE3	1.69	0.74
2:B:83:MET:HE1	2:B:224:LEU:HG	1.71	0.73
1:A:289:PHE:HZ	1:A:362:VAL:HG21	1.54	0.72
1:A:75:ASP:OD1	1:A:76:PHE:N	2.19	0.71
1:A:290:LEU:HD12	1:A:346:PHE:CE2	2.26	0.71
2:B:156:ASP:O	2:B:160:LYS:HG2	1.91	0.70
2:D:205:GLN:C	2:D:207:THR:H	1.99	0.70
1:A:65:LEU:HD12	1:A:222:ASP:HB2	1.74	0.70
1:C:213:ILE:CG2	1:C:363:LYS:HE2	2.23	0.69
2:B:148:VAL:HG13	1:C:136:MET:HE1	1.73	0.69
1:C:213:ILE:HG21	1:C:363:LYS:HE2	1.75	0.69
2:B:201:LEU:O	2:B:205:GLN:HB3	1.92	0.69
2:D:80:HIS:HA	2:D:83:MET:HE2	1.76	0.68
2:B:199:MET:O	2:B:203:GLU:HG3	1.93	0.68
1:C:96:MET:HG3	1:C:122:LEU:HD13	1.75	0.68
2:D:106:LYS:HG3	2:D:111:ARG:NH2	2.09	0.68
1:C:265:LEU:HD23	1:C:309:PHE:CZ	2.28	0.68
2:B:59:LEU:HG	2:B:63:LEU:HD22	1.76	0.67
1:C:67:GLN:OE1	1:C:67:GLN:HA	1.93	0.66
1:C:213:ILE:HG23	6:C:378:HOH:O	1.95	0.66
1:C:123:MET:HE2	1:C:123:MET:CA	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:CG	1:A:335:ARG:HG2	2.20	0.65
1:C:248:SER:O	1:C:251:GLU:HG2	1.95	0.65
1:A:172:GLU:HG3	1:A:295:LEU:HD13	1.78	0.65
1:C:276:VAL:HG21	1:C:334:ARG:HG2	1.78	0.65
1:A:84:PHE:CD1	1:A:196:ILE:HG13	2.32	0.65
2:B:138:PHE:O	2:B:142:VAL:HG23	1.97	0.65
1:C:212:GLU:O	1:C:213:ILE:HD13	1.96	0.65
2:D:195:GLU:HG2	2:D:232:ARG:O	1.96	0.65
1:A:97:ARG:HA	1:A:123:MET:HE1	1.77	0.65
1:C:248:SER:HB3	1:C:251:GLU:CD	2.22	0.65
1:C:349:ALA:HA	1:C:355:ILE:HD11	1.78	0.64
2:B:205:GLN:NE2	2:B:206:HIS:N	2.46	0.64
1:A:146:LEU:HB3	1:A:147:PRO:HD3	1.80	0.63
1:C:306:LYS:HE3	1:C:312:PHE:O	1.99	0.63
1:A:97:ARG:CA	1:A:123:MET:HE1	2.29	0.63
1:C:302:VAL:HG23	1:C:303:VAL:HG22	1.81	0.63
1:C:80:ALA:O	1:C:83:GLU:HB2	1.98	0.62
1:A:183:LYS:O	1:A:186:VAL:HG22	1.99	0.62
2:B:148:VAL:HG22	1:C:136:MET:HE1	1.82	0.62
1:A:54:LEU:HD13	1:A:275:ILE:HD13	1.83	0.61
1:A:311:GLU:HG3	1:C:187:PRO:HB3	1.83	0.61
1:C:243:ILE:HB	1:C:286:ILE:HD13	1.83	0.60
1:A:97:ARG:O	1:A:123:MET:HE1	2.02	0.59
2:B:205:GLN:CD	2:B:206:HIS:N	2.60	0.59
1:C:131:MET:HE2	1:C:131:MET:HA	1.85	0.59
1:A:280:VAL:HG23	2:B:68:LEU:HD22	1.84	0.59
2:D:205:GLN:C	2:D:205:GLN:CD	2.71	0.59
1:A:289:PHE:CZ	1:A:362:VAL:HG21	2.37	0.59
1:A:331:ARG:HG3	1:A:334:ARG:NH2	2.18	0.59
1:A:61:LYS:HE2	6:A:409:HOH:O	2.03	0.58
2:B:193:VAL:HG22	2:B:196:ARG:HH12	1.68	0.58
1:A:184:LEU:HD22	1:A:189:TYR:CZ	2.38	0.58
1:C:184:LEU:HD22	1:C:189:TYR:CZ	2.36	0.58
1:A:100:VAL:HB	1:A:123:MET:HE3	1.83	0.58
1:A:153:TRP:CE3	1:A:178:LEU:HD13	2.38	0.58
1:A:333:LYS:HE2	1:A:333:LYS:HA	1.86	0.58
2:D:106:LYS:HA	2:D:111:ARG:NE	2.19	0.58
1:C:99:LEU:HD13	1:C:170:LEU:CD2	2.34	0.57
1:C:271:ILE:HA	2:D:165:MET:HE2	1.86	0.57
1:C:48:LEU:HA	1:C:217:PRO:HB2	1.86	0.57
1:A:101:ASP:OD2	1:A:105:LYS:HE3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:HG3	1:C:279:ARG:HH11	1.68	0.57
2:B:156:ASP:OD2	2:B:160:LYS:HE2	2.05	0.57
1:C:97:ARG:HB3	1:C:123:MET:HE1	1.87	0.57
1:C:97:ARG:CB	1:C:123:MET:HE1	2.34	0.57
1:A:96:MET:HG3	1:A:122:LEU:HD22	1.87	0.56
1:A:172:GLU:HG3	1:A:295:LEU:CD1	2.36	0.56
1:C:280:VAL:HG22	2:D:207:THR:CG2	2.35	0.56
1:A:47:ARG:O	1:A:47:ARG:HG2	2.05	0.56
1:A:279:ARG:HD3	2:B:208:ILE:O	2.05	0.56
1:C:278:ASN:OD1	1:C:280:VAL:HB	2.06	0.56
2:D:83:MET:HG3	2:D:228:HIS:CD2	2.41	0.56
2:B:205:GLN:C	2:B:207:THR:H	2.14	0.56
1:A:306:LYS:HG2	1:A:312:PHE:HD2	1.71	0.56
1:C:213:ILE:HB	1:C:216:VAL:HB	1.88	0.56
1:A:96:MET:HG3	1:A:122:LEU:CD2	2.36	0.55
2:D:205:GLN:C	2:D:207:THR:N	2.64	0.55
2:D:226:MET:HE1	2:D:229:LEU:HD12	1.88	0.55
2:B:148:VAL:HG22	1:C:136:MET:CE	2.36	0.55
1:C:277:ASN:CB	1:C:335:ARG:NH1	2.70	0.55
2:D:138:PHE:O	2:D:142:VAL:HG23	2.07	0.55
2:B:80:HIS:O	2:B:84:LEU:HD13	2.08	0.54
1:C:70:ILE:HD13	1:C:193:GLN:CD	2.31	0.54
1:A:65:LEU:CD1	1:A:222:ASP:HB2	2.37	0.54
2:B:224:LEU:HA	2:B:227:ARG:NH1	2.23	0.54
1:A:208:GLU:CD	1:A:219:LYS:HE3	2.32	0.54
2:B:70:PHE:CD1	2:B:153:GLN:HG2	2.42	0.54
2:D:67:ALA:HB1	2:D:208:ILE:HG23	1.89	0.54
2:B:205:GLN:C	2:B:207:THR:N	2.64	0.54
1:C:123:MET:HA	1:C:123:MET:CE	2.25	0.54
1:C:122:LEU:HD12	1:C:152:LEU:CD1	2.38	0.53
1:A:78:GLN:O	1:A:82:GLU:HB2	2.08	0.53
2:D:188:ALA:HA	2:D:191:ARG:NH1	2.22	0.53
1:A:174:VAL:HG23	1:A:175:LYS:N	2.23	0.53
2:D:94:LYS:HE3	2:D:98:ASP:OD2	2.09	0.53
1:C:65:LEU:HD21	1:C:209:TYR:HB3	1.89	0.53
1:C:258:GLU:OE2	1:C:258:GLU:N	2.41	0.53
1:C:256:LEU:HD12	1:C:262:THR:HB	1.90	0.53
1:C:140:ARG:HG3	1:C:141:VAL:N	2.23	0.53
1:C:248:SER:O	1:C:251:GLU:CG	2.56	0.53
1:A:314:GLY:O	1:A:316:PRO:HD3	2.09	0.52
1:C:134:GLN:HB3	1:C:136:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:LYS:HA	2:D:111:ARG:CZ	2.39	0.52
1:A:78:GLN:HG3	1:A:190:ILE:HD13	1.91	0.52
1:C:111:GLY:H	1:C:155:ASP:CG	2.17	0.52
2:B:170:GLN:HB2	6:B:243:HOH:O	2.08	0.52
2:D:109:VAL:CG1	2:D:214:LYS:HA	2.40	0.52
1:A:105:LYS:NZ	2:B:22:SER:O	2.41	0.52
1:C:277:ASN:ND2	1:C:335:ARG:NH1	2.56	0.52
1:C:103:ARG:NH2	1:C:104:GLU:HG3	2.25	0.52
2:B:46:PHE:O	2:B:158:ARG:HD3	2.08	0.52
1:C:277:ASN:CG	1:C:335:ARG:NH1	2.69	0.51
2:B:202:GLU:O	2:B:205:GLN:HG3	2.09	0.51
1:C:192:SER:O	1:C:195:ASP:HB2	2.09	0.51
2:B:211:ASP:HB3	2:B:214:LYS:CB	2.35	0.51
1:A:277:ASN:OD1	1:A:335:ARG:HG2	2.09	0.51
2:D:103:PHE:O	2:D:104:LEU:HD23	2.10	0.51
1:A:257:MET:SD	1:A:257:MET:C	2.94	0.51
1:A:131:MET:HE2	1:A:136:MET:HE3	1.92	0.50
2:B:148:VAL:CG1	1:C:136:MET:HE1	2.40	0.50
1:C:213:ILE:O	1:C:216:VAL:HB	2.11	0.50
2:D:209:SER:OG	2:D:214:LYS:HD3	2.12	0.50
1:C:287:ILE:HD12	1:C:362:VAL:HG13	1.94	0.50
2:B:32:GLU:C	2:B:34:GLU:H	2.19	0.50
2:D:60:MET:HE2	2:D:198:LEU:CA	2.41	0.50
1:C:292:LYS:HG2	4:C:402:GDP:C6	2.47	0.49
1:A:320:ARG:HE	1:A:324:LYS:NZ	2.11	0.49
2:B:193:VAL:CA	2:B:196:ARG:NH1	2.69	0.49
2:D:97:LEU:O	2:D:101:HIS:CD2	2.65	0.49
1:A:112:ASP:OD1	1:A:114:LYS:HG3	2.13	0.49
2:B:118:VAL:C	2:B:120:PHE:H	2.20	0.49
2:D:112:VAL:HB	2:D:113:PRO:HD2	1.95	0.49
2:B:223:GLY:O	2:B:224:LEU:C	2.56	0.49
2:B:193:VAL:HG22	2:B:196:ARG:NH1	2.28	0.49
2:B:106:LYS:HD2	2:B:106:LYS:O	2.14	0.48
1:A:290:LEU:HD12	1:A:346:PHE:HE2	1.77	0.48
1:C:203:THR:HB	5:C:602:ALF:F2	2.03	0.48
1:A:48:LEU:HD12	1:A:217:PRO:O	2.12	0.48
2:B:83:MET:HE1	2:B:224:LEU:CG	2.42	0.48
1:C:114:LYS:HD2	1:C:115:ASN:N	2.28	0.48
1:A:69:ARG:HD3	1:A:76:PHE:CZ	2.48	0.48
2:B:198:LEU:HD22	2:B:226:MET:HG3	1.96	0.48
1:A:94:LYS:O	1:A:98:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:GLN:O	1:C:196:ILE:HG12	2.14	0.48
2:D:109:VAL:HG11	2:D:214:LYS:HA	1.96	0.48
1:A:334:ARG:NH1	1:A:342:LEU:HB2	2.29	0.48
1:C:311:GLU:CD	1:C:311:GLU:N	2.59	0.48
1:C:97:ARG:CA	1:C:123:MET:HE1	2.44	0.48
2:D:49:LEU:HD13	2:D:49:LEU:O	2.14	0.47
2:D:106:LYS:HA	2:D:111:ARG:NH2	2.29	0.47
1:A:306:LYS:HE3	1:A:312:PHE:O	2.15	0.47
2:D:49:LEU:HD13	2:D:49:LEU:C	2.40	0.47
1:A:312:PHE:HE2	1:A:316:PRO:HG3	1.79	0.47
2:B:205:GLN:HB2	2:B:208:ILE:CD1	2.45	0.47
1:C:211:PHE:O	1:C:218:PHE:HB2	2.14	0.47
2:D:112:VAL:HB	2:D:146:GLN:HE22	1.80	0.47
1:A:128:ARG:HH12	2:B:32:GLU:CD	2.23	0.47
1:A:279:ARG:HB3	2:B:207:THR:O	2.14	0.47
2:B:29:GLU:HA	2:B:32:GLU:CG	2.35	0.47
2:B:206:HIS:CE1	2:B:207:THR:HG23	2.49	0.47
2:B:76:LEU:HD21	2:B:222:ILE:HG13	1.97	0.47
1:C:96:MET:CG	1:C:122:LEU:HD13	2.44	0.47
1:C:309:PHE:HB3	1:C:311:GLU:OE1	2.15	0.47
1:C:146:LEU:HB3	1:C:147:PRO:HD3	1.97	0.47
1:C:172:GLU:H	1:C:172:GLU:HG2	1.39	0.47
1:C:305:ILE:N	6:C:387:HOH:O	2.48	0.47
1:C:96:MET:HG3	1:C:122:LEU:CD1	2.44	0.46
1:C:130:PRO:O	1:C:134:GLN:HG2	2.15	0.46
1:A:292:LYS:HD2	1:A:295:LEU:HD12	1.97	0.46
2:B:179:VAL:HG12	2:B:180:GLY:N	2.30	0.46
2:B:215:SER:O	2:B:219:VAL:HG23	2.16	0.46
1:C:358:VAL:O	1:C:362:VAL:HG23	2.15	0.46
2:D:148:VAL:O	2:D:151:GLY:N	2.46	0.46
2:B:205:GLN:C	2:B:205:GLN:OE1	2.58	0.46
1:A:300:VAL:O	1:A:317:HIS:HA	2.16	0.46
1:C:79:ARG:O	1:C:83:GLU:HG3	2.15	0.46
2:D:63:LEU:HD23	2:D:222:ILE:HG23	1.96	0.46
1:C:52:LEU:HD21	1:C:236:CYS:HB2	1.97	0.46
1:C:331:ARG:HE	1:C:342:LEU:HB3	1.81	0.46
1:A:251:GLU:CD	1:A:264:ARG:HH11	2.23	0.46
2:B:160:LYS:HB3	2:B:165:MET:HB2	1.98	0.46
1:C:211:PHE:N	1:C:211:PHE:CD1	2.83	0.46
1:A:198:LEU:O	1:A:199:ALA:C	2.56	0.46
2:D:60:MET:CE	2:D:198:LEU:HA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ASP:CG	2:B:185:SER:HG	2.23	0.45
1:A:347:THR:HG22	1:A:358:VAL:HG21	1.99	0.45
2:B:81:ALA:O	2:B:84:LEU:HB2	2.15	0.45
1:C:85:ARG:HG2	1:C:89:TYR:CE2	2.51	0.45
2:D:77:CYS:HA	2:D:103:PHE:CE1	2.51	0.45
1:A:256:LEU:HD11	1:A:267:GLU:CD	2.41	0.45
1:C:52:LEU:HD23	1:C:221:VAL:HB	1.97	0.45
1:A:210:ASP:HA	1:A:218:PHE:O	2.16	0.45
1:A:112:ASP:CG	1:A:114:LYS:HG3	2.42	0.45
1:C:277:ASN:CG	1:C:335:ARG:HH11	2.24	0.45
2:D:202:GLU:HG2	2:D:219:VAL:CG1	2.46	0.45
1:A:97:ARG:HD2	1:A:125:PHE:HB3	1.99	0.45
1:C:150:ARG:O	1:C:154:GLU:HG3	2.17	0.45
2:D:55:ARG:HA	2:D:55:ARG:NE	2.31	0.45
2:D:188:ALA:O	2:D:192:HIS:CD2	2.70	0.45
2:B:200:HIS:CE1	2:B:204:MET:HE3	2.52	0.45
2:D:214:LYS:O	2:D:218:VAL:HG23	2.17	0.45
1:C:128:ARG:NH1	1:C:128:ARG:HG2	2.32	0.44
2:D:108:ALA:O	2:D:111:ARG:N	2.50	0.44
1:A:326:LEU:O	1:A:330:PHE:HD1	2.00	0.44
1:C:61:LYS:HE3	1:C:223:VAL:O	2.17	0.44
1:C:57:GLY:HA2	5:C:602:ALF:F4	2.07	0.44
2:D:100:TYR:CD1	2:D:104:LEU:HB2	2.52	0.44
1:C:280:VAL:HA	2:D:207:THR:CG2	2.48	0.44
1:C:331:ARG:HG3	1:C:342:LEU:CD2	2.42	0.44
1:A:214:LYS:C	1:A:216:VAL:H	2.26	0.44
1:A:349:ALA:HA	1:A:355:ILE:HD11	2.00	0.44
1:C:279:ARG:HG3	1:C:279:ARG:NH1	2.33	0.44
1:C:96:MET:CG	1:C:122:LEU:CD1	2.95	0.44
1:A:48:LEU:HD12	1:A:217:PRO:C	2.42	0.44
1:A:244:LEU:HD21	1:A:362:VAL:HG11	1.99	0.44
1:C:227:ARG:NH1	2:D:162:LEU:HD23	2.33	0.44
2:B:71:GLU:O	2:B:74:PRO:HD2	2.18	0.43
1:C:244:LEU:HD22	1:C:289:PHE:CZ	2.53	0.43
2:D:46:PHE:CZ	2:D:58:HIS:HB3	2.52	0.43
2:D:225:TYR:O	2:D:228:HIS:HB3	2.18	0.43
1:A:110:TRP:CZ2	1:A:116:GLN:HA	2.53	0.43
1:A:291:ASN:CG	1:A:292:LYS:H	2.25	0.43
2:B:193:VAL:CG2	2:B:196:ARG:HH12	2.31	0.43
1:A:153:TRP:CZ3	1:A:178:LEU:HD13	2.53	0.43
1:C:61:LYS:HB2	1:C:61:LYS:HE2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HD11	1:C:174:VAL:HG21	2.01	0.43
2:D:80:HIS:O	2:D:83:MET:HB3	2.18	0.43
1:A:71:ILE:HD13	1:A:356:ARG:HA	2.00	0.43
2:B:154:LEU:O	2:B:158:ARG:HG3	2.18	0.43
2:D:104:LEU:O	2:D:105:GLU:C	2.62	0.43
2:B:50:GLU:OE1	2:B:53:LYS:HE2	2.19	0.43
2:B:224:LEU:HA	2:B:227:ARG:HH12	1.83	0.43
1:C:75:ASP:OD1	1:C:76:PHE:N	2.52	0.43
1:C:204:LYS:HE2	2:D:31:PHE:CE2	2.53	0.43
1:C:208:GLU:HG2	1:C:221:VAL:HG22	2.01	0.43
1:A:165:ARG:HA	1:A:168:PHE:CZ	2.54	0.43
1:C:291:ASN:CG	1:C:292:LYS:H	2.26	0.43
2:B:177:ALA:O	2:B:178:TRP:C	2.61	0.43
2:D:50:GLU:HA	2:D:53:LYS:HE2	2.00	0.43
2:D:188:ALA:O	2:D:192:HIS:HD2	2.01	0.43
2:D:202:GLU:HG2	2:D:219:VAL:HG13	2.00	0.43
1:C:257:MET:SD	1:C:257:MET:C	3.02	0.42
1:A:49:VAL:HG11	1:A:218:PHE:CE2	2.55	0.42
1:A:100:VAL:CG1	1:A:123:MET:HE3	2.49	0.42
2:B:118:VAL:C	2:B:120:PHE:N	2.78	0.42
1:C:51:ILE:HD12	1:C:218:PHE:HE2	1.84	0.42
1:A:68:MET:HG3	1:A:220:MET:SD	2.59	0.42
1:C:213:ILE:HG22	1:C:363:LYS:HE2	1.98	0.42
2:D:106:LYS:HG3	2:D:111:ARG:CZ	2.49	0.42
2:B:148:VAL:CG2	1:C:136:MET:HE1	2.47	0.42
2:D:54:ARG:O	2:D:56:PRO:HD3	2.19	0.42
2:D:201:LEU:HD21	2:D:222:ILE:HD12	2.01	0.42
1:A:61:LYS:NZ	4:A:401:GDP:O2B	2.43	0.42
1:A:118:HIS:HB3	1:A:148:ALA:HB1	2.02	0.42
1:C:212:GLU:C	1:C:213:ILE:HD13	2.44	0.42
2:D:55:ARG:NH1	2:D:190:GLU:OE1	2.53	0.42
2:B:63:LEU:HD12	2:B:63:LEU:HA	1.86	0.42
2:B:134:VAL:HG12	2:B:138:PHE:CE2	2.55	0.42
1:C:300:VAL:CG1	1:C:322:VAL:HG21	2.50	0.42
1:A:184:LEU:HD22	1:A:189:TYR:CE1	2.54	0.42
2:B:166:THR:HB	2:B:167:PRO:HD2	2.02	0.42
1:A:76:PHE:HA	6:A:396:HOH:O	2.19	0.42
1:A:251:GLU:OE2	1:A:254:GLN:OE1	2.37	0.42
1:A:280:VAL:O	1:A:280:VAL:HG12	2.18	0.42
1:C:96:MET:O	1:C:100:VAL:HG23	2.19	0.42
1:A:97:ARG:HA	1:A:123:MET:CE	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:HG2	1:A:254:GLN:NE2	2.35	0.41
1:A:256:LEU:HD12	1:A:262:THR:HB	2.01	0.41
1:C:263:ASN:OD1	1:C:265:LEU:N	2.52	0.41
1:A:203:THR:HB	5:A:601:ALF:F2	2.09	0.41
1:A:216:VAL:HA	1:A:217:PRO:HD3	1.88	0.41
1:C:276:VAL:CG2	1:C:334:ARG:HG2	2.48	0.41
1:A:97:ARG:C	1:A:123:MET:HE1	2.46	0.41
1:A:304:SER:HB3	1:A:307:ASP:OD2	2.19	0.41
1:C:128:ARG:HG2	1:C:128:ARG:HH11	1.86	0.41
2:D:106:LYS:HA	2:D:111:ARG:HE	1.86	0.41
2:D:226:MET:CE	2:D:229:LEU:HD12	2.49	0.41
1:A:230:ARG:CZ	1:A:271:ILE:HD11	2.50	0.41
1:C:265:LEU:HD23	1:C:309:PHE:CE1	2.55	0.41
1:C:277:ASN:HB2	1:C:335:ARG:HH12	1.86	0.41
2:D:205:GLN:CD	2:D:206:HIS:N	2.78	0.41
2:B:117:ASN:O	2:B:120:PHE:HB3	2.21	0.41
1:C:270:ASN:HB3	2:D:163:MET:CE	2.41	0.41
1:C:326:LEU:O	1:C:330:PHE:HD1	2.04	0.41
1:C:176:TYR:CD2	1:C:198:LEU:HD13	2.55	0.41
1:C:274:THR:HG1	2:D:160:LYS:HZ3	1.62	0.41
1:C:213:ILE:CG1	1:C:218:PHE:CD1	3.04	0.41
2:D:65:HIS:CE1	2:D:69:GLN:HG3	2.55	0.41
1:A:105:LYS:HD2	2:B:23:ILE:HG12	2.02	0.41
1:A:174:VAL:CG2	1:A:175:LYS:N	2.83	0.41
1:C:72:HIS:CE1	6:C:378:HOH:O	2.73	0.41
1:C:112:ASP:OD1	1:C:114:LYS:HG3	2.21	0.41
2:D:74:PRO:HB3	2:D:146:GLN:OE1	2.20	0.41
1:C:140:ARG:CG	1:C:141:VAL:N	2.84	0.41
1:A:105:LYS:HZ3	2:B:22:SER:C	2.27	0.40
1:A:366:ILE:O	1:A:366:ILE:HG22	2.21	0.40
2:B:106:LYS:HD2	2:B:106:LYS:C	2.46	0.40
1:A:233:TRP:CZ3	1:A:275:ILE:HD11	2.55	0.40
1:C:51:ILE:HA	1:C:242:SER:O	2.21	0.40
2:B:31:PHE:O	2:B:34:GLU:HG2	2.21	0.40
2:B:182:ASP:HB3	2:B:185:SER:OG	2.21	0.40
2:D:47:GLN:NE2	2:D:158:ARG:HD3	2.35	0.40
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.87	0.40
1:A:251:GLU:OE2	1:A:264:ARG:NH1	2.54	0.40
2:B:59:LEU:HD23	2:B:226:MET:HE1	2.03	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	318/362 (88%)	304 (96%)	14 (4%)	0	100 100
1	C	314/362 (87%)	297 (95%)	16 (5%)	1 (0%)	36 50
2	B	174/246 (71%)	160 (92%)	11 (6%)	3 (2%)	7 10
2	D	155/246 (63%)	142 (92%)	9 (6%)	4 (3%)	4 4
All	All	961/1216 (79%)	903 (94%)	50 (5%)	8 (1%)	16 25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	148	VAL
2	D	109	VAL
2	B	203	GLU
2	B	211	ASP
2	B	33	ASN
1	C	75	ASP
2	D	206	HIS
2	D	145	SER

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	294/328 (90%)	283 (96%)	11 (4%)	30 51
1	C	290/328 (88%)	276 (95%)	14 (5%)	23 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	157/207 (76%)	149 (95%)	8 (5%)	21 37
2	D	142/207 (69%)	136 (96%)	6 (4%)	26 45
All	All	883/1070 (82%)	844 (96%)	39 (4%)	25 43

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	79	ARG
1	A	99	LEU
1	A	122	LEU
1	A	138	GLU
1	A	172	GLU
1	A	173	SER
1	A	196	ILE
1	A	306	LYS
1	A	320	ARG
1	A	336	ASP
2	B	51	GLN
2	B	55	ARG
2	B	63	LEU
2	B	82	ASP
2	B	144	GLN
2	B	189	ARG
2	B	205	GLN
2	B	210	THR
1	C	65	LEU
1	C	99	LEU
1	C	127	THR
1	C	172	GLU
1	C	173	SER
1	C	211	PHE
1	C	231	LYS
1	C	236	CYS
1	C	268	SER
1	C	302	VAL
1	C	303	VAL
1	C	306	LYS
1	C	311	GLU
1	C	364	ASP
2	D	50	GLU

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Mol	Chain	Res	Type
2	D	102	SER
2	D	144	GLN
2	D	162	LEU
2	D	207	THR
2	D	233	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	160	ASN
1	A	254	GLN
1	A	323	GLN
1	A	344	HIS
1	A	368	HIS
1	A	370	ASN
2	B	101	HIS
2	B	146	GLN
2	B	147	GLN
2	B	153	GLN
2	B	174	GLN
2	B	200	HIS
1	C	78	GLN
1	C	107	HIS
1	C	118	HIS
1	C	144	GLN
1	C	160	ASN
1	C	193	GLN
1	C	254	GLN
1	C	283	ASN
1	C	317	HIS
2	D	47	GLN
2	D	101	HIS
2	D	146	GLN
2	D	147	GLN
2	D	153	GLN
2	D	174	GLN
2	D	192	HIS
2	D	206	HIS
2	D	228	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	601	4	4,4,4	1.39	0	-		
4	GDP	A	401	3,5	29,30,30	1.02	2 (6%)	45,47,47	2.02	12 (26%)
4	GDP	C	402	3,5	29,30,30	1.00	2 (6%)	45,47,47	2.03	13 (28%)
5	ALF	C	602	4	4,4,4	1.34	0	-		

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
4	GDP	A	401	3,5	-	3/16/32/32	0/3/3/3
4	GDP	C	402	3,5	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	GDP	O4'-C1'	2.72	1.48	1.42
4	A	401	GDP	O4'-C1'	2.49	1.47	1.42
4	C	402	GDP	PB-O2B	2.26	1.63	1.54
4	A	401	GDP	PB-O2B	2.15	1.62	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	GDP	O3'-C3'-C4'	5.94	128.15	111.08
4	C	402	GDP	O3'-C3'-C4'	5.89	128.00	111.08
4	A	401	GDP	C2-N3-C4	5.65	122.03	112.30
4	C	402	GDP	C2-N3-C4	5.40	121.60	112.30
4	C	402	GDP	C5-C4-N3	-4.74	120.85	128.39
4	A	401	GDP	C5-C4-N3	-4.73	120.86	128.39
4	C	402	GDP	N9-C4-N3	3.69	133.32	125.95
4	A	401	GDP	N9-C4-N3	3.57	133.10	125.95
4	C	402	GDP	C8-N7-C5	2.85	109.33	104.26
4	A	401	GDP	O3B-PB-O2B	2.80	118.30	107.80
4	A	401	GDP	C2-N1-C6	-2.62	120.36	125.11
4	C	402	GDP	O3B-PB-O2B	2.60	117.55	107.80
4	A	401	GDP	C6-C5-N7	2.58	134.98	130.29
4	C	402	GDP	C6-C5-N7	2.56	134.94	130.29
4	A	401	GDP	C8-N7-C5	2.55	108.80	104.26
4	C	402	GDP	O6-C6-C5	-2.41	120.16	126.53
4	C	402	GDP	PA-O5'-C5'	-2.41	107.54	121.35
4	C	402	GDP	C2-N1-C6	-2.35	120.85	125.11
4	C	402	GDP	O3A-PB-O1B	-2.32	98.84	111.04
4	C	402	GDP	N9-C8-N7	-2.26	109.21	113.40
4	A	401	GDP	O6-C6-C5	-2.22	120.66	126.53
4	A	401	GDP	PA-O5'-C5'	-2.22	108.62	121.35
4	A	401	GDP	O3A-PB-O1B	-2.11	99.92	111.04
4	A	401	GDP	C4-C5-N7	-2.08	107.37	110.67
4	C	402	GDP	O3B-PB-O1B	2.01	118.66	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	GDP	PA-O3A-PB-O2B
4	A	401	GDP	PA-O3A-PB-O3B
4	C	402	GDP	PA-O3A-PB-O3B
4	C	402	GDP	PA-O3A-PB-O2B
4	A	401	GDP	PA-O3A-PB-O1B

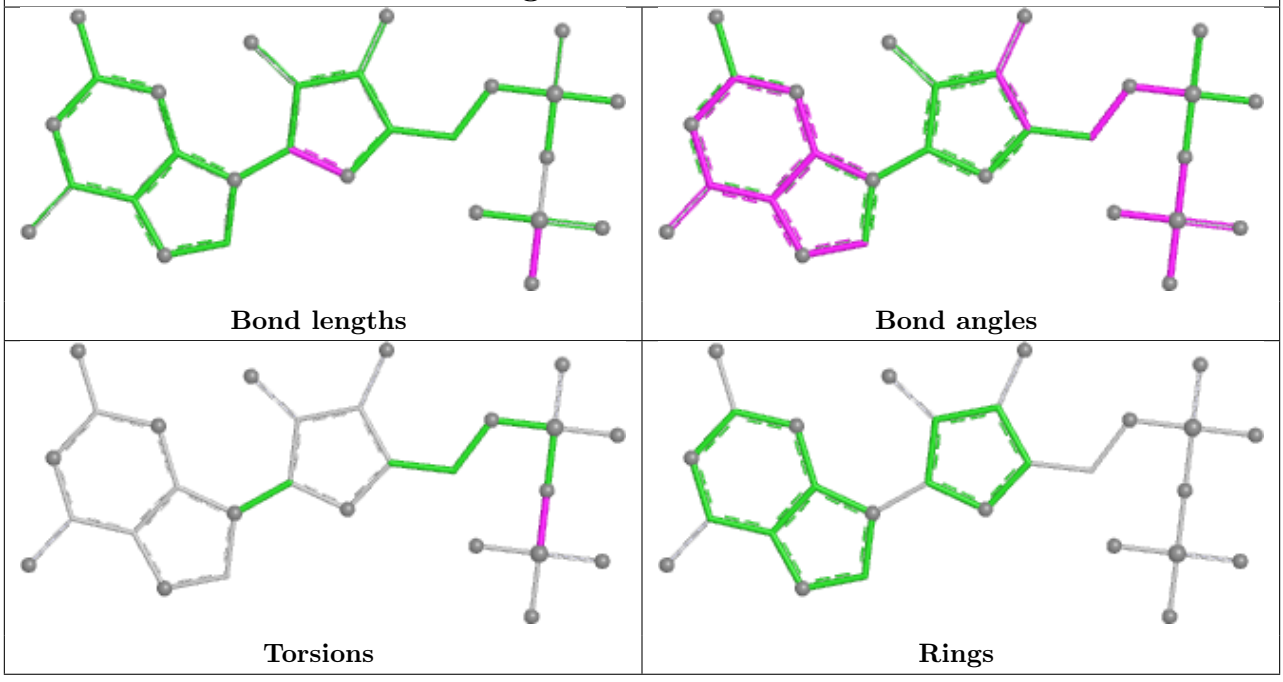
There are no ring outliers.

4 monomers are involved in 5 short contacts:

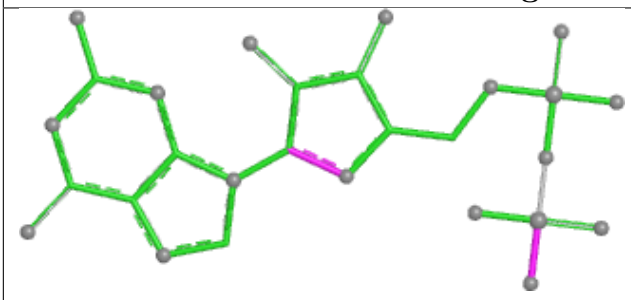
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	ALF	1	0
4	A	401	GDP	1	0
4	C	402	GDP	1	0
5	C	602	ALF	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

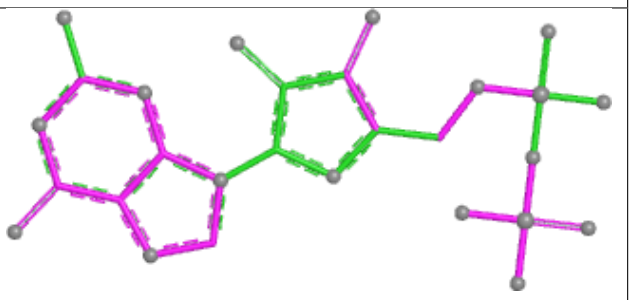
Ligand GDP A 401



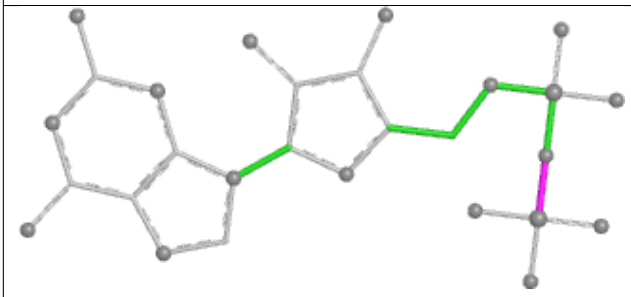
Ligand GDP C 402



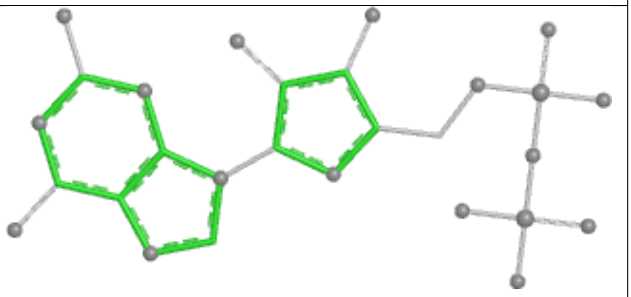
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	322/362 (88%)	-0.11	4 (1%)	76	73	23, 42, 68, 92	0
1	C	318/362 (87%)	-0.12	2 (0%)	85	83	23, 44, 77, 104	0
2	B	182/246 (73%)	0.35	6 (3%)	49	45	27, 54, 95, 107	1 (0%)
2	D	165/246 (67%)	0.35	4 (2%)	59	55	35, 62, 97, 104	1 (0%)
All	All	987/1216 (81%)	0.05	16 (1%)	70	66	23, 47, 86, 107	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	ASN	4.3
1	C	213	ILE	4.2
2	B	118	VAL	3.0
2	B	178	TRP	3.0
2	B	207	THR	2.8
1	A	217	PRO	2.6
1	C	48	LEU	2.6
1	A	318	CYS	2.6
1	A	371	LEU	2.4
1	A	341	PRO	2.4
2	D	85	GLY	2.2
2	D	92	ALA	2.1
2	D	210	THR	2.1
2	D	205	GLN	2.1
2	B	95	ALA	2.1
2	B	85	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

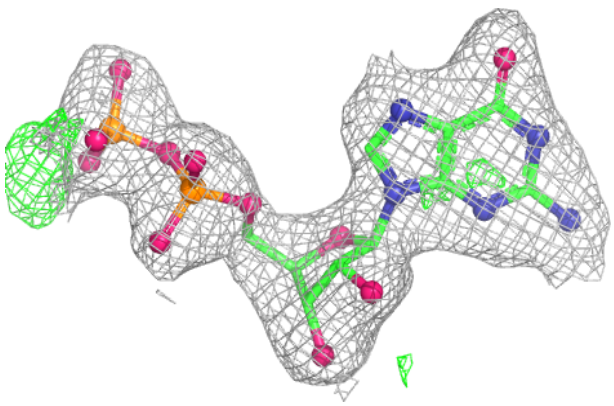
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

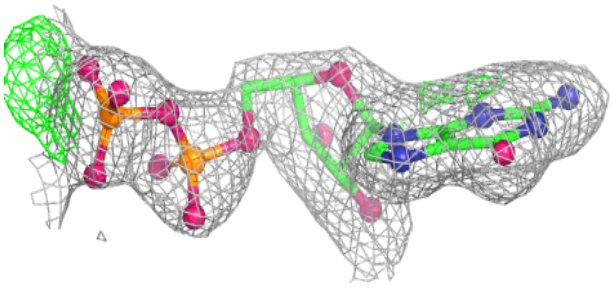
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ALF	C	602	5/5	0.92	0.18	47,47,49,61	0
5	ALF	A	601	5/5	0.94	0.13	33,41,45,51	0
3	MG	C	502	1/1	0.95	0.10	34,34,34,34	0
4	GDP	A	401	28/28	0.97	0.07	19,26,34,40	0
4	GDP	C	402	28/28	0.97	0.07	22,31,39,40	0
3	MG	A	501	1/1	0.98	0.07	30,30,30,30	0

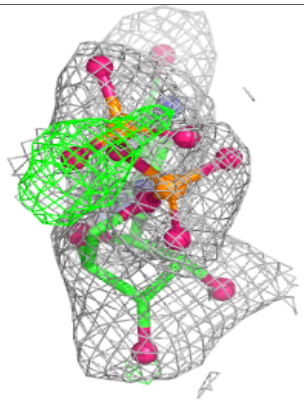
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 401:

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

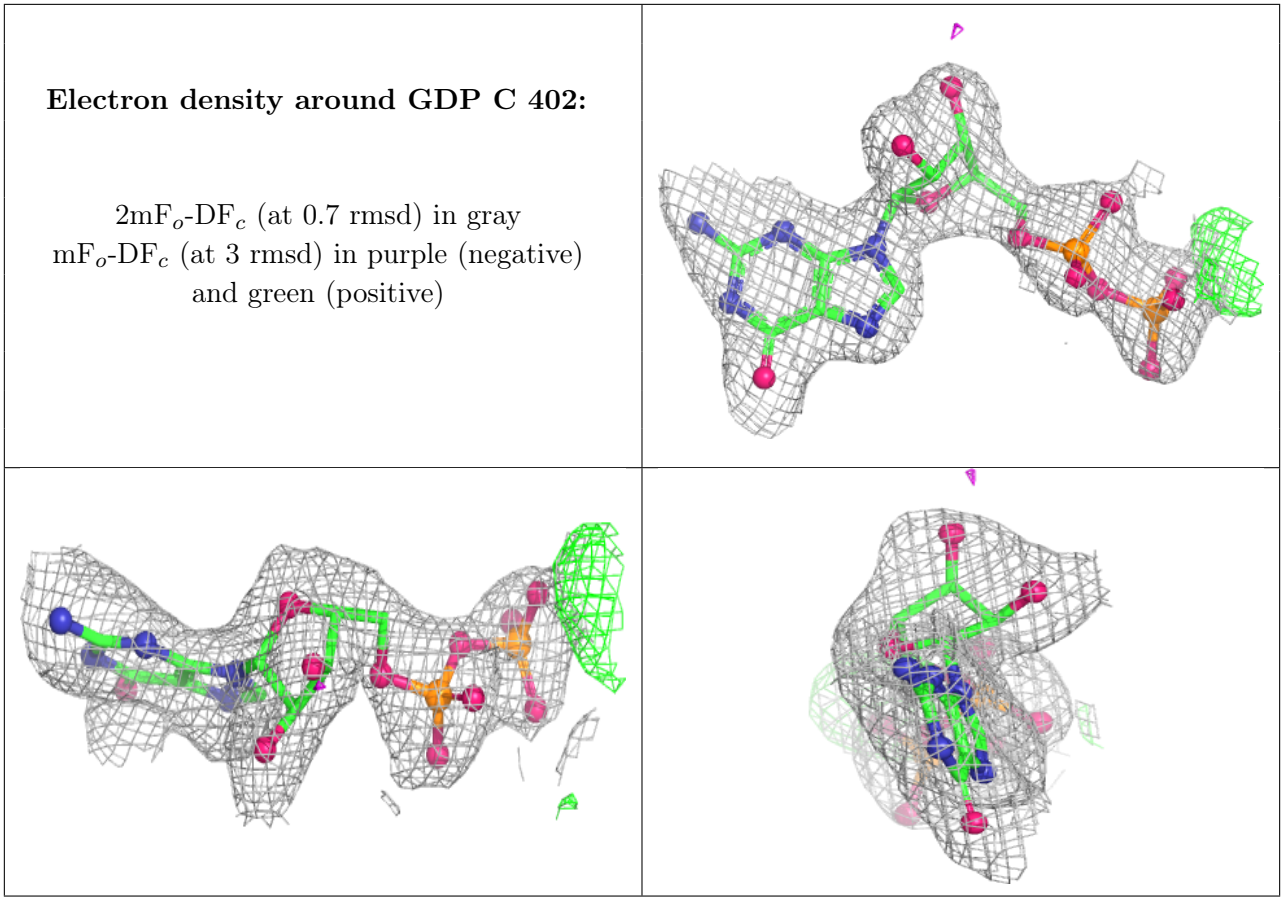






Electron density around GDP C 402:

$2mF_o$-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.