



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:29 PM UTC

PDB ID : 2QA5 / pdb_00002qa5
Title : Crystal structure of Sept2 G-domain
Authors : Sirajuddin, M.; Wittinghofer, A.
Deposited on : 2007-06-14
Resolution : 3.40 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

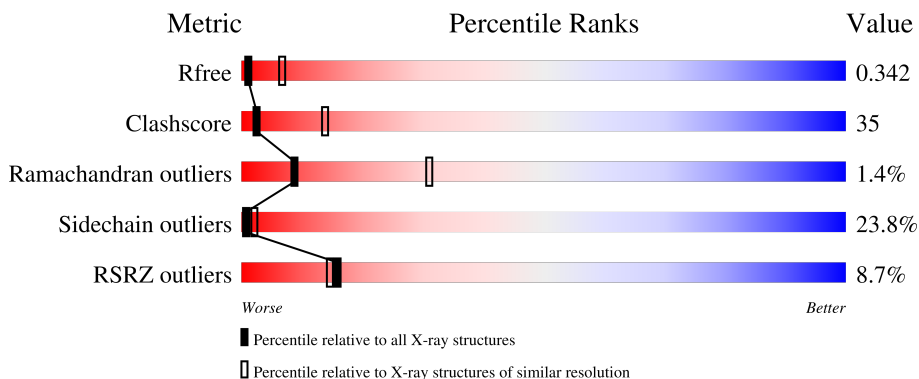
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	

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
2	GDP	B	316	-	-	X	-

2 Entry composition [i](#)

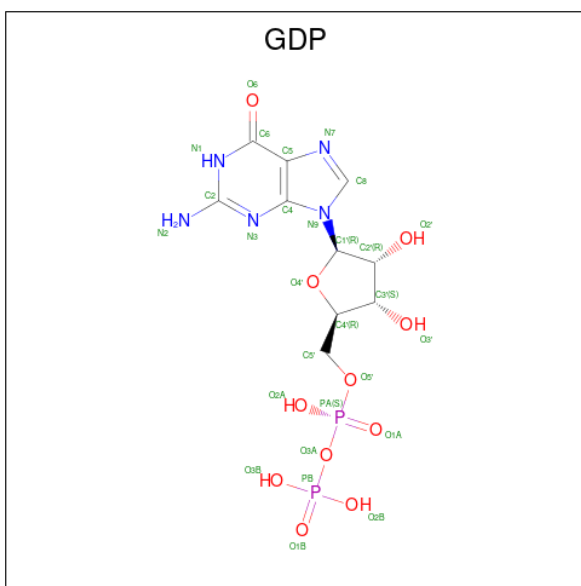
There are 2 unique types of molecules in this entry. The entry contains 3620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

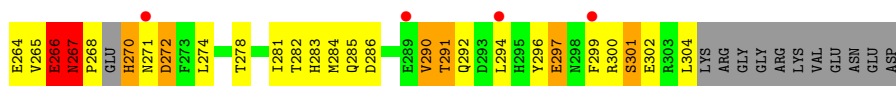
- Molecule 1 is a protein called Septin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	233	Total	C	N	O	S	Se	0	0	0
			1747	1122	292	327	2	4			
1	B	234	Total	C	N	O	S	Se	0	0	0
			1817	1169	306	336	2	4			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.96Å 53.92Å 110.27Å 90.00° 128.37° 90.00°	Depositor
Resolution (Å)	19.79 – 3.40 19.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.79-3.40) 98.4 (19.79-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.13 (at 3.44Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.280 , 0.314 0.310 , 0.342	Depositor DCC
R_{free} test set	502 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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	0.74	4/1766 (0.2%)	1.57	48/2389 (2.0%)
1	B	0.63	1/1840 (0.1%)	1.44	40/2482 (1.6%)
All	All	0.69	5/3606 (0.1%)	1.51	88/4871 (1.8%)

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	4
1	B	0	8
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ASP	C-O	10.23	1.36	1.24
1	A	123	ASP	C-N	-10.20	1.20	1.33
1	A	188	THR	C-N	-7.82	1.23	1.33
1	A	188	THR	C-O	7.19	1.32	1.23
1	B	137	ASN	C-O	5.75	1.30	1.24

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	LEU	N-CA-C	13.86	125.90	111.07
1	B	301	SER	N-CA-C	13.21	125.41	111.14
1	A	59	LEU	N-CA-C	10.72	125.96	112.24
1	A	58	PHE	N-CA-C	10.52	126.20	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ILE	N-CA-C	10.41	120.31	110.53
1	A	263	VAL	CB-CA-C	-10.39	98.06	111.25
1	A	280	LEU	N-CA-C	9.73	121.96	111.36
1	A	263	VAL	N-CA-C	9.57	122.65	107.73
1	A	266	GLU	N-CA-C	9.29	123.91	112.58
1	B	233	ALA	N-CA-C	9.19	120.90	111.07
1	B	284	MSE	N-CA-C	-8.79	100.66	112.26
1	B	143	ASP	CB-CA-C	8.54	124.02	110.19
1	A	50	LYS	N-CA-C	8.51	121.69	111.82
1	A	59	LEU	N-CA-CB	8.46	125.16	112.30
1	B	131	HIS	N-CA-C	8.33	120.14	111.14
1	B	254	ARG	N-CA-C	8.26	123.30	109.76
1	B	82	GLU	N-CA-CB	-8.25	97.82	110.77
1	A	188	THR	CA-C-O	-8.12	112.70	121.56
1	B	135	GLY	N-CA-C	8.02	136.56	113.30
1	A	233	ALA	N-CA-C	7.89	119.96	111.36
1	A	81	ILE	CB-CA-C	-7.87	98.99	110.63
1	A	209	LYS	CB-CA-C	7.83	123.29	110.22
1	A	284	MSE	N-CA-C	-7.75	100.95	111.87
1	A	49	GLY	N-CA-C	7.66	125.95	115.30
1	A	123	ASP	CA-C-O	-7.64	111.76	120.24
1	A	42	VAL	N-CA-C	7.62	118.86	107.51
1	A	279	MSE	N-CA-C	-7.48	103.07	111.07
1	A	301	SER	N-CA-C	7.22	119.23	111.36
1	A	48	LEU	N-CA-C	-7.20	101.80	110.44
1	A	50	LYS	CB-CA-C	-7.17	96.90	110.67
1	B	50	LYS	N-CA-C	7.11	119.11	111.36
1	B	82	GLU	N-CA-C	7.04	119.88	108.34
1	A	209	LYS	N-CA-C	-7.00	97.83	108.96
1	B	136	LEU	N-CA-C	6.96	118.52	111.07
1	B	297	GLU	N-CA-C	6.91	118.81	111.28
1	A	92	GLY	N-CA-C	-6.90	98.44	110.71
1	A	300	ARG	N-CA-C	-6.90	103.84	111.36
1	B	134	SER	N-CA-C	-6.81	94.00	107.69
1	B	254	ARG	CB-CA-C	-6.66	98.30	109.48
1	B	285	GLN	N-CA-C	-6.63	105.06	113.02
1	B	211	TYR	N-CA-C	-6.55	99.23	109.25
1	B	232	LYS	CB-CA-C	6.54	123.23	110.67
1	A	184	ALA	N-CA-C	6.47	120.63	112.87
1	B	281	ILE	CB-CA-C	-6.47	103.57	112.24
1	A	91	ARG	CB-CA-C	6.38	120.56	109.65
1	B	133	GLU	N-CA-C	-6.31	104.32	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	SER	N-CA-C	6.30	118.23	111.36
1	A	82	GLU	CB-CA-C	6.18	120.43	110.16
1	B	297	GLU	CB-CA-C	6.09	120.90	110.79
1	A	81	ILE	N-CA-C	6.08	116.62	108.11
1	B	156	PHE	N-CA-C	6.02	119.30	107.98
1	A	57	LEU	CB-CA-C	-6.01	101.44	110.88
1	B	94	LYS	CB-CA-C	6.00	119.91	110.19
1	A	273	PHE	N-CA-C	-5.99	105.05	112.90
1	B	98	THR	CB-CA-C	5.99	120.69	110.81
1	A	212	HIS	N-CA-C	5.94	117.70	109.15
1	B	126	PHE	N-CA-C	-5.88	104.95	111.36
1	A	162	PRO	CB-CA-C	-5.88	101.86	111.56
1	B	99	VAL	N-CA-C	-5.87	99.95	108.87
1	A	150	PHE	N-CA-C	-5.85	99.20	108.73
1	B	212	HIS	N-CA-C	-5.82	100.35	109.25
1	A	210	ILE	N-CA-C	-5.80	97.27	109.34
1	B	203	ILE	N-CA-C	5.78	116.52	110.62
1	A	84	SER	CB-CA-C	5.70	122.60	110.07
1	B	185	ASP	N-CA-C	-5.67	105.63	112.54
1	B	266	GLU	N-CA-C	5.54	119.03	111.39
1	A	143	ASP	CB-CA-C	-5.49	101.29	110.19
1	A	129	TYR	N-CA-C	5.43	117.28	111.36
1	B	183	LYS	N-CA-C	5.43	118.88	111.39
1	A	94	LYS	N-CA-C	-5.43	97.66	107.75
1	B	145	ARG	N-CA-C	-5.43	100.45	109.46
1	A	121	TYR	N-CA-C	5.41	117.18	111.28
1	A	82	GLU	N-CA-CB	-5.38	102.25	110.65
1	B	296	TYR	CB-CA-C	5.37	119.70	110.79
1	B	96	ARG	N-CA-C	-5.36	98.65	108.02
1	A	147	HIS	CB-CA-C	5.35	120.52	110.63
1	B	127	GLU	N-CA-C	5.31	117.98	111.82
1	A	136	LEU	N-CA-C	5.29	117.13	111.36
1	B	120	SER	N-CA-CB	-5.27	102.34	110.20
1	B	286	ASP	N-CA-C	-5.23	106.16	112.54
1	A	41	MSE	CB-CA-C	-5.21	100.70	109.72
1	B	80	GLN	CB-CA-C	5.19	119.95	109.68
1	B	31	SER	N-CA-C	5.13	116.88	111.28
1	B	53	LEU	N-CA-C	5.13	118.00	111.69
1	B	296	TYR	N-CA-C	-5.11	105.70	111.28
1	A	59	LEU	CB-CA-C	-5.11	103.44	111.51
1	A	241	GLY	N-CA-C	5.10	121.26	111.31
1	A	32	VAL	CB-CA-C	-5.06	105.23	112.22

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	HIS	Peptide
1	A	21	ALA	Peptide
1	A	34	LYS	Peptide
1	A	35	GLY	Peptide
1	B	134	SER	Peptide
1	B	158	HIS	Peptide
1	B	159	GLY	Peptide
1	B	254	ARG	Peptide
1	B	267	ASN	Peptide
1	B	34	LYS	Peptide
1	B	35	GLY	Peptide
1	B	43	VAL	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	1747	0	1638	112	0
1	B	1817	0	1759	132	0
2	A	28	0	12	7	0
2	B	28	0	12	9	0
All	All	3620	0	3421	244	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 35.

All (244) 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:B:48:LEU:HD22	1:B:182:ALA:CB	1.45	1.46
1:A:188:THR:HG22	1:A:191:GLU:CD	1.57	1.27
1:B:130:LEU:HD12	1:B:299:PHE:HD1	1.07	1.17
1:B:238:SER:O	1:B:272:ASP:HB2	1.46	1.14
1:B:48:LEU:CD2	1:B:182:ALA:HB1	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:O	1:B:186:THR:HG22	1.55	1.07
1:A:31:SER:O	1:A:35:GLY:HA2	1.59	1.03
1:B:130:LEU:HD12	1:B:299:PHE:CD1	1.94	1.03
1:B:48:LEU:CD2	1:B:182:ALA:CB	2.40	1.00
1:B:125:GLN:HG2	1:B:144:ASN:O	1.61	1.00
1:A:278:THR:O	1:A:282:THR:HG22	1.61	0.99
1:B:268:PRO:HG3	1:B:271:ASN:O	1.64	0.96
1:A:81:ILE:HG13	1:A:81:ILE:O	1.61	0.95
1:B:48:LEU:HD12	1:B:154:SER:HB2	1.49	0.94
2:B:316:GDP:H8	2:B:316:GDP:H5'	1.34	0.92
1:B:48:LEU:HD22	1:B:182:ALA:HB3	1.47	0.92
1:B:48:LEU:HD22	1:B:182:ALA:HB1	0.91	0.90
1:B:48:LEU:CD1	1:B:154:SER:HB2	2.05	0.87
1:A:188:THR:CG2	1:A:191:GLU:CD	2.44	0.87
1:A:47:GLY:HA3	2:A:316:GDP:O1B	1.75	0.87
1:A:133:GLU:O	1:A:138:ARG:CZ	2.23	0.86
1:B:226:GLU:HA	1:B:229:ARG:NH1	1.90	0.86
1:A:57:LEU:HD12	1:A:57:LEU:O	1.75	0.85
1:B:238:SER:O	1:B:272:ASP:CB	2.24	0.85
1:B:48:LEU:HD11	1:B:155:PRO:HD3	1.59	0.84
1:B:21:ALA:O	1:B:24:PRO:HD2	1.78	0.84
2:B:316:GDP:H5'	2:B:316:GDP:C8	2.13	0.82
1:A:282:THR:HG23	1:A:283:HIS:HD2	1.46	0.80
1:A:147:HIS:HA	1:A:290:VAL:HG21	1.61	0.80
1:B:226:GLU:HA	1:B:229:ARG:HH12	1.47	0.80
1:B:116:LYS:HA	1:B:119:ILE:HD11	1.64	0.79
1:A:169:LYS:O	1:A:172:HIS:CE1	2.37	0.78
1:B:130:LEU:CD1	1:B:299:PHE:HD1	1.94	0.78
1:A:282:THR:HG23	1:A:283:HIS:CD2	2.18	0.78
1:A:172:HIS:HB3	1:A:177:ILE:HD11	1.67	0.77
1:A:23:LEU:N	1:A:24:PRO:HD2	2.00	0.76
1:B:232:LYS:O	1:B:235:ILE:CG2	2.33	0.76
1:A:132:ASP:HB3	1:A:141:ILE:HG22	1.68	0.76
1:B:130:LEU:CD1	1:B:299:PHE:CD1	2.70	0.75
1:B:48:LEU:CD1	1:B:154:SER:HA	2.17	0.74
1:B:48:LEU:HD11	1:B:155:PRO:CD	2.17	0.74
1:A:100:VAL:HG11	1:A:118:ILE:HD11	1.68	0.74
1:B:268:PRO:HA	1:B:270:HIS:N	2.05	0.72
1:A:210:ILE:HG12	1:A:211:TYR:N	2.03	0.72
1:B:278:THR:O	1:B:282:THR:HG22	1.89	0.72
1:B:232:LYS:O	1:B:235:ILE:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:O	1:A:198:ARG:HG3	1.90	0.72
1:B:48:LEU:HD13	1:B:154:SER:HA	1.73	0.71
1:B:54:ILE:HG12	1:B:97:LEU:HD22	1.72	0.70
1:B:268:PRO:CG	1:B:271:ASN:O	2.39	0.70
1:B:185:ASP:CG	2:B:316:GDP:HN21	1.99	0.70
1:A:297:GLU:O	1:A:301:SER:HB2	1.93	0.68
1:A:210:ILE:HG12	1:A:211:TYR:H	1.57	0.67
1:A:188:THR:HG22	1:A:191:GLU:OE2	1.95	0.67
1:A:116:LYS:HA	1:A:119:ILE:HD11	1.75	0.67
1:B:291:THR:HG22	1:B:292:GLN:HG3	1.77	0.67
1:A:188:THR:HG22	1:A:191:GLU:OE1	1.95	0.66
1:B:22:ASN:O	1:B:25:ASN:HB2	1.95	0.66
1:B:48:LEU:CD1	1:B:154:SER:CB	2.74	0.65
1:A:125:GLN:CG	1:A:144:ASN:O	2.44	0.65
1:B:116:LYS:HA	1:B:119:ILE:CD1	2.27	0.65
1:B:256:ARG:CB	1:B:263:VAL:HB	2.27	0.64
1:A:88:ILE:C	1:A:90:GLU:N	2.55	0.64
1:B:35:GLY:O	1:B:36:PHE:CD2	2.51	0.64
1:B:185:ASP:OD2	2:B:316:GDP:N2	2.31	0.63
1:B:267:ASN:HB3	1:B:270:HIS:HB2	1.79	0.63
1:B:125:GLN:CG	1:B:144:ASN:O	2.43	0.63
1:A:266:GLU:HB2	1:A:274:LEU:HG	1.81	0.62
1:A:125:GLN:HG3	1:A:144:ASN:O	1.99	0.62
1:B:240:VAL:HB	1:B:271:ASN:HD22	1.65	0.62
1:B:268:PRO:HG3	1:B:271:ASN:C	2.26	0.61
1:B:297:GLU:O	1:B:301:SER:HB2	2.00	0.61
1:B:161:LYS:HB3	1:B:162:PRO:HD2	1.84	0.60
1:B:194:ARG:O	1:B:198:ARG:HG3	2.02	0.60
1:B:48:LEU:CD2	1:B:182:ALA:HB3	2.21	0.60
1:B:155:PRO:HG3	1:B:182:ALA:O	2.00	0.60
1:B:265:VAL:HG12	1:B:266:GLU:N	2.15	0.60
1:A:47:GLY:CA	2:A:316:GDP:O1B	2.49	0.60
1:A:265:VAL:O	1:A:266:GLU:HG2	2.01	0.60
1:B:175:VAL:HA	1:B:294:LEU:HD13	1.84	0.59
1:A:267:ASN:O	1:A:268:PRO:C	2.46	0.59
1:B:240:VAL:CG2	1:B:271:ASN:ND2	2.66	0.59
1:B:116:LYS:HA	1:B:119:ILE:CG1	2.33	0.59
1:A:119:ILE:HD13	1:A:119:ILE:H	1.67	0.58
1:A:239:VAL:HG11	1:A:276:LEU:HD12	1.84	0.58
1:B:282:THR:HG23	1:B:283:HIS:CD2	2.38	0.58
1:B:48:LEU:HD23	1:B:48:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:CD2	1:B:48:LEU:O	2.52	0.58
1:A:188:THR:HG22	1:A:191:GLU:CG	2.32	0.57
1:A:81:ILE:O	1:A:81:ILE:CG1	2.43	0.57
1:A:41:MSE:HB2	1:A:146:VAL:HG11	1.85	0.57
1:B:176:ASN:ND2	1:B:290:VAL:HG23	2.19	0.57
1:A:57:LEU:HD12	1:A:57:LEU:C	2.29	0.57
1:A:255:GLY:HA2	1:A:265:VAL:HG23	1.87	0.57
1:A:48:LEU:O	1:A:182:ALA:HB1	2.05	0.57
1:B:41:MSE:HE1	1:B:171:ILE:HD11	1.87	0.57
1:A:278:THR:O	1:A:282:THR:CG2	2.45	0.56
1:B:157:GLY:C	1:B:159:GLY:N	2.63	0.56
1:B:300:ARG:O	1:B:304:LEU:HG	2.04	0.56
1:A:267:ASN:HB3	1:A:270:HIS:HB3	1.88	0.56
1:A:31:SER:O	1:A:35:GLY:CA	2.45	0.56
1:B:265:VAL:C	1:B:266:GLU:HG3	2.31	0.56
2:B:316:GDP:C8	2:B:316:GDP:C5'	2.86	0.55
1:A:192:ARG:O	1:A:196:LYS:HG3	2.06	0.55
1:B:131:HIS:O	1:B:134:SER:O	2.25	0.55
1:A:52:THR:HG22	2:A:316:GDP:O1A	2.06	0.55
1:B:133:GLU:C	1:B:135:GLY:HA3	2.32	0.55
1:A:270:HIS:HE1	1:B:260:TRP:HB3	1.71	0.55
1:B:52:THR:HG21	2:B:316:GDP:C8	2.42	0.55
1:A:141:ILE:O	1:A:141:ILE:HG13	2.05	0.54
1:A:134:SER:O	1:A:134:SER:OG	2.25	0.54
1:B:264:GLU:HB3	1:B:270:HIS:CD2	2.42	0.54
1:A:158:HIS:O	1:A:198:ARG:HD3	2.08	0.54
1:A:291:THR:HG22	1:A:292:GLN:HG3	1.90	0.54
1:B:266:GLU:HA	1:B:274:LEU:HG	1.90	0.53
1:B:133:GLU:O	1:B:135:GLY:HA3	2.08	0.53
1:A:119:ILE:HA	1:A:122:ILE:HG12	1.91	0.53
1:B:265:VAL:HG12	1:B:266:GLU:H	1.74	0.53
1:B:21:ALA:O	1:B:24:PRO:CD	2.55	0.53
1:A:188:THR:CG2	1:A:191:GLU:OE2	2.54	0.52
1:A:288:GLN:HB3	1:A:292:GLN:NE2	2.24	0.52
1:A:143:ASP:OD2	1:A:145:ARG:HD3	2.09	0.52
1:B:183:LYS:O	1:B:186:THR:CG2	2.44	0.52
1:B:48:LEU:CD1	1:B:154:SER:CA	2.86	0.52
1:A:52:THR:HG21	2:A:316:GDP:H8	1.74	0.52
1:A:100:VAL:CG1	1:A:118:ILE:HD11	2.40	0.52
1:B:179:PRO:HG3	1:B:210:ILE:HD11	1.90	0.52
1:B:268:PRO:HG3	1:B:272:ASP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:HD3	1:B:236:PRO:O	2.10	0.52
1:B:240:VAL:HB	1:B:271:ASN:ND2	2.24	0.52
1:B:268:PRO:CD	1:B:271:ASN:O	2.57	0.52
1:B:258:TYR:HB3	1:B:260:TRP:CE2	2.46	0.51
1:A:83:ALA:HA	1:A:96:ARG:HA	1.92	0.51
1:A:133:GLU:O	1:A:138:ARG:NH1	2.44	0.51
1:A:188:THR:CG2	1:A:191:GLU:CG	2.89	0.51
1:A:155:PRO:HG3	1:A:182:ALA:O	2.11	0.51
1:A:121:TYR:CD1	1:A:121:TYR:C	2.89	0.51
1:A:143:ASP:CG	1:A:143:ASP:O	2.53	0.51
1:A:23:LEU:N	1:A:24:PRO:CD	2.68	0.51
1:A:203:ILE:HG23	1:A:208:ILE:HG22	1.92	0.51
1:B:274:LEU:O	1:B:278:THR:HG23	2.10	0.51
1:B:132:ASP:HB3	1:B:141:ILE:HG22	1.91	0.50
1:A:151:TYR:HE1	1:A:167:PHE:CD2	2.30	0.50
1:A:52:THR:HG21	2:A:316:GDP:C8	2.46	0.50
1:B:184:ALA:HB2	1:B:238:SER:HB2	1.92	0.50
1:B:264:GLU:HB3	1:B:270:HIS:HD2	1.77	0.50
1:A:243:ASN:OD1	1:A:254:ARG:NH2	2.45	0.50
1:B:43:VAL:HG21	1:B:167:PHE:CZ	2.47	0.50
1:A:286:ASP:O	1:A:290:VAL:HG23	2.12	0.49
1:A:43:VAL:HG22	1:A:100:VAL:HG11	1.93	0.49
1:A:22:ASN:O	1:A:25:ASN:N	2.46	0.49
1:B:179:PRO:HG2	1:B:236:PRO:HB3	1.94	0.49
1:A:100:VAL:HG11	1:A:118:ILE:CD1	2.40	0.49
1:A:206:HIS:C	1:A:208:ILE:N	2.71	0.49
1:A:246:ILE:HG22	1:A:247:GLU:N	2.28	0.48
1:B:258:TYR:C	1:B:260:TRP:H	2.20	0.48
1:B:268:PRO:O	1:B:270:HIS:N	2.46	0.48
1:A:41:MSE:HB2	1:A:146:VAL:CG1	2.42	0.48
1:A:41:MSE:HB3	1:A:149:CYS:HB2	1.94	0.48
1:A:41:MSE:HE2	1:A:149:CYS:SG	2.53	0.48
1:A:260:TRP:CE2	1:B:263:VAL:HG22	2.48	0.48
1:A:292:GLN:O	1:A:296:TYR:CB	2.61	0.48
1:A:238:SER:O	1:A:271:ASN:O	2.32	0.48
1:B:35:GLY:C	1:B:36:PHE:CG	2.92	0.48
1:B:57:LEU:HB3	1:B:58:PHE:CD2	2.49	0.48
1:A:148:CYS:SG	1:A:149:CYS:N	2.86	0.48
1:B:48:LEU:O	1:B:182:ALA:HB1	2.12	0.48
1:B:268:PRO:HD3	1:B:271:ASN:O	2.13	0.48
1:B:48:LEU:HD12	1:B:154:SER:CB	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:CG1	1:B:151:TYR:CE1	2.97	0.47
1:A:137:ASN:O	1:A:138:ARG:HG3	2.14	0.47
1:B:172:HIS:HD2	1:B:209:LYS:HB2	1.80	0.47
1:B:155:PRO:CG	1:B:182:ALA:O	2.62	0.47
1:B:240:VAL:HG21	1:B:271:ASN:ND2	2.30	0.47
1:A:151:TYR:OH	1:A:164:ASP:HA	2.14	0.47
1:A:39:THR:H	1:A:147:HIS:HD2	1.63	0.47
1:B:52:THR:HB	2:B:316:GDP:O1A	2.15	0.47
1:A:45:GLU:H	1:A:50:LYS:CE	2.28	0.46
1:A:173:ASN:HA	1:A:294:LEU:HD22	1.98	0.46
1:B:282:THR:HG23	1:B:283:HIS:HD2	1.79	0.46
1:B:46:SER:HA	1:B:47:GLY:HA2	1.60	0.46
1:A:133:GLU:O	1:A:138:ARG:NH2	2.48	0.46
1:B:265:VAL:CG1	1:B:266:GLU:N	2.79	0.46
1:A:268:PRO:O	1:A:270:HIS:HB2	2.15	0.45
1:B:173:ASN:O	1:B:175:VAL:N	2.49	0.45
1:B:23:LEU:N	1:B:24:PRO:HD2	2.32	0.45
1:B:59:LEU:N	1:B:59:LEU:HD23	2.31	0.45
1:A:55:ASN:CG	1:A:61:ASP:HA	2.42	0.45
1:A:51:SER:HB3	2:A:316:GDP:O3B	2.16	0.45
1:B:123:ASP:OD1	1:B:123:ASP:O	2.34	0.45
1:A:46:SER:HA	1:A:47:GLY:HA2	1.63	0.45
1:A:232:LYS:O	1:A:235:ILE:CG2	2.65	0.45
1:B:43:VAL:HG11	1:B:151:TYR:CE1	2.52	0.44
1:B:39:THR:OG1	1:B:146:VAL:HA	2.17	0.44
1:A:142:ILE:HD12	1:A:142:ILE:O	2.17	0.44
1:A:173:ASN:O	1:A:175:VAL:N	2.51	0.44
1:B:41:MSE:CE	1:B:122:ILE:HG21	2.48	0.44
1:B:21:ALA:C	1:B:24:PRO:HD2	2.40	0.44
1:B:59:LEU:O	1:B:60:THR:HG23	2.18	0.44
1:B:141:ILE:HG13	1:B:141:ILE:O	2.17	0.44
1:A:57:LEU:HA	1:A:273:PHE:HZ	1.83	0.44
1:B:48:LEU:HD11	1:B:154:SER:HA	1.99	0.44
1:A:101:ASP:O	1:A:102:THR:CB	2.64	0.43
1:A:268:PRO:HA	1:A:270:HIS:N	2.32	0.43
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.87	0.43
1:B:116:LYS:HA	1:B:119:ILE:HG12	2.00	0.43
1:B:41:MSE:HB2	1:B:146:VAL:HG11	2.01	0.43
1:A:53:LEU:HD23	1:A:152:PHE:HZ	1.84	0.43
1:B:121:TYR:CD1	1:B:121:TYR:C	2.97	0.43
1:B:265:VAL:CG1	1:B:266:GLU:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PRO:HD3	1:B:210:ILE:HD11	2.01	0.43
1:B:160:LEU:CD2	1:B:165:VAL:HG23	2.49	0.42
1:B:48:LEU:CD1	1:B:155:PRO:HD3	2.38	0.42
1:A:268:PRO:O	1:A:270:HIS:N	2.52	0.42
1:B:148:CYS:SG	1:B:149:CYS:N	2.91	0.42
1:B:302:GLU:C	1:B:304:LEU:H	2.27	0.42
1:A:246:ILE:HG22	1:A:247:GLU:H	1.84	0.42
1:A:267:ASN:HB3	1:A:270:HIS:CD2	2.54	0.42
1:B:45:GLU:H	1:B:50:LYS:HE2	1.83	0.42
1:B:54:ILE:HG12	1:B:97:LEU:CD2	2.47	0.42
1:B:258:TYR:O	1:B:260:TRP:N	2.49	0.41
1:A:149:CYS:HB3	1:A:175:VAL:CG1	2.50	0.41
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.56	0.41
1:B:47:GLY:HA3	2:B:316:GDP:O1B	2.20	0.41
1:A:185:ASP:OD2	2:A:316:GDP:N1	2.43	0.41
1:B:185:ASP:OD1	2:B:316:GDP:N1	2.45	0.41
1:A:22:ASN:O	1:A:25:ASN:HB2	2.20	0.41
1:A:40:LEU:HD12	1:A:148:CYS:O	2.20	0.41
1:A:119:ILE:O	1:A:123:ASP:HB2	2.20	0.41
1:B:156:PHE:CD1	1:B:156:PHE:N	2.85	0.41
1:B:192:ARG:HD2	1:B:238:SER:OG	2.20	0.41
1:B:143:ASP:OD2	1:B:145:ARG:HD3	2.21	0.41
1:A:44:GLY:O	1:A:45:GLU:HG3	2.21	0.41
1:A:57:LEU:C	1:A:57:LEU:CD1	2.93	0.41
1:A:264:GLU:CD	1:A:267:ASN:HD22	2.28	0.41
1:B:43:VAL:HG12	1:B:151:TYR:CE1	2.56	0.41
1:B:160:LEU:HD22	1:B:165:VAL:HG23	2.03	0.41
1:A:188:THR:CG2	1:A:191:GLU:HG3	2.51	0.40
1:A:239:VAL:HG12	1:A:273:PHE:HA	2.03	0.40
1:A:258:TYR:CE1	1:B:185:ASP:O	2.74	0.40
1:B:259:PRO:HG2	1:B:260:TRP:CE3	2.57	0.40
1:A:169:LYS:O	1:A:172:HIS:HE1	1.97	0.40
1:B:157:GLY:C	1:B:159:GLY:H	2.30	0.40
1:B:38:PHE:HA	1:B:147:HIS:HD2	1.87	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	211/315 (67%)	196 (93%)	13 (6%)	2 (1%)	14	42
1	B	214/315 (68%)	195 (91%)	15 (7%)	4 (2%)	6	26
All	All	425/630 (68%)	391 (92%)	28 (7%)	6 (1%)	9	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	HIS
1	A	35	GLY
1	B	267	ASN
1	B	44	GLY
1	B	259	PRO
1	A	44	GLY

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	179/280 (64%)	129 (72%)	50 (28%)	0	1
1	B	195/280 (70%)	156 (80%)	39 (20%)	1	4
All	All	374/560 (67%)	285 (76%)	89 (24%)	1	2

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	39	THR
1	A	43	VAL
1	A	45	GLU
1	A	48	LEU
1	A	51	SER
1	A	54	ILE
1	A	56	SER
1	A	57	LEU
1	A	58	PHE
1	A	59	LEU
1	A	60	THR
1	A	61	ASP
1	A	62	LEU
1	A	95	LEU
1	A	98	THR
1	A	99	VAL
1	A	100	VAL
1	A	117	THR
1	A	119	ILE
1	A	123	ASP
1	A	125	GLN
1	A	142	ILE
1	A	144	ASN
1	A	145	ARG
1	A	149	CYS
1	A	153	ILE
1	A	160	LEU
1	A	163	LEU
1	A	171	ILE
1	A	173	ASN
1	A	177	ILE
1	A	180	VAL
1	A	181	ILE
1	A	200	LEU
1	A	203	ILE
1	A	208	ILE
1	A	210	ILE
1	A	213	LEU
1	A	235	ILE
1	A	242	SER
1	A	244	GLN
1	A	257	LEU

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Mol	Chain	Res	Type
1	A	272	ASP
1	A	276	LEU
1	A	277	ARG
1	A	285	GLN
1	A	287	LEU
1	A	291	THR
1	A	301	SER
1	B	22	ASN
1	B	34	LYS
1	B	39	THR
1	B	40	LEU
1	B	41	MSE
1	B	45	GLU
1	B	54	ILE
1	B	61	ASP
1	B	62	LEU
1	B	80	GLN
1	B	81	ILE
1	B	95	LEU
1	B	98	THR
1	B	99	VAL
1	B	117	THR
1	B	118	ILE
1	B	119	ILE
1	B	120	SER
1	B	125	GLN
1	B	142	ILE
1	B	143	ASP
1	B	153	ILE
1	B	154	SER
1	B	163	LEU
1	B	171	ILE
1	B	175	VAL
1	B	177	ILE
1	B	180	VAL
1	B	186	THR
1	B	187	LEU
1	B	188	THR
1	B	231	LEU
1	B	235	ILE
1	B	257	LEU
1	B	266	GLU

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Mol	Chain	Res	Type
1	B	270	HIS
1	B	272	ASP
1	B	290	VAL
1	B	291	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	25	ASN
1	A	147	HIS
1	A	244	GLN
1	A	267	ASN
1	A	270	HIS
1	A	283	HIS
1	A	295	HIS
1	B	28	HIS
1	B	137	ASN
1	B	172	HIS
1	B	173	ASN
1	B	271	ASN
1	B	283	HIS
1	B	285	GLN

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](#)

2 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
2	GDP	A	316	-	29,30,30	1.14	3 (10%)	45,47,47	1.82	8 (17%)
2	GDP	B	316	-	29,30,30	1.25	3 (10%)	45,47,47	1.71	6 (13%)

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
2	GDP	A	316	-	-	4/16/32/32	0/3/3/3
2	GDP	B	316	-	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	316	GDP	C5-C4	3.14	1.47	1.38
2	B	316	GDP	C6-N1	-3.12	1.33	1.38
2	A	316	GDP	C5-C4	3.03	1.47	1.38
2	B	316	GDP	C5-N7	-2.86	1.33	1.39
2	A	316	GDP	C5-N7	-2.40	1.34	1.39
2	A	316	GDP	C6-N1	-2.32	1.34	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	316	GDP	C5-C4-N3	-6.76	117.63	128.39
2	A	316	GDP	C5-C4-N3	-6.36	118.28	128.39
2	A	316	GDP	C2-N3-C4	5.29	121.42	112.30
2	B	316	GDP	N9-C4-N3	5.00	135.96	125.95
2	B	316	GDP	C2-N3-C4	4.70	120.40	112.30
2	A	316	GDP	N9-C4-N3	4.60	135.15	125.95
2	A	316	GDP	C6-C5-N7	2.98	135.72	130.29
2	A	316	GDP	C3'-C2'-C1'	2.42	106.04	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	316	GDP	C4-C5-N7	-2.38	106.90	110.67
2	A	316	GDP	O6-C6-C5	-2.14	120.89	126.53
2	B	316	GDP	C6-C5-N7	2.13	134.16	130.29
2	A	316	GDP	O3B-PB-O3A	2.09	111.63	104.64
2	B	316	GDP	O6-C6-C5	-2.03	121.18	126.53
2	B	316	GDP	C4-C5-N7	-2.01	107.48	110.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

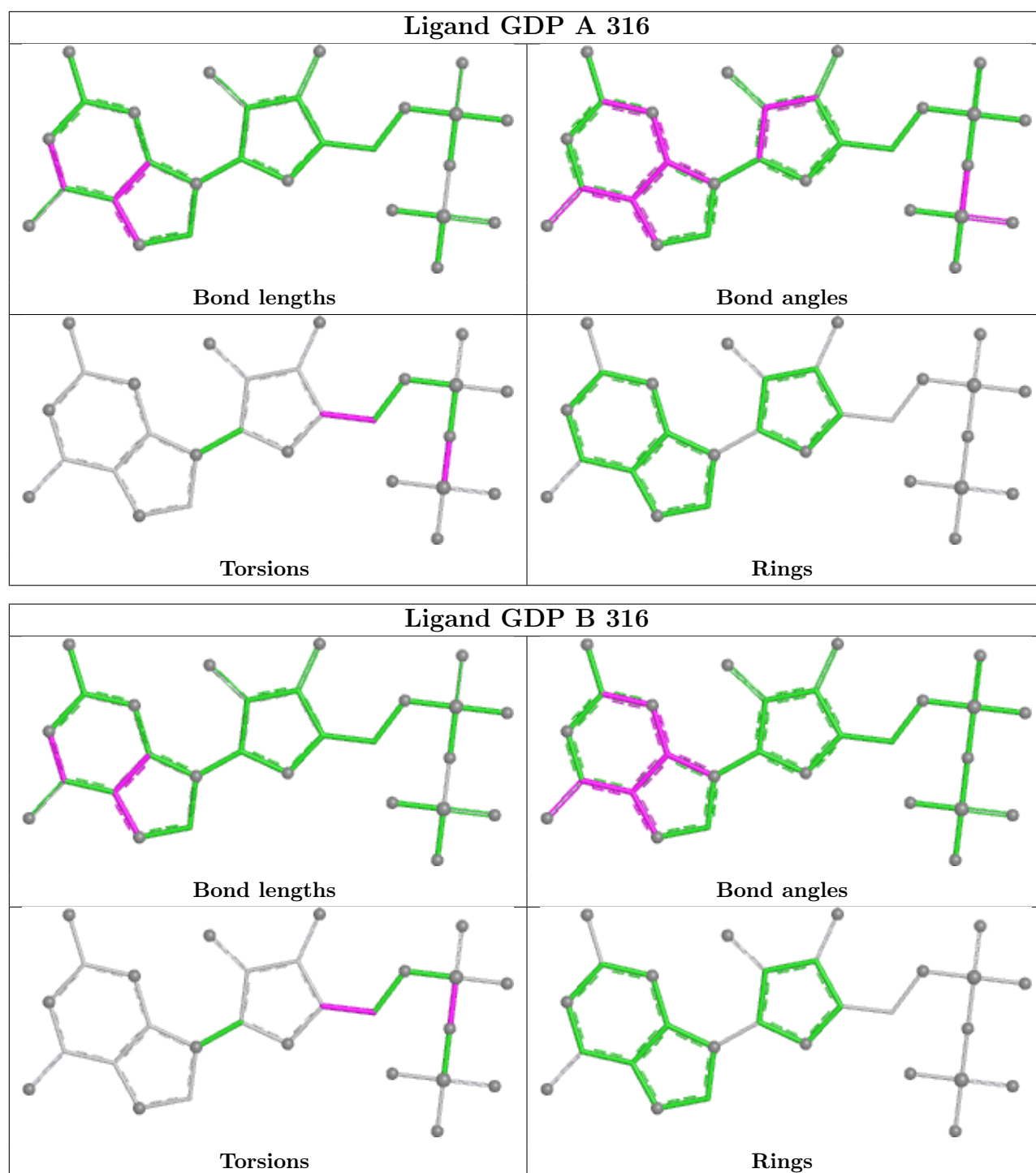
Mol	Chain	Res	Type	Atoms
2	A	316	GDP	PA-O3A-PB-O3B
2	B	316	GDP	C3'-C4'-C5'-O5'
2	B	316	GDP	O4'-C4'-C5'-O5'
2	B	316	GDP	PB-O3A-PA-O2A
2	A	316	GDP	PA-O3A-PB-O1B
2	A	316	GDP	PA-O3A-PB-O2B
2	A	316	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	316	GDP	7	0
2	B	316	GDP	9	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	229/315 (72%)	0.55	15 (6%) 24 19	25, 78, 95, 104	0
1	B	230/315 (73%)	0.71	25 (10%) 10 11	20, 81, 101, 130	0
All	All	459/630 (72%)	0.63	40 (8%) 16 14	20, 80, 100, 130	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	ASN	5.3
1	A	228	THR	3.6
1	B	78	THR	3.6
1	B	20	PHE	3.4
1	B	206	HIS	3.2
1	B	289	GLU	3.0
1	A	187	LEU	3.0
1	B	240	VAL	3.0
1	B	243	ASN	2.9
1	B	45	GLU	2.9
1	A	184	ALA	2.8
1	B	48	LEU	2.8
1	B	119	ILE	2.7
1	B	123	ASP	2.6
1	B	294	LEU	2.6
1	B	35	GLY	2.6
1	B	158	HIS	2.6
1	A	243	ASN	2.6
1	A	241	GLY	2.5
1	A	85	THR	2.5
1	A	20	PHE	2.5
1	B	198	ARG	2.4
1	B	195	LEU	2.4
1	B	159	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	ARG	2.4
1	B	230	LEU	2.4
1	A	84	SER	2.4
1	B	185	ASP	2.3
1	B	160	LEU	2.2
1	A	101	ASP	2.2
1	B	299	PHE	2.2
1	A	35	GLY	2.1
1	A	238	SER	2.1
1	B	137	ASN	2.1
1	A	126	PHE	2.1
1	A	198	ARG	2.1
1	A	247	GLU	2.1
1	B	36	PHE	2.1
1	B	135	GLY	2.0
1	A	240	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

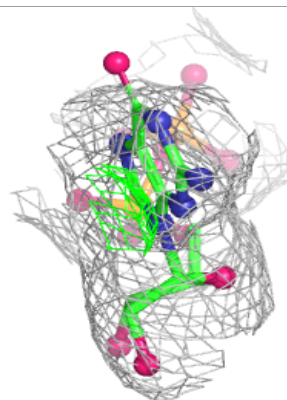
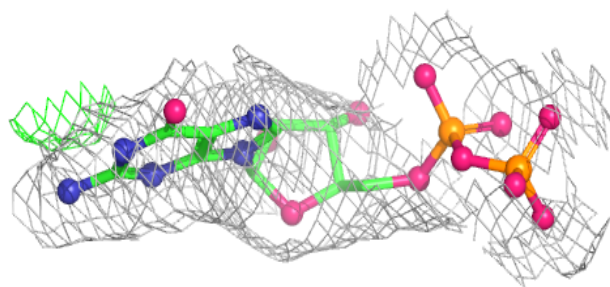
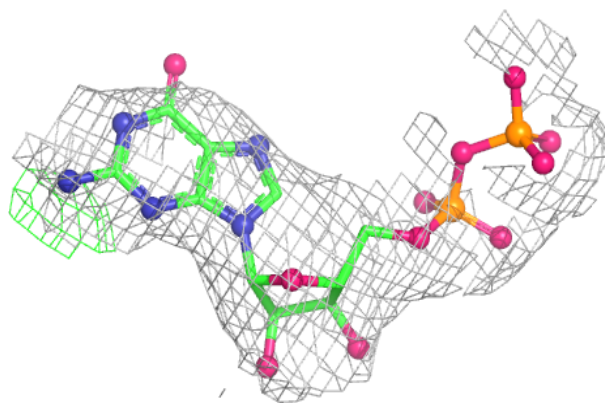
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDP	B	316	28/28	0.91	0.09	63,71,74,74	0
2	GDP	A	316	28/28	0.94	0.08	57,60,62,62	0

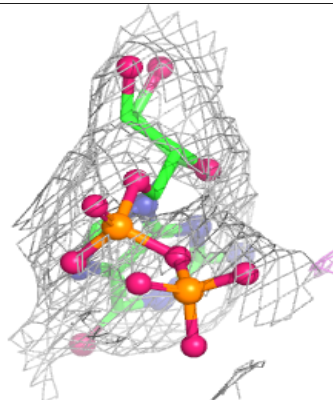
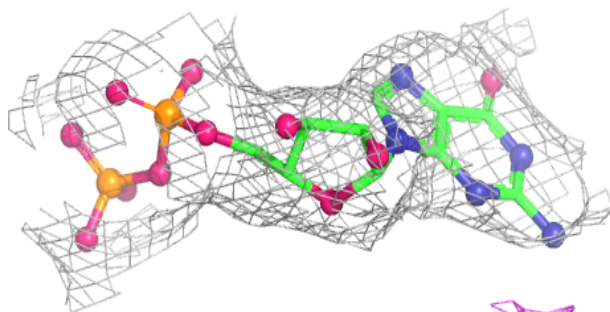
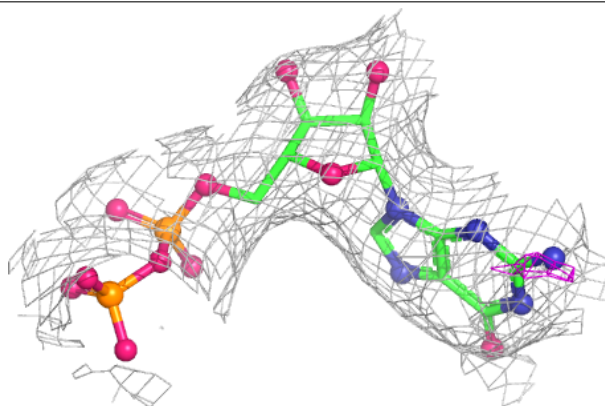
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 316:

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

**Electron density around GDP A 316:**

$2mF_o-DF_c$ (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.