



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:32 PM UTC

PDB ID : 1Y3A / pdb_00001y3a
Title : Structure of G-Alpha-I1 bound to a GDP-selective peptide provides insight into guanine nucleotide exchange
Authors : Johnston, C.A.; Willard, F.S.; Jezyk, M.R.; Fredericks, Z.; Bodor, E.T.; Jones, M.B.; Blaesius, R.; Harden, T.K.; Sondek, J.; Watts, V.J.; Ramer, J.K.; Siderovski, D.P.
Deposited on : 2004-11-24
Resolution : 2.50 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](#) ①) were used in the production of this report:

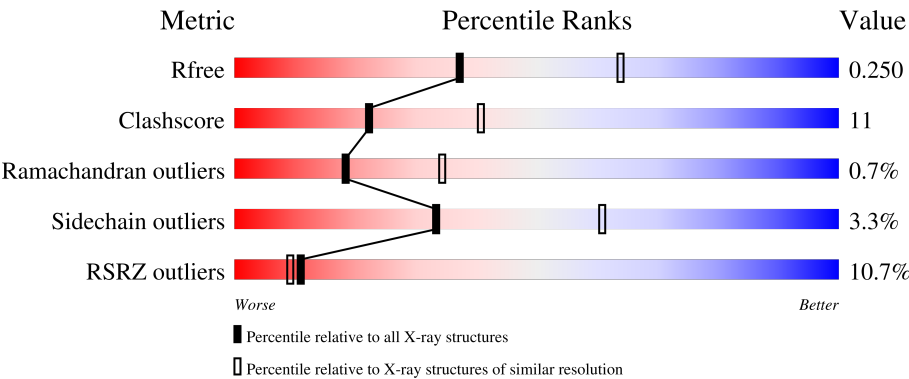
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	329	10% 70% 18% • 9%
1	B	329	6% 72% 19% •• 7%
1	C	329	9% 69% 20% • 9%
1	D	329	13% 69% 22% • 8%
2	E	16	19% 31% 44% 25%

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Mol	Chain	Length	Quality of chain
2	F	16	19% 50% 19% 6% 25%
2	G	16	6% 56% 19% 25%
2	H	16	31% 44% 31% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10424 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(i), alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2413	1540	407	451	15			
1	B	307	Total	C	N	O	S	0	0	0
			2471	1575	414	467	15			
1	C	298	Total	C	N	O	S	0	0	0
			2404	1534	405	450	15			
1	D	304	Total	C	N	O	S	0	0	0
			2452	1562	411	464	15			

- Molecule 2 is a protein called KB752 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			
2	F	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			
2	G	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			
2	H	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

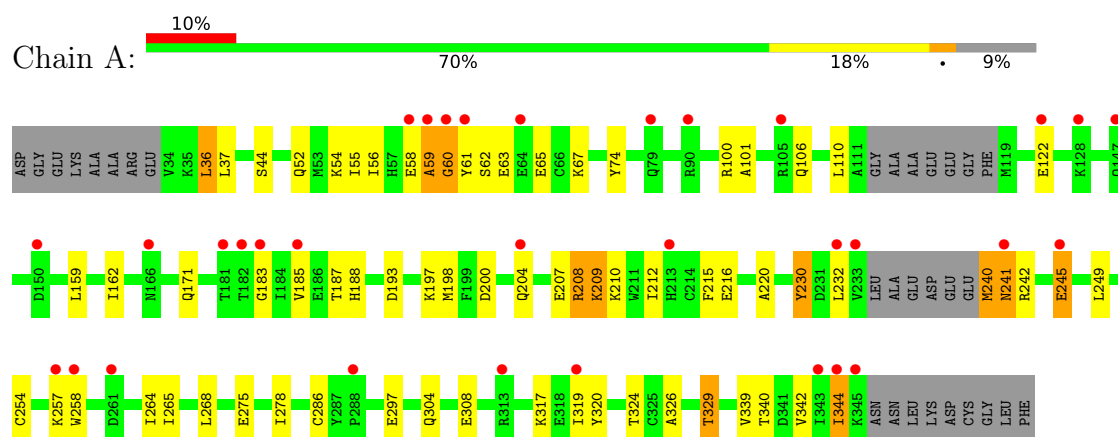
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	29	Total O 29 29	0	0
4	C	30	Total O 30 30	0	0
4	D	25	Total O 25 25	0	0
4	E	2	Total O 2 2	0	0
4	F	1	Total O 1 1	0	0
4	G	2	Total O 2 2	0	0
4	H	1	Total O 1 1	0	0

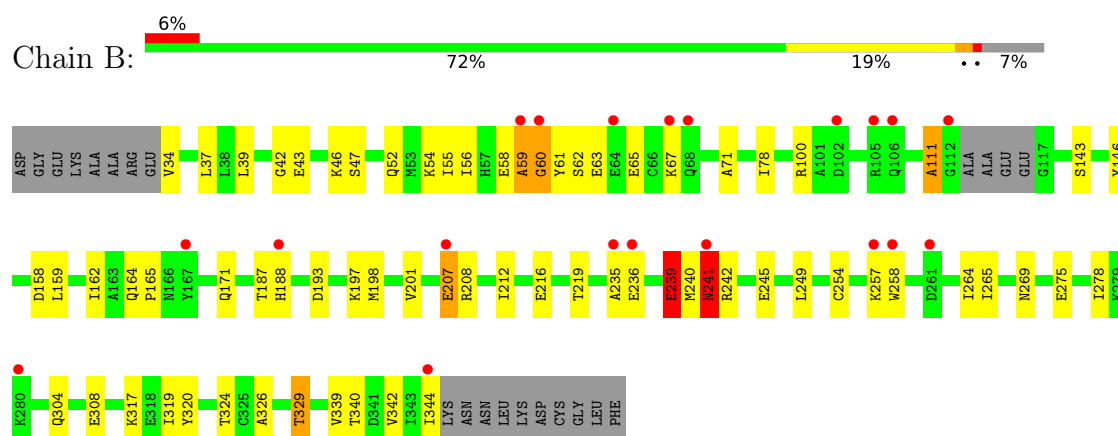
3 Residue-property plots [i](#)

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.

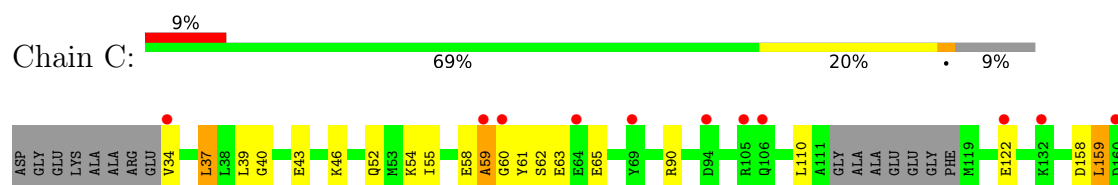
- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

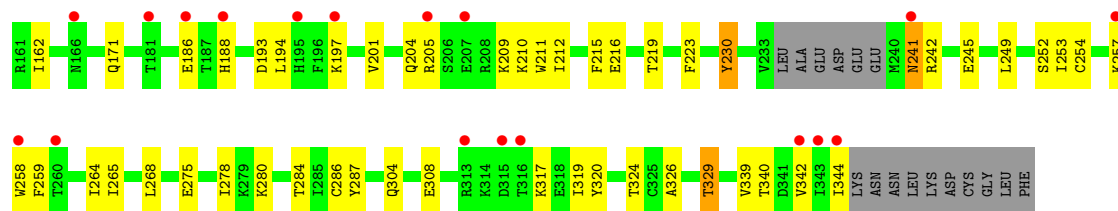


- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

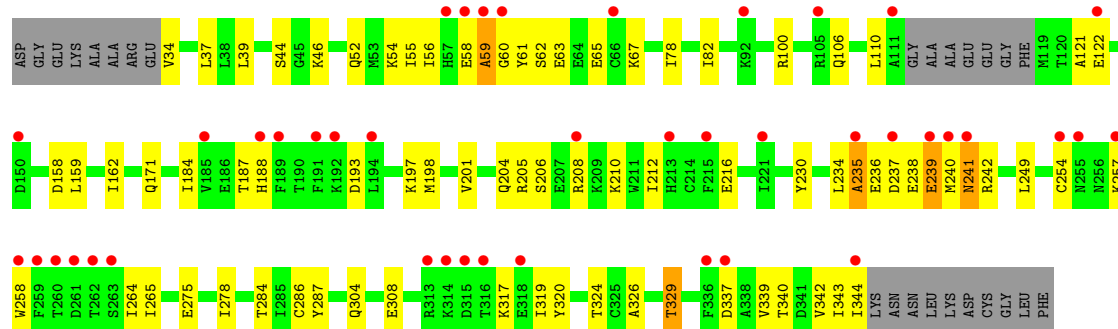


- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit





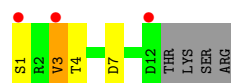
• Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit



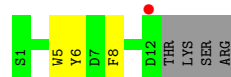
• Molecule 2: KB752 peptide



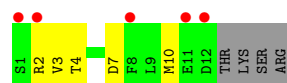
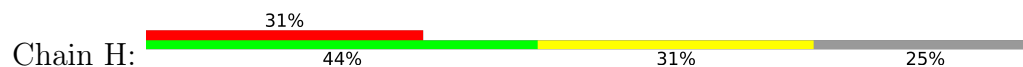
• Molecule 2: KB752 peptide



• Molecule 2: KB752 peptide



• Molecule 2: KB752 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.94Å 112.78Å 109.49Å 90.00° 93.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 96.2 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.280 0.245 , 0.250	Depositor DCC
R_{free} test set	3001 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10424	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% 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	0.48	1/2456 (0.0%)	0.88	8/3306 (0.2%)
1	B	0.53	1/2516 (0.0%)	0.89	8/3389 (0.2%)
1	C	0.47	1/2447 (0.0%)	0.87	4/3295 (0.1%)
1	D	0.49	1/2496 (0.0%)	0.90	4/3363 (0.1%)
2	E	0.38	0/112	0.73	0/151
2	F	0.43	0/112	0.71	0/151
2	G	0.38	0/112	0.66	0/151
2	H	0.38	0/112	0.64	0/151
All	All	0.49	4/10363 (0.0%)	0.88	24/13957 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	ASN	N-CA	9.80	1.57	1.45
1	B	241	ASN	N-CA	8.89	1.57	1.46
1	A	60	GLY	N-CA	5.57	1.54	1.45
1	C	241	ASN	N-CA	5.54	1.53	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	ASN	N-CA-C	-12.80	90.29	110.14
1	B	111	ALA	N-CA-C	9.12	124.14	111.56
1	A	241	ASN	N-CA-C	-6.87	100.31	110.48
1	B	324	THR	N-CA-C	6.58	120.25	109.85
1	A	60	GLY	N-CA-C	-6.37	101.32	112.53
1	A	230	TYR	N-CA-C	6.34	119.00	111.33
1	C	230	TYR	N-CA-C	6.20	118.83	111.33
1	B	239	GLU	N-CA-C	-5.98	99.53	109.46
1	B	245	GLU	N-CA-C	-5.92	104.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	GLY	N-CA-C	-5.89	102.16	112.53
1	B	241	ASN	N-CA-C	5.85	123.25	110.80
1	C	245	GLU	N-CA-C	-5.82	104.93	111.28
1	D	56	ILE	N-CA-C	5.81	116.46	110.82
1	C	324	THR	N-CA-C	5.73	118.90	109.85
1	D	121	ALA	N-CA-C	-5.71	105.05	111.28
1	D	324	THR	N-CA-C	5.52	118.58	109.85
1	A	245	GLU	N-CA-C	-5.51	105.18	111.07
1	C	241	ASN	N-CA-C	5.38	122.25	110.80
1	B	56	ILE	N-CA-C	5.35	116.83	111.00
1	A	324	THR	N-CA-C	5.34	118.29	109.85
1	A	297	GLU	N-CA-C	5.33	116.77	111.07
1	A	56	ILE	N-CA-C	5.16	116.63	111.00
1	B	269	ASN	N-CA-C	5.06	117.93	110.59
1	A	344	ILE	N-CA-C	-5.03	105.42	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2413	0	2411	52	0
1	B	2471	0	2452	43	0
1	C	2404	0	2398	54	1
1	D	2452	0	2437	59	1
2	E	109	0	98	8	0
2	F	109	0	98	5	0
2	G	109	0	98	4	0
2	H	109	0	98	4	0
3	A	28	0	12	2	0
3	B	28	0	12	2	0
3	C	28	0	12	3	0
3	D	28	0	12	3	0
4	A	46	0	0	8	0
4	B	29	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	30	0	0	3	0
4	D	25	0	0	1	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	1	0
4	H	1	0	0	0	0
All	All	10424	0	10138	217	1

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 11.

All (217) 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:D:208:ARG:H	1:D:208:ARG:HD2	1.15	1.09
1:D:55:ILE:HA	1:D:60:GLY:HA2	1.39	1.03
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.38	1.03
1:C:55:ILE:HA	1:C:60:GLY:HA2	1.39	1.03
1:B:55:ILE:HA	1:B:60:GLY:HA2	1.38	1.02
1:A:240:MET:HG2	1:A:241:ASN:H	1.29	0.94
1:A:240:MET:HG2	1:A:241:ASN:N	1.89	0.86
1:D:339:VAL:O	1:D:342:VAL:HG12	1.74	0.85
1:C:339:VAL:O	1:C:342:VAL:HG12	1.77	0.83
1:D:235:ALA:HB3	1:D:238:GLU:HG2	1.61	0.83
1:B:339:VAL:O	1:B:342:VAL:HG12	1.77	0.83
1:A:245:GLU:HB3	4:A:360:HOH:O	1.81	0.80
1:D:264:ILE:HG12	1:D:317:LYS:HE3	1.64	0.79
1:B:264:ILE:HG12	1:B:317:LYS:HE3	1.65	0.79
1:A:339:VAL:O	1:A:342:VAL:HG12	1.81	0.79
1:D:240:MET:HG2	1:D:241:ASN:H	1.51	0.74
1:A:264:ILE:HG12	1:A:317:LYS:HE3	1.70	0.74
1:B:208:ARG:HH12	2:F:3:VAL:HG21	1.53	0.74
1:A:230:TYR:O	1:A:286:CYS:HB2	1.88	0.73
1:C:60:GLY:HA3	4:C:387:HOH:O	1.89	0.72
1:A:183:GLY:HA2	1:A:204:GLN:CD	2.14	0.72
1:C:264:ILE:HG12	1:C:317:LYS:HE3	1.72	0.72
1:C:253:ILE:HD11	2:G:5:TRP:CZ3	2.27	0.70
1:C:90:ARG:NH2	4:C:369:HOH:O	2.22	0.70
1:D:212:ILE:O	1:D:216:GLU:HG3	1.92	0.70
2:F:3:VAL:HG13	2:F:7:ASP:HB2	1.75	0.69
1:A:232:LEU:O	4:A:357:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HD11	1:C:122:GLU:HG2	1.74	0.69
2:E:3:VAL:CG1	2:E:7:ASP:HB2	2.24	0.68
1:B:39:LEU:HD23	1:B:201:VAL:HB	1.77	0.67
1:D:337:ASP:HB2	4:D:371:HOH:O	1.94	0.66
1:A:52:GLN:OE1	1:A:329:THR:HB	1.96	0.66
1:C:212:ILE:O	1:C:216:GLU:HG3	1.94	0.66
1:C:280:LYS:HG2	4:C:365:HOH:O	1.94	0.66
1:A:101:ALA:HB3	4:A:369:HOH:O	1.96	0.66
1:D:240:MET:CG	1:D:241:ASN:H	2.10	0.65
1:D:234:LEU:HD23	1:D:234:LEU:H	1.63	0.63
1:D:208:ARG:HD2	1:D:208:ARG:N	2.00	0.63
1:C:340:THR:O	1:C:344:ILE:HG12	1.99	0.63
1:C:58:GLU:O	1:C:59:ALA:CB	2.47	0.63
1:D:264:ILE:CG1	1:D:317:LYS:HE3	2.29	0.62
1:B:239:GLU:O	1:B:240:MET:HB3	1.99	0.62
1:D:58:GLU:O	1:D:59:ALA:CB	2.47	0.62
1:C:264:ILE:CG1	1:C:317:LYS:HE3	2.30	0.62
1:A:183:GLY:HA2	1:A:204:GLN:NE2	2.14	0.62
1:A:212:ILE:O	1:A:216:GLU:HG3	2.01	0.61
1:B:58:GLU:O	1:B:59:ALA:CB	2.48	0.61
1:A:58:GLU:O	1:A:59:ALA:CB	2.48	0.61
1:B:264:ILE:CG1	1:B:317:LYS:HE3	2.30	0.61
1:D:240:MET:HG2	1:D:241:ASN:N	2.09	0.61
1:A:106:GLN:OE1	4:A:361:HOH:O	2.16	0.61
1:B:239:GLU:O	1:B:239:GLU:HG3	2.00	0.61
1:D:208:ARG:O	1:D:212:ILE:HG12	2.01	0.61
1:A:264:ILE:CG1	1:A:317:LYS:HE3	2.30	0.61
1:B:241:ASN:HB2	4:B:360:HOH:O	2.00	0.61
1:B:52:GLN:OE1	1:B:329:THR:HB	2.00	0.60
1:C:58:GLU:O	1:C:59:ALA:HB3	2.02	0.60
1:D:254:CYS:SG	1:D:319:ILE:HD11	2.42	0.60
1:A:265:ILE:CD1	1:A:339:VAL:HG13	2.31	0.59
1:C:62:SER:OG	1:C:65:GLU:HG3	2.03	0.59
1:B:326:ALA:HB3	3:B:356:GDP:N7	2.18	0.58
1:A:58:GLU:O	1:A:59:ALA:HB3	2.03	0.58
1:A:183:GLY:HA2	1:A:204:GLN:OE1	2.03	0.58
1:D:58:GLU:O	1:D:59:ALA:HB3	2.02	0.58
1:D:62:SER:OG	1:D:65:GLU:HG3	2.03	0.58
1:B:207:GLU:HA	2:F:1:SER:O	2.04	0.58
1:D:52:GLN:OE1	1:D:329:THR:HB	2.03	0.58
1:A:304:GLN:O	1:A:308:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:THR:O	1:D:344:ILE:HG12	2.03	0.58
1:B:58:GLU:O	1:B:59:ALA:HB3	2.03	0.57
1:B:304:GLN:O	1:B:308:GLU:HG3	2.03	0.57
1:C:205:ARG:HD2	4:G:63:HOH:O	2.04	0.57
1:C:204:GLN:H	1:C:204:GLN:CD	2.13	0.57
1:C:209:LYS:HB2	1:D:237:ASP:HB3	1.87	0.57
1:B:212:ILE:O	1:B:216:GLU:HG3	2.05	0.56
1:B:254:CYS:SG	1:B:319:ILE:HD11	2.46	0.56
1:D:39:LEU:HD23	1:D:201:VAL:HB	1.87	0.56
1:D:188:HIS:CE1	1:D:197:LYS:HD2	2.39	0.56
1:A:208:ARG:O	1:A:212:ILE:HG12	2.05	0.56
1:A:212:ILE:HD13	2:E:8:PHE:HZ	1.70	0.56
1:A:254:CYS:SG	1:A:319:ILE:HD11	2.45	0.56
1:C:188:HIS:CE1	1:C:197:LYS:HD2	2.41	0.56
1:B:54:LYS:HA	1:B:58:GLU:HB2	1.87	0.56
1:A:188:HIS:CE1	1:A:197:LYS:HD2	2.40	0.56
1:C:52:GLN:OE1	1:C:329:THR:HB	2.06	0.55
1:B:62:SER:OG	1:B:65:GLU:HG3	2.06	0.55
1:C:215:PHE:CD2	1:C:259:PHE:HZ	2.24	0.55
1:D:230:TYR:O	1:D:286:CYS:HB2	2.07	0.55
1:D:240:MET:CG	1:D:241:ASN:N	2.69	0.55
2:E:3:VAL:HG12	2:E:4:THR:N	2.22	0.55
1:A:265:ILE:HD13	1:A:339:VAL:HG13	1.89	0.55
1:C:39:LEU:HD23	1:C:201:VAL:HB	1.89	0.55
2:H:3:VAL:HG12	2:H:4:THR:O	2.06	0.55
1:D:265:ILE:CD1	1:D:339:VAL:HG13	2.37	0.54
2:E:7:ASP:O	2:E:11:GLU:HG3	2.08	0.54
1:A:54:LYS:HA	1:A:58:GLU:HB2	1.89	0.54
1:D:205:ARG:O	2:H:2:ARG:HD2	2.07	0.53
1:C:254:CYS:SG	1:C:319:ILE:HD11	2.48	0.53
1:D:206:SER:HB3	1:D:210:LYS:HD2	1.89	0.53
1:A:62:SER:OG	1:A:65:GLU:HG3	2.09	0.53
2:F:3:VAL:HG12	2:F:4:THR:O	2.09	0.53
1:C:54:LYS:HA	1:C:58:GLU:HB2	1.91	0.53
1:B:265:ILE:HD13	1:B:339:VAL:HG13	1.91	0.52
1:C:110:LEU:CD1	1:C:122:GLU:HG2	2.39	0.52
1:B:340:THR:O	1:B:344:ILE:HG12	2.09	0.52
2:E:3:VAL:HG11	2:E:7:ASP:HB2	1.92	0.52
1:B:39:LEU:CD2	1:B:201:VAL:HB	2.40	0.51
2:E:3:VAL:HG12	2:E:7:ASP:HB2	1.91	0.51
1:B:188:HIS:CE1	1:B:197:LYS:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ASP:O	1:D:162:ILE:HG12	2.11	0.51
1:D:54:LYS:HA	1:D:58:GLU:HB2	1.91	0.51
1:C:326:ALA:HB3	3:C:357:GDP:N7	2.26	0.51
1:C:34:VAL:HG21	1:C:194:LEU:HD13	1.93	0.51
1:A:36:LEU:HD11	1:A:220:ALA:HB3	1.94	0.50
1:A:61:TYR:H	1:A:171:GLN:NE2	2.09	0.50
1:B:265:ILE:CD1	1:B:339:VAL:HG13	2.41	0.50
1:C:39:LEU:CD2	1:C:201:VAL:HB	2.42	0.50
1:D:265:ILE:HD13	1:D:339:VAL:HG13	1.93	0.50
1:A:257:LYS:HG3	1:A:258:TRP:CD1	2.47	0.50
1:D:257:LYS:HG3	1:D:258:TRP:CD1	2.47	0.50
1:D:304:GLN:O	1:D:308:GLU:HG3	2.12	0.50
1:A:326:ALA:HB3	3:A:355:GDP:N7	2.27	0.49
1:C:55:ILE:HA	1:C:60:GLY:CA	2.28	0.49
1:D:184:ILE:HG13	1:D:204:GLN:HE21	1.76	0.49
1:D:234:LEU:O	1:D:235:ALA:O	2.29	0.49
1:D:239:GLU:O	1:D:240:MET:HB3	2.11	0.49
1:C:320:TYR:CE1	1:C:342:VAL:HG21	2.47	0.49
1:B:208:ARG:NH1	2:F:3:VAL:HG21	2.25	0.49
1:D:326:ALA:HB3	3:D:358:GDP:N7	2.28	0.49
1:A:187:THR:HG22	1:A:198:MET:HB3	1.94	0.48
1:B:257:LYS:HG3	1:B:258:TRP:CD1	2.49	0.48
1:C:34:VAL:HG13	1:C:219:THR:HG21	1.96	0.48
1:D:110:LEU:CD1	1:D:122:GLU:HG2	2.43	0.48
1:C:304:GLN:O	1:C:308:GLU:HG3	2.13	0.48
1:A:340:THR:O	1:A:344:ILE:HG12	2.14	0.48
1:A:209:LYS:HE3	1:A:209:LYS:HA	1.95	0.48
1:B:78:ILE:HG21	1:B:111:ALA:HB1	1.96	0.48
1:C:275:GLU:O	1:C:278:ILE:HG22	2.13	0.48
1:C:257:LYS:HG3	1:C:258:TRP:CD1	2.48	0.48
1:D:61:TYR:H	1:D:171:GLN:NE2	2.11	0.47
1:D:235:ALA:HB3	1:D:238:GLU:CG	2.39	0.47
1:C:40:GLY:HA2	1:C:223:PHE:CE1	2.49	0.47
1:A:36:LEU:CD1	1:A:220:ALA:HB3	2.45	0.47
1:D:44:SER:N	3:D:358:GDP:O3B	2.48	0.47
1:D:238:GLU:O	1:D:238:GLU:HG3	2.15	0.47
1:A:210:LYS:HG3	4:A:396:HOH:O	2.14	0.47
1:D:275:GLU:O	1:D:278:ILE:HG22	2.15	0.47
1:D:46:LYS:HB2	3:D:358:GDP:O1B	2.15	0.46
1:C:46:LYS:HB2	3:C:357:GDP:O1B	2.15	0.46
1:D:55:ILE:HA	1:D:60:GLY:CA	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:HD13	1:C:339:VAL:HG13	1.98	0.46
1:B:320:TYR:CE1	1:B:342:VAL:HG21	2.51	0.46
1:B:158:ASP:O	1:B:162:ILE:HG12	2.16	0.46
1:D:39:LEU:CD2	1:D:201:VAL:HB	2.46	0.46
2:H:3:VAL:HG13	2:H:7:ASP:HB2	1.97	0.46
1:A:106:GLN:HB2	4:A:361:HOH:O	2.15	0.45
1:B:34:VAL:HG13	1:B:219:THR:HG21	1.98	0.45
1:B:63:GLU:O	1:B:67:LYS:HG3	2.16	0.45
1:B:187:THR:HG22	1:B:198:MET:HB3	1.97	0.45
1:A:100:ARG:HA	1:A:100:ARG:NE	2.31	0.45
1:C:230:TYR:O	1:C:286:CYS:HB2	2.16	0.45
1:C:265:ILE:CD1	1:C:339:VAL:HG13	2.46	0.45
1:C:215:PHE:CZ	2:G:5:TRP:HB2	2.52	0.45
1:A:44:SER:N	3:A:355:GDP:O3B	2.50	0.44
1:B:275:GLU:O	1:B:278:ILE:HG22	2.18	0.44
1:C:158:ASP:O	1:C:162:ILE:HG12	2.17	0.44
1:B:55:ILE:HA	1:B:60:GLY:CA	2.27	0.44
1:B:239:GLU:O	1:B:240:MET:CB	2.66	0.44
1:A:63:GLU:O	1:A:67:LYS:HG3	2.18	0.44
1:A:110:LEU:HD13	1:A:122:GLU:HG2	1.99	0.44
1:B:100:ARG:HA	1:B:100:ARG:NE	2.33	0.44
1:C:211:TRP:O	1:C:215:PHE:HD1	2.01	0.44
1:C:212:ILE:HD13	2:G:8:PHE:HZ	1.83	0.44
1:A:215:PHE:HZ	2:E:5:TRP:HB2	1.82	0.43
1:D:63:GLU:O	1:D:67:LYS:HG3	2.18	0.43
1:D:236:GLU:C	1:D:238:GLU:N	2.76	0.43
1:D:78:ILE:O	1:D:82:ILE:HG13	2.18	0.43
1:C:43:GLU:HA	3:C:357:GDP:H5"	2.00	0.43
1:D:187:THR:HG22	1:D:198:MET:HB3	2.00	0.43
1:B:71:ALA:HB3	4:B:369:HOH:O	2.18	0.43
1:A:240:MET:N	4:A:375:HOH:O	2.52	0.43
1:A:106:GLN:HG3	1:A:110:LEU:CD1	2.49	0.43
1:A:185:VAL:HB	1:A:200:ASP:HB3	2.00	0.43
1:B:61:TYR:H	1:B:171:GLN:NE2	2.16	0.43
1:D:100:ARG:NE	1:D:100:ARG:HA	2.34	0.43
1:A:320:TYR:CE1	1:A:342:VAL:HG21	2.53	0.42
1:B:46:LYS:HB2	3:B:356:GDP:O1B	2.19	0.42
1:C:61:TYR:H	1:C:171:GLN:NE2	2.16	0.42
2:H:3:VAL:HG12	2:H:4:THR:N	2.34	0.42
1:A:275:GLU:O	1:A:278:ILE:HG22	2.20	0.42
1:A:55:ILE:HA	1:A:60:GLY:CA	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.84	0.42
1:D:184:ILE:N	1:D:204:GLN:NE2	2.68	0.42
1:D:110:LEU:HD13	1:D:122:GLU:HG2	2.02	0.42
1:D:284:THR:HA	1:D:287:TYR:O	2.20	0.42
2:E:3:VAL:HG12	2:E:4:THR:H	1.83	0.42
1:C:252:SER:HB3	2:G:6:TYR:CE1	2.55	0.41
1:D:34:VAL:HG11	1:D:343:ILE:HD13	2.02	0.41
1:D:234:LEU:H	1:D:234:LEU:CD2	2.31	0.41
1:A:207:GLU:HB2	1:A:210:LYS:HE2	2.02	0.41
1:B:143:SER:HA	1:B:146:TYR:CE1	2.56	0.41
1:C:209:LYS:HD2	1:D:237:ASP:HA	2.02	0.41
1:D:106:GLN:HG3	1:D:110:LEU:HG	2.02	0.41
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.86	0.41
1:C:194:LEU:HD11	1:C:344:ILE:HD13	2.03	0.41
1:C:215:PHE:CD2	1:C:259:PHE:CZ	3.07	0.41
1:A:216:GLU:HB2	4:A:384:HOH:O	2.20	0.41
1:B:42:GLY:O	1:B:43:GLU:HB2	2.21	0.41
1:C:159:LEU:HD23	1:C:159:LEU:HA	1.87	0.41
1:D:320:TYR:CE1	1:D:342:VAL:HG21	2.56	0.41
1:C:186:GLU:OE2	1:C:188:HIS:CE1	2.73	0.41
1:C:278:ILE:HD12	1:C:278:ILE:HA	1.96	0.40
1:B:143:SER:HA	1:B:146:TYR:CZ	2.57	0.40
1:C:37:LEU:HD12	1:C:37:LEU:HA	1.90	0.40
1:A:74:TYR:HE1	1:A:162:ILE:HG22	1.86	0.40
1:B:164:GLN:HA	1:B:165:PRO:HD3	1.93	0.40
1:C:284:THR:HA	1:C:287:TYR:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLU:OE1	1:D:257:LYS:NZ[2_656]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/329 (89%)	291 (99%)	1 (0%)	1 (0%)	36	55
1	B	303/329 (92%)	297 (98%)	2 (1%)	4 (1%)	9	18
1	C	292/329 (89%)	288 (99%)	2 (1%)	2 (1%)	18	34
1	D	300/329 (91%)	292 (97%)	6 (2%)	2 (1%)	18	34
2	E	10/16 (62%)	10 (100%)	0	0	100	100
2	F	10/16 (62%)	10 (100%)	0	0	100	100
2	G	10/16 (62%)	10 (100%)	0	0	100	100
2	H	10/16 (62%)	9 (90%)	1 (10%)	0	100	100
All	All	1228/1380 (89%)	1207 (98%)	12 (1%)	9 (1%)	18	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	C	241	ASN
1	D	235	ALA
1	A	59	ALA
1	B	59	ALA
1	C	59	ALA
1	D	59	ALA
1	B	236	GLU
1	B	235	ALA

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	263/284 (93%)	253 (96%)	10 (4%)	29	56
1	B	268/284 (94%)	258 (96%)	10 (4%)	30	57
1	C	262/284 (92%)	255 (97%)	7 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	267/284 (94%)	260 (97%)	7 (3%)	40	68
2	E	12/16 (75%)	11 (92%)	1 (8%)	10	22
2	F	12/16 (75%)	11 (92%)	1 (8%)	10	22
2	G	12/16 (75%)	12 (100%)	0	100	100
2	H	12/16 (75%)	11 (92%)	1 (8%)	10	22
All	All	1108/1200 (92%)	1071 (97%)	37 (3%)	33	61

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	37	LEU
1	A	159	LEU
1	A	193	ASP
1	A	208	ARG
1	A	209	LYS
1	A	240	MET
1	A	242	ARG
1	A	249	LEU
1	A	329	THR
1	B	37	LEU
1	B	47	SER
1	B	159	LEU
1	B	193	ASP
1	B	207	GLU
1	B	239	GLU
1	B	241	ASN
1	B	242	ARG
1	B	249	LEU
1	B	329	THR
1	C	37	LEU
1	C	159	LEU
1	C	193	ASP
1	C	210	LYS
1	C	242	ARG
1	C	249	LEU
1	C	329	THR
1	D	37	LEU
1	D	159	LEU
1	D	193	ASP

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Mol	Chain	Res	Type
1	D	239	GLU
1	D	242	ARG
1	D	249	LEU
1	D	329	THR
2	E	10	MET
2	F	3	VAL
2	H	10	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	147	GLN
1	A	166	ASN
1	A	171	GLN
1	A	188	HIS
1	A	241	ASN
1	A	333	GLN
1	B	79	GLN
1	B	147	GLN
1	B	166	ASN
1	B	171	GLN
1	B	188	HIS
1	B	241	ASN
1	B	333	GLN
1	C	79	GLN
1	C	147	GLN
1	C	166	ASN
1	C	171	GLN
1	C	188	HIS
1	C	241	ASN
1	C	333	GLN
1	D	79	GLN
1	D	147	GLN
1	D	171	GLN
1	D	188	HIS
1	D	213	HIS
1	D	241	ASN
1	D	333	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GDP	A	355	-	29,30,30	1.49	3 (10%)	45,47,47	2.34	10 (22%)
3	GDP	D	358	-	29,30,30	1.61	4 (13%)	45,47,47	2.35	10 (22%)
3	GDP	C	357	-	29,30,30	1.47	3 (10%)	45,47,47	2.35	10 (22%)
3	GDP	B	356	-	29,30,30	1.71	6 (20%)	45,47,47	2.38	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	355	-	-	3/16/32/32	0/3/3/3
3	GDP	D	358	-	-	3/16/32/32	0/3/3/3
3	GDP	C	357	-	-	3/16/32/32	0/3/3/3
3	GDP	B	356	-	-	3/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	356	GDP	PA-O3A	5.91	1.65	1.59
3	D	358	GDP	PA-O3A	5.89	1.65	1.59
3	C	357	GDP	PA-O3A	4.96	1.64	1.59
3	A	355	GDP	PA-O3A	4.72	1.64	1.59
3	D	358	GDP	C5'-C4'	2.89	1.60	1.51
3	B	356	GDP	C5'-C4'	2.73	1.59	1.51
3	A	355	GDP	C5'-C4'	2.72	1.59	1.51
3	B	356	GDP	C6-N1	2.66	1.43	1.38
3	C	357	GDP	C5'-C4'	2.52	1.59	1.51
3	A	355	GDP	C3'-C4'	2.50	1.59	1.53
3	B	356	GDP	C3'-C4'	2.43	1.59	1.53
3	C	357	GDP	C3'-C4'	2.39	1.59	1.53
3	D	358	GDP	C3'-C4'	2.28	1.58	1.53
3	D	358	GDP	C6-N1	2.13	1.42	1.38
3	B	356	GDP	PA-O2A	-2.06	1.45	1.55
3	B	356	GDP	PB-O1B	-2.02	1.44	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	356	GDP	O2A-PA-O3A	9.34	132.52	107.27
3	A	355	GDP	O2A-PA-O3A	9.13	131.94	107.27
3	D	358	GDP	O2A-PA-O3A	9.06	131.75	107.27
3	C	357	GDP	O2A-PA-O3A	8.81	131.08	107.27
3	C	357	GDP	O5'-PA-O1A	-7.43	79.48	108.94
3	B	356	GDP	O5'-PA-O1A	-7.36	79.75	108.94
3	D	358	GDP	O5'-PA-O1A	-7.35	79.80	108.94
3	A	355	GDP	O5'-PA-O1A	-7.30	80.01	108.94
3	C	357	GDP	O3B-PB-O3A	4.65	120.24	104.64
3	D	358	GDP	O3B-PB-O3A	4.44	119.54	104.64
3	A	355	GDP	O3B-PB-O3A	4.43	119.48	104.64
3	B	356	GDP	O3A-PA-O1A	-4.34	97.65	110.70
3	B	356	GDP	O3B-PB-O3A	4.34	119.18	104.64
3	D	358	GDP	O3A-PA-O1A	-4.08	98.44	110.70
3	C	357	GDP	O3A-PA-O1A	-4.01	98.64	110.70
3	A	355	GDP	O3A-PA-O1A	-3.93	98.89	110.70
3	C	357	GDP	O2A-PA-O1A	3.83	130.28	112.44
3	B	356	GDP	O2A-PA-O1A	3.74	129.82	112.44
3	D	358	GDP	O2A-PA-O1A	3.73	129.79	112.44
3	A	355	GDP	O2A-PA-O1A	3.59	129.14	112.44
3	B	356	GDP	O4'-C4'-C3'	-3.15	98.89	105.15
3	A	355	GDP	O4'-C4'-C3'	-3.13	98.94	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	357	GDP	O4'-C4'-C3'	-3.09	99.01	105.15
3	A	355	GDP	PA-O5'-C5'	3.09	139.05	121.35
3	D	358	GDP	O4'-C4'-C3'	-3.04	99.12	105.15
3	B	356	GDP	PA-O5'-C5'	2.99	138.46	121.35
3	D	358	GDP	PA-O5'-C5'	2.93	138.15	121.35
3	C	357	GDP	PA-O5'-C5'	2.78	137.31	121.35
3	C	357	GDP	O2A-PA-O5'	-2.61	95.72	107.57
3	D	358	GDP	O2A-PA-O5'	-2.59	95.83	107.57
3	B	356	GDP	O2A-PA-O5'	-2.43	96.55	107.57
3	A	355	GDP	O3B-PB-O2B	-2.26	99.33	107.80
3	A	355	GDP	O5'-C5'-C4'	-2.23	101.41	108.99
3	B	356	GDP	O5'-C5'-C4'	-2.21	101.47	108.99
3	D	358	GDP	O3B-PB-O2B	-2.19	99.60	107.80
3	C	357	GDP	O5'-C5'-C4'	-2.16	101.64	108.99
3	D	358	GDP	O5'-C5'-C4'	-2.09	101.87	108.99
3	B	356	GDP	O3B-PB-O2B	-2.09	99.96	107.80
3	A	355	GDP	O2A-PA-O5'	-2.04	98.34	107.57
3	C	357	GDP	O3B-PB-O2B	-2.03	100.19	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	355	GDP	O4'-C4'-C5'-O5'
3	B	356	GDP	O4'-C4'-C5'-O5'
3	C	357	GDP	O4'-C4'-C5'-O5'
3	D	358	GDP	O4'-C4'-C5'-O5'
3	A	355	GDP	C3'-C4'-C5'-O5'
3	B	356	GDP	C3'-C4'-C5'-O5'
3	D	358	GDP	C3'-C4'-C5'-O5'
3	C	357	GDP	C3'-C4'-C5'-O5'
3	A	355	GDP	PB-O3A-PA-O2A
3	B	356	GDP	PB-O3A-PA-O2A
3	C	357	GDP	PB-O3A-PA-O2A
3	D	358	GDP	PB-O3A-PA-O2A

There are no ring outliers.

4 monomers are involved in 10 short contacts:

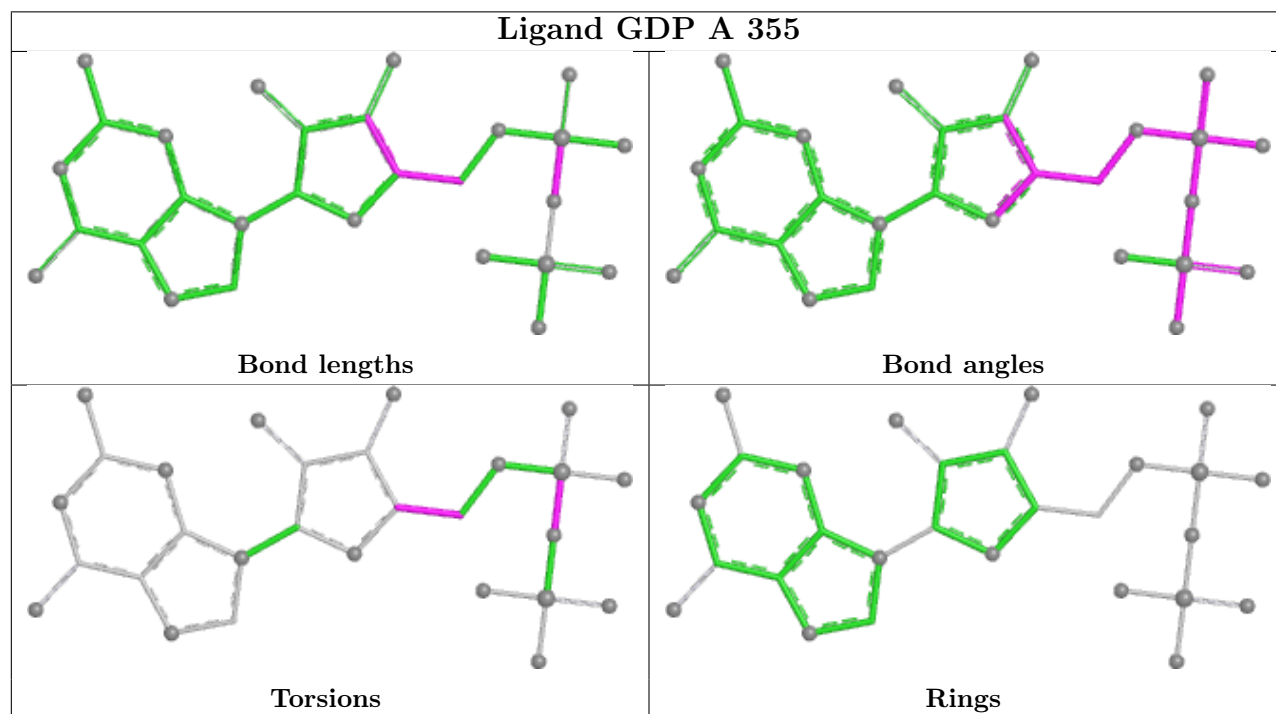
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	355	GDP	2	0

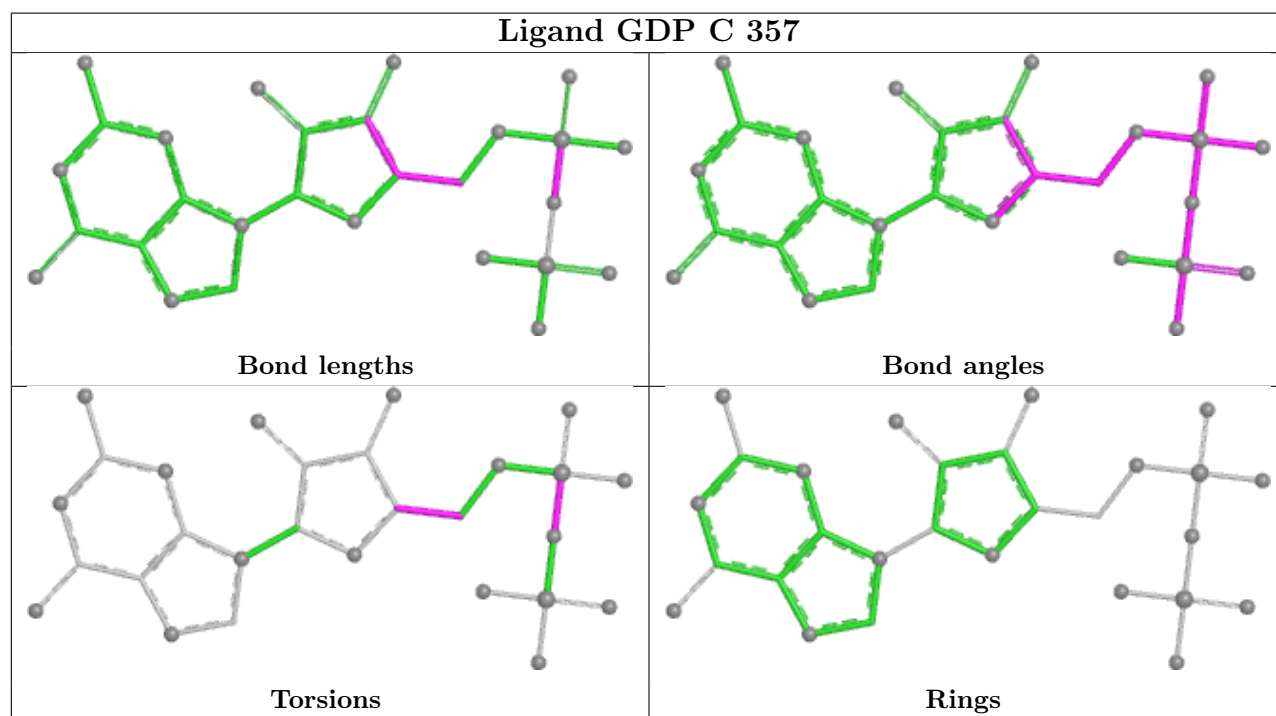
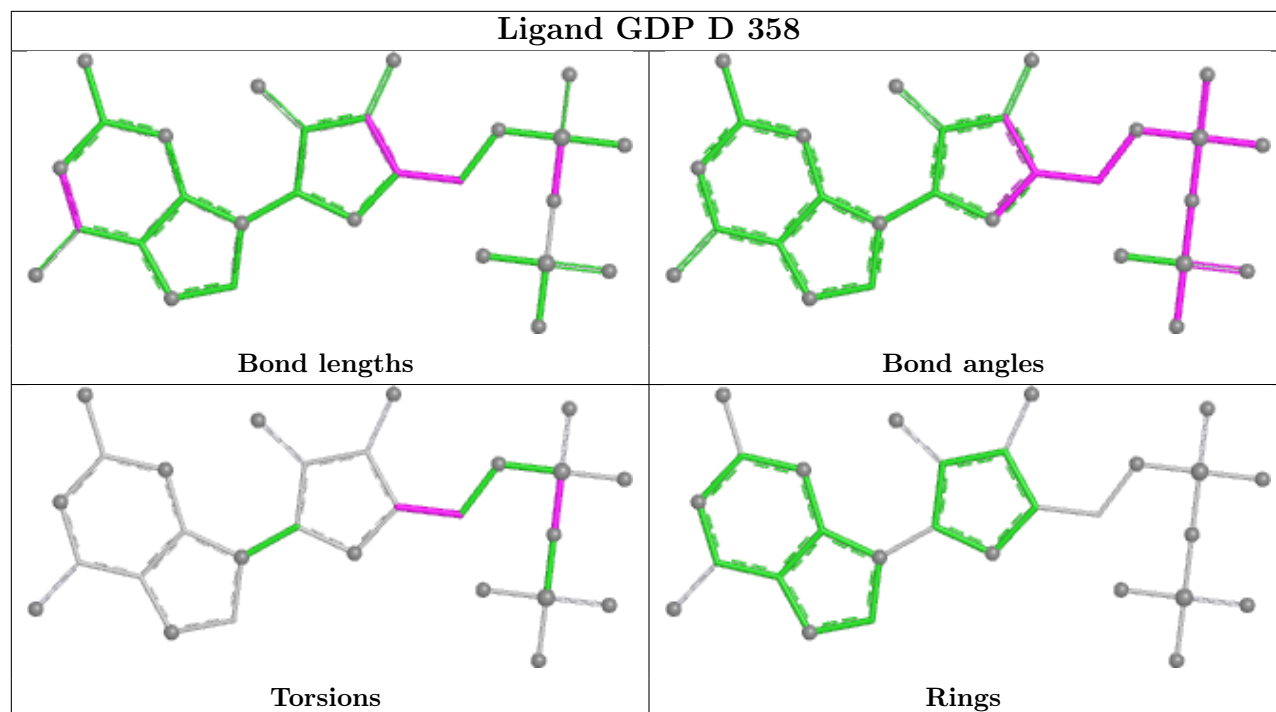
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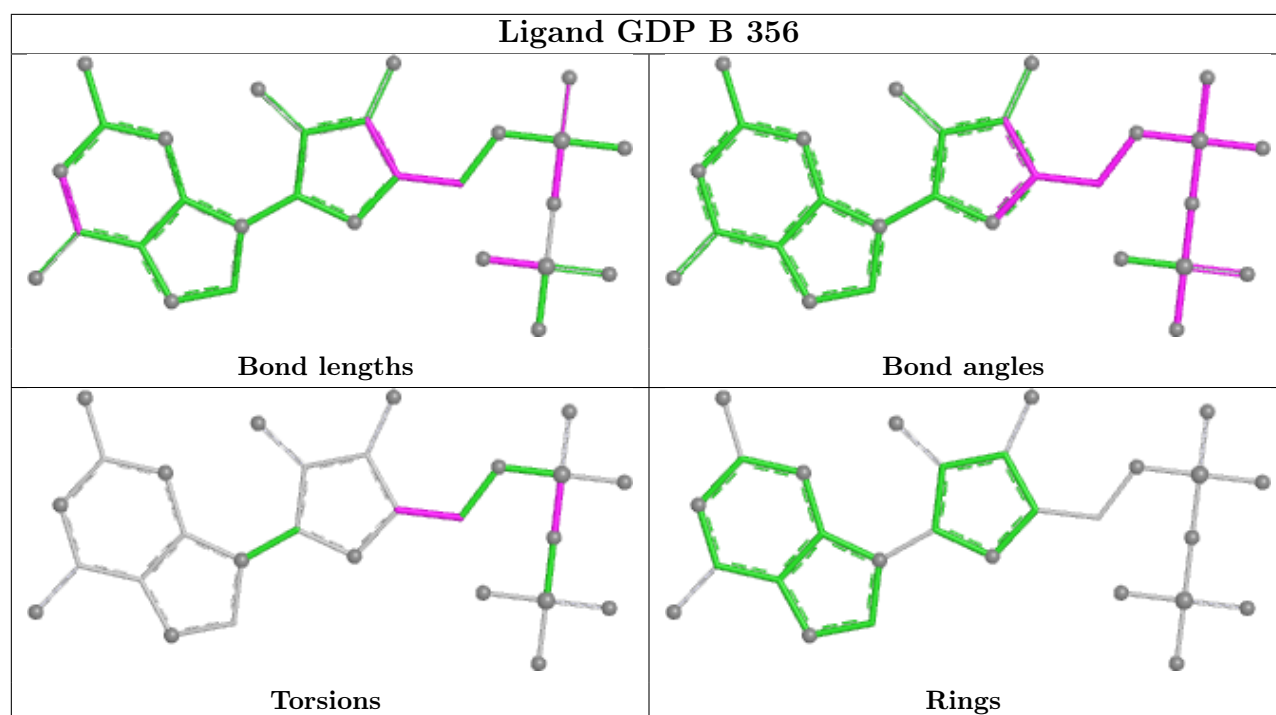
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	358	GDP	3	0
3	C	357	GDP	3	0
3	B	356	GDP	2	0

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 [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	299/329 (90%)	0.69	32 (10%) 11 9	19, 40, 85, 154	0
1	B	307/329 (93%)	0.35	20 (6%) 25 22	16, 37, 78, 136	0
1	C	298/329 (90%)	0.53	29 (9%) 13 11	21, 38, 80, 104	0
1	D	304/329 (92%)	0.68	42 (13%) 6 5	22, 43, 96, 171	0
2	E	12/16 (75%)	1.52	3 (25%) 2 1	43, 64, 84, 142	0
2	F	12/16 (75%)	0.61	3 (25%) 2 1	24, 44, 69, 110	0
2	G	12/16 (75%)	0.71	1 (8%) 17 15	34, 48, 91, 130	0
2	H	12/16 (75%)	1.51	5 (41%) 0 0	43, 66, 100, 148	0
All	All	1256/1380 (91%)	0.58	135 (10%) 11 9	16, 40, 85, 171	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	258	TRP	9.0
1	C	257	LYS	7.8
1	A	64	GLU	7.1
1	A	258	TRP	6.1
1	A	233	VAL	5.6
1	C	316	THR	5.5
1	C	344	ILE	5.4
1	A	345	LYS	5.3
1	A	60	GLY	5.3
1	B	257	LYS	5.2
1	A	181	THR	4.9
1	C	258	TRP	4.8
1	D	122	GLU	4.6
1	D	344	ILE	4.6
1	D	60	GLY	4.5
1	A	257	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	241	ASN	4.1
1	A	183	GLY	4.1
1	A	204	GLN	4.1
1	A	122	GLU	4.0
1	C	60	GLY	4.0
1	C	241	ASN	4.0
1	A	213	HIS	3.9
1	D	257	LYS	3.9
2	G	12	ASP	3.9
2	H	12	ASP	3.9
1	D	261	ASP	3.8
1	A	344	ILE	3.8
1	A	59	ALA	3.7
1	B	105	ARG	3.7
1	A	245	GLU	3.7
1	D	259	PHE	3.7
1	D	336	PHE	3.7
2	F	12	ASP	3.7
1	D	58	GLU	3.6
1	B	344	ILE	3.6
1	C	315	ASP	3.5
1	A	261	ASP	3.5
1	B	236	GLU	3.5
1	D	254	CYS	3.5
1	D	188	HIS	3.5
1	C	59	ALA	3.5
1	A	105	ARG	3.4
1	B	188	HIS	3.3
1	D	59	ALA	3.3
1	B	112	GLY	3.3
1	D	239	GLU	3.3
1	C	105	ARG	3.3
1	A	241	ASN	3.2
1	B	258	TRP	3.2
1	D	66	CYS	3.1
1	A	128	LYS	3.1
1	C	166	ASN	3.1
2	H	2	ARG	3.1
1	C	343	ILE	3.1
2	E	12	ASP	3.0
2	H	8	PHE	2.9
1	A	90	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	64	GLU	2.8
1	C	186	GLU	2.8
1	A	166	ASN	2.7
1	C	342	VAL	2.7
1	D	192	LYS	2.7
2	E	1	SER	2.7
1	D	262	THR	2.7
1	A	313	ARG	2.7
1	D	313	ARG	2.7
1	C	188	HIS	2.7
1	A	182	THR	2.7
1	B	102	ASP	2.6
1	C	197	LYS	2.6
1	A	79	GLN	2.6
1	D	57	HIS	2.6
1	D	315	ASP	2.6
1	A	232	LEU	2.6
1	C	205	ARG	2.5
1	D	111	ALA	2.5
1	B	60	GLY	2.5
1	C	122	GLU	2.5
1	B	207	GLU	2.5
1	C	132	LYS	2.5
1	A	61	TYR	2.4
1	A	343	ILE	2.4
1	D	237	ASP	2.4
1	D	337	ASP	2.4
1	C	34	VAL	2.4
1	B	235	ALA	2.4
1	D	191	PHE	2.4
1	A	185	VAL	2.4
1	B	59	ALA	2.4
1	D	314	LYS	2.4
1	D	318	GLU	2.4
1	D	105	ARG	2.3
1	A	147	GLN	2.3
1	D	92	LYS	2.3
2	E	3	VAL	2.3
1	C	260	THR	2.3
1	A	150	ASP	2.3
1	B	68	GLN	2.3
1	B	106	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	195	HIS	2.2
1	D	316	THR	2.2
1	D	215	PHE	2.2
1	D	221	ILE	2.2
1	A	288	PRO	2.2
1	D	235	ALA	2.2
1	C	106	GLN	2.2
1	D	240	MET	2.2
1	A	58	GLU	2.2
1	B	261	ASP	2.2
1	C	64	GLU	2.2
1	D	185	VAL	2.1
1	B	241	ASN	2.1
1	C	207	GLU	2.1
2	H	11	GLU	2.1
1	D	213	HIS	2.1
1	C	69	TYR	2.1
1	C	94	ASP	2.1
2	F	1	SER	2.1
1	B	67	LYS	2.1
1	B	280	LYS	2.1
1	D	189	PHE	2.1
1	D	194	LEU	2.1
1	D	260	THR	2.1
1	D	208	ARG	2.1
1	B	167	TYR	2.1
1	C	160	ASP	2.1
2	H	1	SER	2.1
1	D	150	ASP	2.1
1	D	263	SER	2.1
1	A	319	ILE	2.0
1	C	181	THR	2.0
1	C	313	ARG	2.0
2	F	3	VAL	2.0
1	D	255	ASN	2.0

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](#)

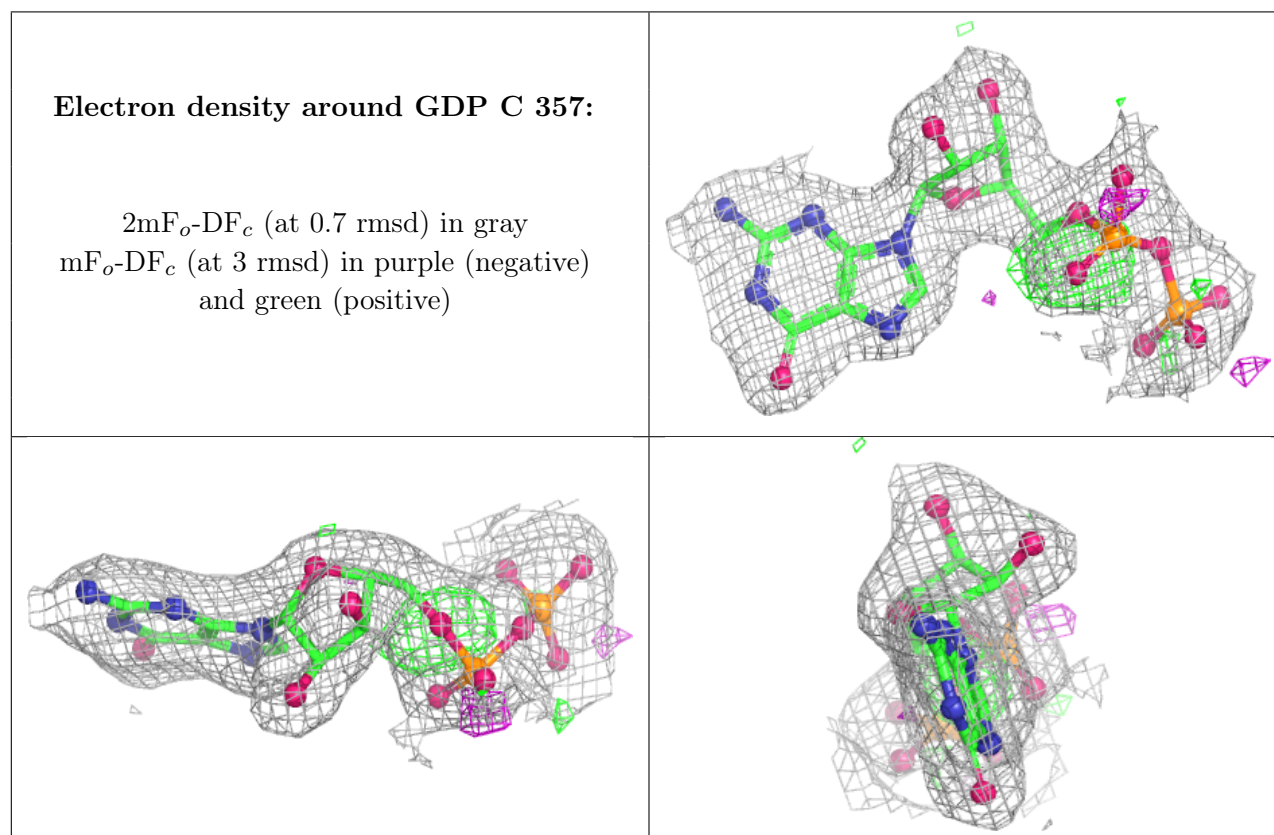
There are no oligosaccharides in this entry.

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, 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.

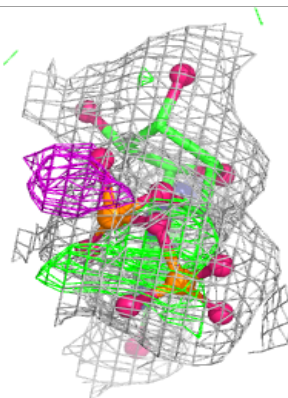
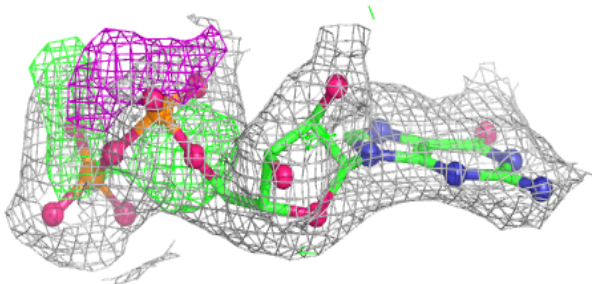
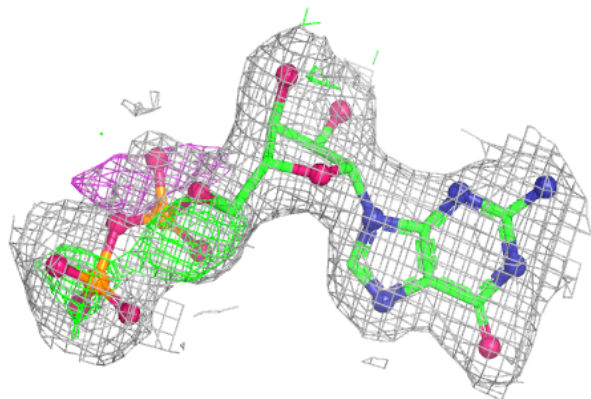
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDP	C	357	28/28	0.90	0.11	25,31,58,58	0
3	GDP	B	356	28/28	0.91	0.12	23,30,48,51	0
3	GDP	A	355	28/28	0.91	0.12	23,31,49,50	0
3	GDP	D	358	28/28	0.91	0.10	28,35,56,59	0

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.

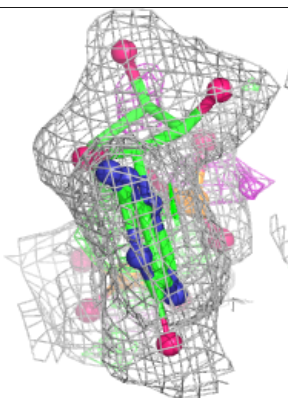
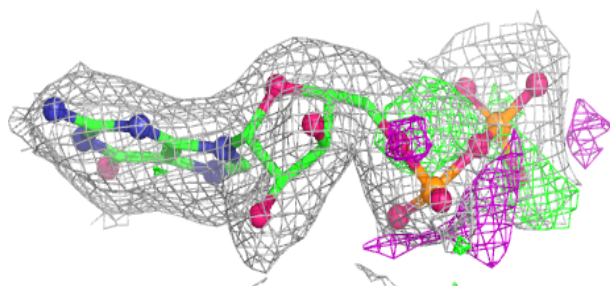
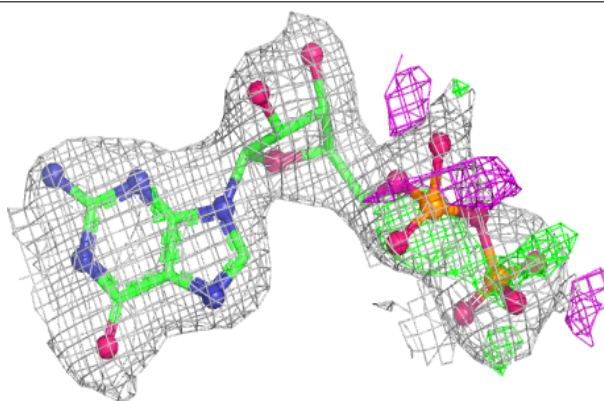


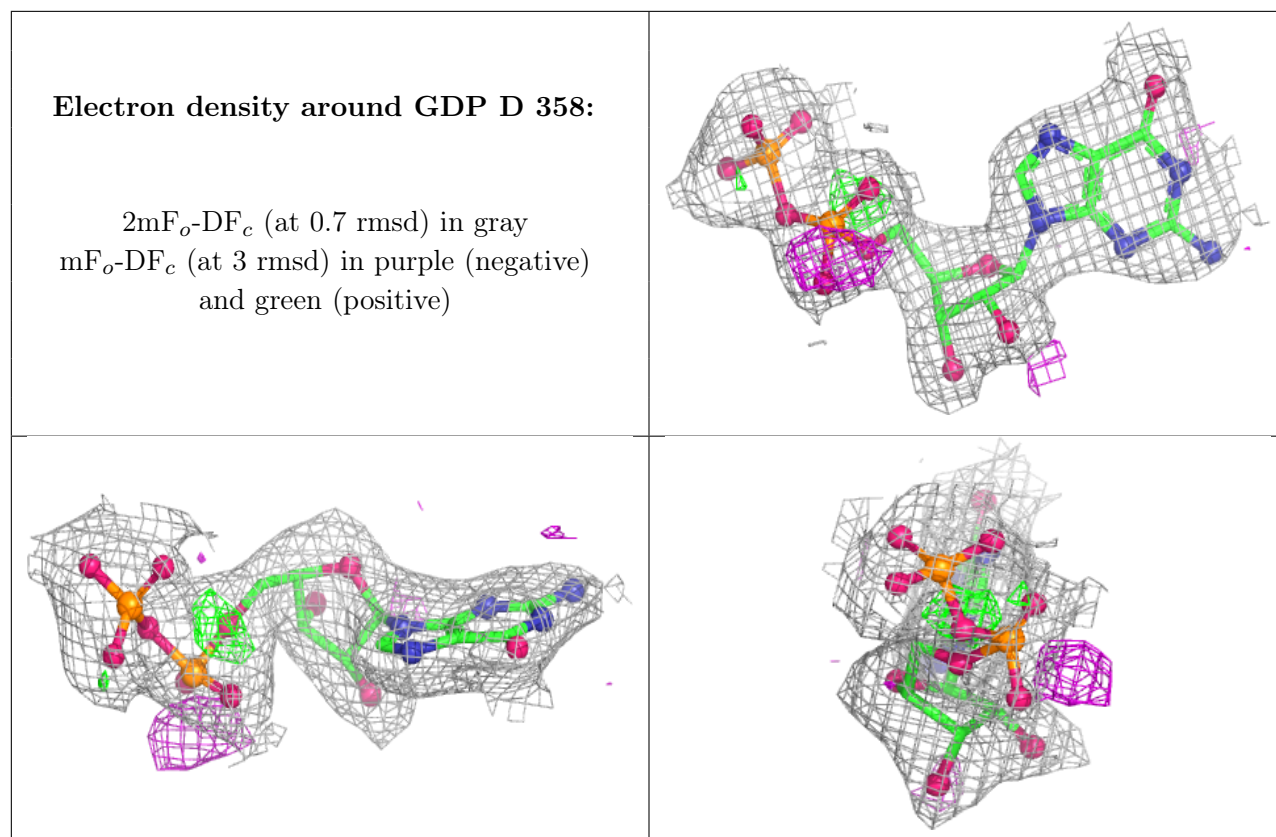
Electron density around GDP B 356:

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

**Electron density around GDP A 355:**

$2mF_o-DF_c$ (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.