



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 11:12 PM UTC

PDB ID : 7TXH / pdb_00007txh
Title : Human MRas Q71R in complex with human Shoc2 LRR domain M173I and human PP1Ca
Authors : Hauseman, Z.J.; Viscomi, J.; Dhembhi, A.; Clark, K.; King, D.A.; Fodor, M.
Deposited on : 2022-02-09
Resolution : 1.95 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)
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

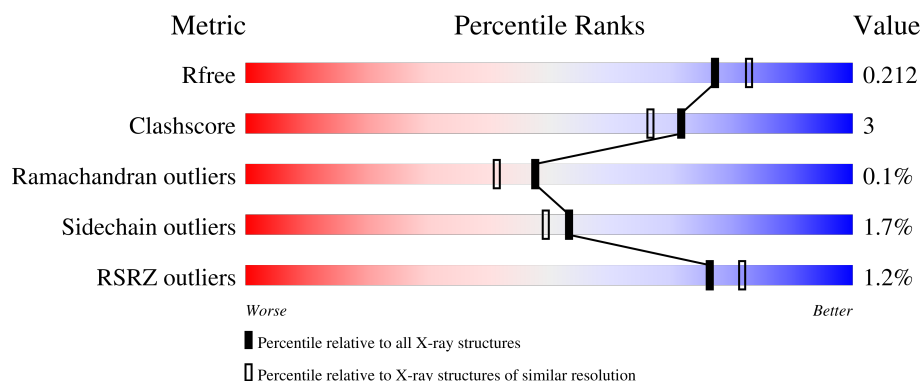
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



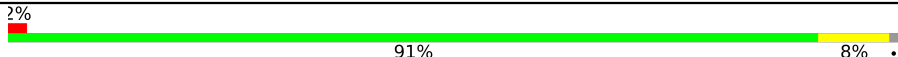
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	180	88% 7% ...
1	D	180	89% 5% 6%
2	B	505	89% 9% ...
2	E	505	91% 7% .
3	C	297	83% 15% .

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Mol	Chain	Length	Quality of chain
3	F	297	 A horizontal bar chart showing the quality of chain F. The bar is green, indicating a high quality. The chart is labeled with '2%' at the start, '91%' in the middle, and '8%' at the end. The bar is divided into three segments: a small red segment at the beginning, a large green segment in the middle, and a small yellow segment at the end.

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
6	GOL	A	203	-	X	-	-
6	GOL	C	504	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17319 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 Ras-related protein M-Ras.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1405	896	241	263	5			
1	D	169	Total	C	N	O	S	0	0	0
			1377	879	237	256	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O14807
A	0	PRO	-	expression tag	UNP O14807
A	71	ARG	GLN	variant	UNP O14807
D	-1	GLY	-	expression tag	UNP O14807
D	0	PRO	-	expression tag	UNP O14807
D	71	ARG	GLN	variant	UNP O14807

- Molecule 2 is a protein called Leucine-rich repeat protein SHOC-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	496	Total	C	N	O	S	0	5	0
			3934	2491	677	748	18			
2	E	496	Total	C	N	O	S	0	11	0
			3961	2511	680	751	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	78	GLY	-	expression tag	UNP Q9UQ13
B	79	PRO	-	expression tag	UNP Q9UQ13
B	173	ILE	MET	engineered mutation	UNP Q9UQ13
E	78	GLY	-	expression tag	UNP Q9UQ13
E	79	PRO	-	expression tag	UNP Q9UQ13
E	173	ILE	MET	engineered mutation	UNP Q9UQ13

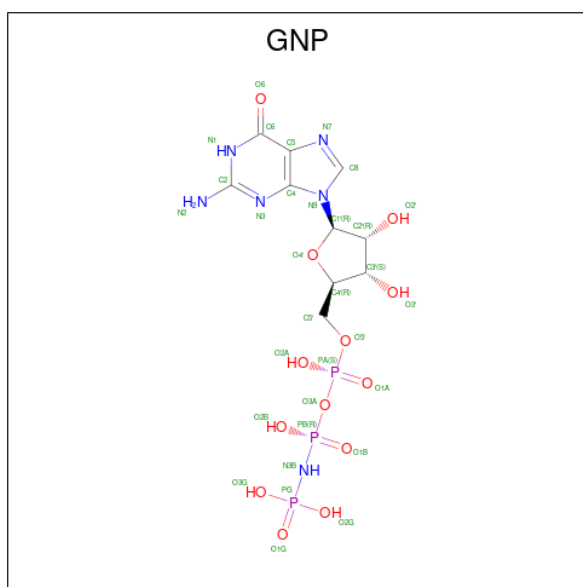
- Molecule 3 is a protein called Serine/threonine-protein phosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	1	0
			2357	1511	395	433	18			
3	F	294	Total	C	N	O	S	0	3	0
			2384	1527	401	438	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	SER	-	expression tag	UNP P62136
C	5	ASN	-	expression tag	UNP P62136
C	6	ALA	-	expression tag	UNP P62136
F	4	SER	-	expression tag	UNP P62136
F	5	ASN	-	expression tag	UNP P62136
F	6	ALA	-	expression tag	UNP P62136

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

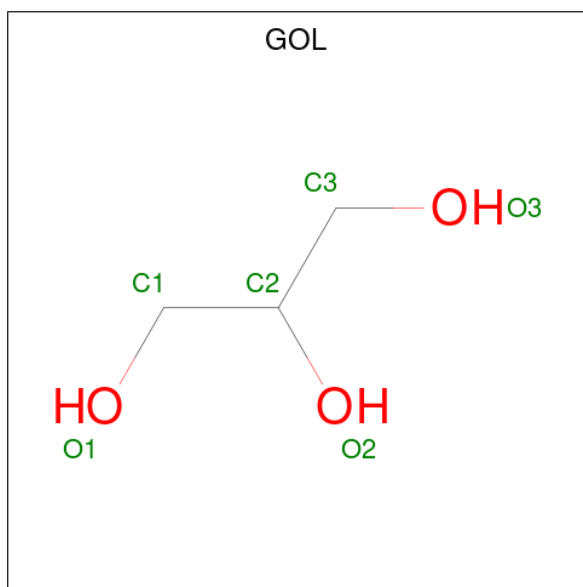


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

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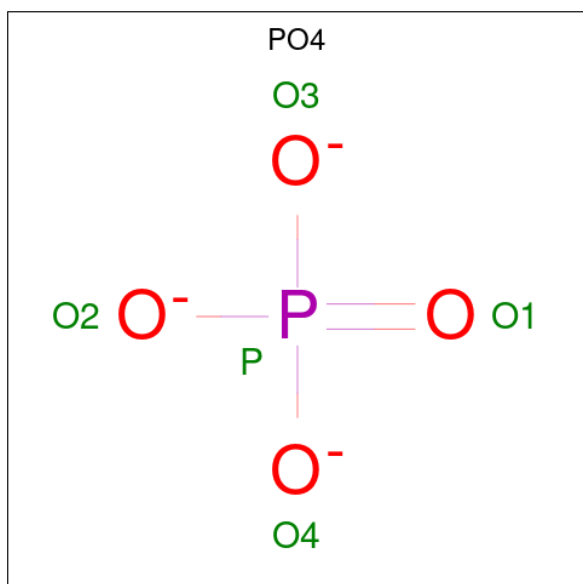
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	Mn	0	0
			2	2		
7	F	2	Total	Mn	0	0
			2	2		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	P	0	0
			5	4	1		
8	E	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		

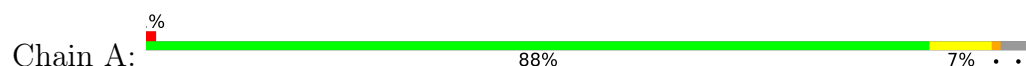
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	149	Total	O	0	0
			149	149		
9	B	402	Total	O	0	0
			402	402		
9	C	144	Total	O	0	0
			144	144		
9	D	256	Total	O	0	0
			256	256		
9	E	532	Total	O	0	0
			532	532		
9	F	232	Total	O	0	0
			232	232		

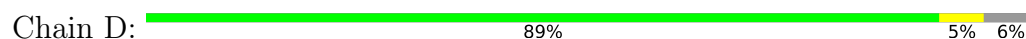
3 Residue-property plots [i](#)

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.

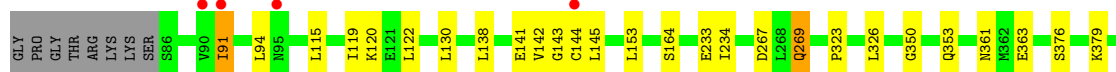
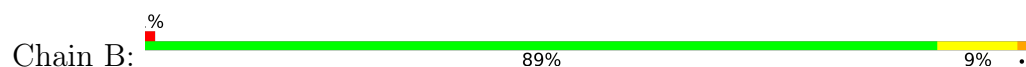
- Molecule 1: Ras-related protein M-Ras



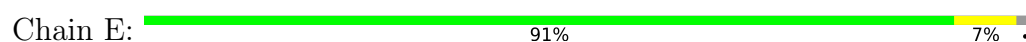
- Molecule 1: Ras-related protein M-Ras



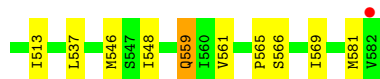
- Molecule 2: Leucine-rich repeat protein SHOC-2

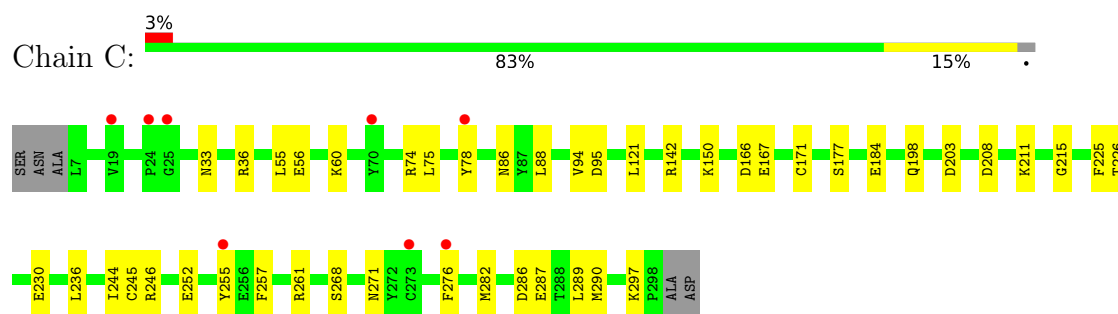


- Molecule 2: Leucine-rich repeat protein SHOC-2

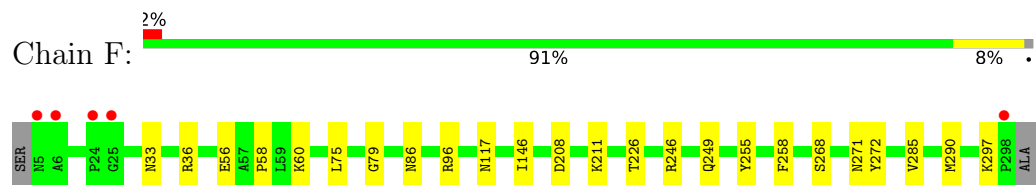


- Molecule 3: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit





- Molecule 3: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.96Å 115.75Å 137.80Å 90.00° 100.31° 90.00°	Depositor
Resolution (Å)	42.26 – 1.95 42.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.26-1.95) 99.8 (42.26-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.11.8, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.167 , 0.210 0.171 , 0.212	Depositor DCC
R_{free} test set	8194 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17319	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: PO4, GOL, GNP, MN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/1435	0.47	0/1940
1	D	0.42	0/1406	0.54	0/1899
2	B	0.29	0/4006	0.47	0/5430
2	E	0.33	0/4048	0.50	0/5486
3	C	0.29	0/2414	0.48	0/3261
3	F	0.38	0/2447	0.57	0/3305
All	All	0.33	0/15756	0.50	0/21321

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1405	0	1398	10	0
1	D	1377	0	1373	5	0
2	B	3934	0	4106	28	0
2	E	3961	0	4152	22	1
3	C	2357	0	2321	27	0
3	F	2384	0	2351	16	1
4	A	32	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	32	0	13	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	7	0	0
6	B	18	0	24	0	0
6	C	12	0	16	4	0
6	D	12	0	15	1	0
6	E	30	0	40	5	0
6	F	18	0	24	2	0
7	C	2	0	0	0	0
7	F	2	0	0	0	0
8	C	10	0	0	0	0
8	E	5	0	0	0	0
8	F	5	0	0	0	0
9	A	149	0	0	0	0
9	B	402	0	0	2	0
9	C	144	0	0	0	0
9	D	256	0	0	2	0
9	E	532	0	0	6	1
9	F	232	0	0	2	0
All	All	17319	0	15853	104	2

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 3.

All (104) 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:66:LEU:HD21	1:A:81:TYR:HB3	1.75	0.69
3:F:96:ARG:NH1	3:F:272:TYR:OH	2.27	0.68
2:B:115:LEU:HD21	2:B:119:ILE:HD13	1.77	0.65
2:E:569:ILE:HD12	6:E:604:GOL:H12	1.79	0.65
2:E:138:LEU:HG	2:E:142:VAL:HG21	1.80	0.64
2:B:323:PRO:HG2	2:B:326:LEU:HB2	1.80	0.63
1:A:8:SER:HB2	1:A:11:LEU:HD21	1.81	0.62
2:E:95[B]:ASN:OD1	2:E:98:ARG:NH1	2.28	0.62
2:E:226:LYS:NZ	9:E:707:HOH:O	2.34	0.61
2:E:566:SER:HA	6:E:604:GOL:H11	1.85	0.59
3:C:75:LEU:HD11	3:C:268:SER:HB3	1.84	0.58
2:B:457:GLU:OE2	3:C:150:LYS:NZ	2.32	0.58
3:C:271:ASN:ND2	3:C:276:PHE:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:249:GLN:HE21	6:F:506:GOL:H31	1.70	0.56
1:D:177:GLN:NE2	9:D:1304:HOH:O	2.35	0.56
3:C:74:ARG:NH1	3:C:297:LYS:O	2.36	0.55
2:E:559:GLN:H	2:E:559:GLN:CD	2.14	0.54
2:E:351:PRO:HB2	2:E:377:ARG:HD2	1.90	0.54
2:E:327:LEU:HB2	2:E:353:GLN:HB2	1.89	0.54
2:B:434[A]:ASN:ND2	2:B:457:GLU:OE1	2.41	0.54
3:C:33:ASN:HA	3:C:36:ARG:HG2	1.90	0.54
3:F:75:LEU:HD11	3:F:268:SER:HB3	1.89	0.54
2:B:120:LYS:HB2	2:B:141:GLU:HB3	1.90	0.54
2:B:91:ILE:HA	2:B:94:LEU:HD12	1.90	0.54
2:B:376:SER:O	2:B:379:LYS:NZ	2.39	0.53
2:B:573:LYS:HE2	2:B:578:TYR:O	2.09	0.53
3:C:86:ASN:ND2	6:C:504:GOL:H11	2.26	0.51
1:A:66:LEU:CD2	1:A:81:TYR:HB3	2.41	0.49
2:B:120:LYS:HG3	2:B:144:CYS:SG	2.53	0.49
3:F:86:ASN:ND2	3:F:117:ASN:HB3	2.27	0.49
3:C:255:TYR:OH	3:F:255:TYR:OH	2.04	0.49
2:E:448:ARG:HD2	9:E:847:HOH:O	2.12	0.49
3:C:55:LEU:HD22	6:C:504:GOL:H31	1.95	0.49
2:E:113:HIS:CE1	2:E:134:LYS:HD2	2.47	0.48
1:A:114:LYS:HD3	1:A:119:PHE:CZ	2.49	0.48
2:E:350:GLY:O	2:E:353:GLN:HG2	2.13	0.48
3:F:33:ASN:OD1	3:F:36[B]:ARG:NH2	2.46	0.48
2:B:350:GLY:O	2:B:353:GLN:HG2	2.14	0.48
3:F:211:LYS:HD3	3:F:258:PHE:HE1	1.79	0.48
2:B:138:LEU:HG	2:B:142:VAL:HG21	1.96	0.48
6:D:204:GOL:H2	9:E:1137:HOH:O	2.14	0.48
2:E:456:GLU:OE2	9:E:701:HOH:O	2.20	0.47
3:C:56:GLU:H	6:C:504:GOL:H32	1.79	0.47
3:C:215:GLY:N	3:C:230:GLU:OE2	2.36	0.47
2:E:537:LEU:HD21	2:E:546:MET:SD	2.55	0.47
2:B:486:LEU:HD11	2:B:501:LEU:HD11	1.98	0.46
3:C:255:TYR:HE2	3:C:257:PHE:CE2	2.34	0.46
2:B:267:ASP:OD1	2:B:269:GLN:NE2	2.44	0.46
3:C:177:SER:HB2	3:C:203:ASP:HB2	1.96	0.46
3:C:257:PHE:CG	3:C:261:ARG:HG2	2.49	0.46
1:A:121:MET:HG3	1:A:150:ILE:HG21	1.97	0.46
3:C:286:ASP:OD2	3:C:290:MET:HB2	2.14	0.46
1:D:128:VAL:HG11	1:D:154:GLU:HB3	1.97	0.46
2:E:288[B]:ARG:NH2	9:E:702:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:56:GLU:O	6:F:505:GOL:H31	2.16	0.45
3:C:230:GLU:H	3:C:230:GLU:CD	2.25	0.45
1:A:9:ASP:OD1	1:A:9:ASP:N	2.49	0.45
3:F:211:LYS:NZ	9:F:616:HOH:O	2.48	0.45
2:E:565:PRO:HB2	6:E:604:GOL:H32	1.99	0.44
1:A:8:SER:HG	1:A:60:TRP:CD1	2.35	0.44
2:B:549:GLU:H	2:B:549:GLU:CD	2.26	0.44
3:C:56:GLU:H	6:C:504:GOL:C3	2.31	0.44
2:E:456:GLU:HG2	2:E:457:GLU:HG3	1.99	0.44
2:B:464:PRO:O	2:B:467:ILE:HG13	2.18	0.44
2:E:120:LYS:HB3	2:E:141:GLU:HB3	2.00	0.43
2:B:143:GLY:HA3	2:B:164:SER:HB2	1.99	0.43
2:B:119:ILE:HG12	2:B:145:LEU:HD11	2.00	0.43
2:B:233:GLU:OE1	9:B:701:HOH:O	2.21	0.43
2:B:522:LEU:O	2:B:546:MET:HA	2.19	0.43
2:B:269:GLN:H	2:B:269:GLN:HG3	1.34	0.43
3:F:36[B]:ARG:HD3	9:F:712:HOH:O	2.18	0.43
2:E:401:TRP:HA	6:E:603:GOL:H12	2.01	0.42
2:B:383:LYS:HB3	2:B:383:LYS:HE2	1.56	0.42
3:C:287:GLU:OE1	3:C:287:GLU:N	2.51	0.42
2:E:169:LYS:NZ	9:E:733:HOH:O	2.51	0.42
3:C:166:ASP:HB2	3:C:289:LEU:HD21	2.01	0.42
3:C:261:ARG:HE	3:F:297:LYS:NZ	2.17	0.42
2:E:315:GLU:HA	2:E:339:ALA:O	2.20	0.42
3:C:94:VAL:O	3:C:95:ASP:HB2	2.20	0.42
3:C:60:LYS:HB3	3:C:282:MET:HE3	2.01	0.41
3:C:171:CYS:HA	3:C:245:CYS:O	2.20	0.41
2:B:130:LEU:HB2	2:B:153:LEU:HD23	2.02	0.41
2:B:233:GLU:OE1	2:B:233:GLU:N	2.53	0.41
3:F:211:LYS:H	3:F:211:LYS:HG2	1.67	0.41
2:E:379:LYS:HD2	6:E:603:GOL:H32	2.01	0.41
1:A:35:GLN:C	1:A:36:LYS:HG2	2.45	0.41
1:A:175:ILE:O	1:A:178:GLN:HG2	2.20	0.41
2:B:267:ASP:OD1	2:B:269:GLN:HG3	2.20	0.41
2:B:379:LYS:HB2	9:B:776:HOH:O	2.19	0.41
2:E:467[B]:ILE:HG13	2:E:470:LEU:HD12	2.03	0.41
2:B:383:LYS:HG2	2:B:406:GLU:HB2	2.02	0.41
1:D:114:LYS:HE2	1:D:119:PHE:CZ	2.56	0.41
1:D:119:PHE:O	1:D:121:MET:HG3	2.20	0.41
3:F:60:LYS:HE3	3:F:79:GLY:O	2.21	0.41
3:C:78:TYR:CZ	3:F:290:MET:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:ASP:O	3:C:226:THR:HA	2.21	0.41
3:F:208:ASP:O	3:F:226:THR:HA	2.21	0.41
3:C:88:LEU:HD11	3:C:121:LEU:HG	2.03	0.40
3:F:58:PRO:HA	3:F:285:VAL:O	2.21	0.40
1:A:6:VAL:HA	3:C:225:PHE:HE2	1.86	0.40
3:C:236:LEU:HD21	3:C:244:ILE:HG13	2.04	0.40
2:B:570:GLN:O	2:B:574:MET:HG2	2.22	0.40
1:D:132:HIS:HD2	9:D:1527:HOH:O	2.05	0.40
2:B:361:ASN:OD1	2:B:363:GLU:HG2	2.22	0.40

All (2) 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)
2:E:581:MET:O	3:F:36[B]:ARG:NH1[2_556]	2.19	0.01
9:E:1104:HOH:O	9:E:1181:HOH:O[2_646]	2.19	0.01

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	171/180 (95%)	167 (98%)	3 (2%)	1 (1%)	21	12
1	D	167/180 (93%)	166 (99%)	1 (1%)	0	100	100
2	B	499/505 (99%)	469 (94%)	30 (6%)	0	100	100
2	E	505/505 (100%)	479 (95%)	26 (5%)	0	100	100
3	C	291/297 (98%)	277 (95%)	14 (5%)	0	100	100
3	F	295/297 (99%)	284 (96%)	11 (4%)	0	100	100
All	All	1928/1964 (98%)	1842 (96%)	85 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER

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	156/160 (98%)	155 (99%)	1 (1%)	78	79
1	D	152/160 (95%)	150 (99%)	2 (1%)	61	58
2	B	466/468 (100%)	455 (98%)	11 (2%)	43	36
2	E	472/468 (101%)	466 (99%)	6 (1%)	61	58
3	C	259/261 (99%)	252 (97%)	7 (3%)	39	32
3	F	262/261 (100%)	259 (99%)	3 (1%)	65	64
All	All	1767/1778 (99%)	1737 (98%)	30 (2%)	53	49

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
2	B	91	ILE
2	B	122	LEU
2	B	234	ILE
2	B	269	GLN
2	B	433	SER
2	B	436	LEU
2	B	548	ILE
2	B	559[A]	GLN
2	B	559[B]	GLN
2	B	561	VAL
2	B	573	LYS
3	C	142	ARG
3	C	167	GLU
3	C	184	GLU
3	C	198	GLN
3	C	211	LYS
3	C	246	ARG

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Mol	Chain	Res	Type
3	C	252	GLU
1	D	36	LYS
1	D	97	LYS
2	E	379	LYS
2	E	490	ILE
2	E	513	ILE
2	E	548	ILE
2	E	559	GLN
2	E	561	VAL
3	F	146	ILE
3	F	246	ARG
3	F	271	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	239	ASN
2	B	368	ASN
3	C	27	ASN
3	C	117	ASN
2	E	262	GLN
2	E	269	GLN
2	E	480	ASN
2	E	495	ASN
3	F	198	GLN
3	F	237	HIS

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

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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
6	GOL	B	601	-	5,5,5	1.39	1 (20%)	5,5,5	0.90	0
8	PO4	F	503	7	4,4,4	1.06	0	6,6,6	0.70	0
6	GOL	E	605	-	5,5,5	0.97	0	5,5,5	1.01	0
6	GOL	D	203	-	5,5,5	1.38	0	5,5,5	1.38	1 (20%)
6	GOL	E	603	-	5,5,5	0.86	0	5,5,5	1.11	0
6	GOL	A	203	-	5,5,5	1.80	3 (60%)	5,5,5	0.79	0
4	GNP	D	201	5	34,34,34	1.20	5 (14%)	47,54,54	0.81	1 (2%)
6	GOL	B	603	-	5,5,5	0.94	0	5,5,5	1.14	0
6	GOL	F	506	-	5,5,5	0.87	0	5,5,5	0.99	0
6	GOL	F	505	-	5,5,5	1.31	0	5,5,5	1.10	0
6	GOL	C	504	-	5,5,5	0.90	0	5,5,5	1.19	1 (20%)
6	GOL	E	601	-	5,5,5	1.36	1 (20%)	5,5,5	0.78	0
4	GNP	A	201	5	34,34,34	1.27	4 (11%)	47,54,54	0.92	2 (4%)
6	GOL	C	505	-	5,5,5	0.75	0	5,5,5	1.14	0
8	PO4	E	606	-	4,4,4	0.94	0	6,6,6	0.42	0
6	GOL	D	204	-	5,5,5	1.04	0	5,5,5	1.10	0
8	PO4	C	506	-	4,4,4	0.92	0	6,6,6	0.45	0
6	GOL	E	604	-	5,5,5	1.17	0	5,5,5	0.95	0
6	GOL	E	602	-	5,5,5	1.11	0	5,5,5	0.97	0
8	PO4	C	503	7	4,4,4	0.87	0	6,6,6	0.59	0
6	GOL	F	504	-	5,5,5	0.89	0	5,5,5	1.08	0
6	GOL	B	602	-	5,5,5	1.14	1 (20%)	5,5,5	1.08	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
6	GOL	E	602	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GNP	D	201	5	-	3/18/38/38	0/3/3/3
6	GOL	F	505	-	-	2/4/4/4	-
6	GOL	C	504	-	-	3/4/4/4	-
6	GOL	E	601	-	-	0/4/4/4	-
6	GOL	B	601	-	-	1/4/4/4	-
4	GNP	A	201	5	-	3/18/38/38	0/3/3/3
6	GOL	B	603	-	-	0/4/4/4	-
6	GOL	C	505	-	-	0/4/4/4	-
6	GOL	F	504	-	-	2/4/4/4	-
6	GOL	E	605	-	-	0/4/4/4	-
6	GOL	D	203	-	-	0/4/4/4	-
6	GOL	E	603	-	-	0/4/4/4	-
6	GOL	D	204	-	-	2/4/4/4	-
6	GOL	F	506	-	-	0/4/4/4	-
6	GOL	A	203	-	-	3/4/4/4	-
6	GOL	E	604	-	-	0/4/4/4	-
6	GOL	B	602	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	GNP	PB-O3A	4.23	1.64	1.59
4	D	201	GNP	PB-O3A	3.39	1.63	1.59
4	A	201	GNP	PG-N3B	3.04	1.71	1.63
4	A	201	GNP	PB-O1B	2.93	1.50	1.46
4	D	201	GNP	PG-O1G	2.88	1.50	1.46
4	D	201	GNP	PB-O1B	2.83	1.50	1.46
4	D	201	GNP	PG-N3B	2.73	1.70	1.63
6	E	601	GOL	C3-C2	2.40	1.60	1.51
6	A	203	GOL	O2-C2	-2.39	1.36	1.43
4	A	201	GNP	PG-O1G	2.33	1.49	1.46
4	D	201	GNP	PA-O2A	-2.28	1.44	1.55
6	B	601	GOL	O2-C2	-2.21	1.36	1.43
6	A	203	GOL	C3-C2	2.14	1.59	1.51
6	A	203	GOL	C1-C2	2.13	1.59	1.51
6	B	602	GOL	C1-C2	2.02	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	GNP	O1G-PG-N3B	-3.45	106.69	111.77
4	D	201	GNP	O1G-PG-N3B	-3.16	107.12	111.77
4	A	201	GNP	O2G-PG-O3G	2.37	113.97	107.59
6	C	504	GOL	C3-C2-C1	-2.21	103.68	111.80
6	D	203	GOL	C3-C2-C1	-2.12	104.02	111.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

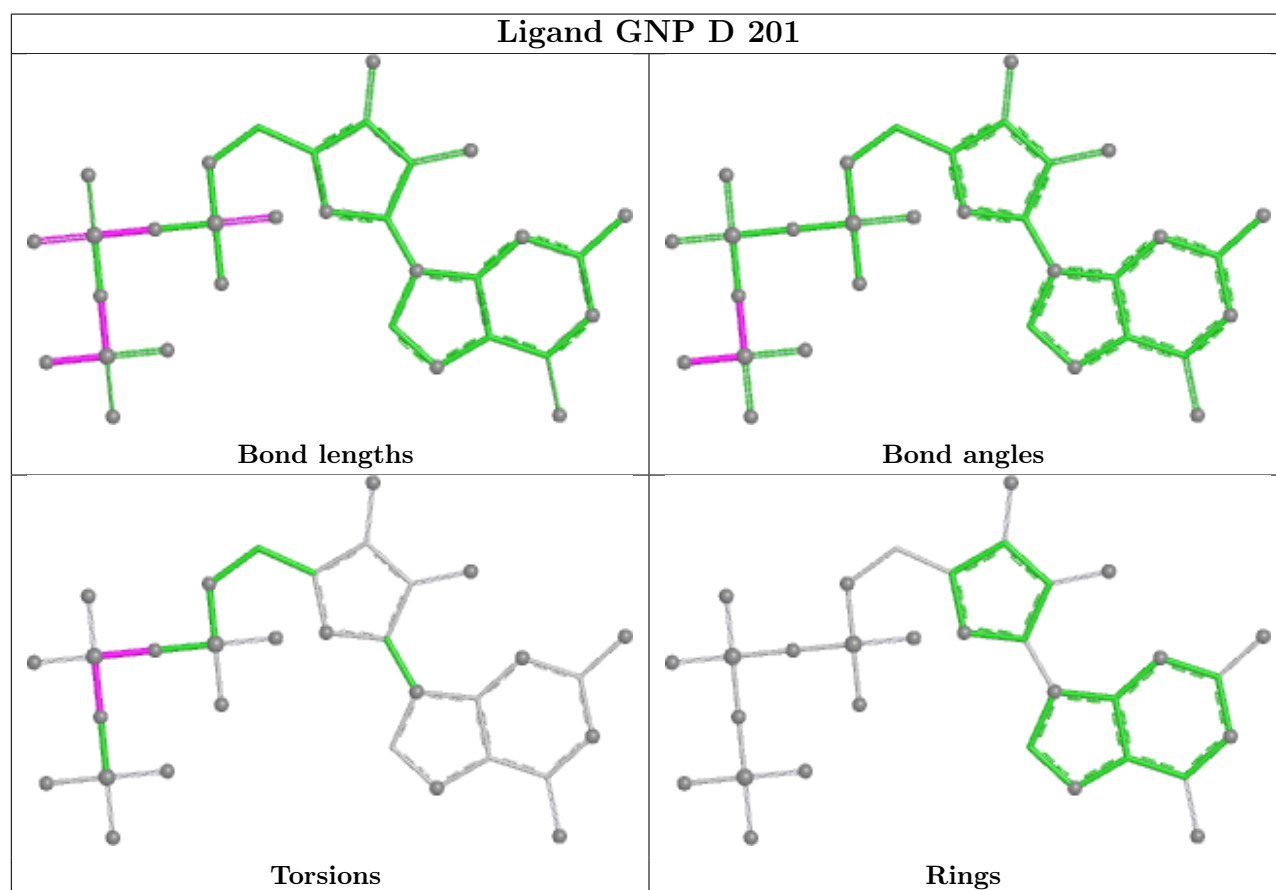
Mol	Chain	Res	Type	Atoms
4	A	201	GNP	PG-N3B-PB-O1B
4	A	201	GNP	PA-O3A-PB-O2B
4	D	201	GNP	PG-N3B-PB-O1B
4	D	201	GNP	PA-O3A-PB-O2B
6	A	203	GOL	C1-C2-C3-O3
6	A	203	GOL	O2-C2-C3-O3
6	B	602	GOL	O1-C1-C2-C3
6	C	504	GOL	O1-C1-C2-O2
6	C	504	GOL	O1-C1-C2-C3
6	D	204	GOL	C1-C2-C3-O3
6	F	504	GOL	C1-C2-C3-O3
6	F	505	GOL	O1-C1-C2-C3
6	F	505	GOL	O1-C1-C2-O2
6	B	602	GOL	O1-C1-C2-O2
6	D	204	GOL	O2-C2-C3-O3
6	A	203	GOL	O1-C1-C2-O2
6	C	504	GOL	O2-C2-C3-O3
6	F	504	GOL	O2-C2-C3-O3
4	A	201	GNP	PA-O3A-PB-O1B
4	D	201	GNP	PA-O3A-PB-O1B
6	B	601	GOL	C1-C2-C3-O3

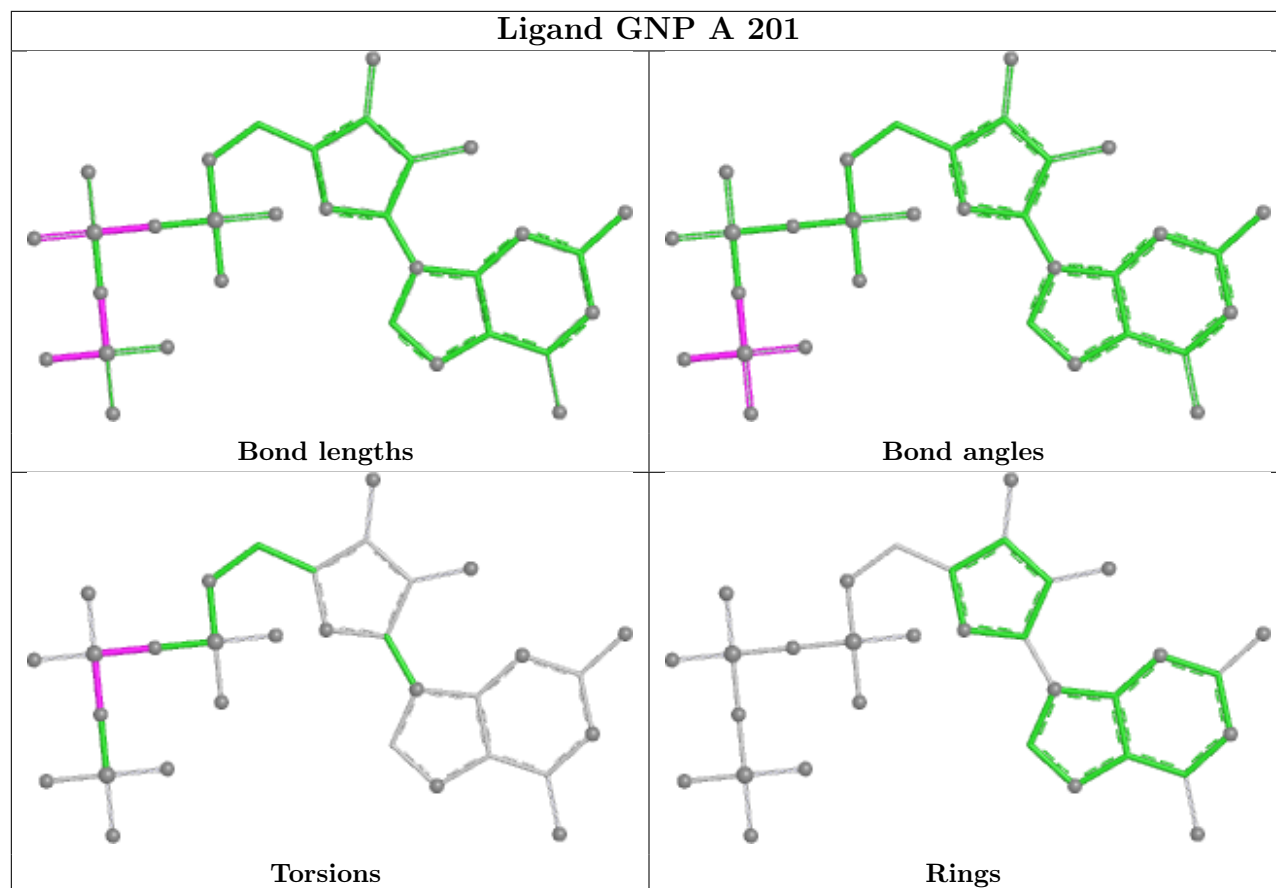
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	603	GOL	2	0
6	F	506	GOL	1	0
6	F	505	GOL	1	0
6	C	504	GOL	4	0
6	D	204	GOL	1	0
6	E	604	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	173/180 (96%)	-0.05	2 (1%) 76 82	25, 36, 59, 120	0
1	D	169/180 (93%)	-0.50	0 100 100	18, 25, 39, 71	0
2	B	496/505 (98%)	0.06	6 (1%) 76 82	19, 37, 58, 90	5 (1%)
2	E	496/505 (98%)	-0.34	2 (0%) 88 91	14, 30, 43, 68	11 (2%)
3	C	292/297 (98%)	0.35	8 (2%) 56 62	23, 40, 67, 119	1 (0%)
3	F	294/297 (98%)	-0.31	5 (1%) 69 76	17, 28, 50, 103	3 (1%)
All	All	1920/1964 (97%)	-0.12	23 (1%) 76 82	14, 33, 56, 120	20 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	78	TYR	3.5
2	B	91	ILE	3.5
2	E	582	VAL	3.4
3	C	24	PRO	3.3
1	A	6	VAL	3.1
3	C	255	TYR	3.1
3	C	273	CYS	2.9
2	B	580	ALA	2.7
3	F	6	ALA	2.7
3	C	276	PHE	2.7
3	F	24	PRO	2.6
2	B	144	CYS	2.3
3	C	70	TYR	2.2
2	B	581	MET	2.2
3	C	19	VAL	2.2
3	C	25	GLY	2.2
2	B	95	ASN	2.2
1	A	9	ASP	2.2
2	B	90	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	88	ALA	2.1
3	F	25	GLY	2.1
3	F	298	PRO	2.1
3	F	5	ASN	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.

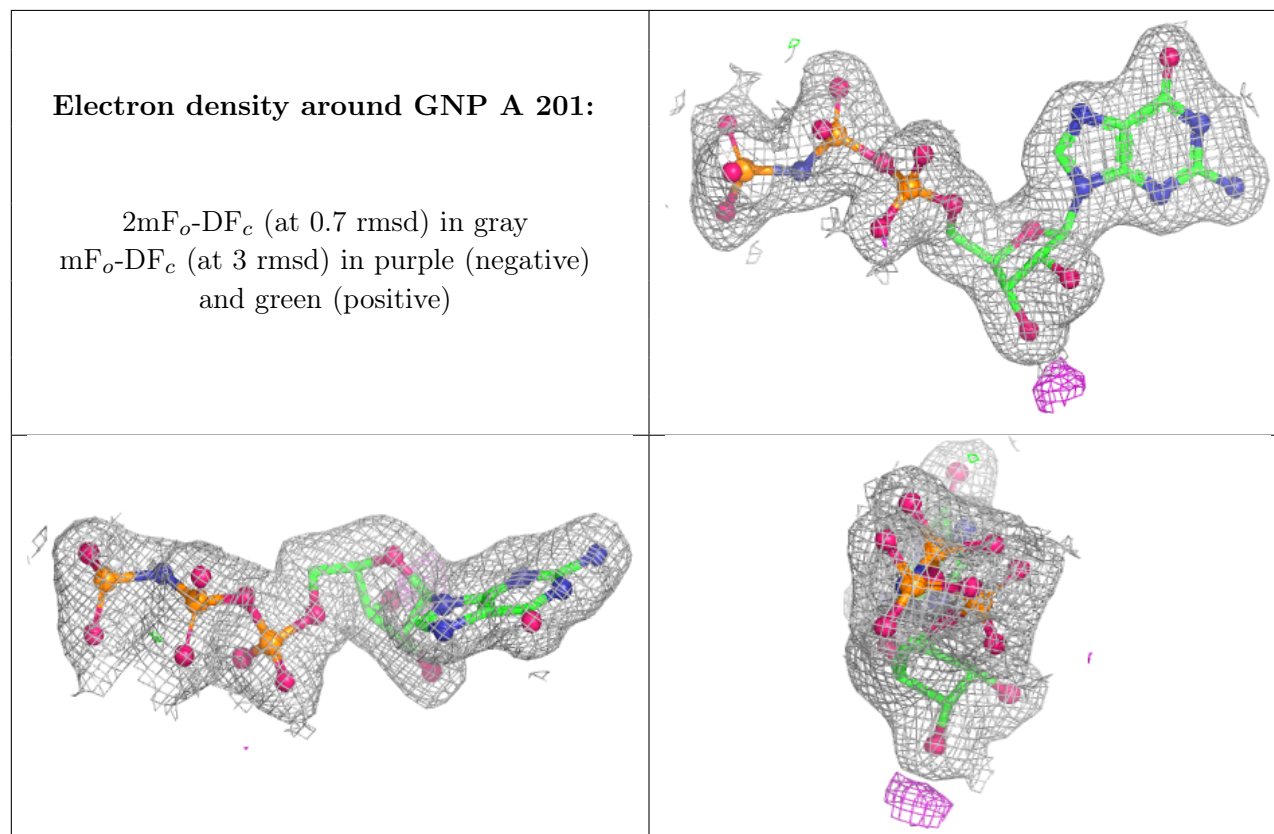
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PO4	C	506	5/5	0.61	0.11	94,99,105,115	0
8	PO4	E	606	5/5	0.77	0.08	85,90,99,106	0
7	MN	C	501	1/1	0.82	0.15	81,81,81,81	0
7	MN	F	501	1/1	0.82	0.16	74,74,74,74	0
6	GOL	F	504	6/6	0.83	0.13	45,49,51,54	0
6	GOL	F	506	6/6	0.83	0.12	54,57,58,61	0
6	GOL	B	603	6/6	0.84	0.12	42,48,51,59	0
6	GOL	E	603	6/6	0.84	0.13	49,50,54,59	0
6	GOL	E	604	6/6	0.84	0.13	59,59,61,62	0
6	GOL	C	505	6/6	0.86	0.11	44,47,51,52	0
6	GOL	D	204	6/6	0.86	0.12	40,45,46,46	0
6	GOL	D	203	6/6	0.87	0.14	23,28,30,37	0
6	GOL	A	203	6/6	0.88	0.18	29,33,34,38	0
6	GOL	B	601	6/6	0.88	0.11	34,44,44,49	0
6	GOL	E	605	6/6	0.89	0.11	62,68,70,72	0
6	GOL	B	602	6/6	0.90	0.12	30,37,40,41	0
6	GOL	C	504	6/6	0.90	0.10	43,46,51,57	0
6	GOL	E	602	6/6	0.91	0.10	36,39,42,45	0
6	GOL	F	505	6/6	0.92	0.08	29,38,47,47	0

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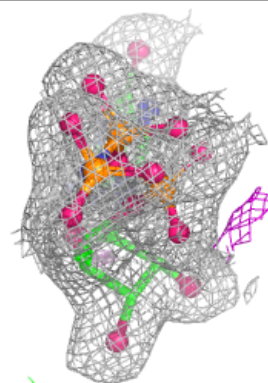
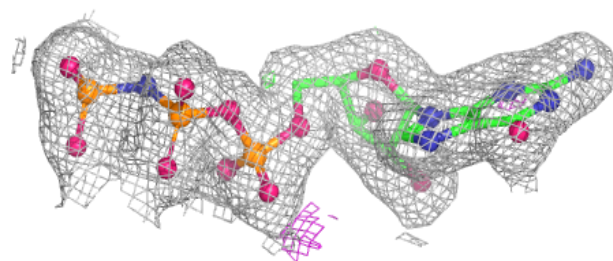
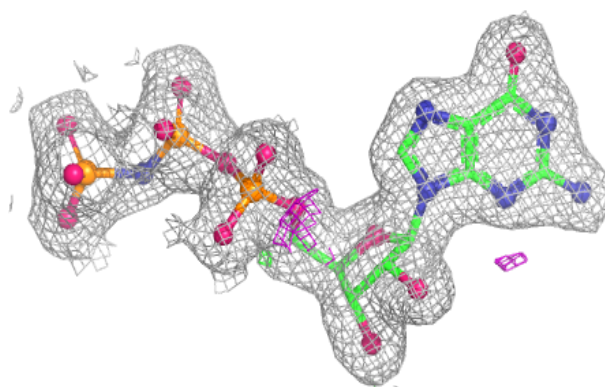
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	E	601	6/6	0.93	0.11	26,29,34,35	0
8	PO4	C	503	5/5	0.93	0.12	44,46,49,52	0
8	PO4	F	503	5/5	0.97	0.06	27,34,36,36	0
4	GNP	A	201	32/32	0.98	0.04	22,26,28,29	0
7	MN	F	502	1/1	0.99	0.02	25,25,25,25	0
4	GNP	D	201	32/32	0.99	0.04	17,20,22,23	0
5	MG	A	202	1/1	0.99	0.01	24,24,24,24	0
7	MN	C	502	1/1	0.99	0.07	36,36,36,36	0
5	MG	D	202	1/1	0.99	0.04	19,19,19,19	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 GNP D 201:

$2mF_o-DF_c$ (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.