



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 PM UTC

PDB ID : 9RK8 / pdb_00009rk8
Title : Crystal Structure of compound 3-mediated ternary complex of KRAS G12V C118S GDP with pVHL:ElonginC:ElonginB
Authors : Zollman, D.; Karolak, N.K.; Ciulli, A.
Deposited on : 2025-06-13
Resolution : 2.63 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

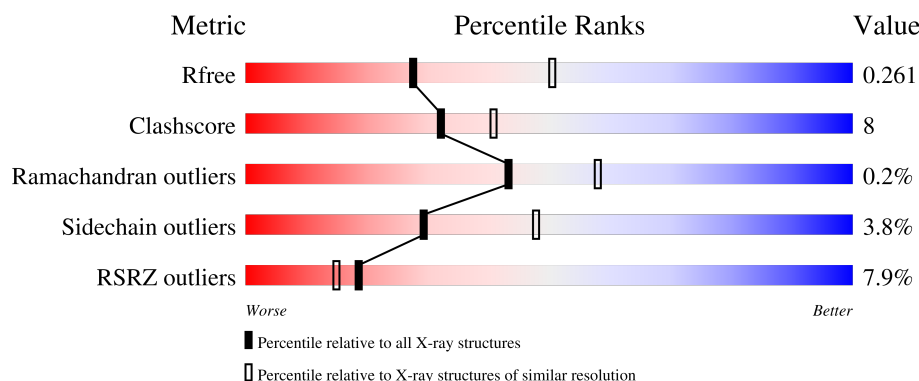
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	104	5% 69% 26% • •
1	E	104	20% 68% 23% • 7%
2	B	97	5% 70% 18% 12%
2	F	97	2% 75% 11% • 12%
3	C	162	4% 77% 12% • 9%

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Mol	Chain	Length	Quality of chain
3	G	162	 3% 72% 20% 8%
4	D	170	 17% 75% 22% ..
4	H	170	 4% 78% 19% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7992 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			765	486	125	149	5			
1	E	97	Total	C	N	O	S	0	0	0
			722	465	123	130	4			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total	C	N	O	S	0	0	0
			662	430	105	121	6			
2	F	85	Total	C	N	O	S	0	0	0
			681	440	109	126	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
F	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	147	Total	C	N	O	S	0	1	0
			1174	748	213	211	2			
3	G	149	Total	C	N	O	S	0	1	0
			1214	773	223	216	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
G	52	GLY	-	expression tag	UNP P40337
G	53	SER	-	expression tag	UNP P40337

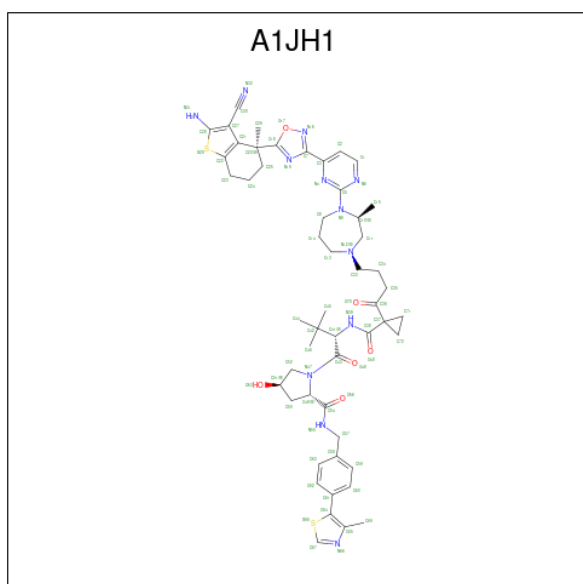
- Molecule 4 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1256	787	212	251	6			
4	H	167	Total	C	N	O	S	0	0	0
			1312	822	225	260	5			

There are 6 discrepancies between the modelled and reference sequences:

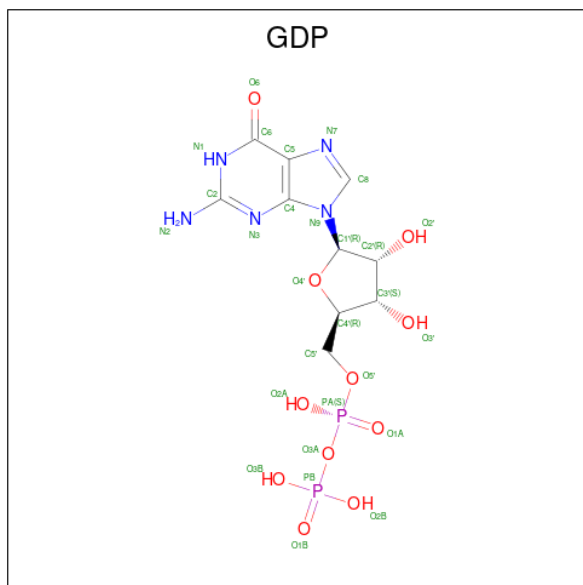
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP P01116
D	12	VAL	GLY	engineered mutation	UNP P01116
D	118	SER	CYS	engineered mutation	UNP P01116
H	0	GLY	-	expression tag	UNP P01116
H	12	VAL	GLY	engineered mutation	UNP P01116
H	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 5 is (2 {S},4 {R})-1-[(2 {S})-2-[[1-[4-[(3 {S})-4-[4-[5-[(4 {S})-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5 {H}-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1-yl]butanoyl]cyclopropyl]carbonylamino]-3,3-dimethyl-butanoyl]-{N}-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: A1JH1) (formula: C₅₂H₆₄N₁₂O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			72	52	12	6	2		
5	G	1	Total	C	N	O	S	0	0
			72	52	12	6	2		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	H	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	O	0	0
			1	1		
8	H	2	Total	O	0	0
			2	2		

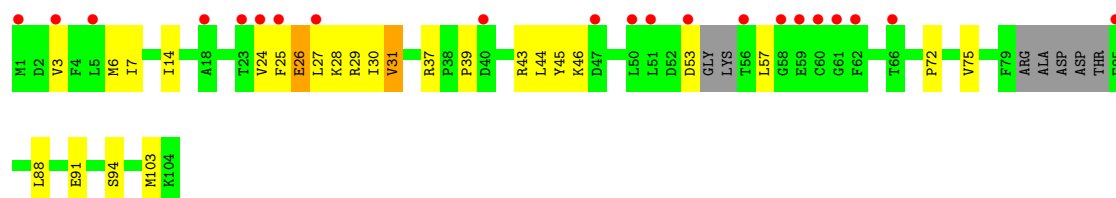
3 Residue-property plots [i](#)

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.

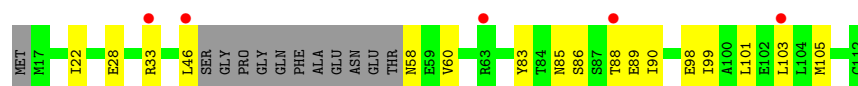
- Molecule 1: Elongin-B



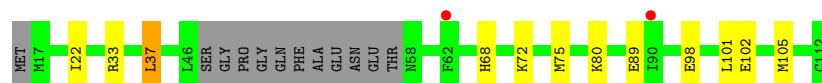
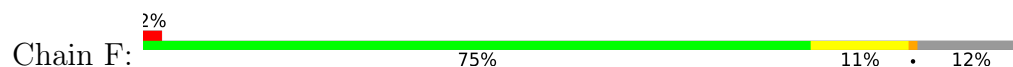
- Molecule 1: Elongin-B



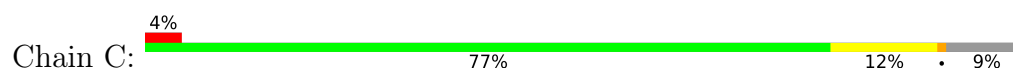
- Molecule 2: Elongin-C

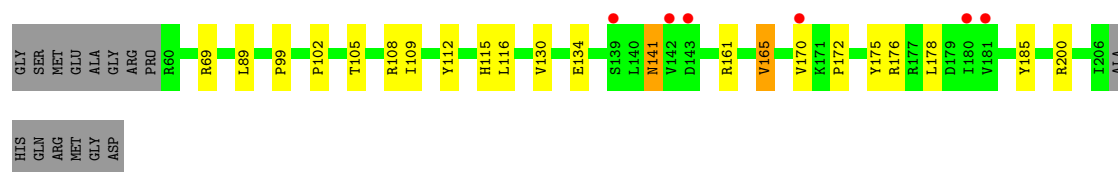


- Molecule 2: Elongin-C

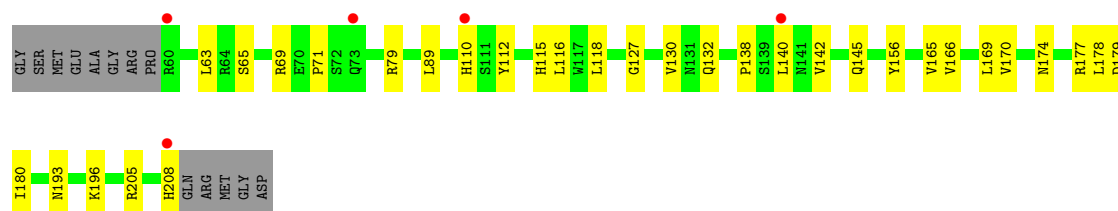


- Molecule 3: von Hippel-Lindau disease tumor suppressor

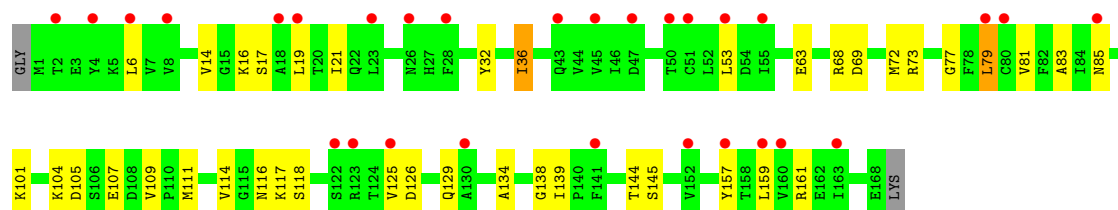
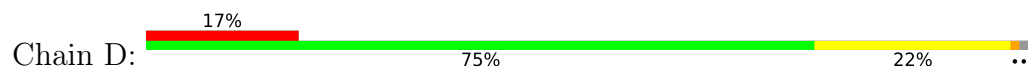




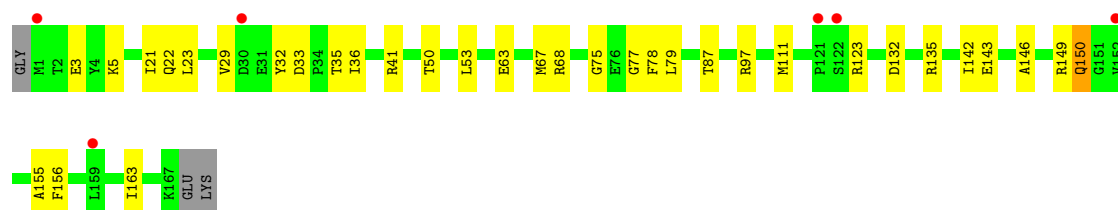
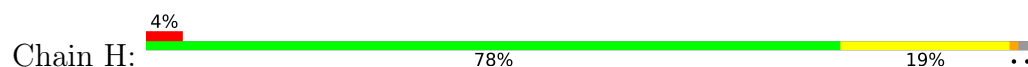
- Molecule 3: von Hippel-Lindau disease tumor suppressor



- Molecule 4: GTPase KRas



- Molecule 4: GTPase KRas



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.19Å 109.43Å 251.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.18 – 2.63 50.18 – 2.63	Depositor EDS
% Data completeness (in resolution range)	72.6 (50.18-2.63) 72.8 (50.18-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.263 0.232 , 0.261	Depositor DCC
R_{free} test set	1411 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	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	7992	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: MG, A1JH1, 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	0.18	0/780	0.41	0/1058
1	E	0.17	0/736	0.46	0/998
2	B	0.15	0/676	0.39	0/915
2	F	0.15	0/695	0.35	0/937
3	C	0.16	0/1209	0.38	0/1657
3	G	0.24	0/1250	0.48	0/1708
4	D	0.20	0/1276	0.41	0/1734
4	H	0.19	0/1333	0.41	0/1805
All	All	0.19	0/7955	0.42	0/10812

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	765	0	740	18	0
1	E	722	0	698	20	0
2	B	662	0	650	10	0
2	F	681	0	683	9	0
3	C	1174	0	1141	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1214	0	1205	20	1
4	D	1256	0	1149	25	0
4	H	1312	0	1270	20	0
5	C	72	0	0	2	0
5	G	72	0	0	0	0
6	D	28	0	12	1	0
6	H	28	0	12	1	1
7	D	1	0	0	0	0
7	H	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
8	H	2	0	0	0	0
All	All	7992	0	7560	125	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 8.

All (125) 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)
3:C:108:ARG:HD3	3:G:132:GLN:HE22	1.42	0.83
3:G:65:SER:HB2	3:G:115:HIS:HA	1.61	0.82
1:A:7:ILE:HG22	1:A:75:VAL:HB	1.64	0.78
3:G:193:ASN:HB3	3:G:196:LYS:HG2	1.66	0.76
3:G:71:PRO:HB3	3:G:110[B]:HIS:HE1	1.51	0.76
4:H:22:GLN:HG3	4:H:149:ARG:HG3	1.70	0.73
1:E:103:MET:HE1	2:F:101:LEU:HG	1.71	0.71
1:E:7:ILE:HG22	1:E:75:VAL:HB	1.73	0.70
4:H:63:GLU:HB3	4:H:68:ARG:HD3	1.72	0.70
1:A:24:VAL:HB	1:A:53:ASP:HA	1.75	0.68
4:D:118:SER:H	4:D:145:SER:HB3	1.60	0.67
4:H:97:ARG:HG3	4:H:111:MET:HE1	1.78	0.64
4:D:63:GLU:HB3	4:D:68:ARG:HG3	1.79	0.63
3:G:174:ASN:HA	3:G:177:ARG:HD3	1.82	0.61
2:B:22:ILE:HD12	2:B:28:GLU:HG2	1.83	0.60
3:C:170:VAL:HG21	3:C:178:LEU:HD11	1.84	0.60
4:D:101:LYS:HD2	4:D:107:GLU:HA	1.84	0.59
4:H:22:GLN:CG	4:H:149:ARG:HG3	2.32	0.59
1:A:27:LEU:O	1:A:31:VAL:HG23	2.02	0.59
3:G:71:PRO:HB3	3:G:110[B]:HIS:CE1	2.34	0.59
1:A:38:PRO:C	1:A:40:ASP:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:ASN:HA	4:D:144:THR:O	2.04	0.58
2:F:68:HIS:NE2	2:F:102:GLU:OE1	2.36	0.58
1:E:24:VAL:HB	1:E:53:ASP:HA	1.84	0.57
4:D:81:VAL:HG12	4:D:114:VAL:HB	1.87	0.57
1:E:28:LYS:HB3	1:E:39:PRO:HB3	1.87	0.57
1:A:28:LYS:HB3	1:A:39:PRO:HB3	1.87	0.57
3:G:142:VAL:O	3:G:145:GLN:HG2	2.05	0.56
1:E:94:SER:OG	2:F:68:HIS:ND1	2.28	0.56
3:G:89:LEU:HD23	3:G:116:LEU:HB3	1.88	0.55
1:A:23:THR:HA	1:A:56:THR:HA	1.88	0.55
1:E:27:LEU:O	1:E:31:VAL:HG13	2.07	0.55
3:C:115:HIS:ND1	5:C:301:A1JH1:O53	2.40	0.55
4:D:69:ASP:HB3	4:D:73:ARG:HH21	1.71	0.55
1:E:29:ARG:HD3	1:E:39:PRO:HG3	1.88	0.54
4:D:79:LEU:HD13	4:D:159:LEU:HD22	1.90	0.54
4:H:77:GLY:HA3	4:H:163:ILE:HD11	1.91	0.53
1:E:28:LYS:HE2	1:E:44:LEU:HD23	1.90	0.52
4:D:104:LYS:HG3	4:D:109:VAL:HG11	1.91	0.52
2:B:86:SER:HB3	2:B:90:ILE:HD11	1.90	0.52
3:C:161:ARG:O	3:C:165:VAL:HG13	2.10	0.52
3:C:89:LEU:HD12	3:C:116:LEU:HD23	1.92	0.51
1:E:3:VAL:HG11	1:E:57:LEU:HD13	1.91	0.51
3:G:63:LEU:HD21	3:G:205:ARG:NH1	2.26	0.51
1:A:65:GLN:N	1:A:65:GLN:OE1	2.44	0.51
2:F:89:GLU:OE2	3:G:79:ARG:NE	2.44	0.50
2:B:33:ARG:CZ	2:B:46:LEU:HD13	2.42	0.50
3:G:89:LEU:HD21	3:G:118:LEU:HD23	1.93	0.50
3:G:127:GLY:O	3:G:156:TYR:OH	2.25	0.50
4:H:21:ILE:HD11	4:H:32:TYR:CD2	2.47	0.50
4:H:142:ILE:HD12	4:H:155:ALA:HA	1.92	0.50
1:A:37:ARG:NH1	1:A:41:GLU:OE1	2.40	0.49
1:A:26:GLU:O	1:A:30:ILE:HG12	2.13	0.49
4:H:33:ASP:OD1	4:H:35:THR:OG1	2.31	0.49
4:H:123:ARG:NH2	4:H:143:GLU:OE2	2.45	0.49
4:H:132:ASP:OD1	4:H:135:ARG:NH2	2.36	0.49
1:E:25:PHE:O	1:E:28:LYS:HB2	2.13	0.49
4:D:17:SER:O	4:D:21:ILE:HG13	2.13	0.48
4:D:21:ILE:HD11	4:D:32:TYR:CE2	2.49	0.48
1:E:94:SER:HG	2:F:68:HIS:HD1	1.56	0.48
3:C:134:GLU:OE2	3:C:200:ARG:NH2	2.48	0.47
1:A:76:GLY:HA2	1:A:90:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:ARG:O	2:F:37:LEU:HD13	2.14	0.47
2:B:33:ARG:NH1	2:B:58:ASN:OD1	2.47	0.47
3:G:166:VAL:O	3:G:170:VAL:HG22	2.15	0.47
3:C:99:PRO:HG3	4:D:105:ASP:HA	1.98	0.46
3:C:102:PRO:HG2	3:C:105:THR:OG1	2.15	0.46
1:E:45:TYR:CD2	1:E:88:LEU:HD22	2.49	0.46
4:H:21:ILE:HD12	4:H:29:VAL:HG11	1.97	0.46
1:A:7:ILE:HD12	1:A:31:VAL:HG22	1.97	0.46
4:H:33:ASP:CG	4:H:36:ILE:HD13	2.41	0.46
4:H:67:MET:HE2	4:H:67:MET:HB3	1.69	0.46
4:H:5:LYS:HG3	4:H:75:GLY:HA2	1.96	0.46
4:H:146:ALA:N	6:H:301:GDP:O6	2.48	0.46
4:D:68:ARG:HH11	4:D:72:MET:HE3	1.80	0.46
3:C:141:ASN:HD22	3:C:141:ASN:N	2.14	0.45
4:D:157:TYR:O	4:D:161:ARG:HG3	2.16	0.45
4:H:78:PHE:HB2	4:H:111:MET:HG2	1.98	0.45
3:C:112:TYR:HB2	3:C:115:HIS:NE2	2.31	0.45
3:G:65:SER:HB3	3:G:89:LEU:O	2.16	0.45
3:G:115:HIS:O	3:G:138:PRO:HD2	2.16	0.45
1:A:103:MET:HE1	2:B:101:LEU:HG	1.99	0.45
1:E:26:GLU:H	1:E:26:GLU:HG2	1.64	0.45
4:D:83:ALA:HB1	4:D:117:LYS:HD2	1.99	0.45
4:D:126:ASP:H	4:D:129:GLN:NE2	2.15	0.44
4:H:23:LEU:HD22	4:H:156:PHE:CG	2.52	0.44
1:A:42:GLN:HB2	1:A:77:LEU:HD11	1.99	0.44
4:D:14:VAL:HG11	4:D:81:VAL:HG23	2.00	0.44
2:B:83:TYR:HB3	2:B:90:ILE:HD12	2.00	0.44
3:G:112:TYR:HB2	3:G:115:HIS:NE2	2.32	0.44
4:D:36:ILE:HD13	4:D:36:ILE:HA	1.81	0.43
4:D:77:GLY:C	4:D:159:LEU:HD21	2.43	0.43
2:B:98:GLU:H	2:B:98:GLU:CD	2.26	0.43
1:E:7:ILE:CG1	1:E:14:ILE:HB	2.49	0.43
1:E:6:MET:HA	1:E:14:ILE:O	2.18	0.43
3:G:165:VAL:O	3:G:169:LEU:HG	2.19	0.43
4:D:111:MET:HG3	4:D:139:ILE:HG21	2.00	0.42
4:D:16:LYS:HG2	4:D:81:VAL:HG21	2.01	0.42
4:D:118:SER:N	4:D:145:SER:HB3	2.30	0.42
2:F:101:LEU:HD11	3:G:178:LEU:HD22	2.01	0.42
1:A:1:MET:HA	1:A:1:MET:HE2	2.01	0.42
3:C:172:PRO:HA	3:C:175:TYR:CD2	2.55	0.42
1:A:38:PRO:C	1:A:40:ASP:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:PRO:HD2	2:F:75:MET:HE3	2.02	0.42
2:B:99:ILE:HG22	2:B:103:LEU:HB2	2.02	0.42
4:D:6:LEU:HD22	4:D:159:LEU:HD23	2.00	0.42
1:E:45:TYR:HD2	1:E:88:LEU:HD22	1.84	0.42
3:C:108:ARG:HD3	3:G:132:GLN:NE2	2.21	0.42
4:H:79:LEU:HD23	4:H:79:LEU:HA	1.79	0.42
3:C:69:ARG:HG2	5:C:301:A1JH1:C71	2.50	0.42
1:E:43:ARG:HD3	1:E:45:TYR:HE1	1.85	0.42
1:A:7:ILE:CG1	1:A:14:ILE:HB	2.50	0.41
4:D:117:LYS:HG2	6:D:301:GDP:C5	2.56	0.41
2:F:72:LYS:HD2	2:F:72:LYS:HA	1.84	0.41
4:H:150:GLN:HE21	4:H:150:GLN:HB3	1.64	0.41
1:A:62:PHE:CZ	1:A:75:VAL:HG22	2.56	0.41
2:B:101:LEU:O	2:B:105:MET:HG3	2.20	0.41
3:C:176:ARG:HA	3:C:185:TYR:CD1	2.55	0.41
4:D:134:ALA:O	4:D:138:GLY:N	2.54	0.41
1:E:103:MET:HG3	3:G:170:VAL:HG13	2.03	0.41
4:H:41:ARG:HA	4:H:53:LEU:O	2.21	0.40
1:A:6:MET:HA	1:A:14:ILE:O	2.21	0.40
2:B:88:THR:OG1	2:B:89:GLU:N	2.54	0.40
4:D:68:ARG:NH1	4:D:72:MET:HE3	2.37	0.40
1:E:37:ARG:HA	1:E:37:ARG:HD3	1.93	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)
3:G:69:ARG:NH2	6:H:301:GDP:O2A[3_654]	1.30	0.90

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	96/104 (92%)	89 (93%)	5 (5%)	2 (2%)	5	7
1	E	91/104 (88%)	88 (97%)	3 (3%)	0	100	100
2	B	81/97 (84%)	78 (96%)	3 (4%)	0	100	100
2	F	81/97 (84%)	78 (96%)	3 (4%)	0	100	100
3	C	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
3	G	148/162 (91%)	144 (97%)	4 (3%)	0	100	100
4	D	166/170 (98%)	161 (97%)	5 (3%)	0	100	100
4	H	165/170 (97%)	162 (98%)	3 (2%)	0	100	100
All	All	974/1066 (91%)	942 (97%)	30 (3%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLY
1	A	39	PRO

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	83/92 (90%)	82 (99%)	1 (1%)	63	78
1	E	73/92 (79%)	68 (93%)	5 (7%)	14	23
2	B	72/86 (84%)	70 (97%)	2 (3%)	38	58
2	F	77/86 (90%)	72 (94%)	5 (6%)	15	26
3	C	130/148 (88%)	126 (97%)	4 (3%)	35	55
3	G	137/148 (93%)	132 (96%)	5 (4%)	31	50
4	D	125/150 (83%)	119 (95%)	6 (5%)	23	37
4	H	142/150 (95%)	138 (97%)	4 (3%)	38	58
All	All	839/952 (88%)	807 (96%)	32 (4%)	29	48

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
2	B	60	VAL
2	B	85	ASN
3	C	109	ILE
3	C	130	VAL
3	C	141	ASN
3	C	165	VAL
4	D	19	LEU
4	D	36	ILE
4	D	53	LEU
4	D	79	LEU
4	D	85	ASN
4	D	125	VAL
1	E	26	GLU
1	E	30	ILE
1	E	31	VAL
1	E	46	LYS
1	E	91	GLU
2	F	22	ILE
2	F	37	LEU
2	F	80	LYS
2	F	98	GLU
2	F	105	MET
3	G	130	VAL
3	G	140	LEU
3	G	179	ASP
3	G	180	ILE
3	G	208	HIS
4	H	3	GLU
4	H	50	THR
4	H	87	THR
4	H	150	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	141	ASN
3	G	203	GLN
4	H	150	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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	A1JH1	C	301	-	77,80,80	0.99	3 (3%)	97,120,120	0.94	3 (3%)
6	GDP	H	301	7	29,30,30	1.16	2 (6%)	45,47,47	1.73	7 (15%)
6	GDP	D	301	7	29,30,30	1.18	3 (10%)	45,47,47	1.80	8 (17%)
5	A1JH1	G	301	-	77,80,80	0.98	3 (3%)	97,120,120	1.02	4 (4%)

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
5	A1JH1	C	301	-	-	2/59/108/108	0/9/9/9
6	GDP	H	301	7	-	3/16/32/32	0/3/3/3
6	GDP	D	301	7	-	3/16/32/32	0/3/3/3
5	A1JH1	G	301	-	-	11/59/108/108	0/9/9/9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	301	A1JH1	C5-N9	5.61	1.46	1.36
5	C	301	A1JH1	C5-N9	5.56	1.46	1.36
5	C	301	A1JH1	O17-C18	5.10	1.39	1.33
5	G	301	A1JH1	O17-C18	5.02	1.39	1.33
5	C	301	A1JH1	C11-N12	3.39	1.50	1.46
6	D	301	GDP	C5-C4	3.19	1.47	1.38
6	H	301	GDP	C5-C4	3.12	1.47	1.38
5	G	301	A1JH1	C11-N12	3.10	1.49	1.46
6	H	301	GDP	C6-N1	-2.42	1.34	1.38
6	D	301	GDP	C6-N1	-2.40	1.34	1.38
6	D	301	GDP	C5-N7	-2.01	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	301	A1JH1	O17-C18-N19	-6.53	111.06	115.25
5	C	301	A1JH1	O17-C18-N19	-6.31	111.19	115.25
6	D	301	GDP	C5-C4-N3	-6.10	118.69	128.39
6	H	301	GDP	C5-C4-N3	-5.90	119.00	128.39
6	D	301	GDP	C2-N3-C4	5.02	120.94	112.30
6	H	301	GDP	C2-N3-C4	4.92	120.77	112.30
6	D	301	GDP	N9-C4-N3	4.51	134.97	125.95
6	H	301	GDP	N9-C4-N3	4.32	134.60	125.95
5	C	301	A1JH1	C18-N19-C7	3.74	105.14	101.53
5	G	301	A1JH1	C18-N19-C7	3.66	105.06	101.53
6	H	301	GDP	C6-C5-N7	3.38	136.43	130.29
6	D	301	GDP	C6-C5-N7	3.24	136.18	130.29
6	H	301	GDP	C4-C5-N7	-2.58	106.58	110.67
6	D	301	GDP	C4-C5-N7	-2.56	106.61	110.67
5	G	301	A1JH1	C54-C49-N47	2.53	119.40	112.50
5	C	301	A1JH1	C72-C37-C38	-2.27	110.30	115.26
6	D	301	GDP	O2A-PA-O3A	2.19	113.19	107.27
6	H	301	GDP	O6-C6-C5	-2.14	120.87	126.53
5	G	301	A1JH1	C72-C37-C38	-2.13	110.61	115.26
6	D	301	GDP	C3'-C2'-C1'	2.12	105.48	101.46
6	D	301	GDP	O6-C6-C5	-2.10	121.00	126.53
6	H	301	GDP	O2A-PA-O3A	2.01	112.72	107.27

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	A1JH1	C35-C36-C37-C71
5	G	301	A1JH1	C34-C33-N12-C11
5	G	301	A1JH1	C35-C36-C37-C71
5	G	301	A1JH1	C35-C36-C37-C72
5	G	301	A1JH1	O70-C36-C37-C71
5	G	301	A1JH1	O70-C36-C37-C72
5	G	301	A1JH1	C50-C49-C54-N55
5	G	301	A1JH1	C50-C49-C54-O56
6	D	301	GDP	C5'-O5'-PA-O3A
6	D	301	GDP	C5'-O5'-PA-O2A
6	H	301	GDP	C5'-O5'-PA-O3A
6	H	301	GDP	C5'-O5'-PA-O1A
6	H	301	GDP	C5'-O5'-PA-O2A
5	G	301	A1JH1	N47-C49-C54-O56
5	G	301	A1JH1	N47-C49-C54-N55
5	G	301	A1JH1	C34-C33-N12-C13
5	C	301	A1JH1	O70-C36-C37-C71
6	D	301	GDP	C5'-O5'-PA-O1A
5	G	301	A1JH1	O70-C36-C37-C38

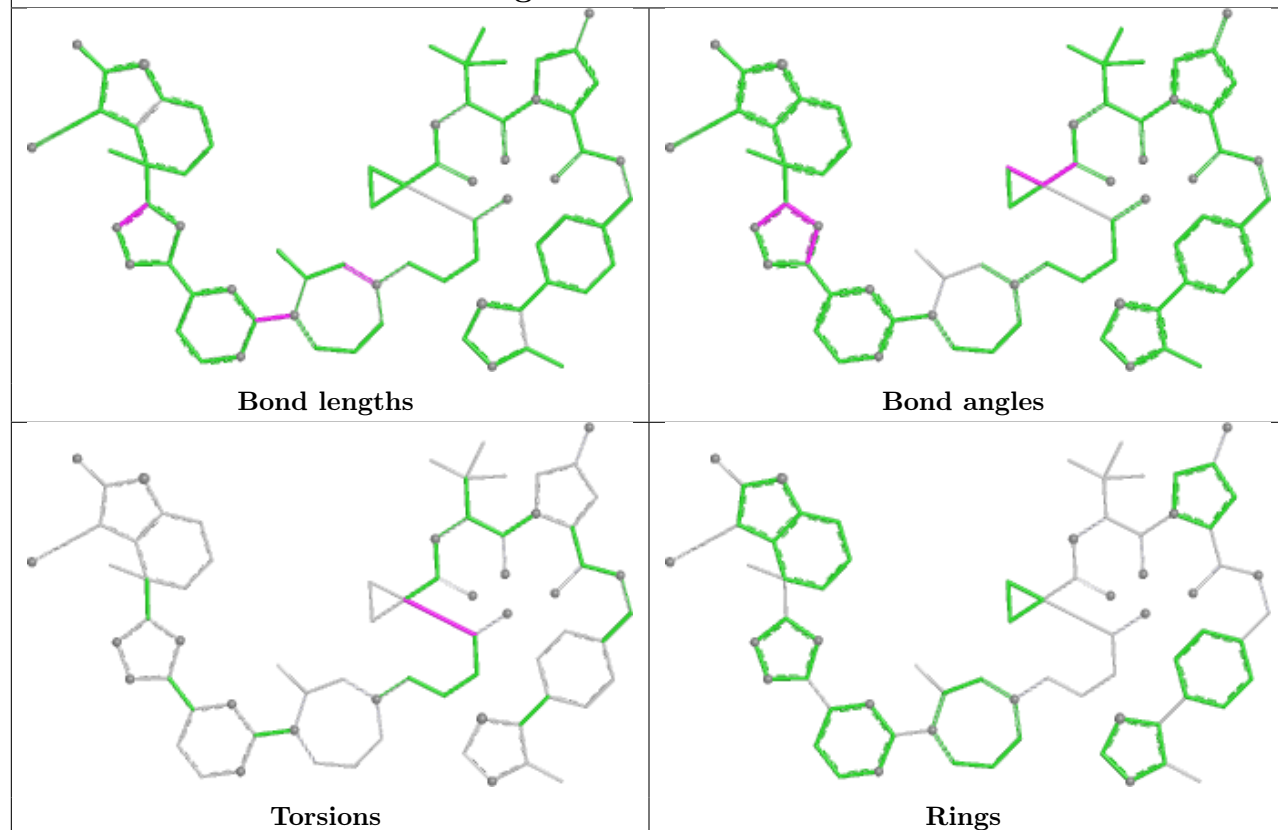
There are no ring outliers.

3 monomers are involved in 5 short contacts:

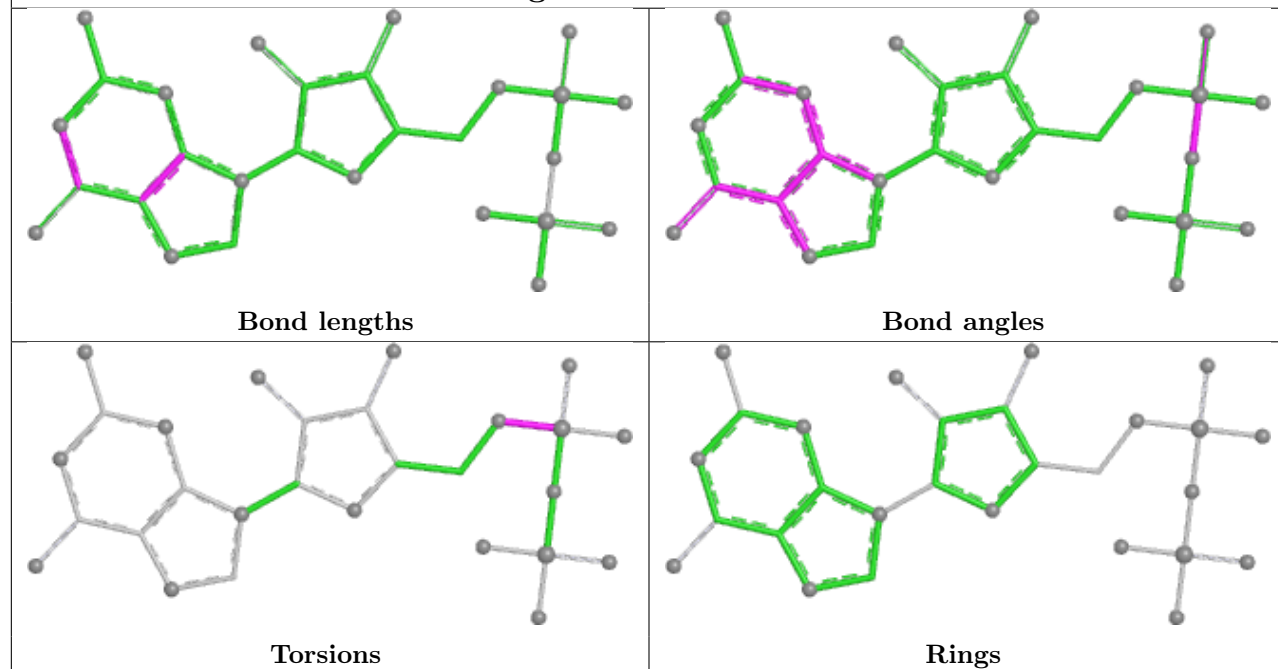
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	A1JH1	2	0
6	H	301	GDP	1	1
6	D	301	GDP	1	0

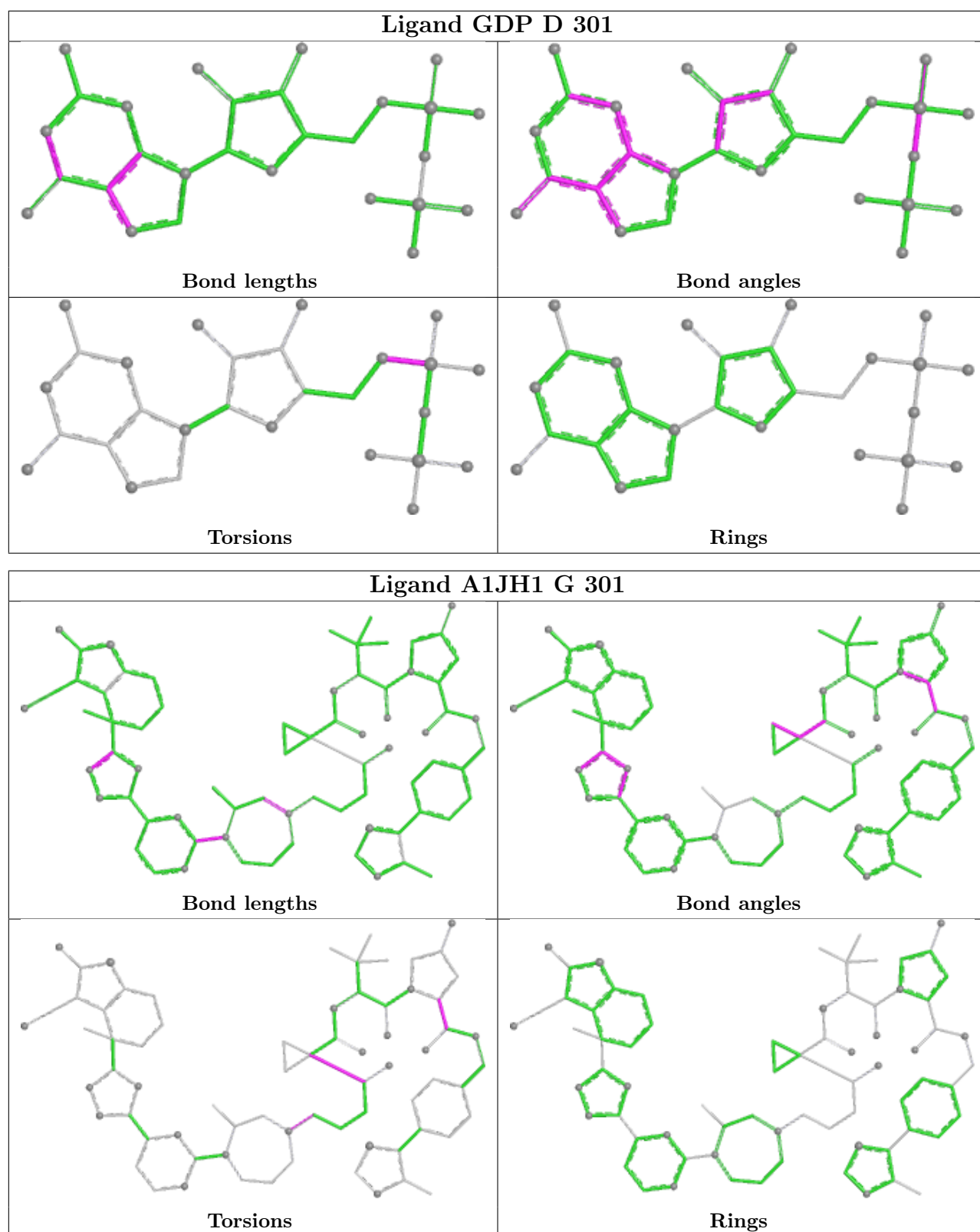
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand A1JH1 C 301



Ligand GDP H 301





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	100/104 (96%)	0.70	5 (5%) 34 28	52, 75, 98, 108	0
1	E	97/104 (93%)	1.15	21 (21%) 2 1	53, 87, 109, 124	0
2	B	85/97 (87%)	0.62	5 (5%) 28 23	44, 70, 87, 96	0
2	F	85/97 (87%)	0.45	2 (2%) 59 55	44, 62, 76, 88	0
3	C	147/162 (90%)	0.36	6 (4%) 41 35	29, 52, 89, 110	1 (0%)
3	G	149/162 (91%)	0.27	5 (3%) 48 42	26, 46, 73, 101	1 (0%)
4	D	168/170 (98%)	1.16	29 (17%) 4 3	47, 86, 117, 135	0
4	H	167/170 (98%)	0.56	6 (3%) 46 40	39, 59, 81, 100	0
All	All	998/1066 (93%)	0.66	79 (7%) 18 15	26, 66, 102, 135	2 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	122	SER	4.4
1	A	35	LEU	4.3
4	H	122	SER	4.0
4	D	6	LEU	3.8
1	E	24	VAL	3.6
4	D	55	ILE	3.5
1	E	53	ASP	3.5
1	E	23	THR	3.5
4	D	159	LEU	3.4
2	F	62	PHE	3.3
1	A	27	LEU	3.2
1	E	3	VAL	3.2
1	E	47	ASP	3.1
1	E	51	LEU	3.1
1	E	58	GLY	3.0
4	D	130	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	19	LEU	2.9
4	D	79	LEU	2.9
4	D	8	VAL	2.9
4	D	163	ILE	2.8
4	D	47	ASP	2.8
2	B	46	LEU	2.8
4	D	23	LEU	2.8
4	D	157	TYR	2.8
4	D	50	THR	2.7
4	D	152	VAL	2.7
2	F	90	ILE	2.7
1	A	57	LEU	2.7
2	B	88	THR	2.7
4	D	18	ALA	2.7
4	D	4	TYR	2.6
4	H	159	LEU	2.6
1	E	59	GLU	2.6
2	B	63	ARG	2.6
4	D	43	GLN	2.6
3	G	208	HIS	2.6
3	C	139	SER	2.5
4	D	80	CYS	2.5
3	G	140	LEU	2.5
1	E	56	THR	2.5
4	H	30	ASP	2.5
4	D	53	LEU	2.4
1	E	27	LEU	2.4
1	E	18	ALA	2.4
3	C	180	ILE	2.4
1	E	50	LEU	2.4
1	E	66	THR	2.4
3	C	143	ASP	2.4
1	E	25	PHE	2.4
1	A	84	THR	2.3
4	D	45	VAL	2.3
1	E	62	PHE	2.3
2	B	103	LEU	2.3
1	E	40	ASP	2.3
4	D	51	CYS	2.3
4	D	125	VAL	2.3
3	C	142	VAL	2.2
1	A	103	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	60	CYS	2.2
4	H	121	PRO	2.2
3	G	110[A]	HIS	2.2
2	B	33	ARG	2.2
4	D	141	PHE	2.2
4	D	85	ASN	2.1
1	E	5	LEU	2.1
4	D	160	VAL	2.1
3	G	60	ARG	2.1
1	E	61	GLY	2.1
3	C	170	VAL	2.1
4	H	1	MET	2.1
3	C	181	VAL	2.1
4	D	2	THR	2.1
1	E	1	MET	2.1
3	G	73	GLN	2.1
1	E	85	PHE	2.1
4	D	28	PHE	2.1
4	H	152	VAL	2.0
4	D	26	ASN	2.0
4	D	123	ARG	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

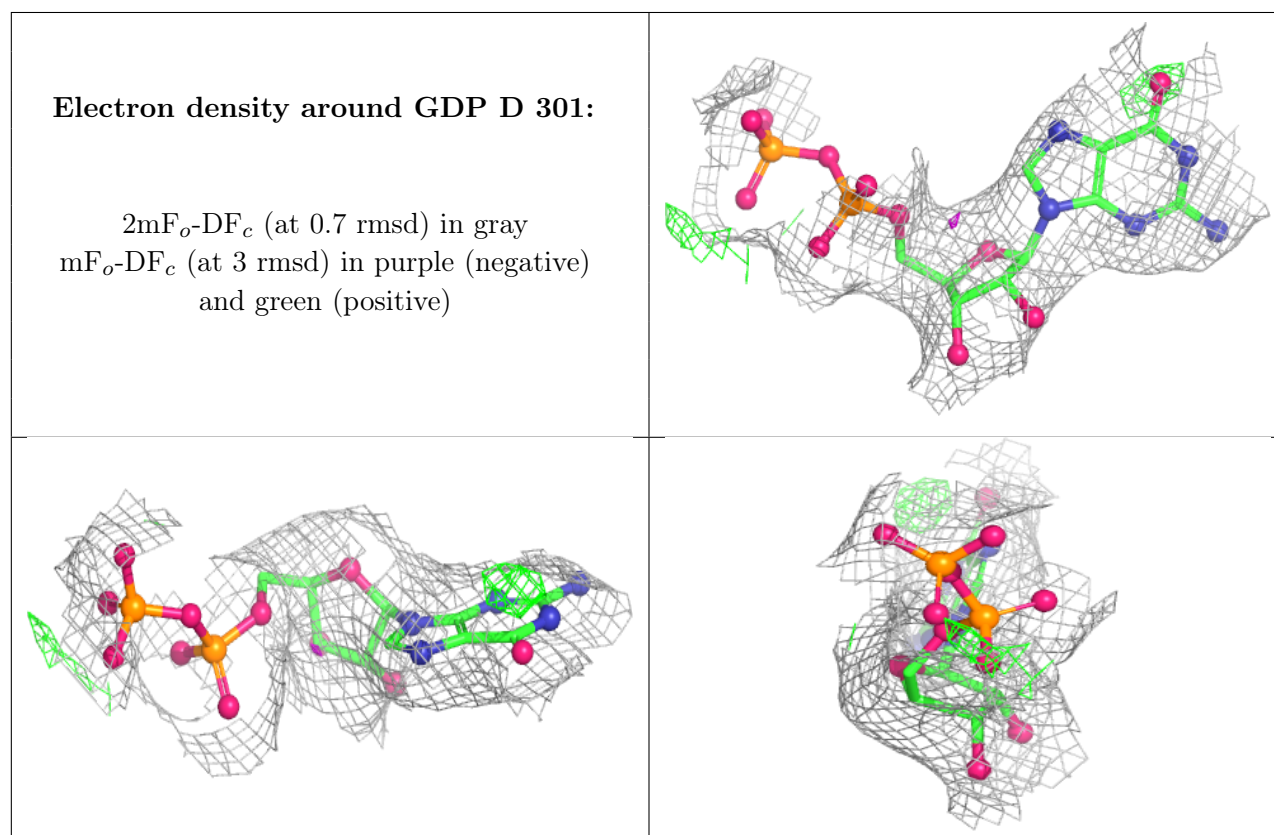
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	D	302	1/1	0.79	0.20	79,79,79,79	0
6	GDP	D	301	28/28	0.83	0.12	78,103,111,112	0

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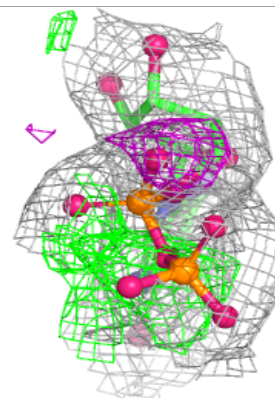
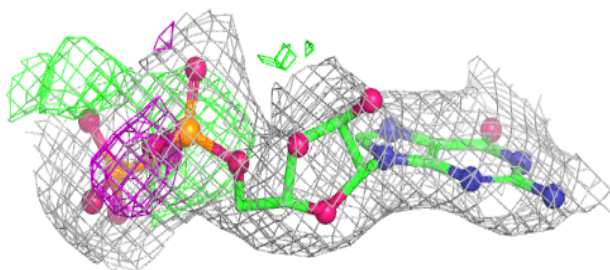
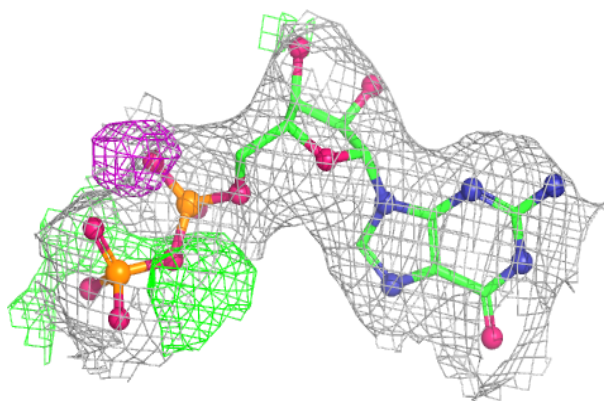
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GDP	H	301	28/28	0.92	0.10	37,52,61,69	0
5	A1JH1	C	301	72/72	0.93	0.11	39,49,61,64	0
7	MG	H	302	1/1	0.93	0.19	45,45,45,45	0
5	A1JH1	G	301	72/72	0.94	0.10	30,41,47,56	0

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.

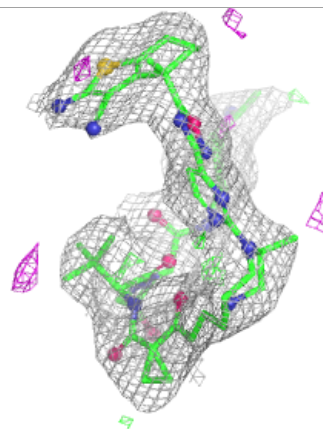
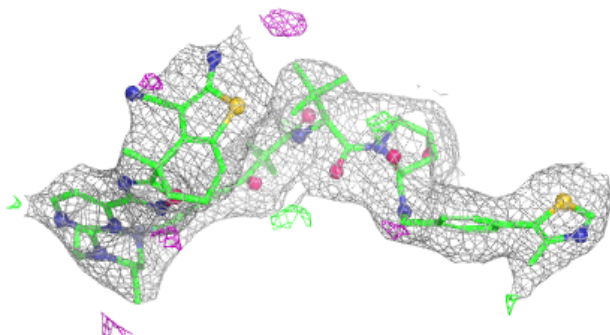
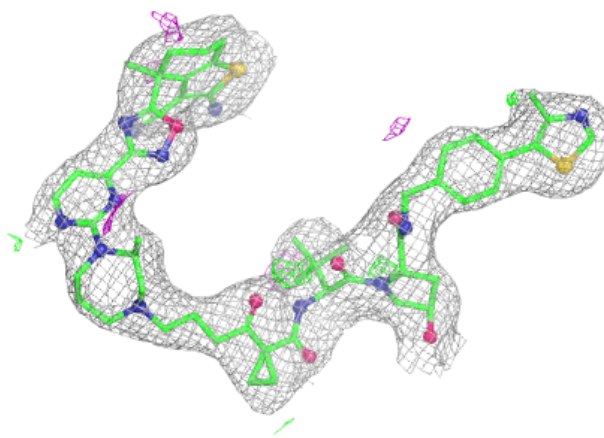


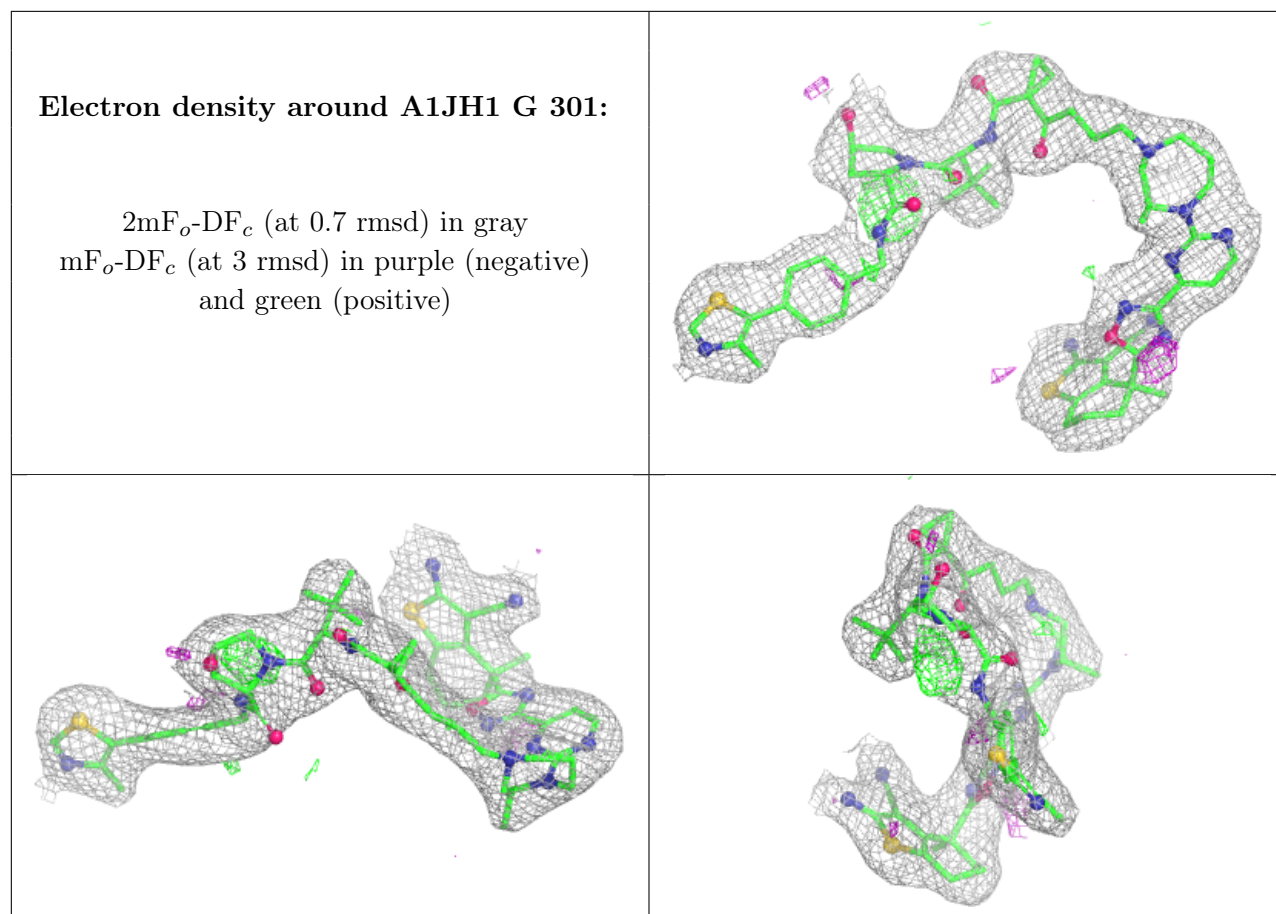
Electron density around GDP H 301:

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

**Electron density around A1JH1 C 301:**

$2mF_o-DF_c$ (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.