Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 03:13 PM JST

PDB ID	:	6JC7
Title	:	Crystal structure of aminotransferase CrmG from Actinoalloteichus sp. WH1-2216-6 in complex with amino donor L-Ala
Authors	:	Xu, J.; Su, K.; Liu, J.
Deposited on	:	2019-01-28
Resolution	:	2.20 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:

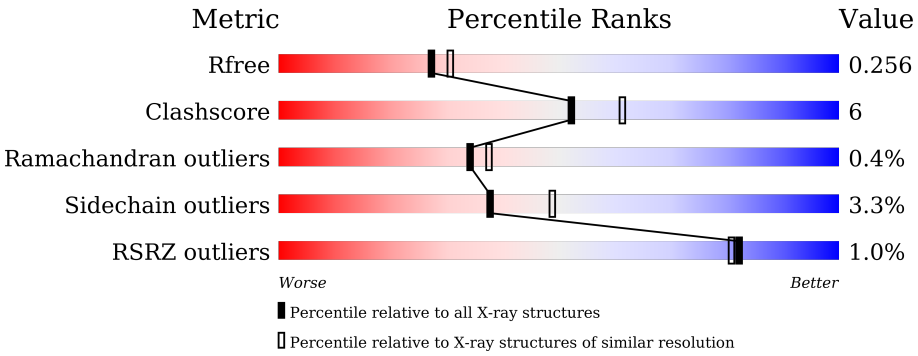
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	523	83% 13%
1	B	523	84% 12%
1	C	523	84% 12%
1	D	523	86% 11%

2 Entry composition

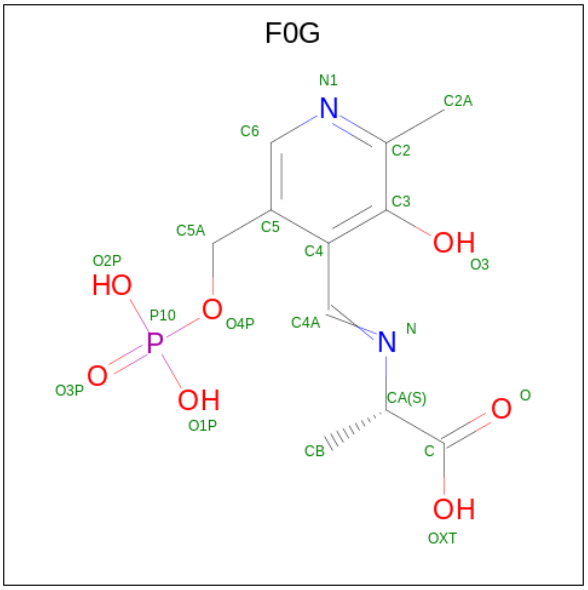
There are 5 unique types of molecules in this entry. The entry contains 16438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CrmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			3949	2470	714	754	11			
1	B	511	Total	C	N	O	S	0	0	0
			3949	2470	714	754	11			
1	C	510	Total	C	N	O	S	0	0	0
			3942	2466	713	752	11			
1	D	512	Total	C	N	O	S	0	0	0
			3958	2476	716	755	11			

- Molecule 2 is (E)-N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-alanine (three-letter code: F0G) (formula: $C_{11}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

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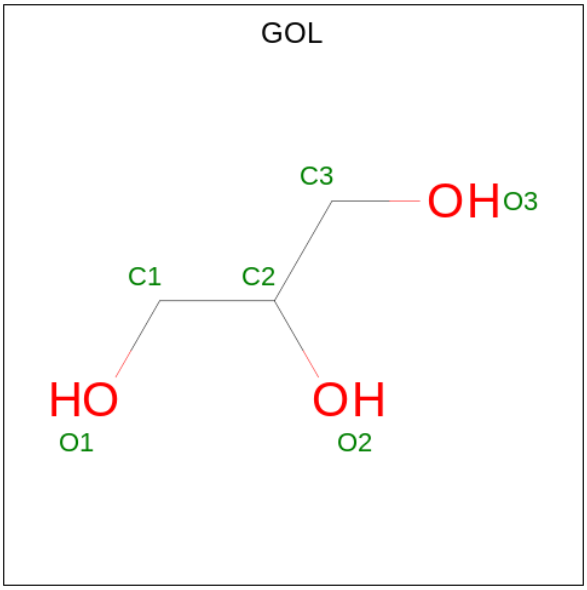
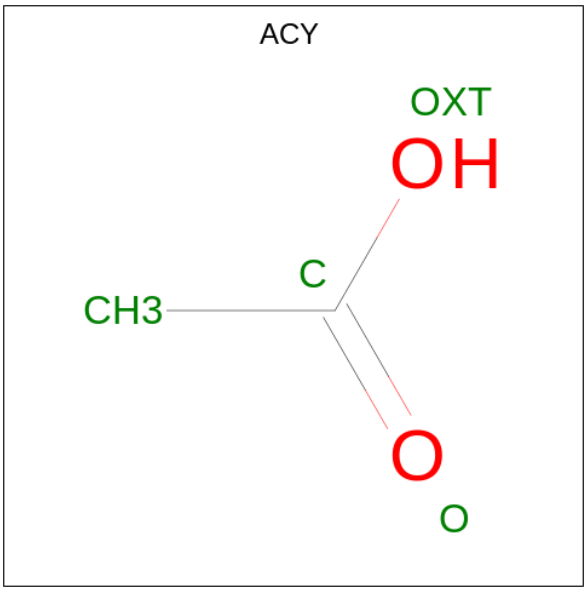
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

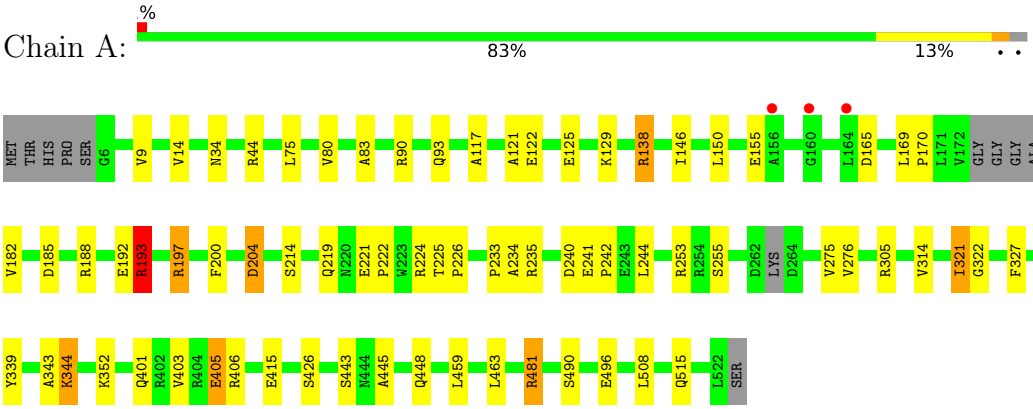
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	117	Total O 117 117	0	0
5	B	139	Total O 139 139	0	0
5	C	127	Total O 127 127	0	0
5	D	121	Total O 121 121	0	0

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.

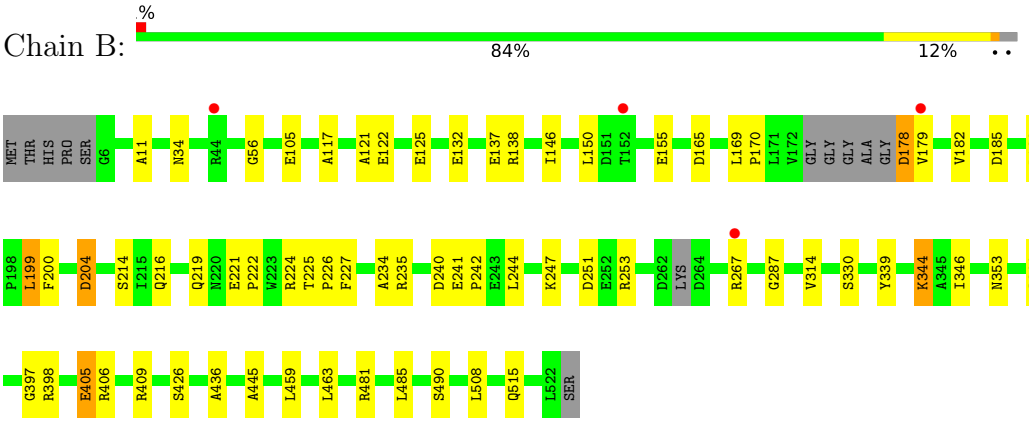
• Molecule 1: CrmG

Chain A:



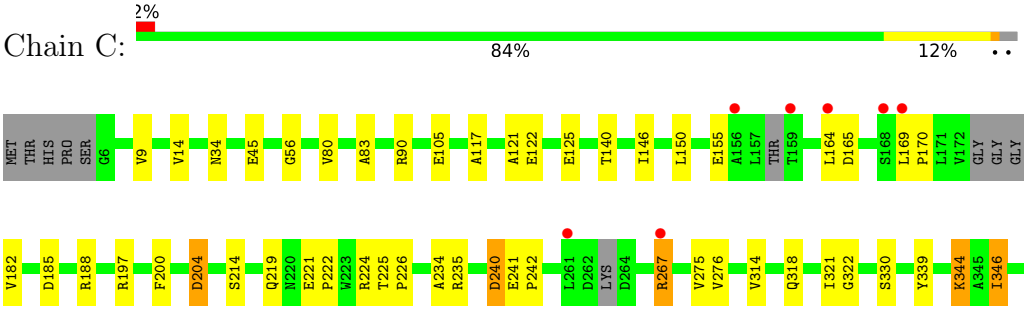
• Molecule 1: CrmG

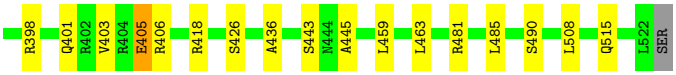
Chain B:



• Molecule 1: CrmG

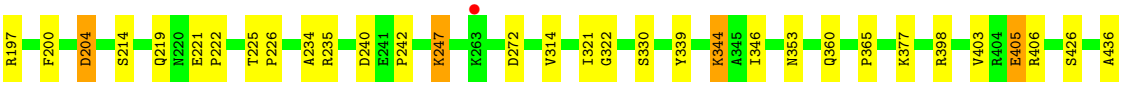
Chain C:





• Molecule 1: CrmG

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.76Å 83.65Å 87.97Å 106.48° 109.07° 95.12°	Depositor
Resolution (Å)	30.00 – 2.20 78.58 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.20) 92.9 (78.58-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.204 , 0.254 0.209 , 0.256	Depositor DCC
R_{free} test set	4960 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.156 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16438	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, F0G, GOL

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	0.76	0/4015	0.91	2/5439 (0.0%)
1	B	0.74	1/4015 (0.0%)	0.91	3/5439 (0.1%)
1	C	0.73	0/4007	0.90	2/5426 (0.0%)
1	D	0.75	1/4025 (0.0%)	0.90	1/5453 (0.0%)
All	All	0.75	2/16062 (0.0%)	0.91	8/21757 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	GLU	CD-OE1	-5.99	1.19	1.25
1	D	132	GLU	CD-OE1	-5.29	1.19	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	339	TYR	CB-CG-CD1	6.25	124.75	121.00
1	A	339	TYR	CB-CG-CD1	6.19	124.71	121.00
1	B	339	TYR	CB-CG-CD1	6.11	124.67	121.00
1	C	339	TYR	CB-CG-CD1	5.99	124.59	121.00
1	A	193	ARG	CG-CD-NE	5.96	124.33	111.80
1	B	481	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	90	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	ALA	Peptide

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	3949	0	3923	55	0
1	B	3949	0	3923	40	0
1	C	3942	0	3915	46	0
1	D	3958	0	3937	41	0
2	A	21	0	0	3	0
2	B	21	0	0	2	0
2	C	21	0	0	4	0
2	D	21	0	0	3	0
3	A	24	0	32	2	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	B	12	0	9	1	0
4	C	4	0	3	1	0
5	A	117	0	0	6	0
5	B	139	0	0	7	0
5	C	127	0	0	5	0
5	D	121	0	0	4	0
All	All	16438	0	15758	175	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (175) 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)
2:D:601:F0G:O3	2:D:601:F0G:N	1.93	0.91
2:A:601:F0G:O3	2:A:601:F0G:N	1.96	0.91
2:B:601:F0G:N	2:B:601:F0G:O3	2.12	0.77
1:D:138:ARG:HG2	1:D:138:ARG:HH21	1.50	0.76
1:A:93:GLN:NE2	5:A:704:HOH:O	2.20	0.73
1:D:344:LYS:O	5:D:701:HOH:O	2.06	0.73
1:A:344:LYS:O	5:A:701:HOH:O	2.07	0.72
1:C:56:GLY:O	5:C:701:HOH:O	2.07	0.71
1:A:138:ARG:HH21	1:A:138:ARG:HG2	1.57	0.70
1:C:344:LYS:O	5:C:703:HOH:O	2.10	0.69
1:A:335:ILE:O	5:A:702:HOH:O	2.09	0.69
1:C:45:GLU:OE2	5:C:702:HOH:O	2.09	0.69
1:A:193:ARG:HB2	1:A:193:ARG:HH21	1.57	0.67
1:B:314:VAL:HG11	1:B:330:SER:HB3	1.81	0.63
1:A:90:ARG:HD2	5:A:736:HOH:O	1.98	0.63
2:C:601:F0G:N	2:C:601:F0G:O3	2.30	0.62
1:D:138:ARG:HH21	1:D:138:ARG:CG	2.12	0.62
1:B:56:GLY:O	5:B:701:HOH:O	2.16	0.62
1:A:193:ARG:HH21	1:A:193:ARG:CB	2.13	0.62
1:C:318:GLN:O	5:C:705:HOH:O	2.16	0.62
1:A:314:VAL:HG11	1:A:330:SER:HB3	1.80	0.62
1:C:314:VAL:HG11	1:C:330:SER:HB3	1.81	0.62
1:A:193:ARG:HB2	1:A:193:ARG:NH2	2.15	0.61
1:D:314:VAL:HG11	1:D:330:SER:HB3	1.83	0.60
1:A:138:ARG:HH21	1:A:138:ARG:CG	2.14	0.60
1:D:113:ASN:HD22	1:D:360:GLN:HG2	1.67	0.60
1:A:193:ARG:HH21	1:A:193:ARG:CG	2.15	0.59
1:A:481:ARG:CZ	1:C:443:SER:HB3	2.33	0.58
1:B:397:GLY:HA2	5:B:765:HOH:O	2.05	0.57
1:A:225:THR:N	1:A:226:PRO:CD	2.68	0.57
1:A:443:SER:HB3	1:C:481:ARG:CZ	2.35	0.57
1:B:225:THR:N	1:B:226:PRO:CD	2.67	0.57
1:B:409:ARG:O	5:B:703:HOH:O	2.18	0.57
1:C:225:THR:N	1:C:226:PRO:CD	2.68	0.57
1:A:405:GLU:OE2	1:A:406:ARG:HD2	2.05	0.56
1:D:405:GLU:OE2	1:D:406:ARG:HD2	2.05	0.56
1:B:146:ILE:O	1:B:150:LEU:HG	2.06	0.56
1:D:225:THR:N	1:D:226:PRO:CD	2.69	0.56
3:A:605:GOL:O1	5:A:703:HOH:O	2.15	0.56
1:C:344:LYS:NZ	2:C:601:F0G:C4A	2.69	0.56
1:C:146:ILE:O	1:C:150:LEU:HG	2.06	0.55
1:A:146:ILE:O	1:A:150:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:GLU:OE2	1:C:406:ARG:HD2	2.06	0.55
1:A:200:PHE:O	1:A:234:ALA:HA	2.07	0.55
1:D:146:ILE:O	1:D:150:LEU:HG	2.06	0.55
1:D:200:PHE:O	1:D:234:ALA:HA	2.07	0.55
1:B:200:PHE:O	1:B:234:ALA:HA	2.07	0.55
1:B:405:GLU:OE2	1:B:406:ARG:HD2	2.05	0.55
1:C:200:PHE:O	1:C:234:ALA:HA	2.06	0.54
1:D:185:ASP:OD1	1:D:188:ARG:NH2	2.40	0.54
1:B:216:GLN:OE1	5:B:702:HOH:O	2.17	0.54
1:A:185:ASP:OD1	1:A:188:ARG:NH2	2.41	0.54
1:A:352:LYS:HD3	1:B:375:PHE:HB3	1.90	0.54
1:A:305:ARG:CZ	3:A:605:GOL:H32	2.38	0.53
1:C:185:ASP:OD1	1:C:188:ARG:NH2	2.41	0.53
1:A:344:LYS:NZ	2:A:601:F0G:C4A	2.71	0.53
1:A:9:VAL:O	1:B:360:GLN:NE2	2.38	0.52
1:D:344:LYS:HZ1	2:D:601:F0G:C4A	2.21	0.52
1:A:244:LEU:HD21	1:C:418:ARG:NH2	2.23	0.52
1:B:185:ASP:OD1	1:B:188:ARG:NH2	2.42	0.52
1:A:344:LYS:HZ1	2:A:601:F0G:C4A	2.23	0.51
1:B:137:GLU:OE2	1:B:137:GLU:HA	2.09	0.51
1:C:275:VAL:HG23	1:C:276:VAL:HG23	1.92	0.51
1:B:459:LEU:O	1:B:463:LEU:HG	2.11	0.51
1:B:405:GLU:OE2	1:B:406:ARG:CD	2.59	0.51
1:C:459:LEU:O	1:C:463:LEU:HG	2.11	0.51
1:D:459:LEU:O	1:D:463:LEU:HG	2.10	0.50
1:B:287:GLY:N	5:B:709:HOH:O	2.35	0.50
1:C:405:GLU:OE2	1:C:406:ARG:CD	2.59	0.50
1:C:14:VAL:HG21	1:D:365:PRO:HB2	1.93	0.50
1:A:405:GLU:OE2	1:A:406:ARG:CD	2.60	0.50
1:B:169:LEU:N	1:B:170:PRO:CD	2.75	0.50
1:A:197:ARG:HD3	1:A:233:PRO:CD	2.41	0.50
1:B:344:LYS:NZ	2:B:601:F0G:C4A	2.75	0.49
1:C:224:ARG:C	1:C:226:PRO:HD2	2.33	0.49
1:D:155:GLU:HA	1:D:155:GLU:OE1	2.12	0.49
1:D:99:ASN:O	5:D:702:HOH:O	2.20	0.49
1:D:169:LEU:N	1:D:170:PRO:CD	2.75	0.49
1:D:344:LYS:NZ	2:D:601:F0G:C4A	2.75	0.49
1:B:155:GLU:HA	1:B:155:GLU:OE1	2.12	0.49
1:A:169:LEU:N	1:A:170:PRO:CD	2.76	0.49
1:A:459:LEU:O	1:A:463:LEU:HG	2.12	0.49
1:C:155:GLU:OE1	1:C:155:GLU:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASP:O	1:A:182:VAL:HG23	2.13	0.49
1:D:405:GLU:OE2	1:D:406:ARG:CD	2.60	0.48
1:A:155:GLU:HA	1:A:155:GLU:OE1	2.14	0.48
1:D:121:ALA:O	1:D:125:GLU:HG3	2.14	0.48
1:B:34:ASN:ND2	1:B:490:SER:OG	2.47	0.48
1:C:121:ALA:O	1:C:125:GLU:HG3	2.13	0.47
1:A:204:ASP:HA	1:A:219:GLN:OE1	2.14	0.47
1:B:247:LYS:NZ	1:B:251:ASP:OD2	2.47	0.47
1:B:138:ARG:NE	5:B:713:HOH:O	2.40	0.47
1:C:169:LEU:N	1:C:170:PRO:CD	2.77	0.47
1:D:178:ASP:O	1:D:182:VAL:HG23	2.15	0.47
1:D:204:ASP:HA	1:D:219:GLN:OE1	2.15	0.47
1:A:14:VAL:HG21	1:B:365:PRO:HB2	1.96	0.47
1:C:169:LEU:N	1:C:170:PRO:HD2	2.29	0.47
1:C:178:ASP:O	1:C:182:VAL:HG23	2.15	0.47
1:B:121:ALA:O	1:B:125:GLU:HG3	2.15	0.46
1:B:178:ASP:O	1:B:182:VAL:HG23	2.15	0.46
1:A:34:ASN:ND2	1:A:490:SER:OG	2.48	0.46
1:A:275:VAL:HG23	1:A:276:VAL:HG23	1.98	0.46
1:B:241:GLU:HB3	1:B:244:LEU:HD13	1.98	0.46
1:C:14:VAL:HG21	1:D:365:PRO:CB	2.46	0.46
1:D:247:LYS:HD3	1:D:247:LYS:C	2.36	0.46
1:A:121:ALA:O	1:A:125:GLU:HG3	2.16	0.45
1:A:221:GLU:N	1:A:222:PRO:HD2	2.31	0.45
1:C:204:ASP:HA	1:C:219:GLN:OE1	2.15	0.45
1:D:34:ASN:ND2	1:D:490:SER:OG	2.49	0.45
1:A:75:LEU:HA	5:B:814:HOH:O	2.15	0.45
1:A:224:ARG:C	1:A:226:PRO:HD2	2.35	0.45
1:C:9:VAL:O	1:D:360:GLN:NE2	2.44	0.45
1:C:344:LYS:HZ1	2:C:601:F0G:C4A	2.29	0.45
1:D:221:GLU:N	1:D:222:PRO:HD2	2.31	0.45
1:C:365:PRO:HB2	1:D:14:VAL:HG21	1.98	0.45
1:B:169:LEU:N	1:B:170:PRO:HD2	2.32	0.45
1:B:204:ASP:HA	1:B:219:GLN:OE1	2.16	0.45
1:C:34:ASN:ND2	1:C:490:SER:OG	2.49	0.45
1:C:140:THR:HG23	5:C:708:HOH:O	2.16	0.45
1:A:193:ARG:NH2	1:A:255:SER:O	2.49	0.45
1:C:221:GLU:N	1:C:222:PRO:HD2	2.32	0.45
1:D:137:GLU:OE2	1:D:137:GLU:HA	2.17	0.44
1:B:221:GLU:N	1:B:222:PRO:HD2	2.32	0.44
1:D:169:LEU:N	1:D:170:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ALA:HA	1:D:485:LEU:O	2.17	0.44
1:C:165:ASP:HB3	1:C:267:ARG:HG3	2.00	0.43
1:A:80:VAL:CG1	1:A:83:ALA:HB2	2.48	0.43
1:B:436:ALA:HA	1:B:485:LEU:O	2.18	0.43
1:D:377:LYS:HD3	5:D:802:HOH:O	2.18	0.43
1:C:360:GLN:NE2	1:D:9:VAL:O	2.45	0.43
1:D:165:ASP:C	1:D:165:ASP:OD1	2.57	0.43
1:C:80:VAL:CG1	1:C:83:ALA:HB2	2.49	0.43
1:C:436:ALA:HA	1:C:485:LEU:O	2.18	0.43
1:A:169:LEU:N	1:A:170:PRO:HD2	2.33	0.43
1:B:224:ARG:C	1:B:226:PRO:HD2	2.39	0.43
1:D:113:ASN:ND2	1:D:360:GLN:HG2	2.30	0.43
1:D:117:ALA:HB1	1:D:122:GLU:HB3	2.01	0.43
1:A:129:LYS:HE2	1:B:227:PHE:CZ	2.54	0.43
1:C:344:LYS:HZ3	2:C:601:F0G:C4A	2.30	0.43
1:D:463:LEU:HD22	1:D:508:LEU:HD11	2.01	0.43
1:B:117:ALA:HB1	1:B:122:GLU:HB3	2.01	0.42
1:A:117:ALA:HB1	1:A:122:GLU:HB3	2.01	0.42
1:A:463:LEU:HD22	1:A:508:LEU:HD11	2.01	0.42
1:C:117:ALA:HB1	1:C:122:GLU:HB3	2.01	0.42
1:C:165:ASP:OD1	1:C:165:ASP:C	2.57	0.42
1:C:463:LEU:HD22	1:C:508:LEU:HD11	2.01	0.42
1:A:165:ASP:C	1:A:165:ASP:OD1	2.58	0.42
1:B:165:ASP:OD1	1:B:165:ASP:C	2.57	0.42
1:C:322:GLY:O	1:C:403:VAL:HG11	2.20	0.42
1:A:44:ARG:HB2	1:A:44:ARG:NH1	2.35	0.42
1:A:197:ARG:HD3	1:A:233:PRO:HD3	2.01	0.42
1:B:463:LEU:HD22	1:B:508:LEU:HD11	2.01	0.42
1:B:197:ARG:NH1	1:B:199:LEU:HD11	2.34	0.42
1:C:240:ASP:C	1:C:242:PRO:HD3	2.39	0.42
1:D:138:ARG:HD2	5:D:753:HOH:O	2.19	0.41
1:A:322:GLY:O	1:A:403:VAL:HG11	2.20	0.41
1:A:496:GLU:HB2	5:A:777:HOH:O	2.20	0.41
1:D:322:GLY:O	1:D:403:VAL:HG11	2.21	0.41
1:B:445:ALA:HB1	1:B:515:GLN:OE1	2.21	0.41
1:D:240:ASP:C	1:D:242:PRO:HD3	2.40	0.41
1:C:346:ILE:HG23	1:C:353:ASN:HB3	2.02	0.41
1:A:445:ALA:HB1	1:A:515:GLN:OE1	2.21	0.41
1:C:105:GLU:OE2	4:C:603:ACY:O	2.39	0.41
1:D:346:ILE:HG23	1:D:353:ASN:HB3	2.02	0.41
1:A:241:GLU:HB3	1:A:244:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLU:OE2	4:B:603:ACY:OXT	2.39	0.41
1:A:80:VAL:HG12	1:A:83:ALA:HB2	2.02	0.41
1:A:240:ASP:C	1:A:242:PRO:HD3	2.41	0.40
1:D:225:THR:N	1:D:226:PRO:HD3	2.36	0.40
1:A:193:ARG:HH21	1:A:193:ARG:HG2	1.85	0.40
1:C:164:LEU:C	1:C:164:LEU:HD13	2.42	0.40
1:A:321:ILE:HD13	1:A:327:PHE:CZ	2.56	0.40
1:B:240:ASP:C	1:B:242:PRO:HD3	2.42	0.40
1:C:445:ALA:HB1	1:C:515:GLN:OE1	2.22	0.40
1:B:346:ILE:HG23	1:B:353:ASN:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	505/523 (97%)	486 (96%)	16 (3%)	3 (1%)	25	26
1	B	505/523 (97%)	483 (96%)	20 (4%)	2 (0%)	34	37
1	C	502/523 (96%)	482 (96%)	18 (4%)	2 (0%)	34	37
1	D	508/523 (97%)	487 (96%)	19 (4%)	2 (0%)	34	37
All	All	2020/2092 (97%)	1938 (96%)	73 (4%)	9 (0%)	34	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	LYS
1	B	344	LYS
1	C	344	LYS
1	D	344	LYS
1	A	343	ALA

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Mol	Chain	Res	Type
1	D	179	VAL
1	A	179	VAL
1	B	179	VAL
1	C	179	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/422 (98%)	399 (96%)	16 (4%)	32	41
1	B	415/422 (98%)	403 (97%)	12 (3%)	42	54
1	C	414/422 (98%)	400 (97%)	14 (3%)	37	47
1	D	416/422 (99%)	403 (97%)	13 (3%)	40	51
All	All	1660/1688 (98%)	1605 (97%)	55 (3%)	38	49

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	A	178	ASP
1	A	192	GLU
1	A	193	ARG
1	A	197	ARG
1	A	204	ASP
1	A	214	SER
1	A	235	ARG
1	A	253	ARG
1	A	321	ILE
1	A	401	GLN
1	A	405	GLU
1	A	415	GLU
1	A	426	SER
1	A	448	GLN
1	A	481	ARG
1	B	178	ASP

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Mol	Chain	Res	Type
1	B	192	GLU
1	B	197	ARG
1	B	199	LEU
1	B	204	ASP
1	B	214	SER
1	B	235	ARG
1	B	253	ARG
1	B	267	ARG
1	B	398	ARG
1	B	405	GLU
1	B	426	SER
1	C	178	ASP
1	C	197	ARG
1	C	204	ASP
1	C	214	SER
1	C	235	ARG
1	C	240	ASP
1	C	241	GLU
1	C	267	ARG
1	C	321	ILE
1	C	346	ILE
1	C	398	ARG
1	C	401	GLN
1	C	405	GLU
1	C	426	SER
1	D	138	ARG
1	D	178	ASP
1	D	197	ARG
1	D	204	ASP
1	D	214	SER
1	D	235	ARG
1	D	247	LYS
1	D	272	ASP
1	D	321	ILE
1	D	398	ARG
1	D	405	GLU
1	D	426	SER
1	D	481	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	34	ASN
1	B	34	ASN
1	B	216	GLN
1	C	34	ASN
1	D	34	ASN
1	D	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	F0G	D	601	-	20,21,21	2.48	5 (25%)	26,30,30	3.57	12 (46%)
3	GOL	A	603	-	5,5,5	0.16	0	5,5,5	0.38	0
2	F0G	B	601	-	20,21,21	2.91	8 (40%)	26,30,30	3.20	12 (46%)
3	GOL	C	602	-	5,5,5	0.11	0	5,5,5	0.31	0
4	ACY	C	603	-	3,3,3	1.16	0	3,3,3	0.95	0
3	GOL	A	605	-	5,5,5	0.18	0	5,5,5	0.52	0
2	F0G	C	601	-	20,21,21	1.82	5 (25%)	26,30,30	2.69	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	602	-	5,5,5	0.19	0	5,5,5	0.31	0
2	F0G	A	601	-	20,21,21	2.02	5 (25%)	26,30,30	2.62	9 (34%)
3	GOL	D	602	-	5,5,5	0.28	0	5,5,5	0.61	0
4	ACY	B	604	-	3,3,3	1.01	0	3,3,3	0.92	0
4	ACY	B	602	-	3,3,3	1.26	0	3,3,3	0.51	0
3	GOL	A	604	-	5,5,5	0.20	0	5,5,5	0.47	0
4	ACY	B	603	-	3,3,3	1.35	0	3,3,3	0.55	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
2	F0G	D	601	-	-	4/15/15/15	0/1/1/1
3	GOL	A	603	-	-	2/4/4/4	-
2	F0G	B	601	-	-	3/15/15/15	0/1/1/1
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
2	F0G	C	601	-	-	1/15/15/15	0/1/1/1
3	GOL	A	602	-	-	4/4/4/4	-
2	F0G	A	601	-	-	3/15/15/15	0/1/1/1
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	A	604	-	-	1/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	F0G	C4-C5	7.99	1.52	1.42
2	B	601	F0G	C4-C5	7.84	1.51	1.42
2	B	601	F0G	C3-C2	6.35	1.47	1.40
2	A	601	F0G	C3-C2	5.69	1.46	1.40
2	C	601	F0G	C4-C3	4.62	1.47	1.40
2	B	601	F0G	C4-C3	4.49	1.47	1.40
2	D	601	F0G	C3-C2	4.11	1.45	1.40
2	D	601	F0G	C4A-N	4.00	1.34	1.27
2	A	601	F0G	C4-C4A	-3.68	1.39	1.46
2	C	601	F0G	C3-C2	3.35	1.44	1.40
2	C	601	F0G	C4-C5	3.08	1.45	1.42
2	B	601	F0G	P10-O3P	3.06	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	F0G	C4A-N	2.82	1.32	1.27
2	B	601	F0G	C6-C5	2.81	1.43	1.37
2	B	601	F0G	C4A-N	2.81	1.32	1.27
2	C	601	F0G	C2-N1	2.72	1.39	1.33
2	C	601	F0G	C4-C4A	-2.67	1.41	1.46
2	D	601	F0G	C4-C3	2.58	1.44	1.40
2	A	601	F0G	C4-C5	2.45	1.45	1.42
2	A	601	F0G	C2-N1	2.44	1.38	1.33
2	B	601	F0G	O3-C3	2.20	1.42	1.37
2	D	601	F0G	CA-N	2.09	1.49	1.47
2	B	601	F0G	P10-O1P	-2.08	1.46	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	F0G	C4-C3-C2	-10.29	113.82	120.19
2	D	601	F0G	C5-C4-C4A	9.96	137.95	121.56
2	D	601	F0G	C3-C4-C4A	-8.06	105.39	120.41
2	C	601	F0G	C4-C3-C2	-7.61	115.48	120.19
2	A	601	F0G	CA-N-C4A	7.04	130.34	118.00
2	D	601	F0G	CA-N-C4A	6.76	129.84	118.00
2	C	601	F0G	CA-N-C4A	6.34	129.12	118.00
2	C	601	F0G	C4-C4A-N	-5.99	109.70	123.01
2	D	601	F0G	C2A-C2-C3	-5.89	113.62	120.89
2	A	601	F0G	C4-C4A-N	-5.82	110.08	123.01
2	B	601	F0G	C2A-C2-C3	-5.42	114.20	120.89
2	B	601	F0G	C3-C4-C4A	-5.37	110.40	120.41
2	A	601	F0G	C3-C4-C4A	-4.76	111.54	120.41
2	A	601	F0G	C5-C4-C4A	4.57	129.08	121.56
2	B	601	F0G	C5-C4-C4A	4.49	128.94	121.56
2	B	601	F0G	C4-C4A-N	-4.20	113.69	123.01
2	D	601	F0G	C5A-C5-C6	-3.70	113.28	119.37
2	D	601	F0G	C3-C4-C5	-3.61	115.49	118.26
2	C	601	F0G	C2A-C2-C3	-3.48	116.59	120.89
2	D	601	F0G	C4-C4A-N	-3.41	115.42	123.01
2	D	601	F0G	OXT-C-O	-3.41	116.35	124.09
2	B	601	F0G	O4P-C5A-C5	-3.34	102.99	109.35
2	B	601	F0G	O3-C3-C2	3.17	124.40	117.49
2	D	601	F0G	C2A-C2-N1	2.98	123.49	117.67
2	A	601	F0G	C2A-C2-C3	-2.97	117.22	120.89
2	A	601	F0G	O3-C3-C2	2.74	123.47	117.49
2	B	601	F0G	CA-N-C4A	2.72	122.76	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	F0G	C4-C3-C2	-2.69	118.52	120.19
2	D	601	F0G	O3-C3-C2	2.66	123.28	117.49
2	A	601	F0G	OXT-C-O	-2.62	118.13	124.09
2	C	601	F0G	CB-CA-N	2.61	113.50	108.54
2	B	601	F0G	C3-C4-C5	2.54	120.21	118.26
2	A	601	F0G	C2A-C2-N1	2.47	122.50	117.67
2	B	601	F0G	C3-C2-N1	2.44	123.92	120.77
2	C	601	F0G	C2A-C2-N1	2.27	122.11	117.67
2	C	601	F0G	C3-C4-C4A	-2.21	116.30	120.41
2	D	601	F0G	O4P-P10-O3P	2.16	112.54	106.47
2	A	601	F0G	O2P-P10-O1P	2.15	115.84	107.64
2	B	601	F0G	C2A-C2-N1	2.12	121.82	117.67
2	B	601	F0G	C6-N1-C2	2.10	123.05	119.17
2	C	601	F0G	C6-N1-C2	2.06	122.99	119.17

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	F0G	CB-CA-N-C4A
2	D	601	F0G	CB-CA-N-C4A
2	D	601	F0G	OXT-C-CA-CB
2	D	601	F0G	O-C-CA-CB
3	A	602	GOL	C1-C2-C3-O3
3	A	603	GOL	O1-C1-C2-C3
3	A	605	GOL	O1-C1-C2-C3
3	A	605	GOL	O1-C1-C2-O2
3	D	602	GOL	O1-C1-C2-C3
2	B	601	F0G	CB-CA-N-C4A
3	A	602	GOL	O2-C2-C3-O3
3	A	603	GOL	O1-C1-C2-O2
2	A	601	F0G	CB-CA-N-C4A
2	A	601	F0G	OXT-C-CA-CB
2	A	601	F0G	O-C-CA-CB
3	A	602	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	D	602	GOL	O1-C1-C2-O2
2	D	601	F0G	OXT-C-CA-N
2	B	601	F0G	OXT-C-CA-CB
2	B	601	F0G	O-C-CA-CB
3	A	602	GOL	O1-C1-C2-C3

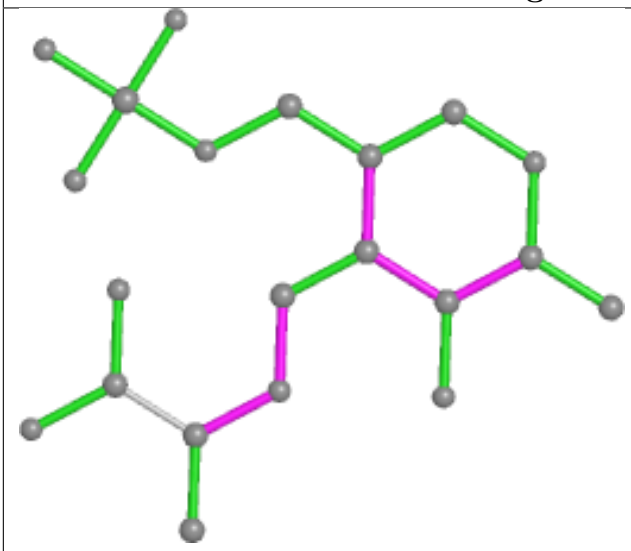
There are no ring outliers.

7 monomers are involved in 16 short contacts:

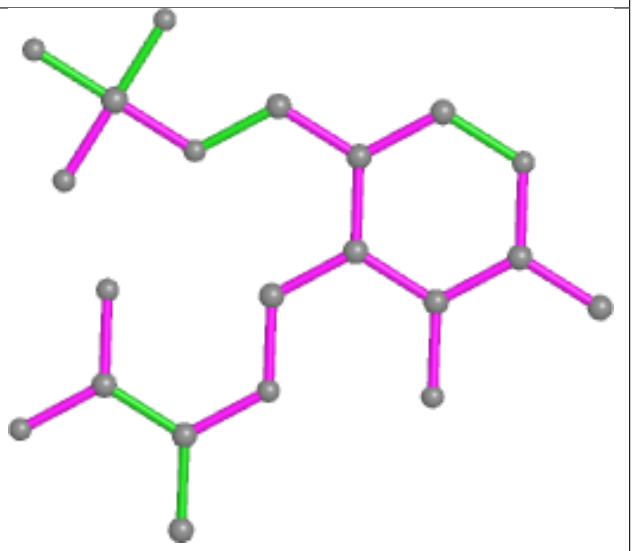
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	F0G	3	0
2	B	601	F0G	2	0
4	C	603	ACY	1	0
3	A	605	GOL	2	0
2	C	601	F0G	4	0
2	A	601	F0G	3	0
4	B	603	ACY	1	0

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

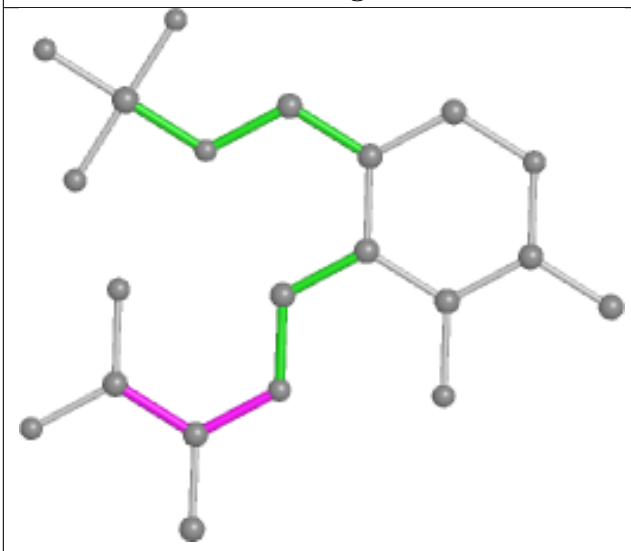
Ligand F0G D 601



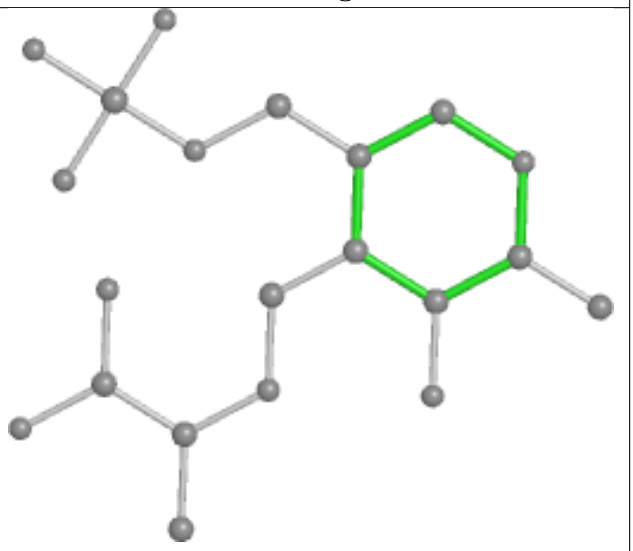
Bond lengths



Bond angles

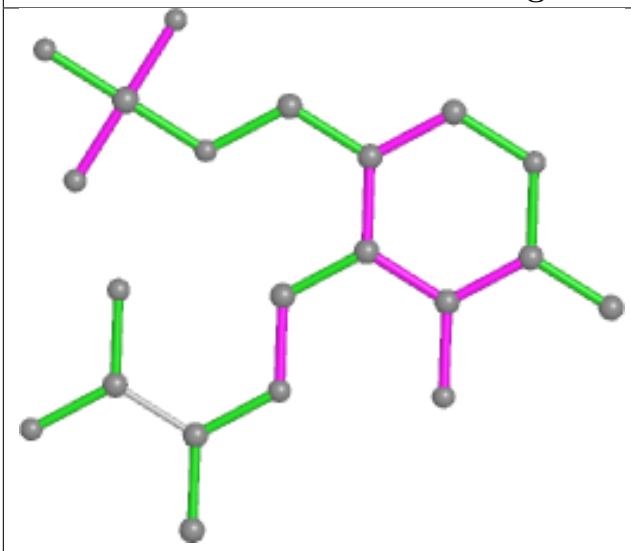


Torsions

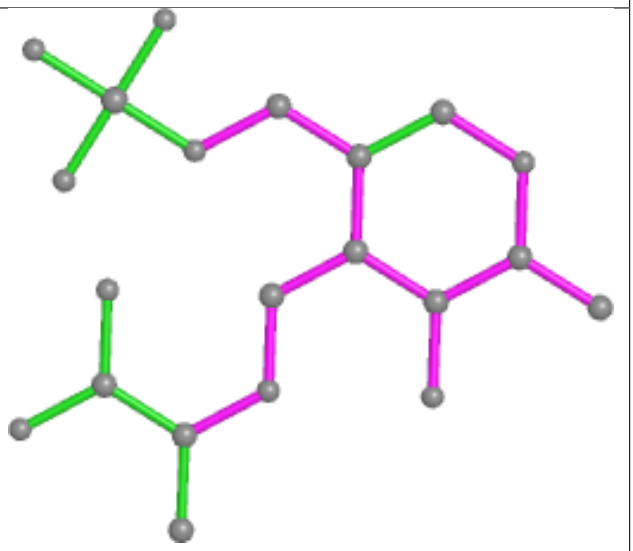


Rings

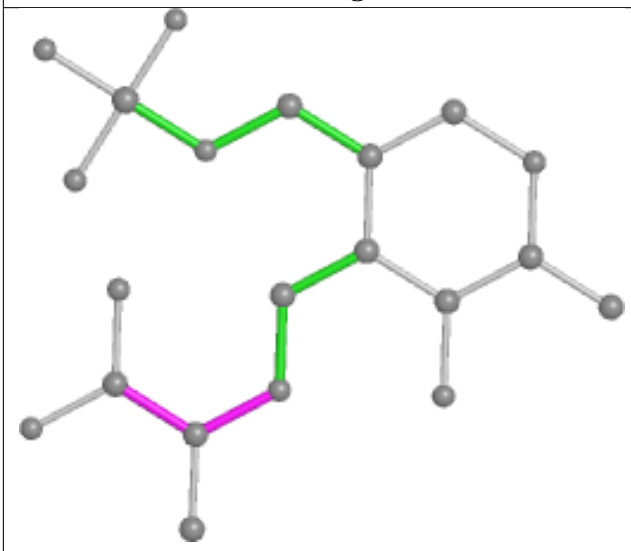
Ligand F0G B 601



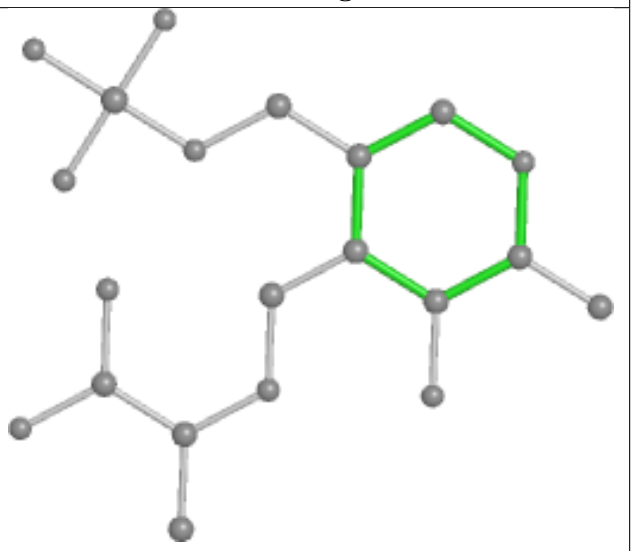
Bond lengths



Bond angles

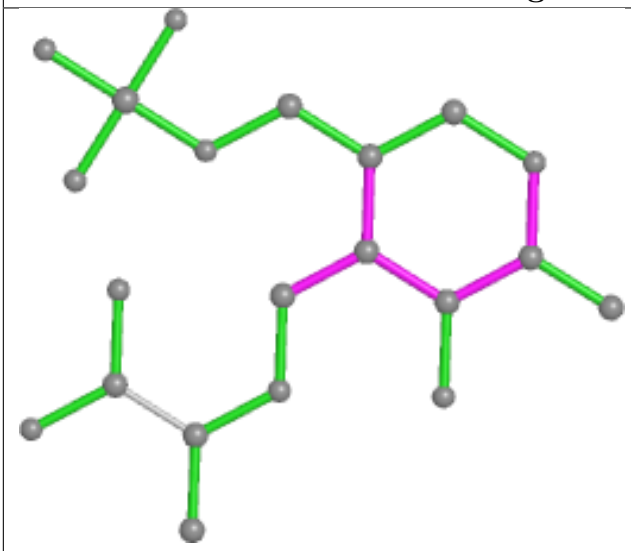


Torsions

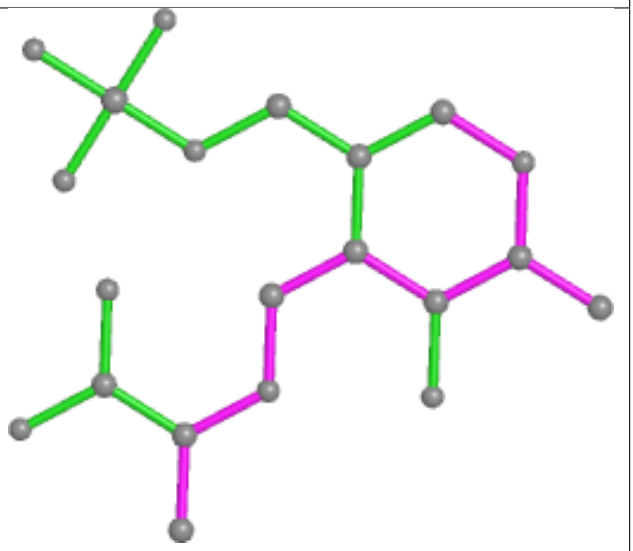


Rings

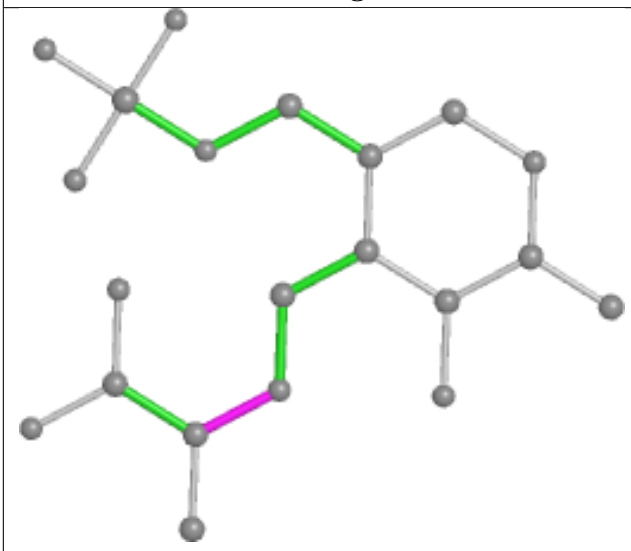
Ligand F0G C 601



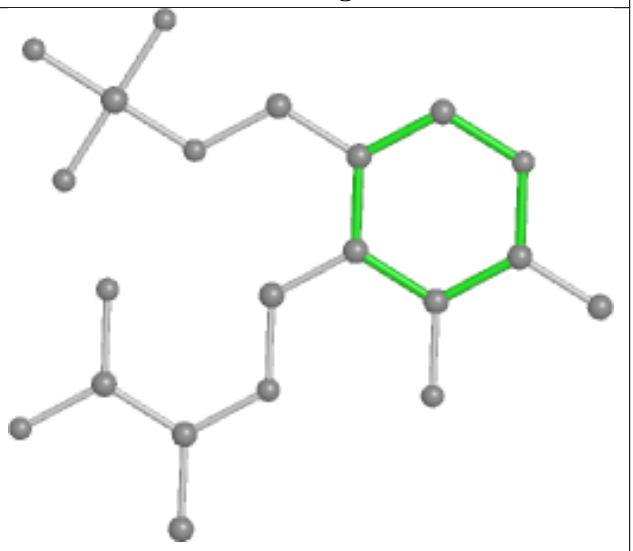
Bond lengths



Bond angles

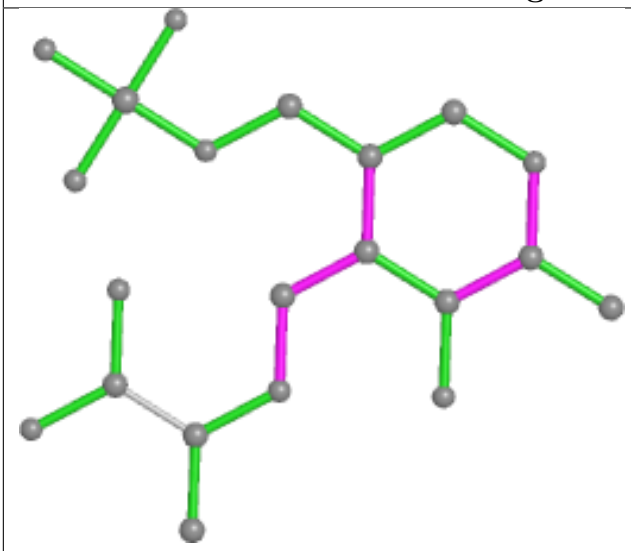


Torsions

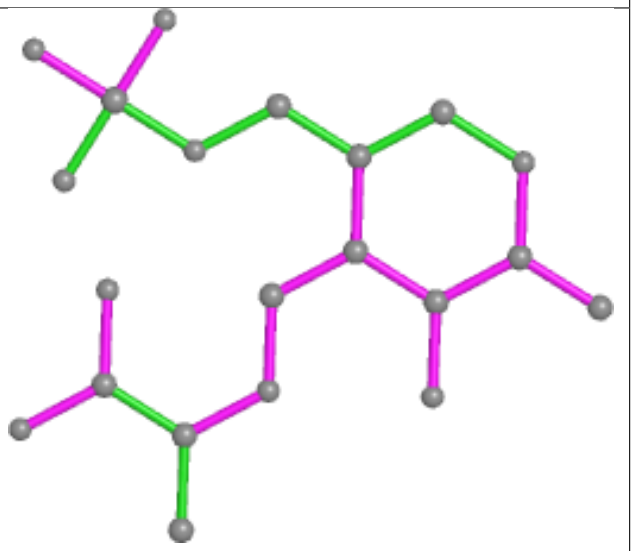


Rings

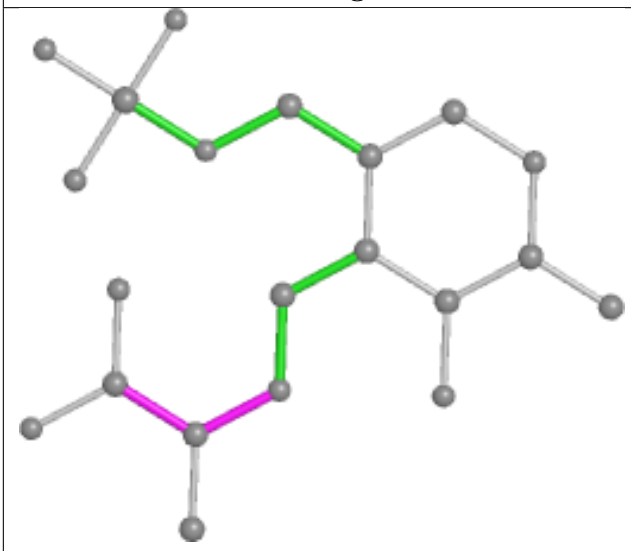
Ligand F0G A 601



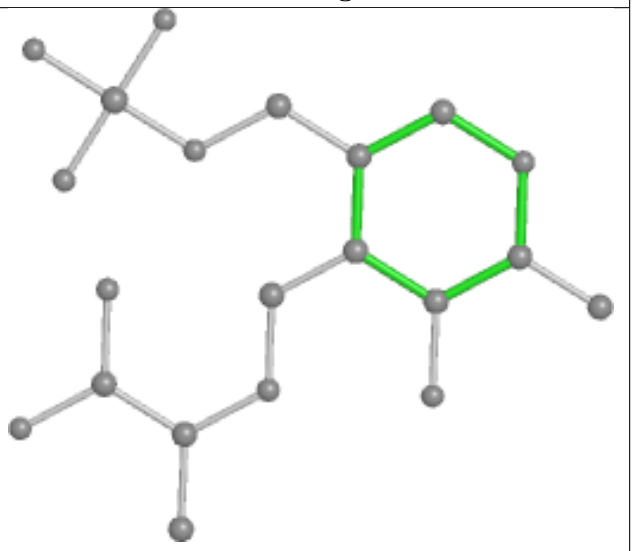
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	511/523 (97%)	-0.24	4 (0%)	86	85	22, 38, 69, 91	0
1	B	511/523 (97%)	-0.19	4 (0%)	86	85	21, 38, 71, 98	0
1	C	510/523 (97%)	-0.13	8 (1%)	72	70	24, 38, 73, 95	0
1	D	512/523 (97%)	-0.22	4 (0%)	86	85	24, 38, 67, 94	0
All	All	2044/2092 (97%)	-0.20	20 (0%)	82	81	21, 38, 70, 98	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	ARG	4.4
1	C	164	LEU	3.6
1	D	158	THR	3.1
1	A	160	GLY	3.1
1	B	179	VAL	2.8
1	A	164	LEU	2.8
1	D	263	LYS	2.7
1	C	169	LEU	2.6
1	D	164	LEU	2.5
1	C	168	SER	2.5
1	D	161	THR	2.4
1	C	156	ALA	2.3
1	B	267	ARG	2.3
1	B	44	ARG	2.2
1	A	179	VAL	2.2
1	C	159	THR	2.2
1	C	179	VAL	2.1
1	B	152	THR	2.0
1	C	261	LEU	2.0
1	A	156	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

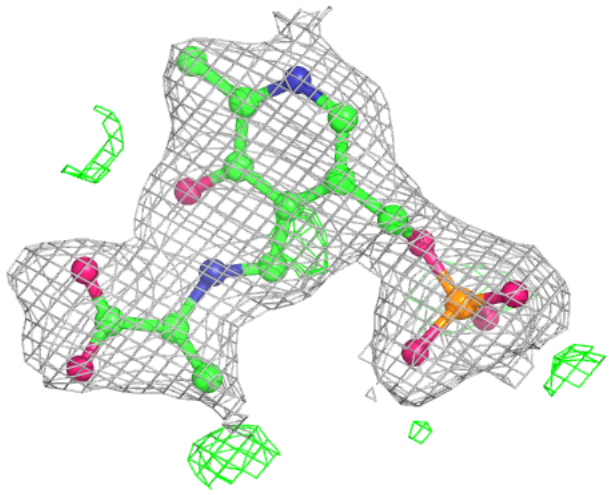
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

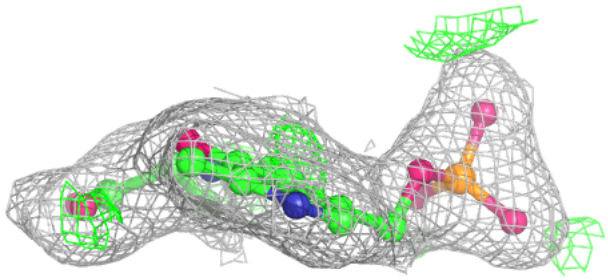
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACY	B	604	4/4	0.69	0.17	50,54,55,56	0
3	GOL	A	602	6/6	0.76	0.19	55,57,59,63	0
4	ACY	C	603	4/4	0.85	0.15	45,45,48,48	0
3	GOL	A	604	6/6	0.86	0.13	49,57,60,62	0
3	GOL	D	602	6/6	0.86	0.10	42,44,48,50	0
3	GOL	C	602	6/6	0.87	0.15	51,55,58,60	0
4	ACY	B	603	4/4	0.87	0.14	44,48,48,52	0
4	ACY	B	602	4/4	0.88	0.10	40,47,47,53	0
3	GOL	A	605	6/6	0.91	0.12	44,53,56,57	0
3	GOL	A	603	6/6	0.94	0.15	49,52,55,56	0
2	F0G	A	601	21/21	0.96	0.12	27,34,59,65	0
2	F0G	B	601	21/21	0.96	0.13	26,36,63,64	0
2	F0G	C	601	21/21	0.97	0.11	24,33,66,70	0
2	F0G	D	601	21/21	0.97	0.13	28,38,59,63	0

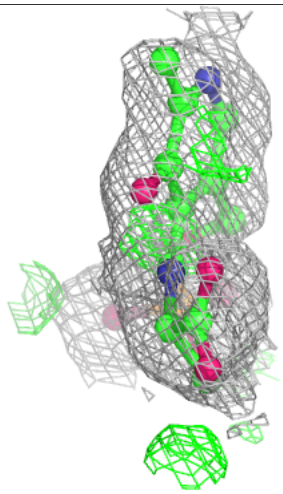
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around F0G A 601:

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

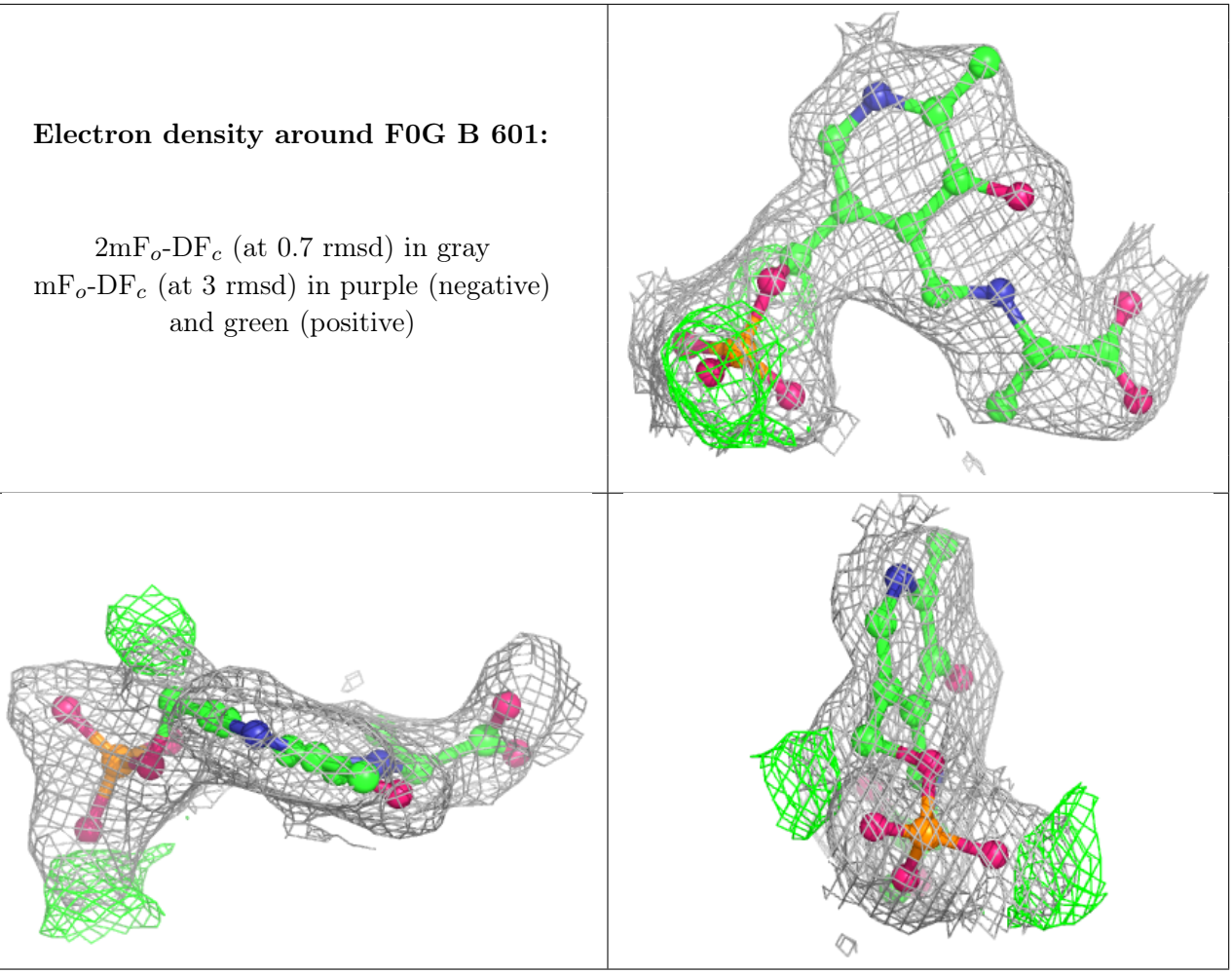






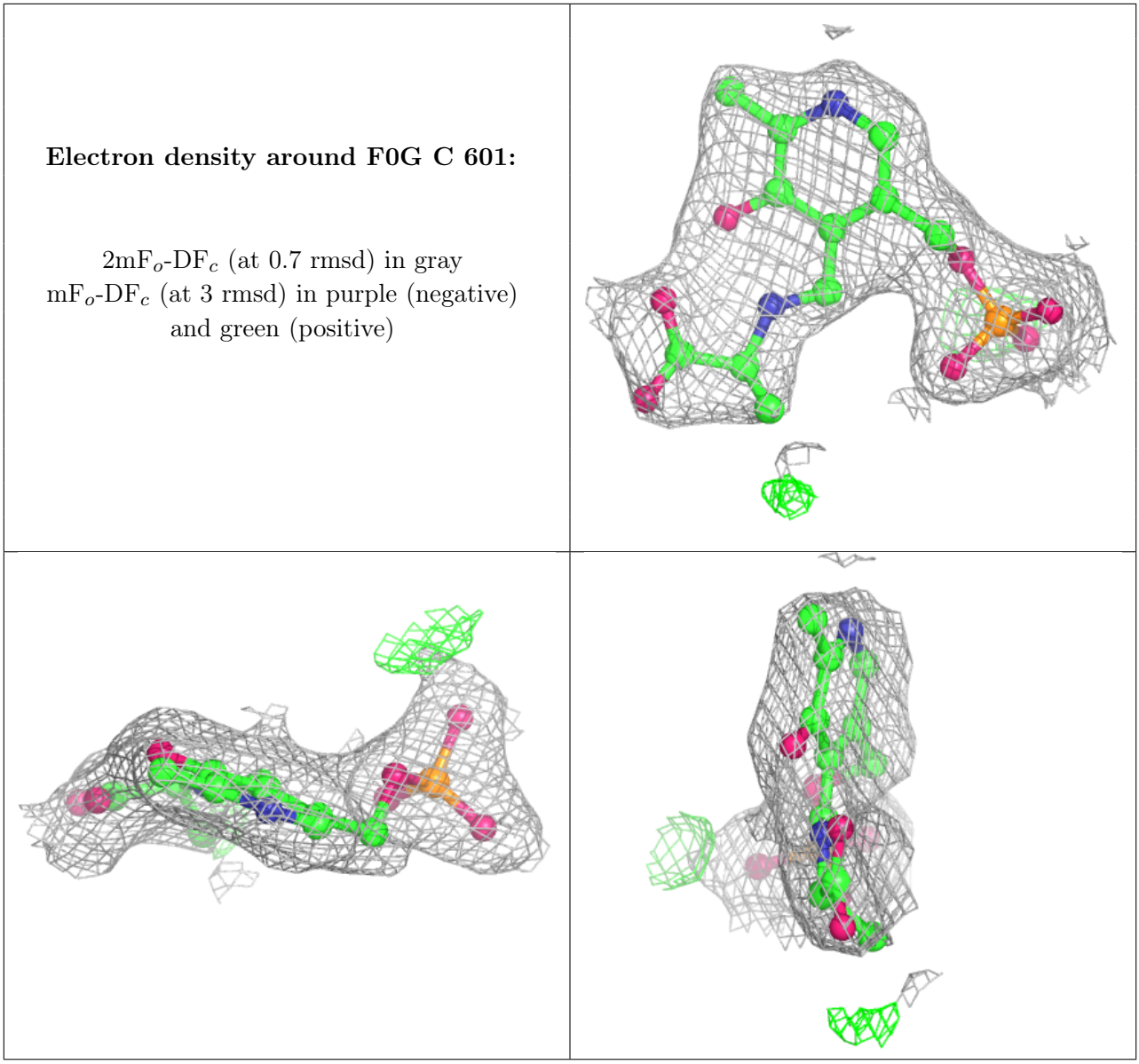
Electron density around F0G B 601:

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



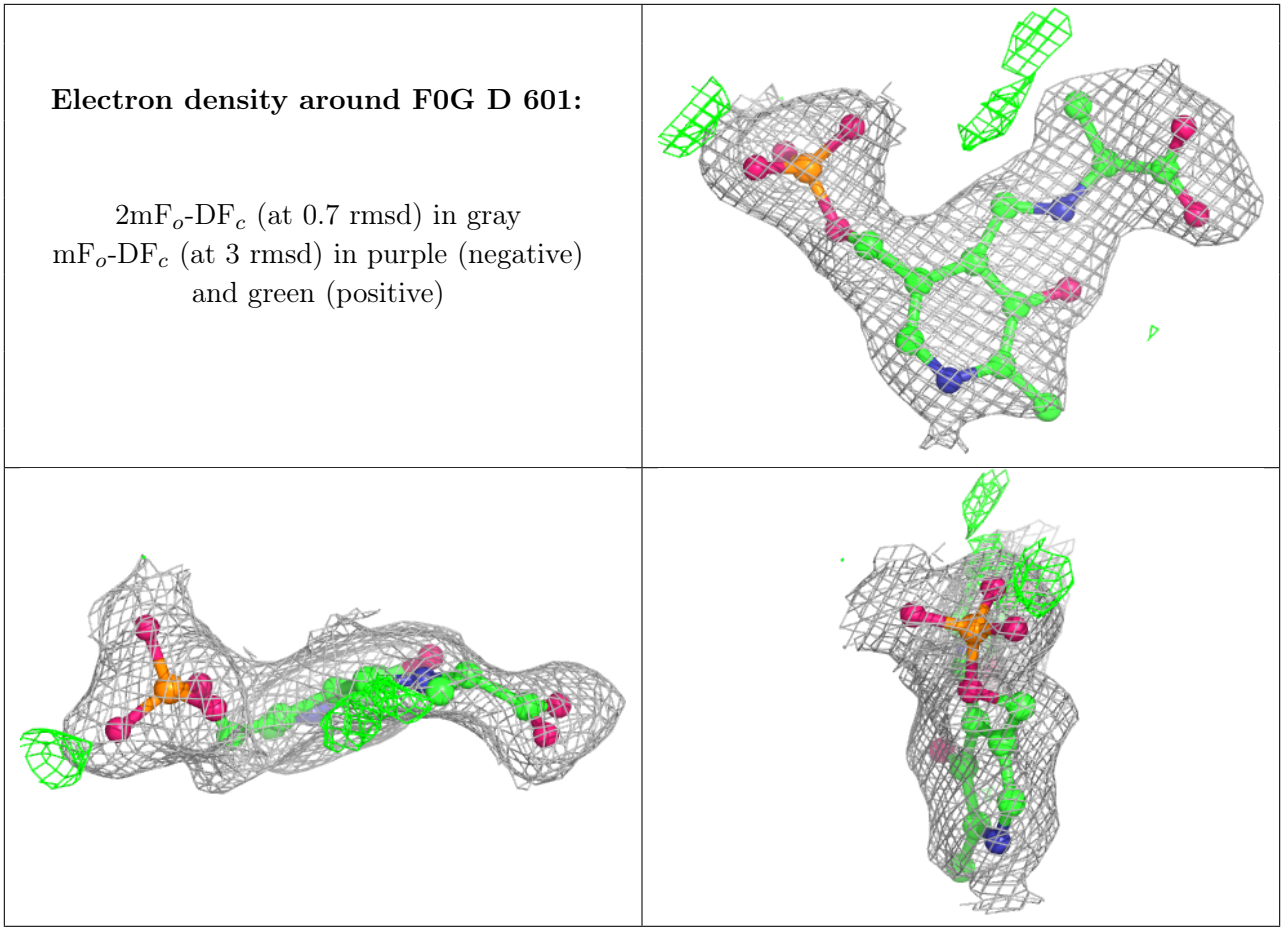
Electron density around F0G C 601:

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



Electron density around F0G D 601:

$2mF_o$-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

There are no such residues in this entry.