Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 05:33 PM JST

PDB ID	:	5GN5
Title	:	Crystal structure of glycerol kinase from Trypanosoma brucei gambiense complexed with cumarin derivative-17
Authors	:	Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Tsuge, T.; May, B.; Sato, T.; Kido, Y.; Takeshi, N.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Watanabe, Y.; Moore, A.L.; Harada, S.; Kita, K.
Deposited on	:	2016-07-19
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

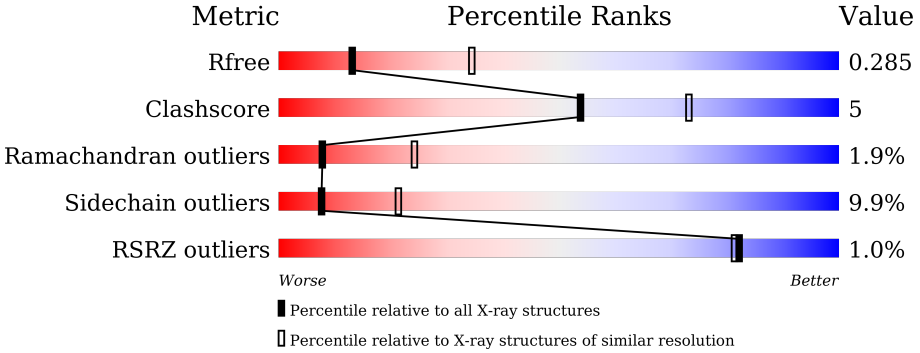
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	514	78% 19% •
1	B	514	2% 76% 21% •
1	C	514	82% 15% • •
1	D	514	2% 78% 19% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	6XZ	B	601	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16138 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 Glycerol kinase.

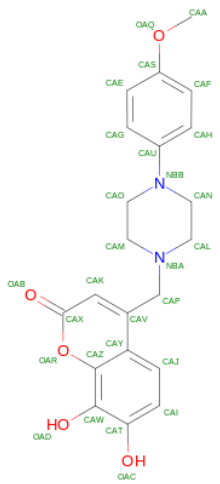
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	3951	2493	694	731	33	0	0	0
1	B	513	3951	2493	694	731	33	0	0	0
1	C	513	3951	2493	694	731	33	0	0	0
1	D	513	3951	2493	694	731	33	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-1	ALA	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-1	ALA	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-1	ALA	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is 4-[[4-(4-methoxyphenyl)piperazin-1-yl]methyl]-7,8-bis(oxidanyl)chromen-2-one (three-letter code: 6XZ) (formula: $C_{21}H_{22}N_2O_5$).

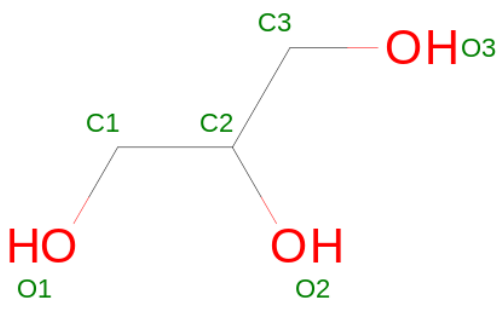
6XZ



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	28	21	2	5	0	0
2	B	1	28	21	2	5	0	0
2	C	1	28	21	2	5	0	0
2	D	1	28	21	2	5	0	0

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

GOL



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

- Molecule 4 is water.

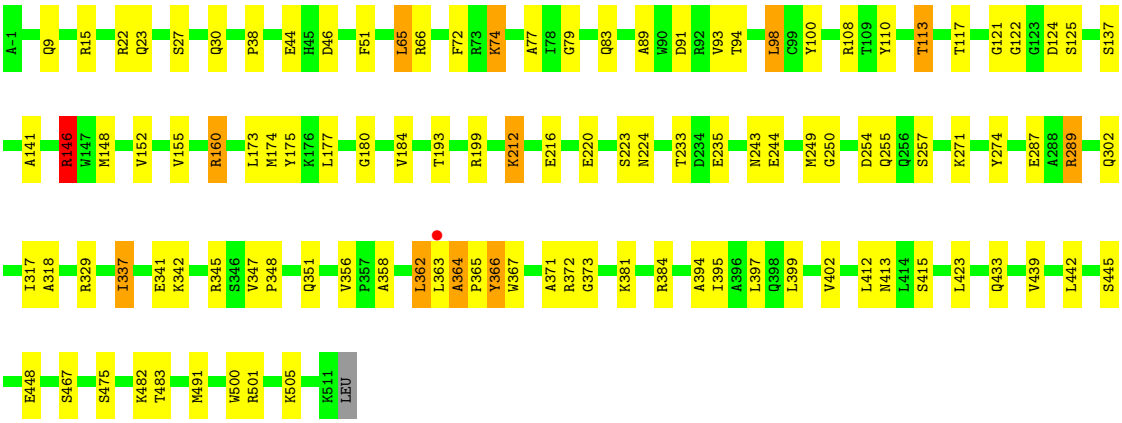
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
4	B	38	38	38	0	0
4	C	51	51	51	0	0
4	D	47	47	47	0	0

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.

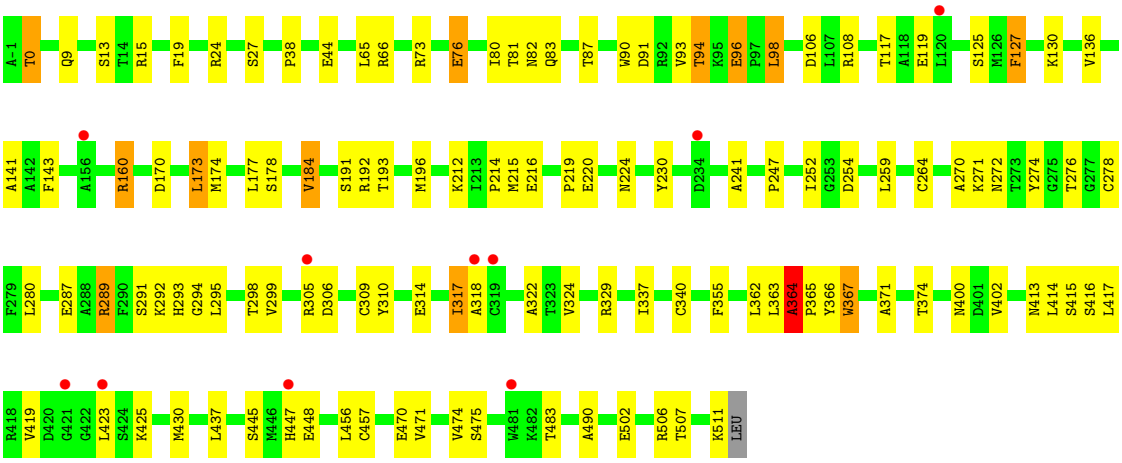
• Molecule 1: Glycerol kinase

Chain A: 78% 19%



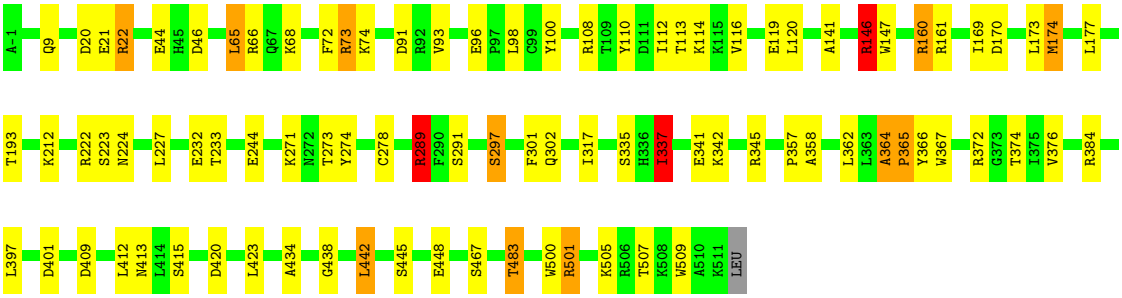
• Molecule 1: Glycerol kinase

Chain B: 2% 76% 21%



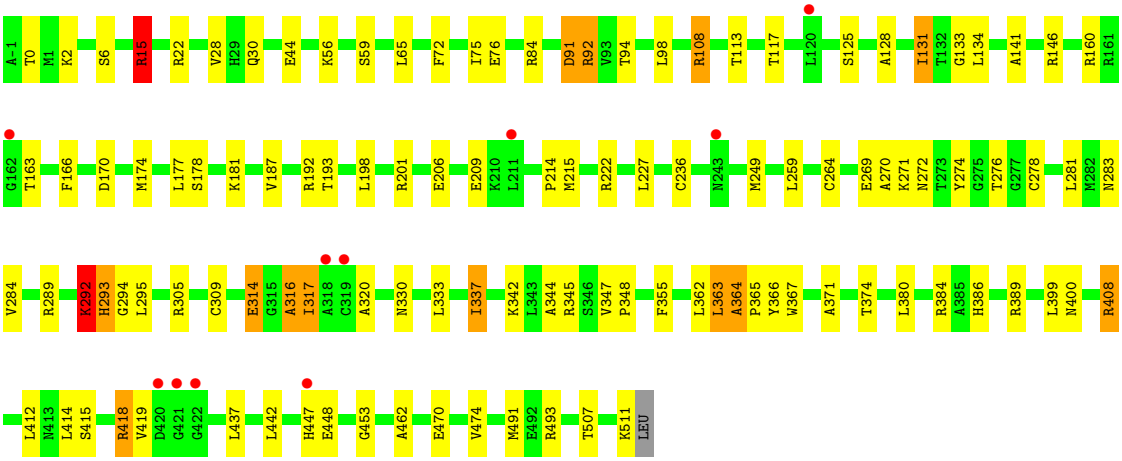
• Molecule 1: Glycerol kinase

Chain C: 82% 15%



- Molecule 1: Glycerol kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.03Å 63.20Å 154.85Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 19.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-2.85) 89.0 (19.99-2.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.194 , 0.286 0.198 , 0.285	Depositor DCC
R_{free} test set	2454 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16138	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6XZ, 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	0/4032	0.95	7/5456 (0.1%)
1	B	0.71	0/4032	0.90	1/5456 (0.0%)
1	C	0.75	1/4032 (0.0%)	0.94	11/5456 (0.2%)
1	D	0.71	0/4032	0.94	6/5456 (0.1%)
All	All	0.73	1/16128 (0.0%)	0.93	25/21824 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	D	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	367	TRP	CB-CG	-6.53	1.38	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	420	ASP	CB-CG-OD2	6.47	124.13	118.30
1	D	192	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	384	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	364	ALA	N-CA-C	-5.86	95.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	22	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	108	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	493	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	D	15	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	146	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	222	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	C	161	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	46	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	160	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	384	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	108	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	22	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	289	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	73	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	384	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	22	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	384	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	408	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	46	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	TYR	Peptide
1	A	83	GLN	Peptide
1	B	274	TYR	Peptide
1	B	291	SER	Peptide
1	B	293	HIS	Peptide
1	D	316	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3951	0	3966	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3951	0	3966	51	0
1	C	3951	0	3966	36	0
1	D	3951	0	3966	42	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	1	0
2	D	28	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	62	0	0	0	0
4	B	38	0	0	2	0
4	C	51	0	0	1	0
4	D	47	0	0	0	0
All	All	16138	0	15896	170	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 5.

All (170) 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:110:TYR:O	1:A:113:THR:HG22	1.92	0.69
1:B:416:SER:HA	4:B:722:HOH:O	1.92	0.69
1:B:192:ARG:NH1	1:B:314:GLU:OE1	2.25	0.67
1:C:224:ASN:HD22	1:C:302:GLN:H	1.43	0.67
1:A:341:GLU:OE2	1:A:345:ARG:NH2	2.30	0.63
1:A:141:ALA:HB3	1:A:193:THR:HA	1.79	0.63
1:C:170:ASP:O	1:C:174:MET:HB2	2.00	0.62
1:C:141:ALA:HB3	1:C:193:THR:HA	1.82	0.60
1:B:141:ALA:HB3	1:B:193:THR:HA	1.84	0.60
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.37	0.59
1:A:318:ALA:HB2	1:A:363:LEU:HD12	1.84	0.59
1:C:44:GLU:HG2	1:C:100:TYR:HB3	1.84	0.58
1:D:316:ALA:HB3	1:D:363:LEU:HD13	1.86	0.58
1:D:374:THR:OG1	1:D:507:THR:HG22	2.03	0.58
1:D:91:ASP:HB3	1:D:94:THR:HG22	1.85	0.57
1:A:364:ALA:HB1	1:A:365:PRO:CD	2.34	0.57
1:B:91:ASP:HB3	1:B:94:THR:HG22	1.86	0.57
1:B:289:ARG:CZ	1:B:289:ARG:HA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ALA:HB2	1:B:363:LEU:HD21	1.87	0.56
1:A:358:ALA:O	1:A:372:ARG:HA	2.04	0.56
1:A:224:ASN:HD22	1:A:302:GLN:H	1.52	0.55
1:B:364:ALA:HB1	1:B:402:VAL:CG2	2.37	0.55
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.90	0.54
1:B:90:TRP:HA	1:B:98:LEU:HD22	1.89	0.54
1:C:289:ARG:O	1:C:297:SER:OG	2.25	0.54
1:A:89:ALA:HB2	1:A:148:MET:CE	2.37	0.54
1:A:254:ASP:OD2	1:A:255:GLN:N	2.41	0.54
1:D:293:HIS:O	1:D:295:LEU:N	2.41	0.53
1:A:362:LEU:HD22	1:A:371:ALA:CB	2.39	0.53
1:B:419:VAL:HG21	1:B:430:MET:SD	2.48	0.53
1:D:133:GLY:HA3	1:D:198:LEU:HD12	1.91	0.53
1:D:283:ASN:OD1	1:D:283:ASN:C	2.48	0.53
1:D:292:LYS:HD2	1:D:292:LYS:N	2.24	0.52
1:B:363:LEU:O	1:B:363:LEU:HD12	2.08	0.52
1:D:92:ARG:HB2	1:D:163:THR:HB	1.92	0.52
1:A:223:SER:HB2	1:A:302:GLN:HG2	1.92	0.52
1:B:82:ASN:ND2	1:B:83:GLN:O	2.41	0.51
1:C:401:ASP:OD2	1:C:501:ARG:NH1	2.42	0.51
1:D:270:ALA:HB3	1:D:414:LEU:HD11	1.93	0.51
1:A:91:ASP:HB2	1:A:98:LEU:HD11	1.92	0.51
1:A:152:VAL:HG12	1:A:155:VAL:HG23	1.92	0.51
1:D:259:LEU:HD12	1:D:264:CYS:HB2	1.93	0.51
1:A:362:LEU:HD22	1:A:371:ALA:HB2	1.93	0.51
1:C:376:VAL:HG12	1:D:374:THR:HG22	1.93	0.51
1:D:44:GLU:HG2	1:D:108:ARG:HH22	1.76	0.51
1:C:364:ALA:HB1	1:C:365:PRO:HD3	1.93	0.51
1:B:278:CYS:CB	1:B:317:ILE:HG23	2.41	0.50
1:A:365:PRO:HD3	1:A:402:VAL:HG22	1.92	0.50
1:B:259:LEU:HD12	1:B:264:CYS:HB2	1.93	0.50
1:A:44:GLU:OE1	1:A:100:TYR:HB2	2.11	0.50
1:B:272:ASN:HB3	1:B:419:VAL:HG12	1.93	0.50
1:B:400:ASN:HA	1:B:437:LEU:HD21	1.93	0.50
1:C:374:THR:HG21	1:C:507:THR:HA	1.93	0.49
2:C:601:6XZ:OAC	3:C:602:GOL:O1	2.30	0.49
1:C:65:LEU:HD13	1:C:72:PHE:CD2	2.47	0.49
1:C:376:VAL:HA	1:D:374:THR:HG22	1.94	0.49
1:B:178:SER:HA	1:B:230:TYR:O	2.13	0.49
1:B:364:ALA:O	1:B:365:PRO:C	2.51	0.49
1:A:79:GLY:HA2	1:A:250:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:THR:HG23	1:B:322:ALA:HB2	1.95	0.48
1:D:278:CYS:SG	1:D:320:ALA:HB3	2.53	0.48
1:D:201:ARG:HD3	1:D:309:CYS:SG	2.53	0.48
1:B:44:GLU:HG3	1:B:108:ARG:HH22	1.79	0.48
1:B:224:ASN:O	1:B:457:CYS:HB3	2.14	0.48
1:B:94:THR:HG23	1:B:96:GLU:HB3	1.95	0.48
1:B:184:VAL:HA	1:B:219:PRO:HB2	1.96	0.47
1:C:291:SER:HA	1:C:409:ASP:OD2	2.15	0.47
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.49	0.47
1:D:178:SER:HB3	1:D:181:LYS:HB2	1.95	0.47
1:C:337:ILE:HD13	1:C:337:ILE:N	2.30	0.47
1:D:128:ALA:O	1:D:131:ILE:HD12	2.15	0.47
1:B:318:ALA:HB2	1:B:363:LEU:HD11	1.97	0.46
1:A:184:VAL:HG12	1:A:220:GLU:HB3	1.98	0.46
1:B:280:LEU:HD23	1:B:402:VAL:CG1	2.46	0.46
1:D:284:VAL:HG21	1:D:289:ARG:HG2	1.96	0.46
1:C:364:ALA:HB1	1:C:365:PRO:CD	2.44	0.46
1:D:347:VAL:HG11	1:D:386:HIS:NE2	2.31	0.46
1:C:341:GLU:OE2	1:C:345:ARG:NH2	2.48	0.45
1:B:511:LYS:N	4:B:703:HOH:O	2.48	0.45
1:B:81:THR:HA	1:B:252:ILE:O	2.15	0.45
1:B:324:VAL:HG21	1:B:423:LEU:HD21	1.98	0.45
1:D:15:ARG:HG2	1:D:30:GLN:HG3	1.99	0.45
1:A:23:GLN:HE22	1:A:475:SER:HB2	1.81	0.45
1:C:74:LYS:HD2	1:C:244:GLU:HG3	1.98	0.45
1:A:117:THR:HG23	1:A:125:SER:HA	1.99	0.45
1:A:397:LEU:HD13	1:A:500:TRP:HB2	1.98	0.45
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.97	0.45
1:D:362:LEU:HB2	1:D:371:ALA:HB3	1.99	0.45
1:B:117:THR:HG23	1:B:125:SER:HA	1.98	0.45
1:D:364:ALA:HB1	1:D:365:PRO:HD3	1.98	0.45
1:A:121:GLY:O	1:A:124:ASP:N	2.45	0.44
1:A:77:ALA:HB1	1:A:249:MET:HG3	1.99	0.44
1:A:89:ALA:CB	1:A:148:MET:CE	2.95	0.44
1:A:364:ALA:CB	1:A:365:PRO:CD	2.96	0.44
1:D:364:ALA:HB1	1:D:365:PRO:CD	2.47	0.44
1:D:198:LEU:O	1:D:198:LEU:HD23	2.17	0.44
1:B:470:GLU:O	1:B:474:VAL:HG23	2.18	0.44
1:A:371:ALA:O	1:A:372:ARG:NH1	2.51	0.44
1:A:27:SER:HB2	1:A:65:LEU:HG	2.00	0.44
1:C:442:LEU:HD12	1:C:483:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.99	0.43
1:D:187:VAL:HG13	1:D:222:ARG:O	2.18	0.43
1:D:269:GLU:OE1	1:D:418:ARG:NH2	2.51	0.43
1:C:20:ASP:O	1:C:22:ARG:N	2.51	0.43
1:C:91:ASP:OD2	1:C:93:VAL:HG22	2.18	0.43
1:D:249:MET:SD	1:D:462:ALA:HB2	2.59	0.43
1:D:92:ARG:CB	1:D:163:THR:HB	2.48	0.43
1:D:141:ALA:HB3	1:D:193:THR:HA	2.00	0.43
1:D:344:ALA:O	1:D:389:ARG:NH1	2.51	0.43
1:B:191:SER:HB3	1:B:299:VAL:HG23	2.01	0.43
1:B:278:CYS:HB2	1:B:317:ILE:HG23	2.00	0.43
1:B:364:ALA:CB	1:B:365:PRO:CD	2.96	0.43
1:A:175:TYR:CE1	1:A:180:GLY:HA2	2.54	0.43
1:D:272:ASN:OD1	1:D:274:TYR:CZ	2.71	0.43
1:A:74:LYS:HD2	1:A:244:GLU:HG3	2.01	0.42
1:B:173:LEU:O	1:B:177:LEU:HB2	2.19	0.42
1:B:254:ASP:OD2	3:B:602:GOL:O2	2.36	0.42
1:B:374:THR:HG21	1:B:507:THR:HA	2.01	0.42
1:B:365:PRO:HD3	1:B:402:VAL:HG22	2.01	0.42
1:C:358:ALA:O	1:C:372:ARG:HA	2.19	0.42
1:C:337:ILE:HD13	1:C:337:ILE:H	1.84	0.42
1:D:59:SER:OG	1:D:236:CYS:O	2.22	0.42
1:A:146:ARG:NH1	1:A:212:LYS:O	2.51	0.42
1:A:287:GLU:OE2	1:A:289:ARG:NH2	2.53	0.42
1:A:347:VAL:HB	1:A:348:PRO:HD2	2.01	0.42
1:C:119:GLU:O	1:C:120:LEU:HD23	2.20	0.42
1:D:44:GLU:CG	1:D:108:ARG:HH22	2.32	0.42
1:A:44:GLU:HG2	1:A:100:TYR:HB3	2.00	0.42
1:D:117:THR:HG23	1:D:125:SER:HA	2.01	0.42
1:A:318:ALA:HB2	1:A:363:LEU:CD1	2.49	0.42
1:C:364:ALA:CB	1:C:365:PRO:CD	2.97	0.42
1:C:483:THR:HG23	4:C:740:HOH:O	2.19	0.42
1:A:66:ARG:HE	1:A:66:ARG:HB3	1.75	0.42
1:A:274:TYR:HB3	1:A:423:LEU:HB2	2.00	0.42
1:B:136:VAL:HG13	1:B:143:PHE:CZ	2.54	0.42
1:A:394:ALA:O	1:A:395:ILE:C	2.57	0.42
1:B:502:GLU:O	1:B:506:ARG:NH1	2.52	0.42
1:D:317:ILE:HG22	1:D:399:LEU:HD21	2.01	0.42
1:B:309:CYS:SG	1:B:310:TYR:N	2.93	0.41
1:B:66:ARG:NH2	1:B:241:ALA:O	2.53	0.41
1:B:414:LEU:HD21	1:B:417:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:HA	1:B:24:ARG:O	2.21	0.41
1:C:108:ARG:HD3	1:C:147:TRP:CZ2	2.55	0.41
1:D:330:ASN:OD1	1:D:330:ASN:N	2.53	0.41
1:B:294:GLY:C	1:B:367:TRP:CZ3	2.94	0.41
1:C:116:VAL:HG13	1:C:120:LEU:HD12	2.03	0.41
1:C:146:ARG:NH1	1:C:212:LYS:O	2.54	0.41
1:C:397:LEU:HD13	1:C:500:TRP:HB2	2.01	0.41
1:A:51:PHE:CE2	1:A:235:GLU:HG2	2.56	0.41
1:A:399:LEU:HD12	1:A:433:GLN:OE1	2.20	0.41
1:B:362:LEU:HB2	1:B:371:ALA:HB3	2.02	0.41
1:C:110:TYR:O	1:C:113:THR:HG22	2.21	0.41
1:B:287:GLU:O	1:B:287:GLU:HG3	2.21	0.41
1:B:456:LEU:HD22	1:B:471:VAL:HG13	2.02	0.41
1:C:169:ILE:O	1:C:173:LEU:HB2	2.21	0.41
1:D:91:ASP:HB3	1:D:94:THR:CG2	2.50	0.41
1:D:400:ASN:HA	1:D:437:LEU:HD21	2.02	0.41
1:D:470:GLU:O	1:D:474:VAL:HG23	2.20	0.41
1:B:270:ALA:HB3	1:B:414:LEU:HD11	2.03	0.40
1:D:364:ALA:CB	1:D:365:PRO:CD	2.99	0.40
1:B:80:ILE:CG2	1:B:81:THR:N	2.84	0.40
1:C:223:SER:HB2	1:C:302:GLN:HG2	2.03	0.40
1:C:224:ASN:ND2	1:C:301:PHE:HA	2.36	0.40
1:C:273:THR:O	1:C:278:CYS:HA	2.21	0.40
1:D:281:LEU:HG	1:D:314:GLU:HG3	2.03	0.40
1:B:76:GLU:O	1:B:247:PRO:HD2	2.22	0.40
1:A:356:VAL:O	1:A:373:GLY:HA2	2.22	0.40
1:B:160:ARG:CZ	1:B:160:ARG:HB2	2.51	0.40
1:C:434:ALA:O	1:C:438:GLY:N	2.53	0.40
1:D:333:LEU:O	1:D:384:ARG:HD2	2.21	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	511/514 (99%)	473 (93%)	32 (6%)	6 (1%)	13	35
1	B	511/514 (99%)	451 (88%)	48 (9%)	12 (2%)	6	20
1	C	511/514 (99%)	472 (92%)	31 (6%)	8 (2%)	9	28
1	D	511/514 (99%)	448 (88%)	51 (10%)	12 (2%)	6	20
All	All	2044/2056 (99%)	1844 (90%)	162 (8%)	38 (2%)	8	24

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ILE
1	B	295	LEU
1	B	364	ALA
1	B	448	GLU
1	B	490	ALA
1	C	337	ILE
1	C	364	ALA
1	D	294	GLY
1	D	364	ALA
1	A	122	GLY
1	A	505	LYS
1	B	127	PHE
1	C	21	GLU
1	D	215	MET
1	D	292	LYS
1	D	305	ARG
1	D	348	PRO
1	D	448	GLU
1	B	0	THR
1	B	215	MET
1	B	415	SER
1	C	365	PRO
1	C	505	LYS
1	C	509	TRP
1	D	214	PRO
1	D	337	ILE
1	A	351	GLN
1	A	364	ALA
1	B	119	GLU
1	B	214	PRO
1	B	305	ARG
1	C	357	PRO
1	D	0	THR

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Mol	Chain	Res	Type
1	D	276	THR
1	D	453	GLY
1	C	112	ILE
1	A	38	PRO
1	B	38	PRO

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	420/421 (100%)	377 (90%)	43 (10%)	7 20
1	B	420/421 (100%)	377 (90%)	43 (10%)	7 20
1	C	420/421 (100%)	387 (92%)	33 (8%)	12 31
1	D	420/421 (100%)	373 (89%)	47 (11%)	6 16
All	All	1680/1684 (100%)	1514 (90%)	166 (10%)	8 21

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	15	ARG
1	A	30	GLN
1	A	65	LEU
1	A	74	LYS
1	A	93	VAL
1	A	94	THR
1	A	98	LEU
1	A	113	THR
1	A	137	SER
1	A	146	ARG
1	A	160	ARG
1	A	173	LEU
1	A	174	MET
1	A	177	LEU
1	A	199	ARG

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Mol	Chain	Res	Type
1	A	212	LYS
1	A	216	GLU
1	A	233	THR
1	A	243	ASN
1	A	257	SER
1	A	271	LYS
1	A	289	ARG
1	A	317	ILE
1	A	329	ARG
1	A	337	ILE
1	A	342	LYS
1	A	362	LEU
1	A	366	TYR
1	A	367	TRP
1	A	381	LYS
1	A	412	LEU
1	A	413	ASN
1	A	415	SER
1	A	439	VAL
1	A	442	LEU
1	A	445	SER
1	A	448	GLU
1	A	467	SER
1	A	482	LYS
1	A	483	THR
1	A	491	MET
1	A	501	ARG
1	B	0	THR
1	B	9	GLN
1	B	13	SER
1	B	15	ARG
1	B	27	SER
1	B	65	LEU
1	B	73	ARG
1	B	76	GLU
1	B	87	THR
1	B	93	VAL
1	B	94	THR
1	B	96	GLU
1	B	98	LEU
1	B	106	ASP
1	B	127	PHE

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Mol	Chain	Res	Type
1	B	130	LYS
1	B	160	ARG
1	B	170	ASP
1	B	173	LEU
1	B	174	MET
1	B	184	VAL
1	B	196	MET
1	B	212	LYS
1	B	216	GLU
1	B	220	GLU
1	B	271	LYS
1	B	289	ARG
1	B	292	LYS
1	B	298	THR
1	B	306	ASP
1	B	317	ILE
1	B	329	ARG
1	B	337	ILE
1	B	340	CYS
1	B	355	PHE
1	B	366	TYR
1	B	367	TRP
1	B	413	ASN
1	B	425	LYS
1	B	445	SER
1	B	447	HIS
1	B	475	SER
1	B	483	THR
1	C	9	GLN
1	C	65	LEU
1	C	66	ARG
1	C	68	LYS
1	C	73	ARG
1	C	96	GLU
1	C	98	LEU
1	C	114	LYS
1	C	146	ARG
1	C	160	ARG
1	C	174	MET
1	C	177	LEU
1	C	227	LEU
1	C	232	GLU

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Mol	Chain	Res	Type
1	C	233	THR
1	C	271	LYS
1	C	289	ARG
1	C	297	SER
1	C	317	ILE
1	C	335	SER
1	C	337	ILE
1	C	342	LYS
1	C	362	LEU
1	C	366	TYR
1	C	412	LEU
1	C	413	ASN
1	C	415	SER
1	C	442	LEU
1	C	445	SER
1	C	448	GLU
1	C	467	SER
1	C	483	THR
1	C	501	ARG
1	D	2	LYS
1	D	6	SER
1	D	15	ARG
1	D	28	VAL
1	D	56	LYS
1	D	65	LEU
1	D	72	PHE
1	D	75	ILE
1	D	76	GLU
1	D	84	ARG
1	D	91	ASP
1	D	92	ARG
1	D	98	LEU
1	D	113	THR
1	D	131	ILE
1	D	134	LEU
1	D	146	ARG
1	D	160	ARG
1	D	166	PHE
1	D	170	ASP
1	D	174	MET
1	D	177	LEU
1	D	206	GLU

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Mol	Chain	Res	Type
1	D	209	GLU
1	D	227	LEU
1	D	271	LYS
1	D	292	LYS
1	D	293	HIS
1	D	314	GLU
1	D	317	ILE
1	D	337	ILE
1	D	342	LYS
1	D	345	ARG
1	D	355	PHE
1	D	363	LEU
1	D	366	TYR
1	D	367	TRP
1	D	380	LEU
1	D	408	ARG
1	D	412	LEU
1	D	415	SER
1	D	418	ARG
1	D	419	VAL
1	D	442	LEU
1	D	447	HIS
1	D	491	MET
1	D	511	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	30	GLN
1	A	39	HIS
1	A	224	ASN
1	A	272	ASN
1	A	351	GLN
1	B	23	GLN
1	B	293	HIS
1	C	23	GLN
1	C	29	HIS
1	C	36	HIS
1	C	39	HIS
1	C	224	ASN
1	C	272	ASN

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Mol	Chain	Res	Type
1	C	336	HIS
1	D	23	GLN
1	D	151	ASN
1	D	293	HIS
1	D	302	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	D	602	-	5,5,5	0.17	0	5,5,5	0.22	0
2	6XZ	B	601	-	31,31,31	1.26	3 (9%)	43,44,44	2.07	14 (32%)
2	6XZ	D	601	-	31,31,31	1.48	5 (16%)	43,44,44	1.91	12 (27%)
2	6XZ	C	601	-	31,31,31	1.27	3 (9%)	43,44,44	2.02	13 (30%)
3	GOL	A	602	-	5,5,5	0.32	0	5,5,5	0.36	0
3	GOL	B	602	-	5,5,5	0.20	0	5,5,5	0.50	0
3	GOL	C	602	-	5,5,5	0.25	0	5,5,5	0.23	0
2	6XZ	A	601	-	31,31,31	1.52	5 (16%)	43,44,44	1.97	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	602	-	-	2/4/4/4	-
2	6XZ	B	601	-	-	9/10/20/20	0/4/4/4
2	6XZ	D	601	-	-	4/10/20/20	0/4/4/4
2	6XZ	C	601	-	-	6/10/20/20	0/4/4/4
3	GOL	A	602	-	-	4/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
2	6XZ	A	601	-	-	4/10/20/20	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	6XZ	CAP-CAV	-3.99	1.46	1.50
2	A	601	6XZ	CAK-CAV	3.50	1.42	1.35
2	A	601	6XZ	CAN-NBB	3.42	1.52	1.46
2	C	601	6XZ	CAK-CAV	3.21	1.41	1.35
2	A	601	6XZ	CAO-NBB	3.14	1.51	1.46
2	B	601	6XZ	CAP-CAV	-2.93	1.47	1.50
2	B	601	6XZ	CAP-NBA	2.93	1.53	1.47
2	C	601	6XZ	CAP-CAV	-2.86	1.47	1.50
2	B	601	6XZ	CAK-CAV	2.62	1.40	1.35
2	D	601	6XZ	CAK-CAV	2.62	1.40	1.35
2	A	601	6XZ	CAL-CAN	2.57	1.61	1.51
2	D	601	6XZ	CAL-CAN	2.25	1.60	1.51
2	D	601	6XZ	CAK-CAX	-2.17	1.40	1.44
2	C	601	6XZ	CAY-CAV	-2.17	1.42	1.46
2	D	601	6XZ	CAP-NBA	2.08	1.51	1.47
2	A	601	6XZ	CAK-CAX	-2.02	1.40	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	6XZ	CAP-CAV-CAY	6.34	127.45	118.19
2	C	601	6XZ	CAP-NBA-CAL	-6.02	101.75	111.09
2	D	601	6XZ	CAP-CAV-CAY	5.46	126.17	118.19
2	D	601	6XZ	CAP-NBA-CAM	-5.07	103.23	111.09
2	A	601	6XZ	OAR-CAX-OAB	4.90	122.68	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	6XZ	CAP-NBA-CAM	-4.72	103.77	111.09
2	A	601	6XZ	CAZ-OAR-CAX	-4.44	118.20	121.99
2	C	601	6XZ	OAR-CAX-OAB	4.34	121.98	116.44
2	C	601	6XZ	CAZ-OAR-CAX	-4.33	118.30	121.99
2	B	601	6XZ	CAN-CAL-NBA	4.27	119.41	110.64
2	A	601	6XZ	CAO-CAM-NBA	-4.23	101.97	110.64
2	D	601	6XZ	OAR-CAX-OAB	4.15	121.73	116.44
2	A	601	6XZ	OAB-CAX-CAK	-4.12	117.42	125.84
2	B	601	6XZ	CAZ-OAR-CAX	-3.60	118.92	121.99
2	C	601	6XZ	OAB-CAX-CAK	-3.55	118.60	125.84
2	C	601	6XZ	CAL-NBA-CAM	3.54	116.80	108.83
2	A	601	6XZ	CAY-CAV-CAK	-3.41	113.61	119.72
2	D	601	6XZ	OAB-CAX-CAK	-3.28	119.14	125.84
2	A	601	6XZ	CAT-CAW-CAZ	3.15	121.56	118.43
2	D	601	6XZ	CAN-CAL-NBA	3.12	117.04	110.64
2	B	601	6XZ	CAA-OAQ-CAS	-3.04	110.91	117.51
2	C	601	6XZ	CAY-CAV-CAK	-2.98	114.37	119.72
2	B	601	6XZ	OAB-CAX-CAK	-2.90	119.92	125.84
2	B	601	6XZ	CAN-NBB-CAU	2.90	125.92	118.09
2	B	601	6XZ	CAY-CAV-CAK	-2.86	114.59	119.72
2	C	601	6XZ	CAN-NBB-CAU	2.83	125.75	118.09
2	A	601	6XZ	CAL-NBA-CAM	2.79	115.11	108.83
2	C	601	6XZ	CAA-OAQ-CAS	-2.76	111.53	117.51
2	B	601	6XZ	CAP-NBA-CAL	-2.68	106.93	111.09
2	A	601	6XZ	CAP-NBA-CAM	-2.67	106.95	111.09
2	A	601	6XZ	CAN-NBB-CAO	2.63	117.32	111.52
2	B	601	6XZ	OAR-CAX-OAB	2.53	119.67	116.44
2	D	601	6XZ	CAT-CAW-CAZ	2.52	120.94	118.43
2	B	601	6XZ	OAR-CAX-CAK	2.51	120.40	117.17
2	C	601	6XZ	CAT-CAW-CAZ	2.46	120.88	118.43
2	B	601	6XZ	CAL-CAN-NBB	-2.44	105.97	110.70
2	C	601	6XZ	CAN-NBB-CAO	2.40	116.81	111.52
2	A	601	6XZ	CAP-CAV-CAY	2.38	121.66	118.19
2	B	601	6XZ	CAM-CAO-NBB	2.37	115.31	110.70
2	C	601	6XZ	CAP-CAV-CAK	2.30	126.57	121.59
2	D	601	6XZ	CAP-NBA-CAL	2.29	114.64	111.09
2	D	601	6XZ	CAL-NBA-CAM	2.24	113.87	108.83
2	D	601	6XZ	CAZ-OAR-CAX	-2.20	120.11	121.99
2	A	601	6XZ	CAN-NBB-CAU	2.18	123.97	118.09
2	B	601	6XZ	CAT-CAW-CAZ	2.16	120.58	118.43
2	D	601	6XZ	CAO-CAM-NBA	2.15	115.05	110.64
2	A	601	6XZ	OAR-CAX-CAK	2.12	119.89	117.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	6XZ	CAN-CAL-NBA	2.10	114.95	110.64
2	C	601	6XZ	CAH-CAU-NBB	-2.10	118.49	121.38
2	D	601	6XZ	CAL-CAN-NBB	2.04	114.65	110.70
2	D	601	6XZ	CAP-CAV-CAK	-2.01	117.23	121.59

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	6XZ	CAV-CAP-NBA-CAM
2	A	601	6XZ	CAV-CAP-NBA-CAL
2	D	601	6XZ	NBA-CAP-CAV-CAK
3	D	602	GOL	O1-C1-C2-C3
2	B	601	6XZ	CAF-CAS-OAQ-CAA
2	B	601	6XZ	CAE-CAS-OAQ-CAA
2	C	601	6XZ	CAF-CAS-OAQ-CAA
2	C	601	6XZ	CAE-CAS-OAQ-CAA
2	A	601	6XZ	CAF-CAS-OAQ-CAA
2	A	601	6XZ	CAE-CAS-OAQ-CAA
2	D	601	6XZ	CAF-CAS-OAQ-CAA
2	D	601	6XZ	CAE-CAS-OAQ-CAA
2	B	601	6XZ	CAH-CAU-NBB-CAO
3	A	602	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	C	602	GOL	O1-C1-C2-C3
2	C	601	6XZ	CAG-CAU-NBB-CAO
3	A	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2
3	C	602	GOL	O1-C1-C2-O2
2	B	601	6XZ	CAG-CAU-NBB-CAO
2	C	601	6XZ	CAH-CAU-NBB-CAO
3	D	602	GOL	O1-C1-C2-O2
2	B	601	6XZ	CAH-CAU-NBB-CAN
2	B	601	6XZ	CAG-CAU-NBB-CAN
2	B	601	6XZ	CAV-CAP-NBA-CAL
2	C	601	6XZ	CAG-CAU-NBB-CAN
2	B	601	6XZ	NBA-CAP-CAV-CAK
2	B	601	6XZ	NBA-CAP-CAV-CAY
2	D	601	6XZ	NBA-CAP-CAV-CAY
3	A	602	GOL	C1-C2-C3-O3
2	C	601	6XZ	CAH-CAU-NBB-CAN
3	A	602	GOL	O2-C2-C3-O3

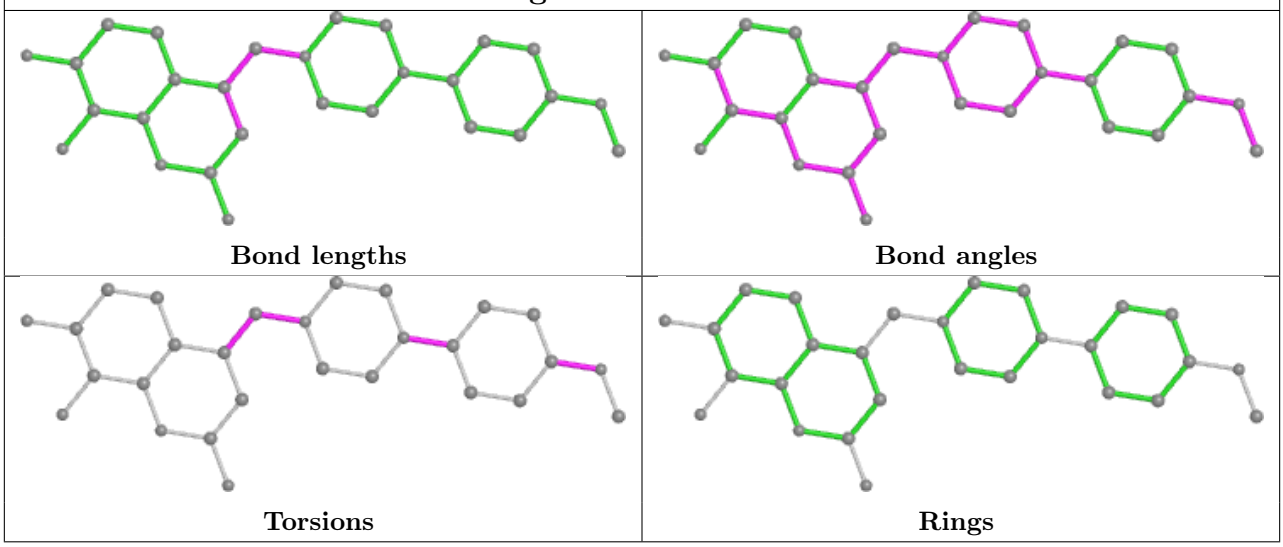
There are no ring outliers.

3 monomers are involved in 2 short contacts:

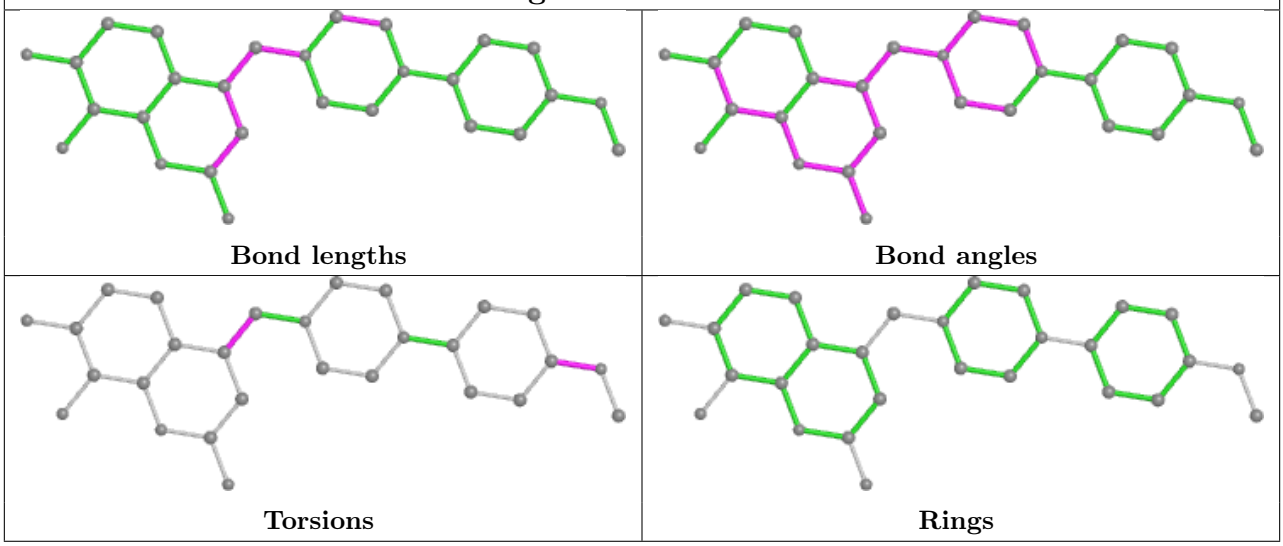
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	6XZ	1	0
3	B	602	GOL	1	0
3	C	602	GOL	1	0

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.

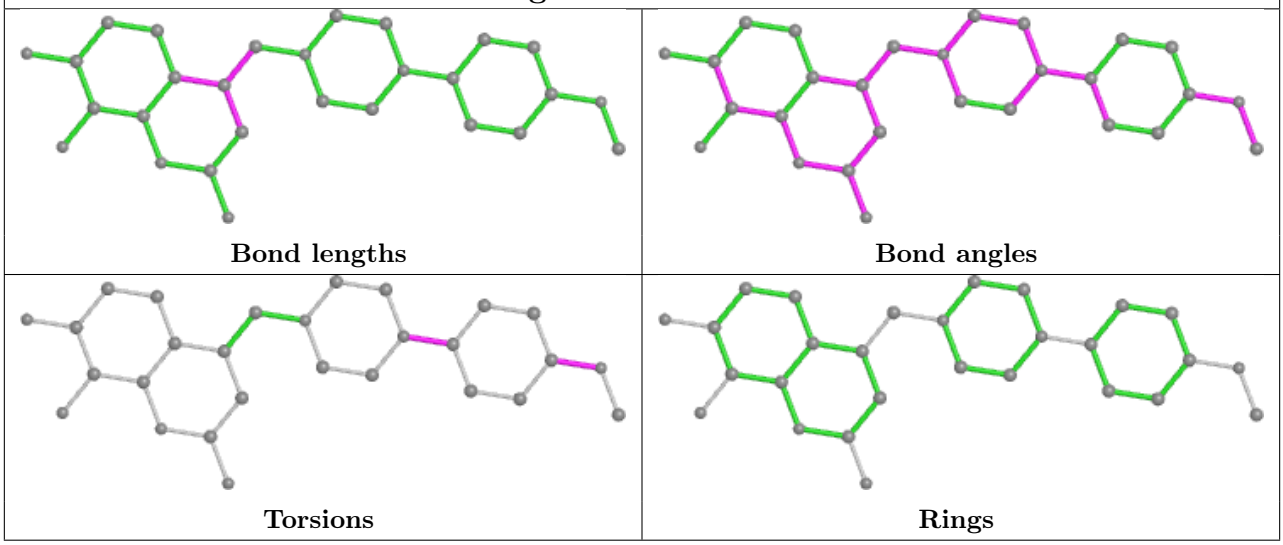
Ligand 6XZ B 601



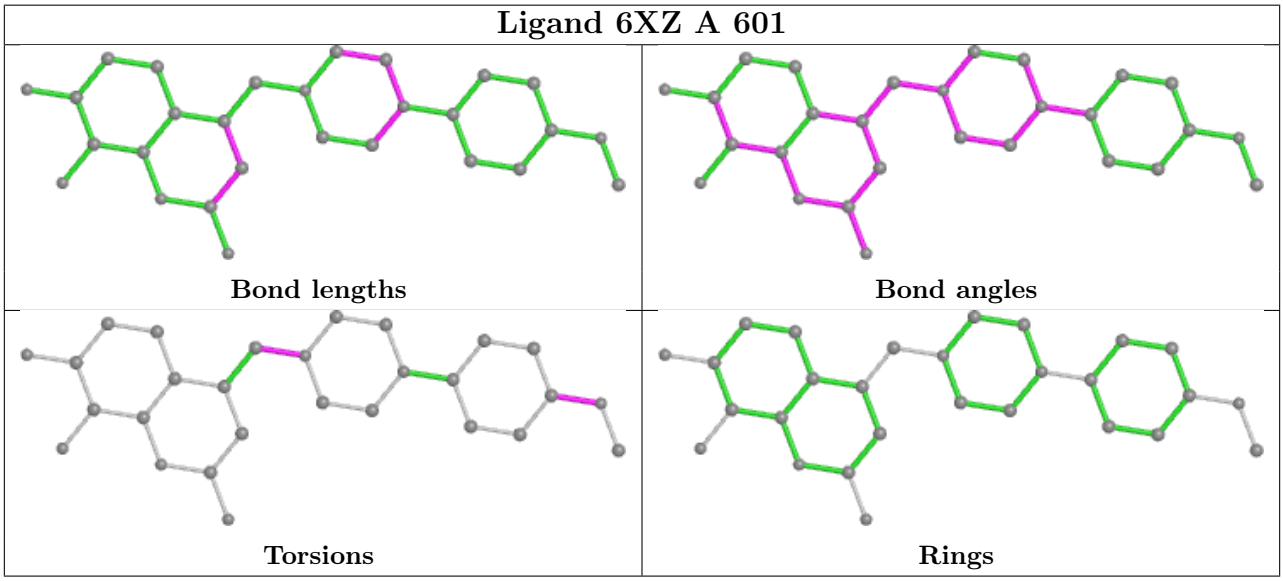
Ligand 6XZ D 601



Ligand 6XZ C 601



Ligand 6XZ A 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	513/514 (99%)	-0.30	1 (0%)	95	95	26, 44, 67, 84	1 (0%)
1	B	513/514 (99%)	0.05	10 (1%)	66	64	26, 65, 93, 110	1 (0%)
1	C	513/514 (99%)	-0.34	0	100	100	26, 45, 67, 80	1 (0%)
1	D	513/514 (99%)	0.03	10 (1%)	66	64	29, 64, 92, 108	1 (0%)
All	All	2052/2056 (99%)	-0.14	21 (1%)	82	81	26, 53, 86, 110	4 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	LEU	4.8
1	B	318	ALA	4.6
1	B	421	GLY	4.2
1	B	234	ASP	3.6
1	B	305	ARG	3.3
1	D	420	ASP	3.2
1	B	481	TRP	2.7
1	B	447	HIS	2.7
1	D	319	CYS	2.7
1	D	211	LEU	2.6
1	D	162	GLY	2.5
1	B	120	LEU	2.4
1	D	447	HIS	2.4
1	B	156	ALA	2.3
1	D	243	ASN	2.3
1	D	422	GLY	2.3
1	A	363	LEU	2.1
1	D	318	ALA	2.1
1	B	319	CYS	2.1
1	D	421	GLY	2.1
1	D	120	LEU	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)

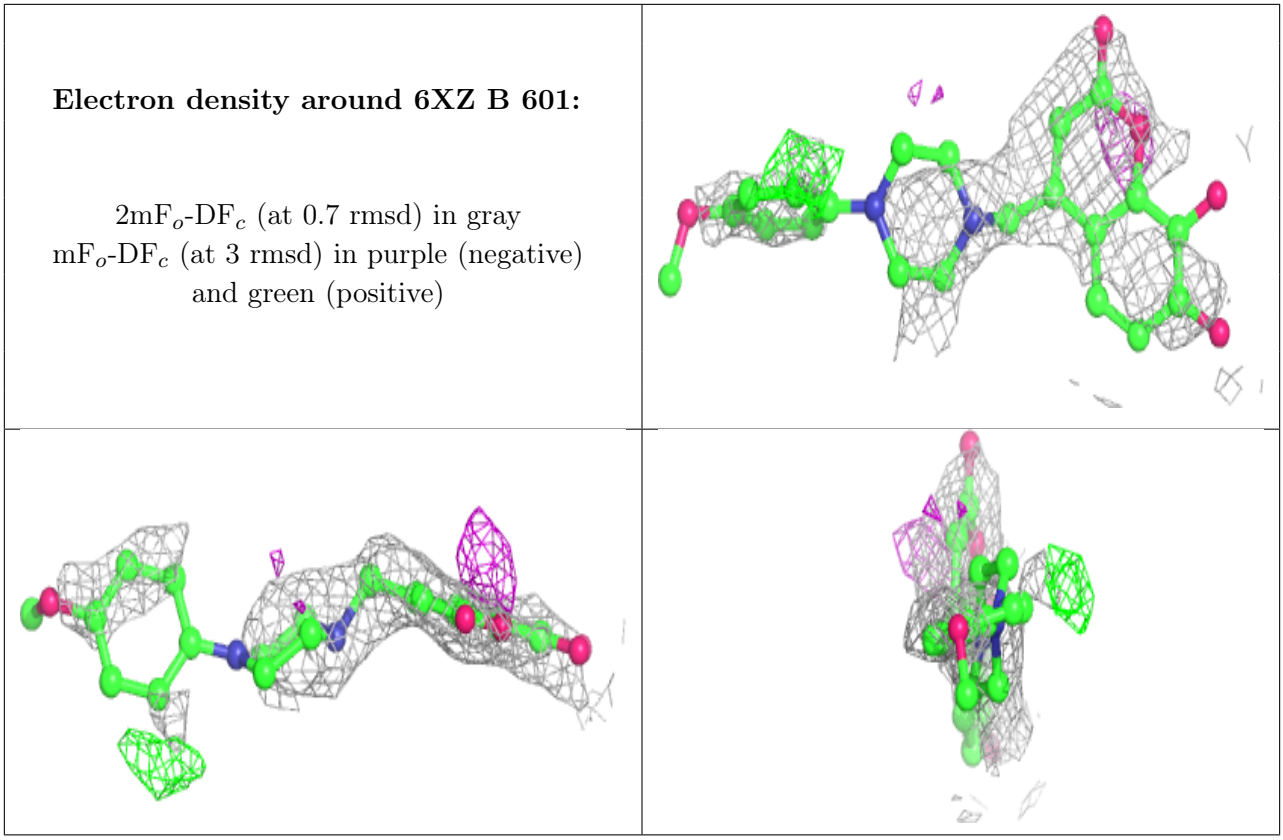
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6XZ	B	601	28/28	0.70	0.49	96,109,123,124	0
2	6XZ	C	601	28/28	0.84	0.39	72,94,102,104	0
2	6XZ	D	601	28/28	0.84	0.40	75,96,105,108	0
2	6XZ	A	601	28/28	0.87	0.39	76,89,103,105	0
3	GOL	D	602	6/6	0.87	0.35	60,63,63,71	0
3	GOL	A	602	6/6	0.93	0.31	62,66,67,71	0
3	GOL	B	602	6/6	0.95	0.23	41,42,42,45	0
3	GOL	C	602	6/6	0.96	0.19	60,60,63,64	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.

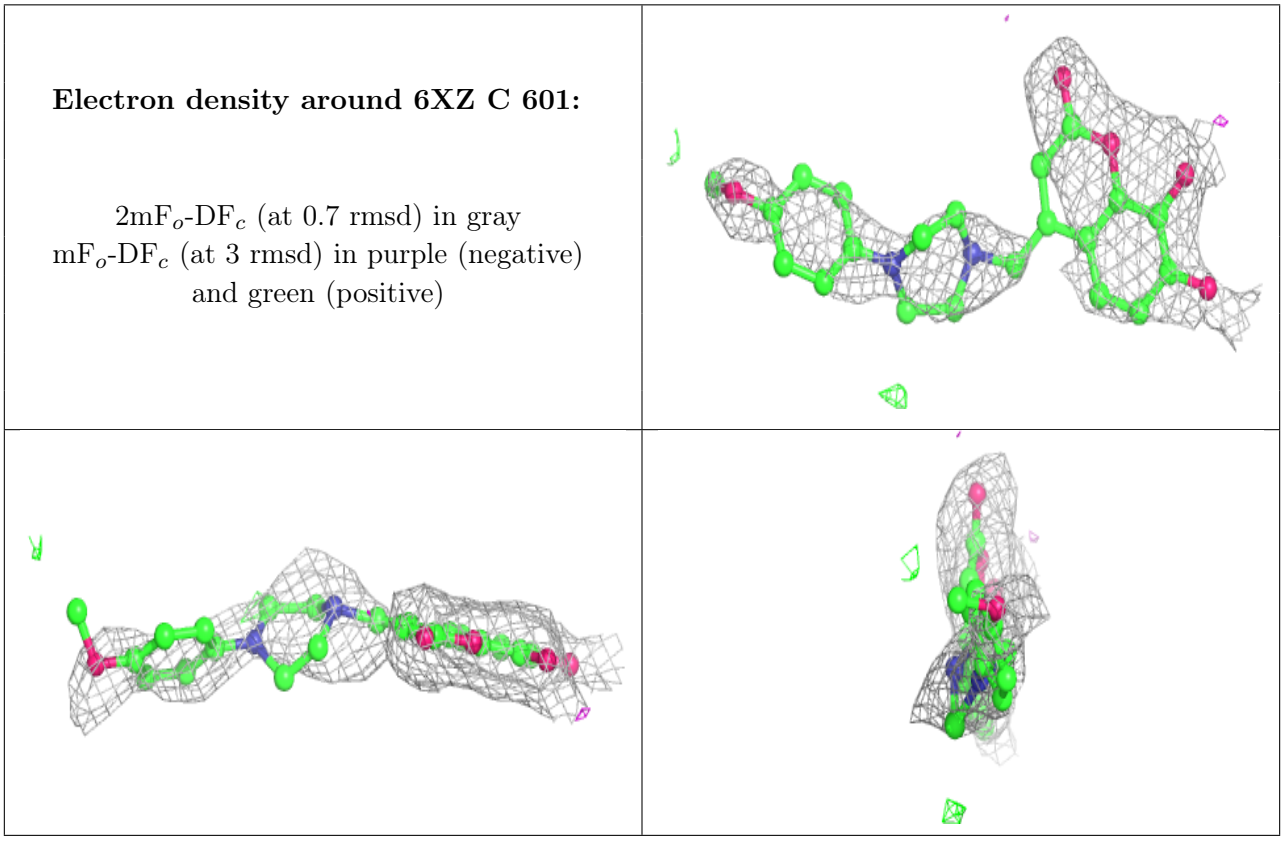
Electron density around 6XZ B 601:

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



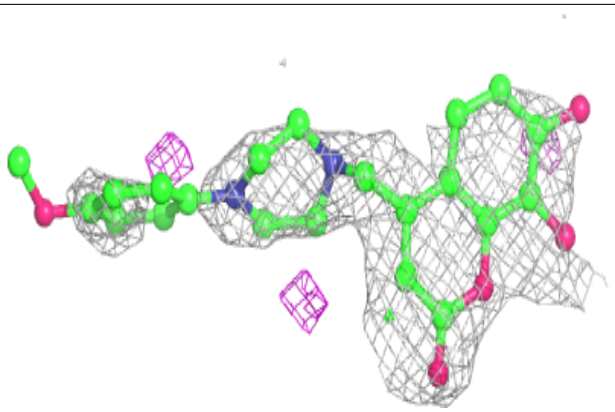
Electron density around 6XZ C 601:

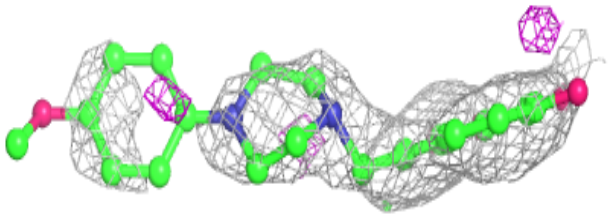
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

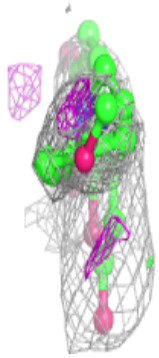


Electron density around 6XZ D 601:

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

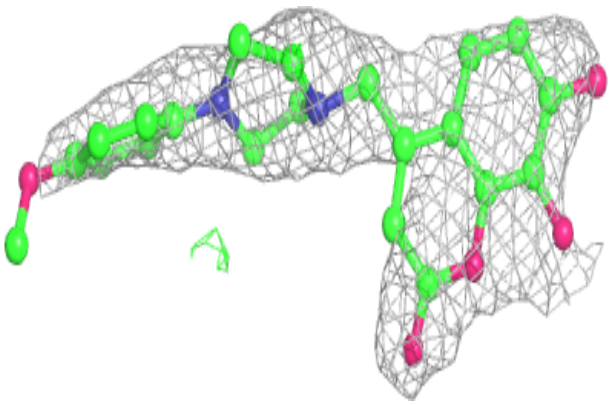


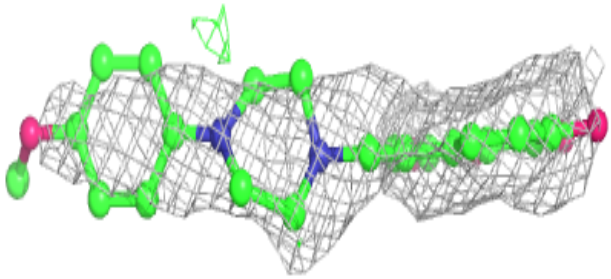


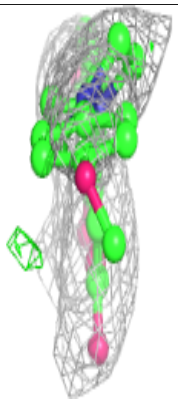


Electron density around 6XZ A 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.