



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:53 PM UTC

PDB ID : 5GN5 / pdb_00005gn5
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

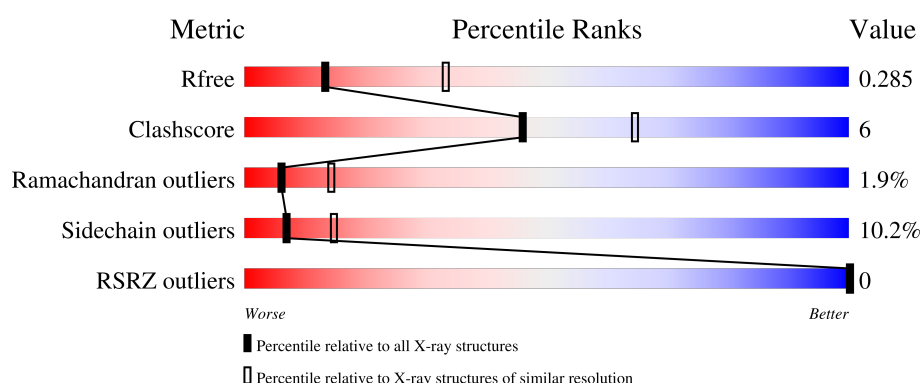
1 Overall quality at a glance

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	514	 78% 20% .
1	B	514	 74% 21% .
1	C	514	 81% 17% .
1	D	514	 74% 23% .

2 Entry composition

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.

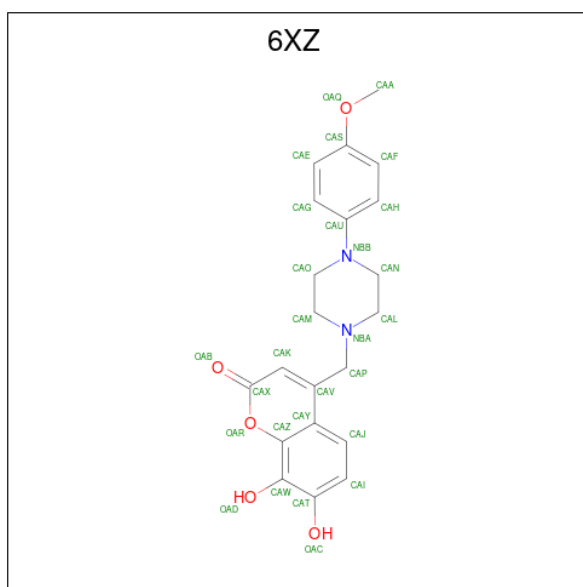
- Molecule 1 is a protein called Glycerol kinase.

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

There are 8 discrepancies between the modelled and reference sequences:

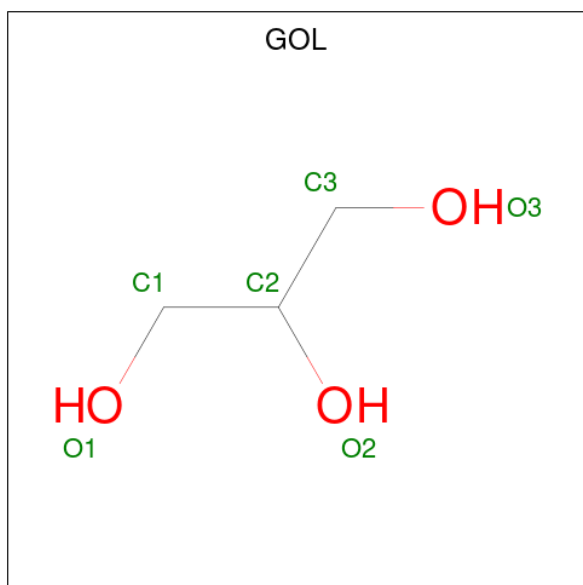
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-1	ALA	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-1	ALA	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-1	ALA	-	expression tag	UNP D3KVM3
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 (CCD ID: 6XZ) (formula: C₂₁H₂₂N₂O₅).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

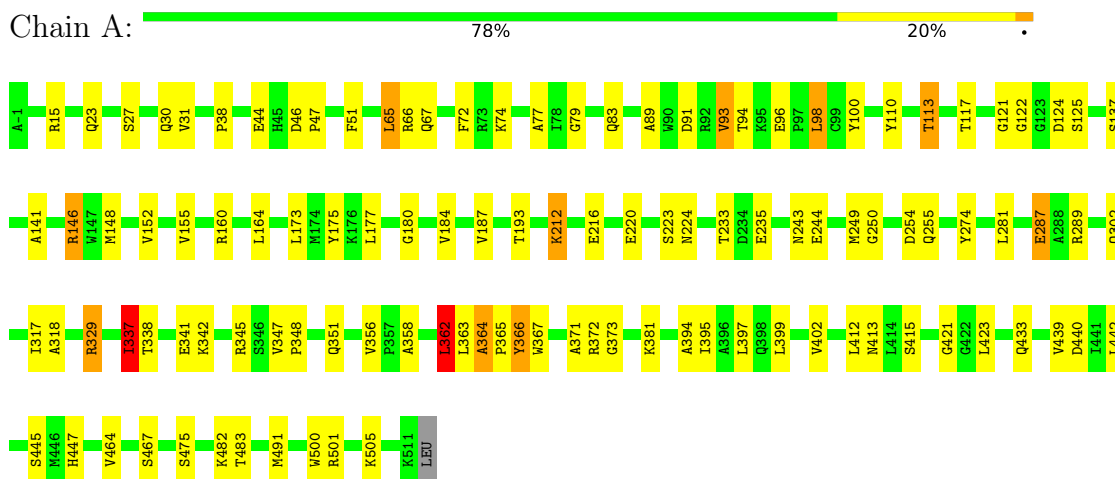
- Molecule 4 is water.

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

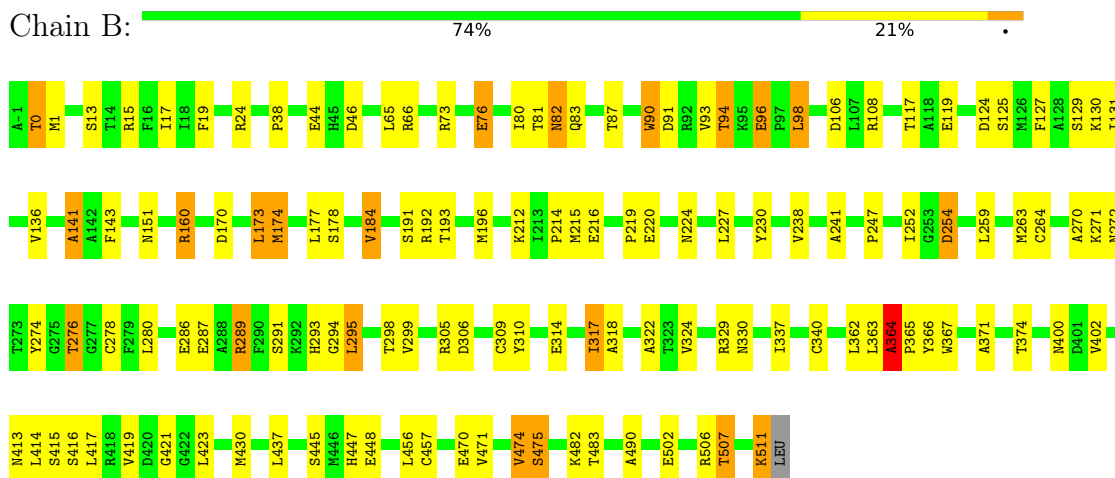
3 Residue-property plots

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.

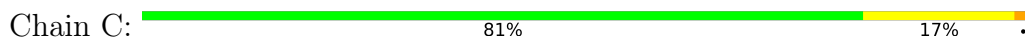
- Molecule 1: Glycerol kinase

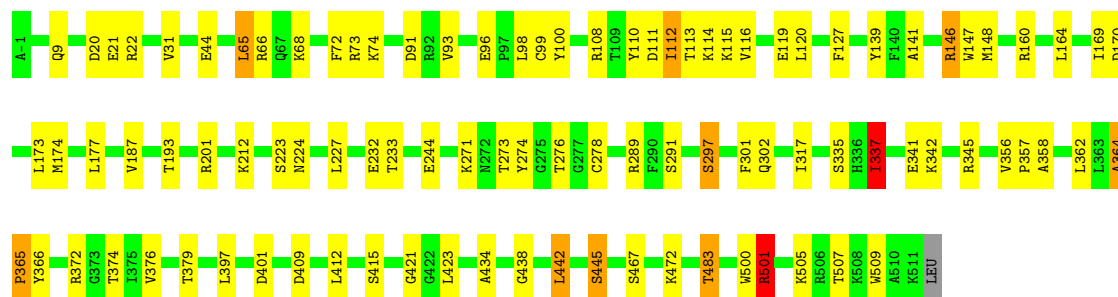


- Molecule 1: Glycerol kinase

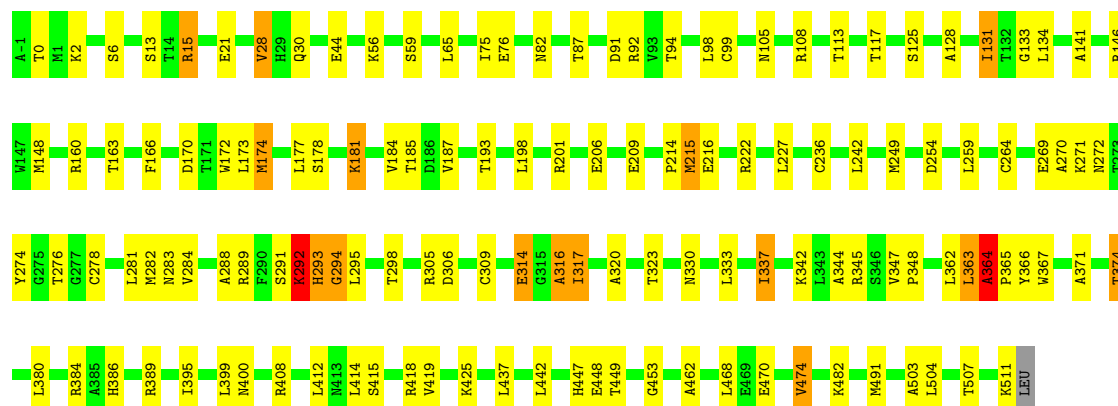


- Molecule 1: Glycerol kinase





• Molecule 1: Glycerol kinase



4 Data and refinement statistics

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 20.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-2.85) 89.0 (20.00-2.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.44%)	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)	0.33 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	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.*

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: GOL, 6XZ

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	1.06	2/4032 (0.0%)	1.17	12/5456 (0.2%)
1	B	1.01	1/4032 (0.0%)	1.16	15/5456 (0.3%)
1	C	1.04	1/4032 (0.0%)	1.15	11/5456 (0.2%)
1	D	1.00	4/4032 (0.1%)	1.16	11/5456 (0.2%)
All	All	1.03	8/16128 (0.0%)	1.16	49/21824 (0.2%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	ASP	CA-C	6.33	1.60	1.52
1	D	13	SER	C-O	-5.72	1.16	1.23
1	A	93	VAL	CA-CB	5.43	1.61	1.54
1	D	298	THR	CA-CB	5.27	1.62	1.53
1	C	201	ARG	CA-C	-5.22	1.46	1.53
1	D	28	VAL	C-O	-5.21	1.18	1.23
1	A	67	GLN	C-O	-5.11	1.17	1.24
1	D	105	ASN	N-CA	5.02	1.51	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	ASP	N-CA-C	7.15	118.72	111.07
1	B	90	TRP	N-CA-C	6.99	119.80	109.24
1	C	164	LEU	N-CA-C	6.95	120.45	110.24
1	A	421	GLY	N-CA-C	-6.69	104.80	112.29
1	D	364	ALA	CA-C-N	-6.63	111.99	119.28
1	D	364	ALA	C-N-CA	-6.63	111.99	119.28
1	B	364	ALA	N-CA-C	-6.62	95.17	109.81
1	B	129	SER	N-CA-C	6.50	120.48	112.54
1	C	127	PHE	N-CA-C	6.43	119.10	111.71
1	B	507	THR	N-CA-C	6.25	119.08	111.82
1	D	185	THR	N-CA-C	-6.24	99.84	109.52
1	B	238	VAL	N-CA-C	6.18	116.34	110.53
1	C	31	VAL	CA-C-N	-6.17	114.38	120.98
1	C	31	VAL	C-N-CA	-6.17	114.38	120.98
1	B	151	ASN	N-CA-C	6.17	120.94	113.17
1	A	31	VAL	CA-C-N	-6.13	114.45	120.52
1	A	31	VAL	C-N-CA	-6.13	114.45	120.52
1	A	464	VAL	N-CA-C	-5.94	104.83	110.42
1	B	46	ASP	CA-C-N	5.92	125.62	119.05
1	B	46	ASP	C-N-CA	5.92	125.62	119.05
1	B	141	ALA	N-CA-C	5.89	117.39	110.97
1	B	330	ASN	N-CA-C	5.86	119.61	112.23
1	D	288	ALA	N-CA-C	5.86	117.86	110.24
1	D	482	LYS	N-CA-C	-5.85	101.35	110.42
1	A	187	VAL	CB-CA-C	-5.81	103.16	112.16
1	B	421	GLY	N-CA-C	5.80	117.80	110.38
1	C	187	VAL	CB-CA-C	-5.71	103.31	112.16
1	C	337	ILE	N-CA-C	5.68	121.16	109.34
1	D	172	TRP	N-CA-C	5.66	118.18	111.33
1	B	1	MET	N-CA-C	5.64	117.88	109.59
1	A	164	LEU	N-CA-C	5.50	118.21	109.96
1	C	139	TYR	N-CA-C	5.41	117.26	111.36
1	D	82	ASN	N-CA-C	5.39	117.28	108.76
1	A	337	ILE	N-CA-C	5.33	120.42	109.34
1	B	82	ASN	N-CA-C	5.31	116.91	108.79
1	A	329	ARG	N-CA-C	5.26	120.70	113.97
1	D	474	VAL	N-CA-CB	5.25	116.34	110.51
1	D	294	GLY	N-CA-C	5.22	125.55	113.18
1	C	501	ARG	N-CA-C	5.19	117.34	111.11
1	C	445	SER	N-CA-C	-5.17	105.09	111.40
1	D	395	ILE	N-CA-C	-5.17	105.67	110.53
1	B	482	LYS	N-CA-C	-5.14	102.44	110.42
1	A	47	PRO	N-CA-C	5.12	120.65	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	379	THR	N-CA-C	-5.12	102.32	109.69
1	C	421	GLY	N-CA-C	-5.11	106.83	112.04
1	A	362	LEU	N-CA-C	5.07	117.40	107.57
1	B	254	ASP	N-CA-C	5.04	116.86	111.36
1	A	46	ASP	CA-C-N	5.03	124.63	119.05
1	A	46	ASP	C-N-CA	5.03	124.63	119.05

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

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	43	0
1	B	3951	0	3966	54	0
1	C	3951	0	3966	39	0
1	D	3951	0	3966	48	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	47	0	0	0	0
All	All	16138	0	15896	183	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 (183) 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:B:174:MET:HE3	1:B:184:VAL:HG23	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:D:283:ASN:OD1	1:D:283:ASN:C	2.48	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
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:D:174:MET:HE3	1:D:184:VAL:HG23	1.89	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:B:263:MET:HE3	1:B:475:SER:HB2	1.88	0.53
1:D:293:HIS:O	1:D:295:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:99:CYS:SG	1:C:148:MET:HE3	2.49	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:D:282:MET:HE2	1:D:414:LEU:CD1	2.41	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:B:364:ALA:O	1:B:365:PRO:C	2.51	0.51
1:D:282:MET:HE2	1:D:414:LEU:HD13	1.91	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:B:263:MET:HE3	1:B:475:SER:CB	2.42	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:A:79:GLY:HA2	1:A:250:GLY:O	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:394:ALA:O	1:A:395:ILE:C	2.57	0.46
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:294:GLY:C	1:B:367:TRP:CZ3	2.94	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:D:503:ALA:O	1:D:504:LEU:C	2.58	0.45
1:C:20:ASP:C	1:C:22:ARG:H	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:254:ASP:OD2	3:B:602:GOL:O2	2.36	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:C:111:ASP:O	1:C:112:ILE:C	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:99:CYS:SG	1:D:148:MET:HE3	2.62	0.40
1:A:89:ALA:HB2	1:A:148:MET:HE2	2.03	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:291:SER:C	1:D:292:LYS:HG3	2.47	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/514 (99%)	473 (93%)	32 (6%)	6 (1%)	10	22
1	B	511/514 (99%)	451 (88%)	48 (9%)	12 (2%)	5	11
1	C	511/514 (99%)	472 (92%)	31 (6%)	8 (2%)	7	17
1	D	511/514 (99%)	448 (88%)	51 (10%)	12 (2%)	5	11
All	All	2044/2056 (99%)	1844 (90%)	162 (8%)	38 (2%)	6	14

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 ⓘ

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%)	379 (90%)	41 (10%)	7	16
1	B	420/421 (100%)	376 (90%)	44 (10%)	6	13
1	C	420/421 (100%)	387 (92%)	33 (8%)	11	24
1	D	420/421 (100%)	366 (87%)	54 (13%)	4	7
All	All	1680/1684 (100%)	1508 (90%)	172 (10%)	7	15

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	30	GLN
1	A	65	LEU
1	A	93	VAL
1	A	94	THR
1	A	96	GLU
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	177	LEU
1	A	212	LYS
1	A	216	GLU
1	A	233	THR

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Mol	Chain	Res	Type
1	A	243	ASN
1	A	281	LEU
1	A	287	GLU
1	A	317	ILE
1	A	329	ARG
1	A	337	ILE
1	A	338	THR
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	440	ASP
1	A	442	LEU
1	A	445	SER
1	A	447	HIS
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	13	SER
1	B	15	ARG
1	B	17	ILE
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	130	LYS
1	B	131	ILE
1	B	160	ARG
1	B	170	ASP

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Mol	Chain	Res	Type
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	227	LEU
1	B	271	LYS
1	B	276	THR
1	B	286	GLU
1	B	289	ARG
1	B	295	LEU
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	366	TYR
1	B	413	ASN
1	B	445	SER
1	B	447	HIS
1	B	474	VAL
1	B	475	SER
1	B	483	THR
1	B	511	LYS
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	115	LYS
1	C	146	ARG
1	C	160	ARG
1	C	177	LEU
1	C	227	LEU
1	C	232	GLU
1	C	233	THR

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Mol	Chain	Res	Type
1	C	271	LYS
1	C	276	THR
1	C	297	SER
1	C	317	ILE
1	C	335	SER
1	C	337	ILE
1	C	342	LYS
1	C	356	VAL
1	C	362	LEU
1	C	366	TYR
1	C	412	LEU
1	C	415	SER
1	C	442	LEU
1	C	445	SER
1	C	467	SER
1	C	472	LYS
1	C	483	THR
1	C	501	ARG
1	D	2	LYS
1	D	6	SER
1	D	15	ARG
1	D	21	GLU
1	D	28	VAL
1	D	56	LYS
1	D	65	LEU
1	D	75	ILE
1	D	76	GLU
1	D	87	THR
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	173	LEU
1	D	174	MET
1	D	177	LEU
1	D	181	LYS
1	D	206	GLU
1	D	209	GLU

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Mol	Chain	Res	Type
1	D	215	MET
1	D	216	GLU
1	D	227	LEU
1	D	242	LEU
1	D	271	LYS
1	D	292	LYS
1	D	293	HIS
1	D	306	ASP
1	D	314	GLU
1	D	317	ILE
1	D	323	THR
1	D	337	ILE
1	D	342	LYS
1	D	345	ARG
1	D	363	LEU
1	D	366	TYR
1	D	367	TRP
1	D	374	THR
1	D	380	LEU
1	D	408	ARG
1	D	412	LEU
1	D	415	SER
1	D	419	VAL
1	D	425	LYS
1	D	442	LEU
1	D	447	HIS
1	D	449	THR
1	D	468	LEU
1	D	491	MET
1	D	511	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	29	HIS
1	A	30	GLN
1	A	151	ASN
1	A	224	ASN
1	A	336	HIS
1	A	351	GLN
1	B	23	GLN

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Mol	Chain	Res	Type
1	B	293	HIS
1	B	351	GLN
1	B	433	GLN
1	C	23	GLN
1	C	224	ASN
1	C	272	ASN
1	C	336	HIS
1	D	23	GLN
1	D	36	HIS
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 oligosaccharides 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	B	602	-	5,5,5	0.20	0	5,5,5	0.55	0
3	GOL	D	602	-	5,5,5	0.17	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	602	-	5,5,5	0.25	0	5,5,5	0.25	0
2	6XZ	D	601	-	31,31,31	1.53	6 (19%)	43,44,44	1.92	10 (23%)
2	6XZ	B	601	-	31,31,31	1.30	3 (9%)	43,44,44	2.08	13 (30%)
3	GOL	A	602	-	5,5,5	0.33	0	5,5,5	0.37	0
2	6XZ	C	601	-	31,31,31	1.31	3 (9%)	43,44,44	2.03	12 (27%)
2	6XZ	A	601	-	31,31,31	1.52	5 (16%)	43,44,44	1.99	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	B	602	-	-	2/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
2	6XZ	D	601	-	-	4/10/20/20	0/4/4/4
2	6XZ	B	601	-	-	9/10/20/20	0/4/4/4
3	GOL	A	602	-	-	4/4/4/4	-
2	6XZ	C	601	-	-	6/10/20/20	0/4/4/4
2	6XZ	A	601	-	-	4/10/20/20	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	6XZ	CAP-CAV	-4.21	1.46	1.51
2	A	601	6XZ	CAK-CAV	3.71	1.42	1.35
2	C	601	6XZ	CAK-CAV	3.40	1.41	1.35
2	A	601	6XZ	CAN-NBB	3.14	1.52	1.46
2	B	601	6XZ	CAP-CAV	-3.10	1.47	1.51
2	C	601	6XZ	CAP-CAV	-3.02	1.47	1.51
2	B	601	6XZ	CAP-NBA	2.96	1.53	1.47
2	A	601	6XZ	CAO-NBB	2.88	1.51	1.46
2	B	601	6XZ	CAK-CAV	2.79	1.40	1.35
2	D	601	6XZ	CAK-CAV	2.79	1.40	1.35
2	A	601	6XZ	CAL-CAN	2.67	1.61	1.51
2	D	601	6XZ	CAL-CAN	2.33	1.60	1.51
2	C	601	6XZ	CAY-CAV	-2.23	1.42	1.46
2	D	601	6XZ	CAK-CAX	-2.11	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	6XZ	CAP-NBA	2.11	1.51	1.47
2	D	601	6XZ	CAH-CAU	2.08	1.43	1.39
2	A	601	6XZ	CAP-CAV	-2.07	1.48	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	6XZ	CAP-CAV-CAY	6.45	127.45	118.19
2	C	601	6XZ	CAP-NBA-CAL	-6.04	101.75	111.14
2	D	601	6XZ	CAP-CAV-CAY	5.56	126.17	118.19
2	D	601	6XZ	CAP-NBA-CAM	-5.09	103.23	111.14
2	A	601	6XZ	OAR-CAX-OAB	4.83	122.68	116.40
2	B	601	6XZ	CAP-NBA-CAM	-4.74	103.77	111.14
2	A	601	6XZ	CAZ-OAR-CAX	-4.57	118.20	121.97
2	C	601	6XZ	CAZ-OAR-CAX	-4.45	118.30	121.97
2	B	601	6XZ	CAN-CAL-NBA	4.34	119.41	110.65
2	A	601	6XZ	CAO-CAM-NBA	-4.30	101.97	110.65
2	C	601	6XZ	OAR-CAX-OAB	4.29	121.98	116.40
2	A	601	6XZ	OAB-CAX-CAK	-4.22	117.42	125.92
2	D	601	6XZ	OAR-CAX-OAB	4.10	121.73	116.40
2	A	601	6XZ	CAY-CAV-CAK	-3.73	113.61	119.61
2	C	601	6XZ	CAL-NBA-CAM	3.70	116.80	108.84
2	B	601	6XZ	CAZ-OAR-CAX	-3.69	118.92	121.97
2	C	601	6XZ	OAB-CAX-CAK	-3.64	118.60	125.92
2	D	601	6XZ	OAB-CAX-CAK	-3.37	119.14	125.92
2	C	601	6XZ	CAY-CAV-CAK	-3.25	114.37	119.61
2	D	601	6XZ	CAN-CAL-NBA	3.17	117.04	110.65
2	B	601	6XZ	CAY-CAV-CAK	-3.12	114.59	119.61
2	B	601	6XZ	CAA-OAQ-CAS	-3.07	110.91	117.50
2	B	601	6XZ	OAB-CAX-CAK	-2.98	119.92	125.92
2	A	601	6XZ	CAL-NBA-CAM	2.91	115.11	108.84
2	B	601	6XZ	CAN-NBB-CAU	2.86	125.92	118.11
2	C	601	6XZ	CAN-NBB-CAU	2.80	125.75	118.11
2	C	601	6XZ	CAA-OAQ-CAS	-2.78	111.53	117.50
2	B	601	6XZ	CAP-NBA-CAL	-2.71	106.93	111.14
2	A	601	6XZ	CAP-NBA-CAM	-2.70	106.95	111.14
2	B	601	6XZ	OAR-CAX-CAK	2.66	120.40	117.16
2	A	601	6XZ	CAN-NBB-CAO	2.56	117.32	111.57
2	B	601	6XZ	OAR-CAX-OAB	2.52	119.67	116.40
2	A	601	6XZ	CAP-CAV-CAY	2.42	121.66	118.19
2	C	601	6XZ	CAP-CAV-CAK	2.35	126.57	121.73
2	C	601	6XZ	CAN-NBB-CAO	2.33	116.81	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	6XZ	CAL-NBA-CAM	2.33	113.87	108.84
2	B	601	6XZ	CAL-CAN-NBB	-2.29	105.97	110.78
2	A	601	6XZ	CAT-CAW-CAZ	2.26	121.56	118.50
2	D	601	6XZ	CAZ-OAR-CAX	-2.26	120.11	121.97
2	D	601	6XZ	CAP-NBA-CAL	2.25	114.64	111.14
2	A	601	6XZ	OAR-CAX-CAK	2.25	119.89	117.16
2	D	601	6XZ	CAP-CAV-CAK	-2.18	117.23	121.73
2	D	601	6XZ	CAO-CAM-NBA	2.18	115.05	110.65
2	A	601	6XZ	CAN-NBB-CAU	2.15	123.97	118.11
2	B	601	6XZ	CAM-CAO-NBB	2.15	115.31	110.78
2	C	601	6XZ	CAN-CAL-NBA	2.13	114.95	110.65
2	C	601	6XZ	CAH-CAU-NBB	-2.09	118.49	121.39

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
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	A	601	6XZ	CAF-CAS-OAQ-CAA
2	A	601	6XZ	CAE-CAS-OAQ-CAA
2	C	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
3	D	602	GOL	O1-C1-C2-C3
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	C	601	6XZ	CAG-CAU-NBB-CAO
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	CAV-CAP-NBA-CAL
2	B	601	6XZ	NBA-CAP-CAV-CAK

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Mol	Chain	Res	Type	Atoms
2	B	601	6XZ	NBA-CAP-CAV-CAY
2	D	601	6XZ	NBA-CAP-CAV-CAY
2	B	601	6XZ	CAH-CAU-NBB-CAN
2	B	601	6XZ	CAG-CAU-NBB-CAN
3	A	602	GOL	C1-C2-C3-O3
2	C	601	6XZ	CAG-CAU-NBB-CAN
2	C	601	6XZ	CAH-CAU-NBB-CAN
3	A	602	GOL	O2-C2-C3-O3

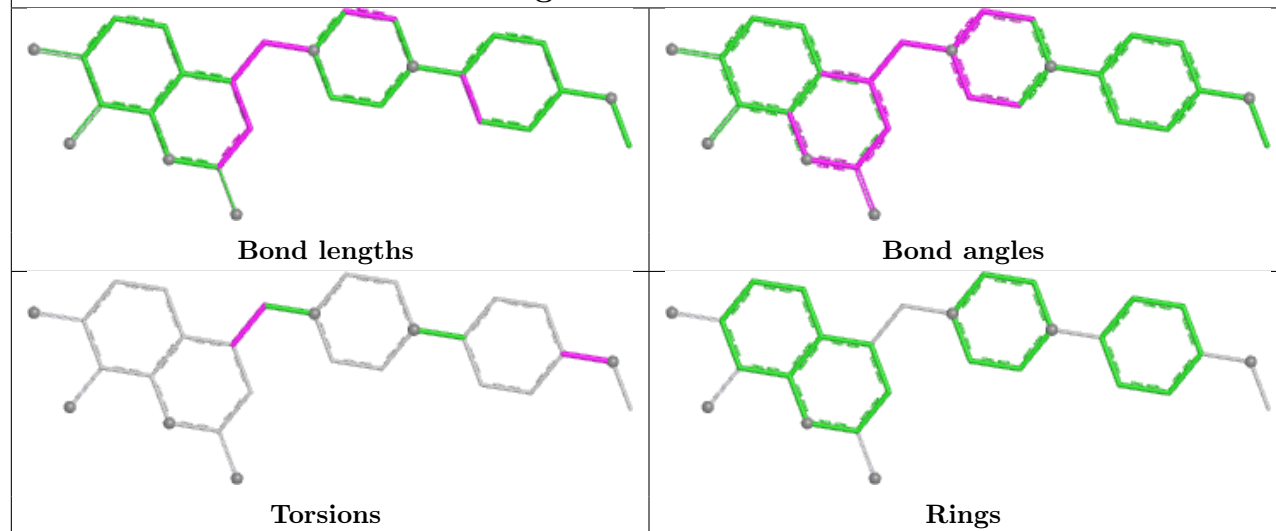
There are no ring outliers.

3 monomers are involved in 2 short contacts:

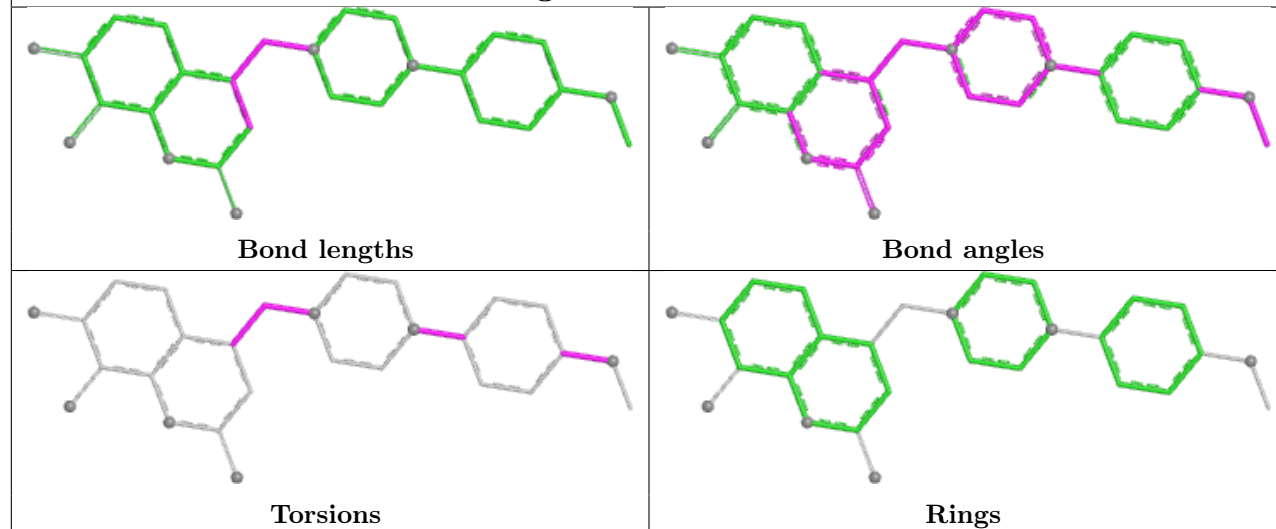
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	1	0
3	C	602	GOL	1	0
2	C	601	6XZ	1	0

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.

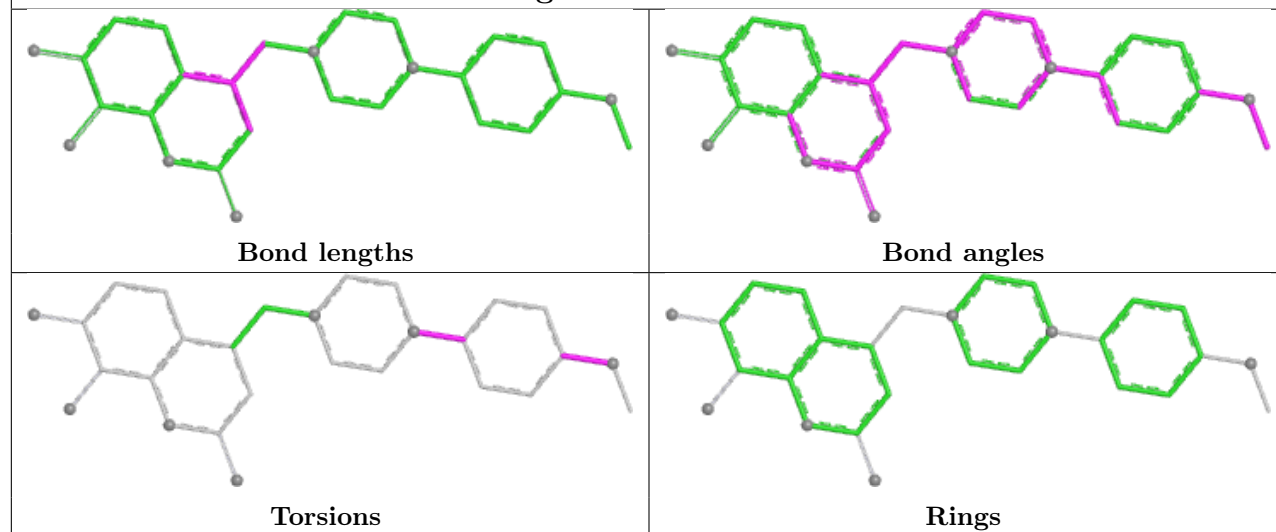
Ligand 6XZ D 601

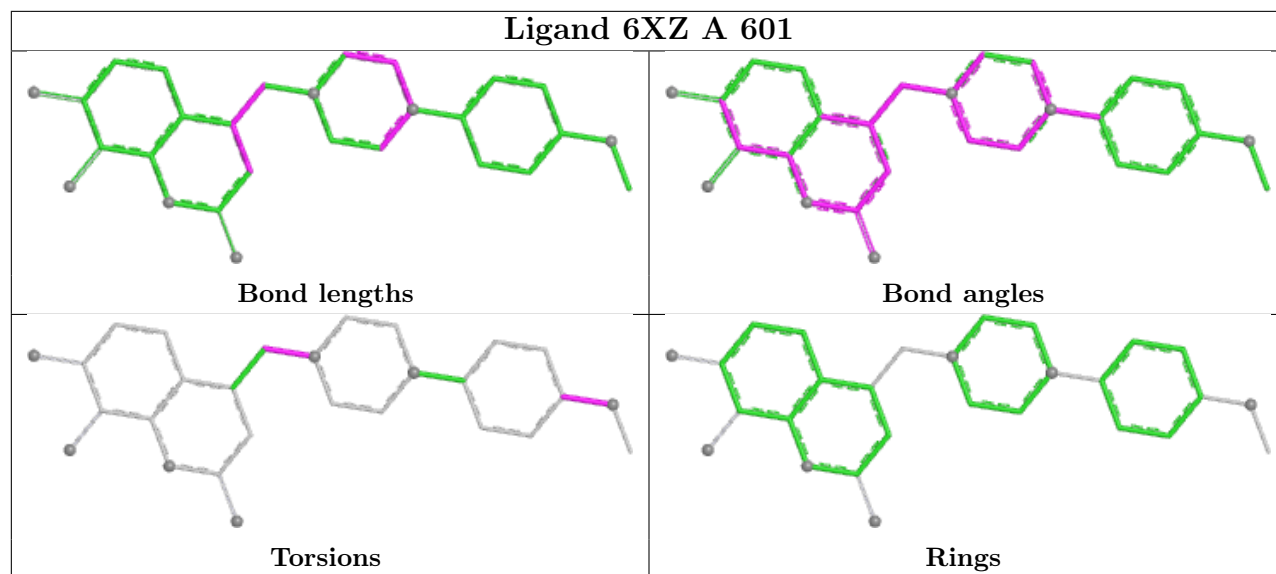


Ligand 6XZ B 601



Ligand 6XZ C 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%)	-1.69	0 100 100	26, 44, 67, 84	1 (0%)
1	B	513/514 (99%)	-1.58	0 100 100	26, 65, 93, 110	1 (0%)
1	C	513/514 (99%)	-1.70	0 100 100	26, 45, 67, 80	1 (0%)
1	D	513/514 (99%)	-1.59	0 100 100	29, 64, 92, 108	1 (0%)
All	All	2052/2056 (99%)	-1.64	0 100 100	26, 52, 86, 110	4 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6XZ	B	601	28/28	0.98	0.06	96,109,123,124	0
2	6XZ	C	601	28/28	0.98	0.05	72,94,102,104	0
2	6XZ	A	601	28/28	0.99	0.04	76,89,103,105	0
2	6XZ	D	601	28/28	0.99	0.05	75,96,105,108	0

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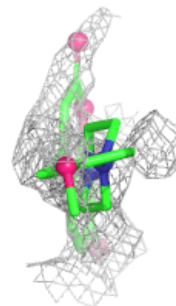
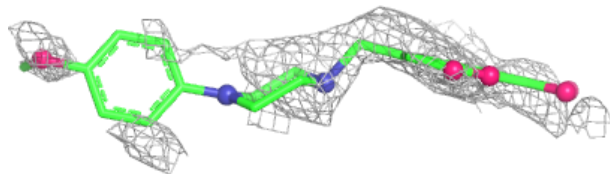
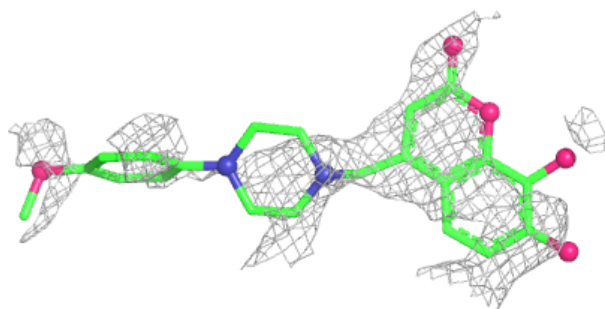
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	602	6/6	0.99	0.04	62,66,67,71	0
3	GOL	B	602	6/6	0.99	0.04	41,42,42,45	0
3	GOL	C	602	6/6	0.99	0.04	60,60,63,64	0
3	GOL	D	602	6/6	0.99	0.06	60,63,63,71	0

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.

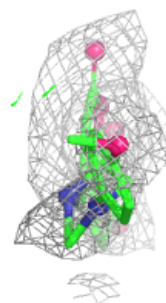
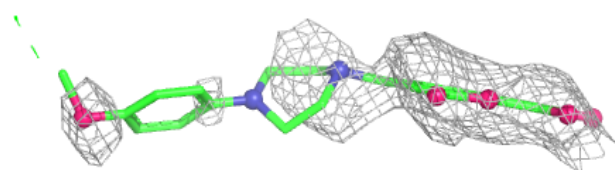
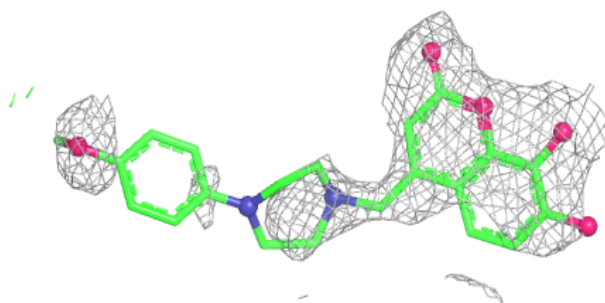
Electron density around 6XZ B 601:

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

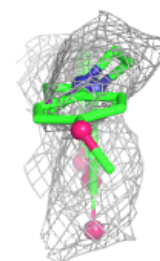
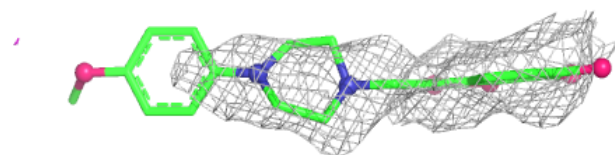
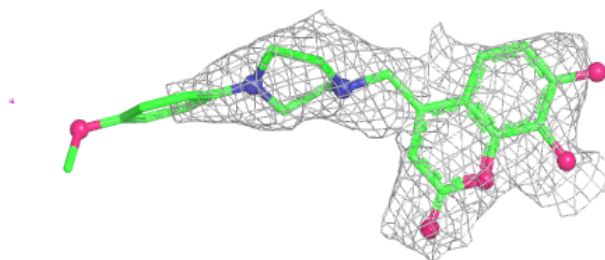


Electron density around 6XZ C 601:

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

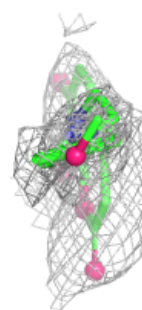
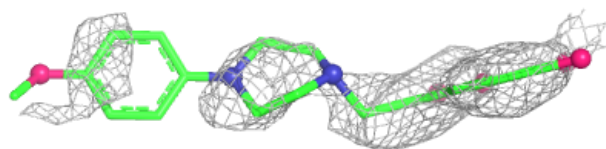
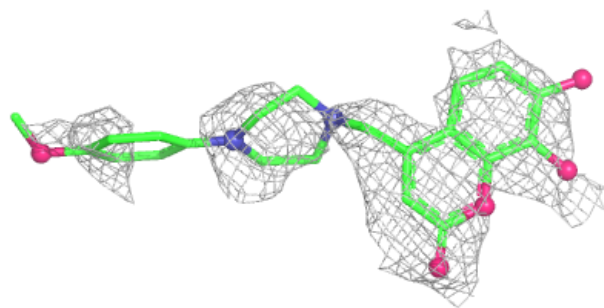
**Electron density around 6XZ A 601:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.