



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:41 AM UTC

PDB ID : 6K3E / pdb_00006k3e
Title : LSD1/Co-Rest structure with an inhibitor
Authors : Wang, J.
Deposited on : 2019-05-17
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

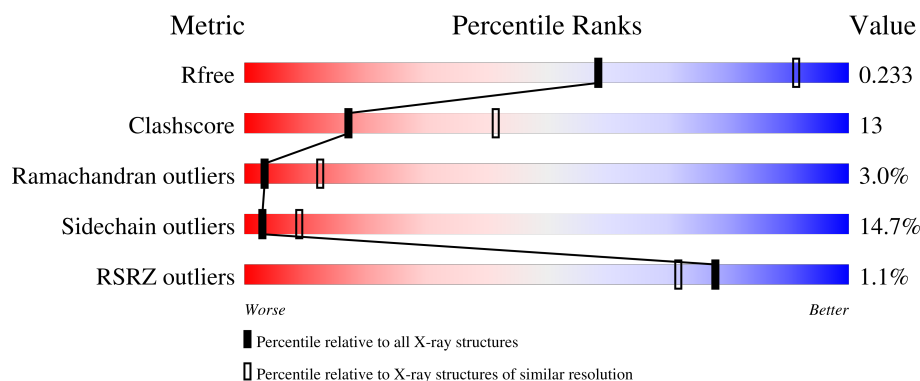
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	662	% 66% 29% 5%
2	B	140	% 44% 35% 15% • 5%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6483 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5177	3297	901	959	20			

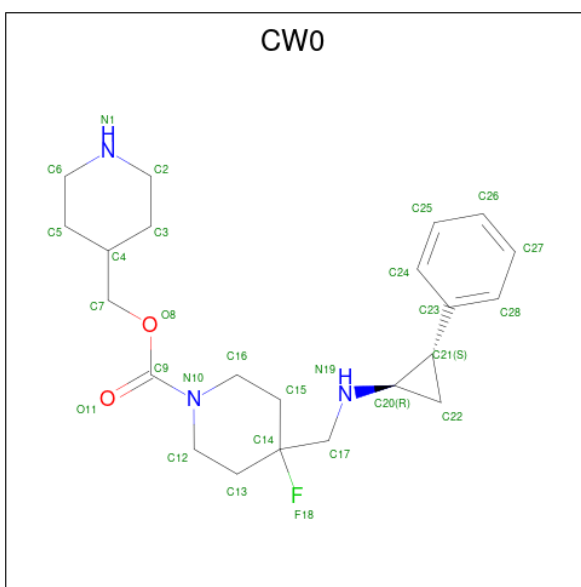
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

There are 7 discrepancies between the modelled and reference sequences:

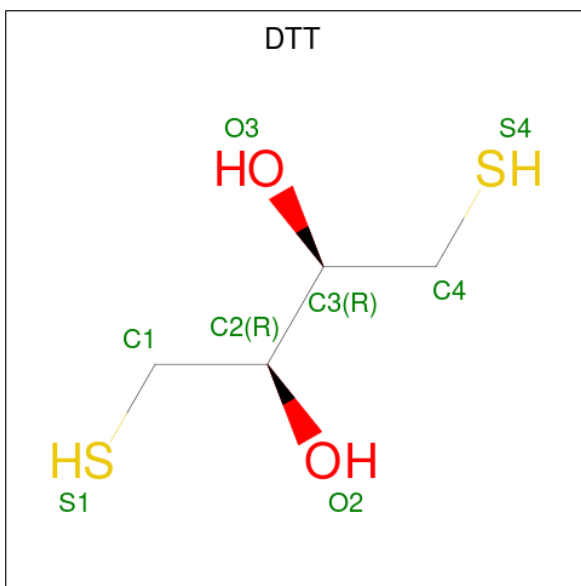
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	GLY	-	expression tag	UNP Q9UKL0
B	302	SER	-	expression tag	UNP Q9UKL0
B	303	SER	-	expression tag	UNP Q9UKL0
B	304	GLY	-	expression tag	UNP Q9UKL0
B	305	SER	-	expression tag	UNP Q9UKL0
B	306	ALA	-	expression tag	UNP Q9UKL0
B	307	SER	-	expression tag	UNP Q9UKL0

- Molecule 3 is piperidin-4-ylmethyl 4-fluoranyl-4-[[[(1 {R},2 {S})-2-phenylcyclopropyl]amino]methyl]piperidine-1-carboxylate (CCD ID: CW0) (formula: C₂₂H₃₂FN₃O₂) (labeled as "Ligand of Interest" by depositor).



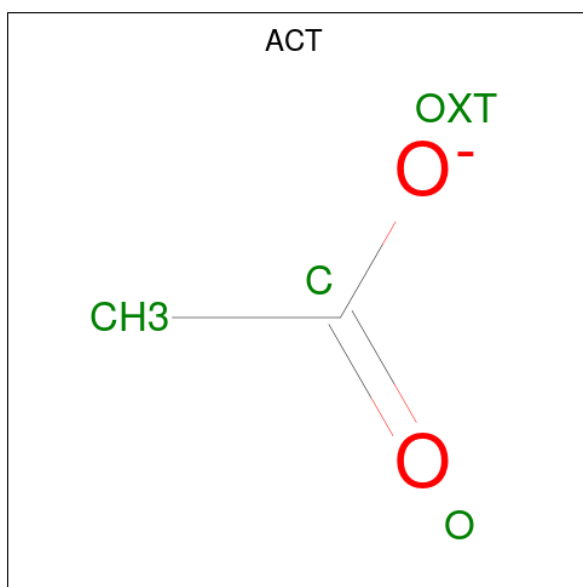
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			28	22	1	3	2		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



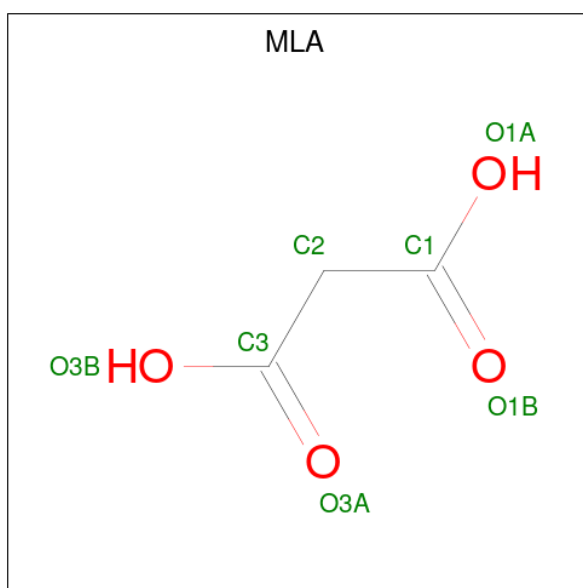
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



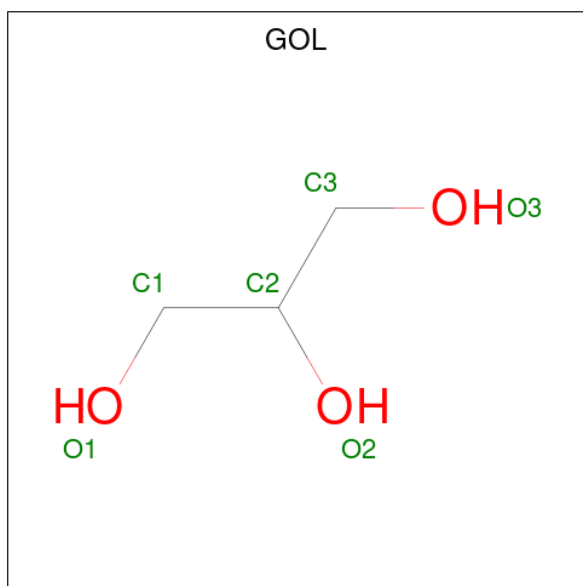
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	A	1	Total	C	O	0	0
			7	3	4		

Continued on next page...

Continued from previous page...

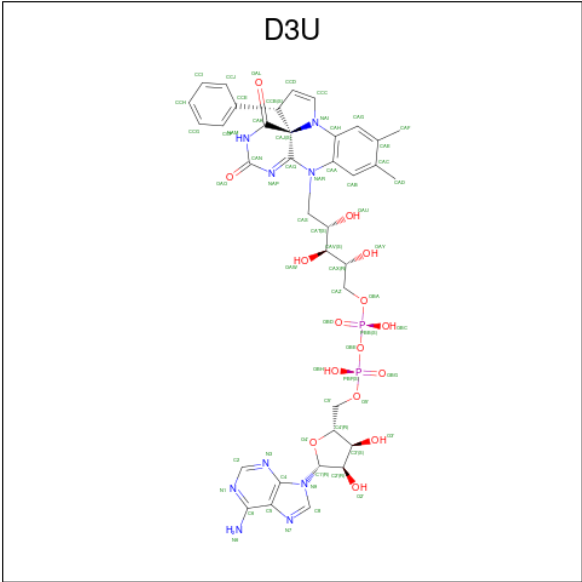
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



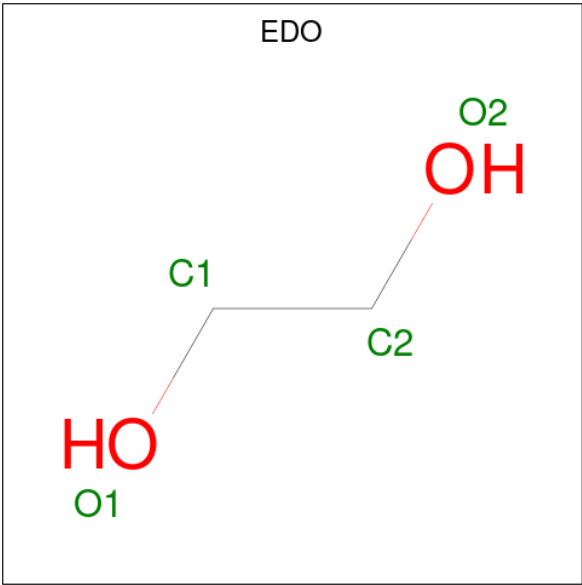
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 2-PCPA derivative (CCD ID: D3U) (formula: $C_{36}H_{41}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			62	36	9	15	2		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



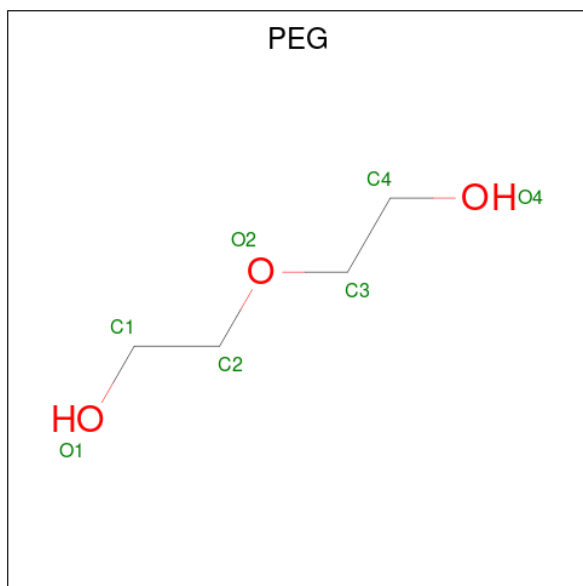
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Cl	0	0
			2	2		

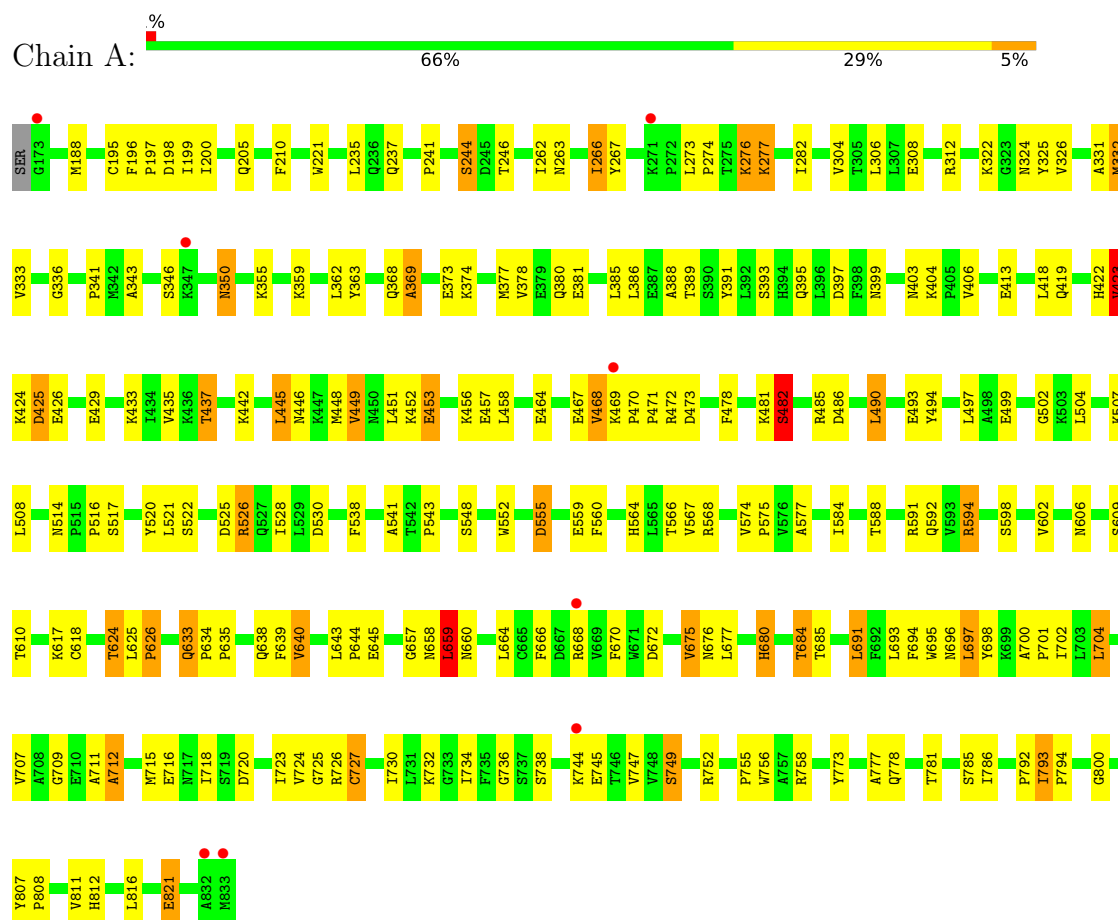
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		

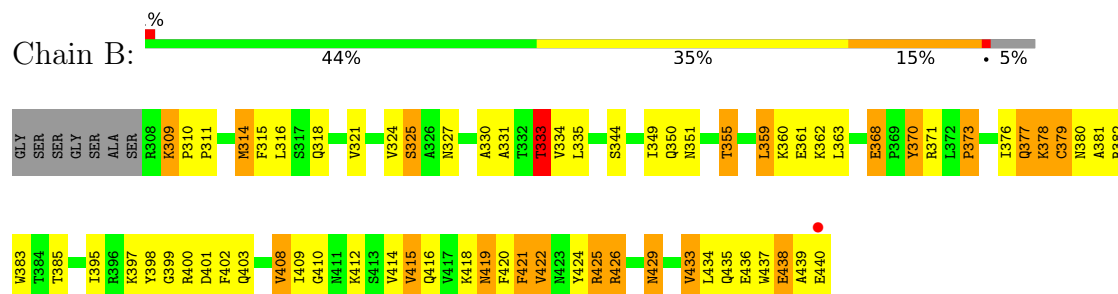
3 Residue-property plots

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: Lysine-specific histone demethylase 1A



• Molecule 2: REST corepressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.51Å 179.44Å 234.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.46 – 2.87 76.46 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (76.46-2.87) 98.7 (76.46-2.87)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.189 , 0.223 (Not available) , 0.233	Depositor DCC
R_{free} test set	2828 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	93.3	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 89.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6483	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CW0, D3U, ACT, CL, MLA, DTT, GOL, PEG

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	1.12	8/5289 (0.2%)	1.56	25/7174 (0.3%)
2	B	1.10	0/1091	1.61	3/1471 (0.2%)
All	All	1.12	8/6380 (0.1%)	1.57	28/8645 (0.3%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	777	ALA	C-O	7.70	1.34	1.24
1	A	618	CYS	C-O	7.06	1.32	1.23
1	A	635	PRO	C-O	-6.37	1.16	1.23
1	A	756	TRP	C-O	5.88	1.31	1.24
1	A	592	GLN	C-O	5.42	1.29	1.23
1	A	695	TRP	C-O	5.42	1.30	1.24
1	A	312	ARG	C-O	5.28	1.30	1.23
1	A	263	ASN	C-O	5.01	1.30	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	PRO	CB-CA-C	-6.57	102.98	111.39
1	A	473	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	712	ALA	O-C-N	5.99	128.24	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	GLU	CA-C-N	5.96	128.74	120.63
1	A	373	GLU	C-N-CA	5.96	128.74	120.63
1	A	625	LEU	CA-C-N	5.93	125.94	119.89
1	A	625	LEU	C-N-CA	5.93	125.94	119.89
1	A	800	GLY	CA-C-O	-5.86	118.41	122.22
1	A	635	PRO	CA-C-O	-5.71	115.12	121.23
1	A	698	TYR	CB-CA-C	5.61	119.05	109.80
1	A	499	GLU	CA-C-N	5.57	128.53	120.79
1	A	499	GLU	C-N-CA	5.57	128.53	120.79
1	A	625	LEU	O-C-N	5.53	125.91	121.38
1	A	425	ASP	CA-CB-CG	5.52	118.12	112.60
2	B	333	THR	CA-CB-OG1	-5.46	101.42	109.60
1	A	624	THR	CA-CB-OG1	5.46	117.78	109.60
2	B	318	GLN	CA-C-N	5.46	127.85	120.38
2	B	318	GLN	C-N-CA	5.46	127.85	120.38
1	A	684	THR	CA-C-N	5.45	128.37	120.79
1	A	684	THR	C-N-CA	5.45	128.37	120.79
1	A	567	VAL	O-C-N	5.42	129.55	122.94
1	A	559	GLU	N-CA-CB	5.33	117.85	110.17
1	A	331	ALA	CA-C-O	-5.28	115.96	121.55
1	A	821	GLU	CB-CG-CD	5.23	121.50	112.60
1	A	555	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	639	PHE	CB-CA-C	5.13	118.22	109.75
1	A	502	GLY	CA-C-N	5.11	127.39	120.65
1	A	502	GLY	C-N-CA	5.11	127.39	120.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	GLY	Peptide
1	A	792	PRO	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	5177	0	5212	122	0
2	B	1076	0	1091	55	0
3	A	28	0	0	1	0
4	A	8	0	10	1	0
5	A	8	0	6	1	0
6	A	21	0	6	2	0
7	A	24	0	32	1	0
8	A	62	0	0	1	0
9	A	48	0	72	0	0
10	A	21	0	30	0	0
11	A	2	0	0	0	0
12	A	8	0	0	0	0
All	All	6483	0	6459	163	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 13.

All (163) 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:566:THR:HG21	1:A:697:LEU:HD12	1.56	0.88
1:A:693:LEU:HD12	1:A:694:PHE:N	1.96	0.81
1:A:308:GLU:OE2	8:A:912:D3U:O3'	1.99	0.80
2:B:381:ALA:HA	2:B:416:GLN:HE22	1.45	0.79
2:B:309:LYS:HE3	2:B:309:LYS:HA	1.67	0.76
2:B:381:ALA:HA	2:B:416:GLN:NE2	2.03	0.74
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.71	0.71
2:B:422:VAL:O	2:B:425:ARG:HB2	1.90	0.71
1:A:385:LEU:O	1:A:388:ALA:HB3	1.91	0.71
1:A:693:LEU:HD12	1:A:694:PHE:H	1.58	0.68
1:A:672:ASP:O	1:A:675:VAL:HG12	1.93	0.68
1:A:350:ASN:O	1:A:350:ASN:ND2	2.28	0.66
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.32	0.64
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.27	0.64
1:A:660:ASN:HA	1:A:749:SER:OG	1.96	0.64
1:A:453:GLU:HA	1:A:453:GLU:OE1	1.97	0.64
2:B:368:GLU:OE2	2:B:371:ARG:NH1	2.28	0.63
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.79	0.63
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.33	0.62
1:A:548:SER:O	1:A:552:TRP:HB3	1.98	0.62
1:A:666:PHE:O	1:A:701:PRO:HG2	2.00	0.62
1:A:807:TYR:N	1:A:808:PRO:HD3	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.41	0.61
1:A:381:GLU:OE2	2:B:314:MET:HE1	2.02	0.60
2:B:424:TYR:O	2:B:426:ARG:N	2.35	0.60
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.82	0.59
1:A:235:LEU:HD21	1:A:246:THR:CG2	2.33	0.58
1:A:793:ILE:N	1:A:793:ILE:HD13	2.19	0.58
1:A:196:PHE:N	1:A:197:PRO:CD	2.67	0.57
1:A:594:ARG:HA	1:A:640:VAL:O	2.04	0.57
2:B:310:PRO:O	2:B:311:PRO:C	2.48	0.57
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.20	0.56
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.88	0.56
1:A:566:THR:HG21	1:A:697:LEU:CD1	2.33	0.56
2:B:381:ALA:CA	2:B:416:GLN:HE22	2.17	0.56
1:A:520:TYR:CE2	1:A:521:LEU:HD12	2.41	0.55
1:A:720:ASP:O	1:A:724:VAL:HG23	2.06	0.55
2:B:309:LYS:HG3	2:B:310:PRO:HD2	1.88	0.55
1:A:677:LEU:HD23	1:A:677:LEU:N	2.22	0.55
1:A:195:CYS:SG	4:A:902:DTT:S4	3.05	0.55
7:A:910:GOL:H32	7:A:911:GOL:C3	2.38	0.54
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.88	0.54
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.06	0.54
1:A:725:GLY:C	1:A:727:CYS:H	2.14	0.54
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.88	0.53
2:B:414:VAL:O	2:B:418:LYS:HG3	2.08	0.53
1:A:725:GLY:O	1:A:727:CYS:N	2.42	0.53
1:A:266:ILE:HD12	1:A:577:ALA:HB1	1.89	0.52
1:A:725:GLY:C	1:A:727:CYS:N	2.66	0.52
1:A:468:VAL:O	1:A:472:ARG:NH1	2.41	0.52
2:B:416:GLN:O	2:B:419:ASN:HB2	2.09	0.52
2:B:359:LEU:HD23	2:B:359:LEU:N	2.25	0.52
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.46	0.51
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.45	0.51
1:A:418:LEU:HD12	2:B:324:VAL:HG21	1.93	0.51
1:A:445:LEU:CD1	2:B:360:LYS:HG3	2.41	0.51
1:A:188:MET:HE3	1:A:210:PHE:CD2	2.46	0.51
1:A:241:PRO:O	1:A:244:SER:HB3	2.11	0.50
1:A:391:TYR:CE1	2:B:310:PRO:HD3	2.45	0.50
1:A:419:GLN:HE22	2:B:315:PHE:H	1.59	0.50
1:A:343:ALA:O	1:A:346:SER:OG	2.30	0.50
1:A:564:HIS:ND1	3:A:901[A]:CW0:C12	2.74	0.50
1:A:812:HIS:O	1:A:816:LEU:HG	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:HG3	5:A:903:ACT:H2	1.92	0.50
1:A:693:LEU:HD12	1:A:693:LEU:C	2.36	0.50
1:A:332:MET:CE	1:A:704:LEU:HD13	2.42	0.50
1:A:325:TYR:O	1:A:326:VAL:HG23	2.12	0.49
2:B:378:LYS:O	2:B:380:ASN:N	2.45	0.49
1:A:464:GLU:O	1:A:467:GLU:HB2	2.12	0.49
2:B:421:PHE:HE1	2:B:434:LEU:HD11	1.77	0.49
2:B:324:VAL:HG12	2:B:324:VAL:O	2.13	0.49
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.42	0.49
2:B:350:GLN:HA	2:B:350:GLN:OE1	2.13	0.49
1:A:235:LEU:HD21	1:A:246:THR:HG22	1.95	0.48
1:A:437:THR:HG22	1:A:508:LEU:CD2	2.43	0.48
1:A:723:ILE:O	1:A:727:CYS:HB2	2.12	0.48
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.95	0.48
2:B:399:GLY:HA3	2:B:437:TRP:CE3	2.49	0.48
1:A:781:THR:OG1	1:A:794:PRO:HB3	2.12	0.48
1:A:332:MET:HG2	1:A:333:VAL:HG23	1.95	0.47
2:B:370:TYR:N	2:B:370:TYR:CD1	2.82	0.47
2:B:400:ARG:O	2:B:402:PHE:N	2.46	0.47
1:A:341:PRO:CG	1:A:816:LEU:HD21	2.44	0.47
1:A:418:LEU:HD11	2:B:324:VAL:HG21	1.97	0.47
1:A:541:ALA:O	1:A:657:GLY:HA3	2.15	0.47
2:B:309:LYS:CG	2:B:310:PRO:HD2	2.44	0.47
1:A:362:LEU:C	1:A:363:TYR:CD1	2.93	0.47
1:A:807:TYR:N	1:A:808:PRO:CD	2.78	0.47
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.97	0.47
2:B:383:TRP:CZ2	2:B:420:PHE:HB2	2.50	0.47
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.49	0.46
1:A:235:LEU:HD21	1:A:246:THR:HG21	1.97	0.46
1:A:276:LYS:HE2	1:A:277:LYS:N	2.30	0.46
2:B:309:LYS:HD3	2:B:310:PRO:CD	2.45	0.46
1:A:793:ILE:N	1:A:793:ILE:CD1	2.78	0.46
2:B:370:TYR:N	2:B:370:TYR:HD1	2.13	0.46
1:A:606:ASN:HD22	1:A:609:SER:H	1.63	0.46
1:A:374:LYS:O	1:A:377:MET:N	2.43	0.46
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.31	0.45
2:B:321:VAL:O	2:B:325:SER:OG	2.35	0.45
1:A:811:VAL:O	1:A:812:HIS:C	2.60	0.45
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.46	0.45
1:A:368:GLN:C	1:A:369:ALA:O	2.59	0.45
1:A:660:ASN:HD21	1:A:716:GLU:CG	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ASN:C	1:A:406:VAL:HG23	2.41	0.45
1:A:493:GLU:O	1:A:497:LEU:HD13	2.17	0.45
1:A:660:ASN:HD21	1:A:716:GLU:HG3	1.81	0.45
1:A:350:ASN:HD22	1:A:350:ASN:C	2.21	0.44
1:A:694:PHE:HA	1:A:704:LEU:O	2.17	0.44
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.99	0.44
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.30	0.44
1:A:530:ASP:OD2	1:A:685:THR:HA	2.18	0.44
1:A:697:LEU:N	1:A:697:LEU:CD2	2.81	0.44
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.53	0.43
1:A:391:TYR:HE1	2:B:309:LYS:HE3	1.83	0.43
2:B:309:LYS:HA	2:B:309:LYS:CE	2.39	0.43
1:A:478:PHE:O	1:A:482:SER:HB3	2.17	0.43
1:A:664:LEU:HD11	1:A:727:CYS:SG	2.58	0.43
2:B:429:ASN:N	2:B:429:ASN:OD1	2.52	0.43
1:A:442:LYS:CE	2:B:355:THR:HG21	2.49	0.43
1:A:448:MET:HE2	2:B:363:LEU:CD1	2.47	0.43
1:A:386:LEU:O	1:A:389:THR:N	2.48	0.43
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.49	0.43
1:A:306:LEU:HD13	1:A:584:ILE:HG12	2.00	0.42
1:A:422:HIS:O	1:A:423:VAL:C	2.61	0.42
1:A:778:GLN:HG2	6:A:906:MLA:C3	2.48	0.42
1:A:391:TYR:CE1	1:A:395:GLN:HG3	2.55	0.42
2:B:408:VAL:HG12	2:B:409:ILE:N	2.34	0.42
2:B:438:GLU:O	2:B:440:GLU:N	2.53	0.42
1:A:341:PRO:HG3	1:A:816:LEU:HD21	2.01	0.42
2:B:415:VAL:CG2	2:B:416:GLN:N	2.83	0.42
1:A:470:PRO:HA	1:A:471:PRO:C	2.45	0.42
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.55	0.42
1:A:273:LEU:O	1:A:274:PRO:C	2.60	0.42
1:A:525:ASP:O	1:A:528:ILE:N	2.53	0.42
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.55	0.42
2:B:377:GLN:HB2	2:B:410:GLY:O	2.20	0.42
1:A:670:PHE:CD1	1:A:670:PHE:O	2.73	0.41
1:A:378:VAL:O	1:A:381:GLU:N	2.53	0.41
1:A:560:PHE:CE1	1:A:807:TYR:HE2	2.39	0.41
1:A:574:VAL:HB	1:A:575:PRO:HD3	2.02	0.41
2:B:433:VAL:O	2:B:436:GLU:HB2	2.20	0.41
1:A:481:LYS:O	1:A:482:SER:C	2.64	0.41
1:A:658:ASN:OD1	1:A:659:LEU:N	2.51	0.41
1:A:732:LYS:O	1:A:736:GLY:N	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:O	1:A:469:LYS:N	2.53	0.41
1:A:643:LEU:HA	1:A:644:PRO:HD2	1.86	0.41
1:A:660:ASN:CA	1:A:749:SER:OG	2.65	0.41
1:A:368:GLN:O	1:A:369:ALA:O	2.38	0.41
1:A:393:SER:O	1:A:397:ASP:HA	2.20	0.41
2:B:380:ASN:OD1	2:B:381:ALA:N	2.54	0.41
2:B:309:LYS:HD3	2:B:310:PRO:HD2	2.03	0.41
2:B:378:LYS:H	2:B:378:LYS:CD	2.33	0.41
1:A:709:GLY:C	1:A:711:ALA:N	2.78	0.41
2:B:333:THR:HG22	2:B:334:VAL:N	2.37	0.41
1:A:424:LYS:O	1:A:426:GLU:N	2.54	0.40
1:A:522:SER:O	1:A:525:ASP:N	2.51	0.40
1:A:633:GLN:HA	1:A:634:PRO:HA	1.90	0.40
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.36	0.40
1:A:449:VAL:C	1:A:451:LEU:H	2.29	0.40
1:A:490:LEU:HD23	1:A:490:LEU:N	2.36	0.40
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.57	0.40
1:A:778:GLN:HG2	6:A:906:MLA:O3A	2.22	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	659/662 (100%)	560 (85%)	85 (13%)	14 (2%)	5	19
2	B	131/140 (94%)	100 (76%)	21 (16%)	10 (8%)	1	2
All	All	790/802 (98%)	660 (84%)	106 (13%)	24 (3%)	3	12

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	ALA
1	A	468	VAL
2	B	379	CYS
2	B	425	ARG
1	A	244	SER
1	A	425	ASP
2	B	429	ASN
2	B	439	ALA
1	A	403	ASN
1	A	726	ARG
2	B	331	ALA
2	B	373	PRO
1	A	507	LYS
1	A	659	LEU
2	B	351	ASN
2	B	401	ASP
2	B	419	ASN
1	A	482	SER
1	A	526	ARG
1	A	322	LYS
1	A	423	VAL
1	A	457	GLU
1	A	516	PRO
2	B	333	THR

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	561/562 (100%)	489 (87%)	72 (13%)	4	12
2	B	117/121 (97%)	89 (76%)	28 (24%)	1	2
All	All	678/683 (99%)	578 (85%)	100 (15%)	3	9

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	199	ILE
1	A	200	ILE
1	A	205	GLN
1	A	237	GLN
1	A	266	ILE
1	A	267	TYR
1	A	276	LYS
1	A	277	LYS
1	A	304	VAL
1	A	324	ASN
1	A	332	MET
1	A	350	ASN
1	A	355	LYS
1	A	359	LYS
1	A	380	GLN
1	A	404	LYS
1	A	423	VAL
1	A	429	GLU
1	A	433	LYS
1	A	437	THR
1	A	445	LEU
1	A	446	ASN
1	A	449	VAL
1	A	452	LYS
1	A	453	GLU
1	A	458	LEU
1	A	482	SER
1	A	485	ARG
1	A	490	LEU
1	A	504	LEU
1	A	514	ASN
1	A	517	SER
1	A	526	ARG
1	A	538	PHE
1	A	543	PRO
1	A	555	ASP
1	A	568	ARG
1	A	588	THR
1	A	591	ARG
1	A	594	ARG
1	A	598	SER
1	A	610	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	617	LYS
1	A	624	THR
1	A	626	PRO
1	A	633	GLN
1	A	638	GLN
1	A	640	VAL
1	A	645	GLU
1	A	659	LEU
1	A	668	ARG
1	A	675	VAL
1	A	676	ASN
1	A	680	HIS
1	A	684	THR
1	A	691	LEU
1	A	696	ASN
1	A	697	LEU
1	A	702	ILE
1	A	704	LEU
1	A	718	ILE
1	A	727	CYS
1	A	738	SER
1	A	744	LYS
1	A	745	GLU
1	A	747	VAL
1	A	749	SER
1	A	785	SER
1	A	786	ILE
1	A	793	ILE
1	A	821	GLU
2	B	309	LYS
2	B	314	MET
2	B	316	LEU
2	B	325	SER
2	B	335	LEU
2	B	344	SER
2	B	355	THR
2	B	359	LEU
2	B	361	GLU
2	B	362	LYS
2	B	368	GLU
2	B	370	TYR
2	B	373	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	376	ILE
2	B	377	GLN
2	B	378	LYS
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	397	LYS
2	B	408	VAL
2	B	415	VAL
2	B	421	PHE
2	B	422	VAL
2	B	426	ARG
2	B	433	VAL
2	B	435	GLN
2	B	438	GLU

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	237	GLN
1	A	259	HIS
1	A	298	GLN
1	A	395	GLN
1	A	410	GLN
1	A	419	GLN
1	A	422	HIS
1	A	459	HIS
1	A	484	HIS
1	A	532	HIS
1	A	535	ASN
1	A	606	ASN
1	A	633	GLN
1	A	717	ASN
1	A	806	ASN
2	B	337	GLN
2	B	348	GLN
2	B	411	ASN
2	B	416	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	EDO	A	914	-	3,3,3	0.35	0	2,2,2	0.53	0
4	DTT	A	902	-	7,7,7	0.52	0	4,8,8	1.21	1 (25%)
9	EDO	A	918	-	3,3,3	0.06	0	2,2,2	0.15	0
10	PEG	A	927	-	6,6,6	0.30	0	5,5,5	0.17	0
7	GOL	A	909	-	5,5,5	0.27	0	5,5,5	0.56	0
7	GOL	A	908	-	5,5,5	0.26	0	5,5,5	0.48	0
9	EDO	A	913	-	3,3,3	0.25	0	2,2,2	0.49	0
10	PEG	A	925	-	6,6,6	0.13	0	5,5,5	0.17	0
5	ACT	A	904	-	3,3,3	1.38	0	3,3,3	0.65	0
9	EDO	A	916	-	3,3,3	0.22	0	2,2,2	0.29	0
9	EDO	A	923	-	3,3,3	0.43	0	2,2,2	0.75	0
10	PEG	A	926	-	6,6,6	0.30	0	5,5,5	0.17	0
9	EDO	A	920	-	3,3,3	0.22	0	2,2,2	0.14	0
5	ACT	A	903	-	3,3,3	1.12	0	3,3,3	1.52	0
3	CW0	A	901[A]	-	30,31,31	1.82	9 (30%)	33,43,43	2.78	15 (45%)
6	MLA	A	907	-	6,6,6	1.27	0	7,7,7	0.90	0
9	EDO	A	919	-	3,3,3	0.23	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLA	A	906	-	6,6,6	1.45	1 (16%)	7,7,7	0.99	0
9	EDO	A	915	-	3,3,3	0.07	0	2,2,2	0.17	0
6	MLA	A	905	-	6,6,6	1.54	0	7,7,7	0.86	0
8	D3U	A	912	-	65,69,69	3.36	27 (41%)	88,107,107	2.03	29 (32%)
7	GOL	A	910	-	5,5,5	0.12	0	5,5,5	0.35	0
9	EDO	A	921	-	3,3,3	0.14	0	2,2,2	0.27	0
7	GOL	A	911	-	5,5,5	0.19	0	5,5,5	0.47	0
9	EDO	A	922	-	3,3,3	0.13	0	2,2,2	0.11	0
9	EDO	A	924	-	3,3,3	0.18	0	2,2,2	0.15	0
9	EDO	A	917	-	3,3,3	0.16	0	2,2,2	0.27	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
9	EDO	A	914	-	-	1/1/1/1	-
4	DTT	A	902	-	-	4/8/8/8	-
9	EDO	A	918	-	-	0/1/1/1	-
10	PEG	A	927	-	-	2/4/4/4	-
7	GOL	A	909	-	-	3/4/4/4	-
7	GOL	A	908	-	-	0/4/4/4	-
9	EDO	A	913	-	-	1/1/1/1	-
10	PEG	A	925	-	-	2/4/4/4	-
9	EDO	A	916	-	-	0/1/1/1	-
9	EDO	A	923	-	-	1/1/1/1	-
10	PEG	A	926	-	-	2/4/4/4	-
9	EDO	A	920	-	-	1/1/1/1	-
3	CW0	A	901[A]	-	-	7/18/44/44	0/4/4/4
6	MLA	A	907	-	-	2/4/4/4	-
9	EDO	A	919	-	-	0/1/1/1	-
6	MLA	A	906	-	-	2/4/4/4	-
9	EDO	A	915	-	-	1/1/1/1	-
6	MLA	A	905	-	-	2/4/4/4	-
8	D3U	A	912	-	-	2/38/103/103	0/8/8/8
7	GOL	A	910	-	-	4/4/4/4	-
9	EDO	A	921	-	-	1/1/1/1	-
7	GOL	A	911	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	922	-	-	1/1/1/1	-
9	EDO	A	924	-	-	1/1/1/1	-
9	EDO	A	917	-	-	0/1/1/1	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	912	D3U	PBB-OBE	10.42	1.70	1.59
8	A	912	D3U	CCB-CCD	-10.11	1.39	1.52
8	A	912	D3U	C2-N1	8.73	1.49	1.33
8	A	912	D3U	CCE-CCB	-8.25	1.44	1.52
8	A	912	D3U	CAK-NAM	6.75	1.48	1.37
8	A	912	D3U	CAF-CAE	-6.17	1.39	1.51
8	A	912	D3U	CAH-NAI	-5.83	1.28	1.40
8	A	912	D3U	CAS-CAT	5.19	1.59	1.52
8	A	912	D3U	PBF-OBH	5.18	1.79	1.55
8	A	912	D3U	CAD-CAC	-5.10	1.41	1.51
8	A	912	D3U	C2-N3	4.24	1.41	1.33
3	A	901[A]	CW0	C22-C20	4.15	1.54	1.49
8	A	912	D3U	CAN-NAM	3.78	1.47	1.39
3	A	901[A]	CW0	C9-N10	3.62	1.41	1.35
8	A	912	D3U	PBB-OBA	3.47	1.73	1.59
8	A	912	D3U	PBB-OBH	3.30	1.62	1.50
8	A	912	D3U	O3'-C3'	3.19	1.50	1.43
8	A	912	D3U	CAJ-CCB	3.14	1.66	1.57
8	A	912	D3U	CAS-NAR	3.07	1.55	1.47
3	A	901[A]	CW0	O11-C9	2.98	1.25	1.21
8	A	912	D3U	CCC-NAI	-2.94	1.35	1.39
8	A	912	D3U	C5-N7	-2.92	1.33	1.39
8	A	912	D3U	CCJ-CCE	2.82	1.43	1.39
3	A	901[A]	CW0	C17-C14	2.75	1.58	1.52
3	A	901[A]	CW0	C20-N19	2.68	1.53	1.47
3	A	901[A]	CW0	C22-C21	2.47	1.54	1.50
8	A	912	D3U	CCG-CCF	2.46	1.43	1.38
3	A	901[A]	CW0	C23-C21	2.35	1.55	1.51
8	A	912	D3U	C8-N9	-2.31	1.33	1.37
8	A	912	D3U	CAQ-NAP	2.31	1.37	1.31
8	A	912	D3U	CAG-CAE	-2.23	1.36	1.39
8	A	912	D3U	OAL-CAK	2.22	1.26	1.22
8	A	912	D3U	O4'-C4'	2.20	1.49	1.45
3	A	901[A]	CW0	C16-N10	2.18	1.50	1.47
3	A	901[A]	CW0	C17-N19	2.14	1.49	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	912	D3U	PBF-OBE	2.12	1.61	1.59
6	A	906	MLA	O3A-C3	2.07	1.28	1.22

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901[A]	CW0	C12-C13-C14	5.86	116.77	112.38
3	A	901[A]	CW0	O8-C9-O11	-5.69	114.86	124.76
8	A	912	D3U	CAH-NAI-CCC	-5.61	115.30	123.64
3	A	901[A]	CW0	C16-C15-C14	-5.50	108.26	112.38
3	A	901[A]	CW0	O8-C9-N10	5.35	121.11	111.77
3	A	901[A]	CW0	C17-N19-C20	5.16	122.29	115.04
8	A	912	D3U	C6-C5-C4	4.76	123.68	117.18
3	A	901[A]	CW0	C15-C14-C13	-4.58	104.99	110.05
8	A	912	D3U	O4'-C1'-C2'	-4.57	96.85	106.62
8	A	912	D3U	N3-C2-N1	-4.21	122.21	128.58
8	A	912	D3U	CAB-CAA-CAH	-3.73	114.35	120.06
8	A	912	D3U	CAH-CAA-NAR	3.54	123.36	119.03
8	A	912	D3U	C4'-O4'-C1'	-3.42	101.92	109.47
8	A	912	D3U	CCI-CCJ-CCE	3.37	124.68	120.65
3	A	901[A]	CW0	C6-C5-C4	-3.26	107.11	112.14
8	A	912	D3U	N9-C8-N7	-3.08	109.57	113.94
8	A	912	D3U	CCH-CCG-CCF	3.02	123.97	120.24
3	A	901[A]	CW0	C2-N1-C6	3.01	118.90	110.40
8	A	912	D3U	OAL-CAK-NAM	2.99	125.44	120.59
8	A	912	D3U	OBE-PBB-OB	-2.99	101.72	110.70
8	A	912	D3U	C5-C4-N3	-2.94	122.66	126.72
3	A	901[A]	CW0	C2-C3-C4	-2.88	107.69	112.14
3	A	901[A]	CW0	C27-C26-C25	-2.87	115.94	119.87
8	A	912	D3U	N6-C6-N1	2.76	124.53	118.38
8	A	912	D3U	CAJ-CAK-NAM	-2.73	113.34	116.97
8	A	912	D3U	PBB-OBA-CAZ	-2.71	105.84	121.35
8	A	912	D3U	C5-C6-N6	-2.70	116.60	123.29
8	A	912	D3U	OBA-CAZ-CAX	2.65	116.43	109.36
3	A	901[A]	CW0	C16-N10-C9	2.64	129.43	121.75
8	A	912	D3U	CAZ-CAX-CAV	-2.57	107.38	112.22
8	A	912	D3U	OBH-PBF-O5'	-2.54	96.06	107.57
8	A	912	D3U	O4'-C4'-C5'	-2.50	101.31	109.33
8	A	912	D3U	NAM-CAN-NAP	-2.46	114.27	119.50
8	A	912	D3U	OAU-CAT-CAV	-2.45	103.51	109.25
8	A	912	D3U	C4-N9-C8	2.39	108.25	105.74
3	A	901[A]	CW0	C26-C27-C28	2.23	122.99	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	912	D3U	OAW-CAV-CAX	-2.22	103.88	108.93
8	A	912	D3U	C5-N7-C8	2.22	106.94	103.45
8	A	912	D3U	CAS-CAT-CAV	2.20	115.64	109.66
8	A	912	D3U	OBH-PBF-OBG	2.19	122.62	112.44
8	A	912	D3U	C6-C5-N7	-2.17	127.90	132.09
3	A	901[A]	CW0	C15-C16-N10	2.16	114.85	110.82
3	A	901[A]	CW0	C28-C23-C24	-2.10	115.70	118.30
3	A	901[A]	CW0	C28-C23-C21	2.10	125.11	121.08
4	A	902	DTT	C2-C1-S1	2.00	120.03	114.43

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901[A]	CW0	C5-C4-C7-O8
3	A	901[A]	CW0	C13-C14-C17-N19
3	A	901[A]	CW0	C15-C14-C17-N19
3	A	901[A]	CW0	C22-C20-N19-C17
3	A	901[A]	CW0	N10-C9-O8-C7
3	A	901[A]	CW0	O11-C9-O8-C7
4	A	902	DTT	S1-C1-C2-O2
4	A	902	DTT	S1-C1-C2-C3
4	A	902	DTT	C2-C3-C4-S4
4	A	902	DTT	O3-C3-C4-S4
7	A	910	GOL	C1-C2-C3-O3
7	A	910	GOL	O2-C2-C3-O3
7	A	910	GOL	O1-C1-C2-O2
10	A	925	PEG	O1-C1-C2-O2
3	A	901[A]	CW0	C3-C4-C7-O8
10	A	926	PEG	O1-C1-C2-O2
10	A	926	PEG	O2-C3-C4-O4
7	A	909	GOL	O1-C1-C2-C3
7	A	909	GOL	C1-C2-C3-O3
7	A	910	GOL	O1-C1-C2-C3
7	A	911	GOL	C1-C2-C3-O3
7	A	909	GOL	O2-C2-C3-O3
9	A	914	EDO	O1-C1-C2-O2
9	A	921	EDO	O1-C1-C2-O2
10	A	925	PEG	O2-C3-C4-O4
9	A	913	EDO	O1-C1-C2-O2
9	A	915	EDO	O1-C1-C2-O2
9	A	922	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	920	EDO	O1-C1-C2-O2
7	A	911	GOL	O1-C1-C2-O2
7	A	911	GOL	O2-C2-C3-O3
10	A	927	PEG	C1-C2-O2-C3
10	A	927	PEG	O2-C3-C4-O4
6	A	905	MLA	C1-C2-C3-O3B
6	A	907	MLA	C1-C2-C3-O3A
9	A	924	EDO	O1-C1-C2-O2
6	A	905	MLA	C1-C2-C3-O3A
6	A	906	MLA	O1A-C1-C2-C3
8	A	912	D3U	O4'-C4'-C5'-O5'
6	A	907	MLA	C1-C2-C3-O3B
6	A	906	MLA	O1B-C1-C2-C3
9	A	923	EDO	O1-C1-C2-O2
8	A	912	D3U	C2'-C1'-N9-C8

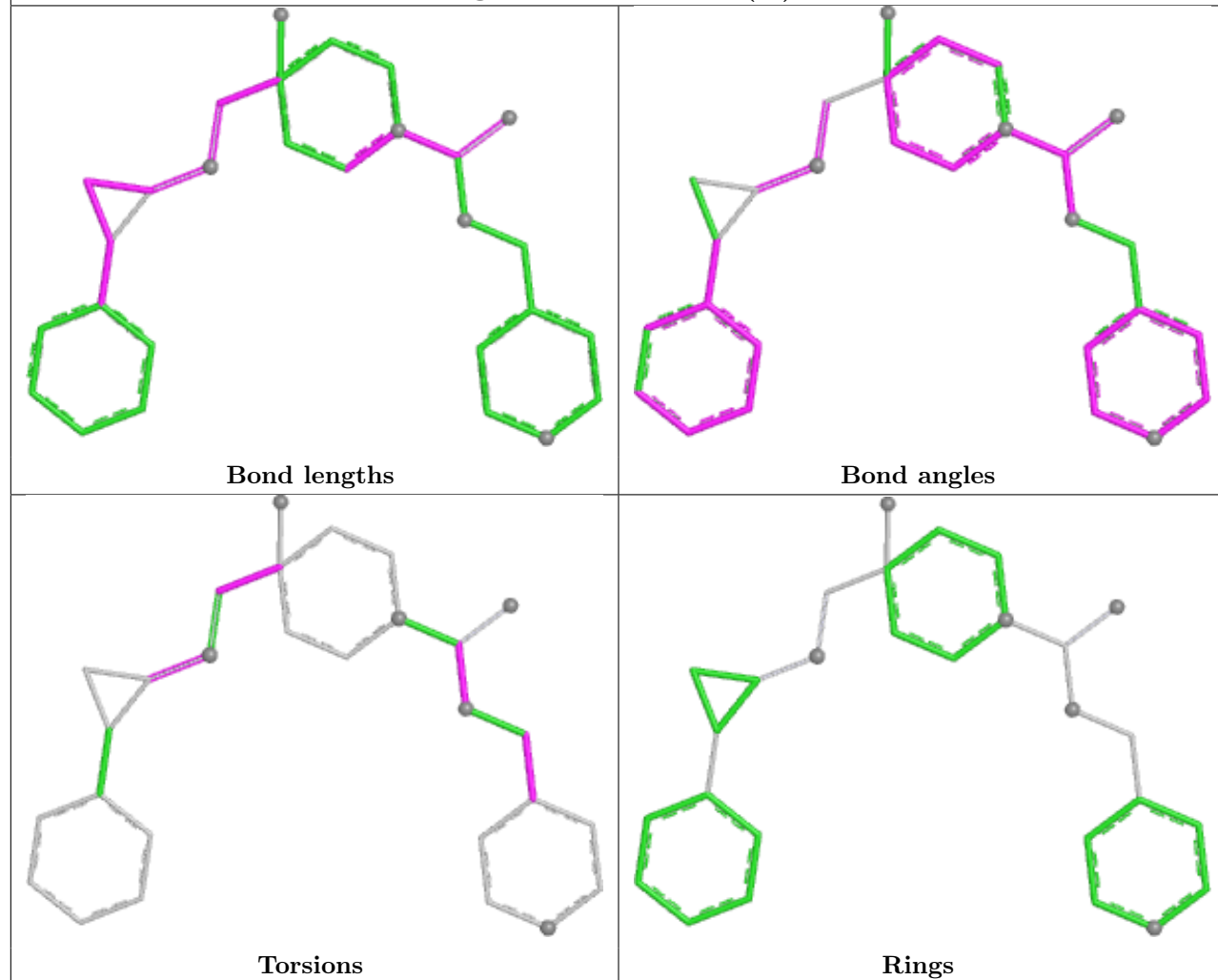
There are no ring outliers.

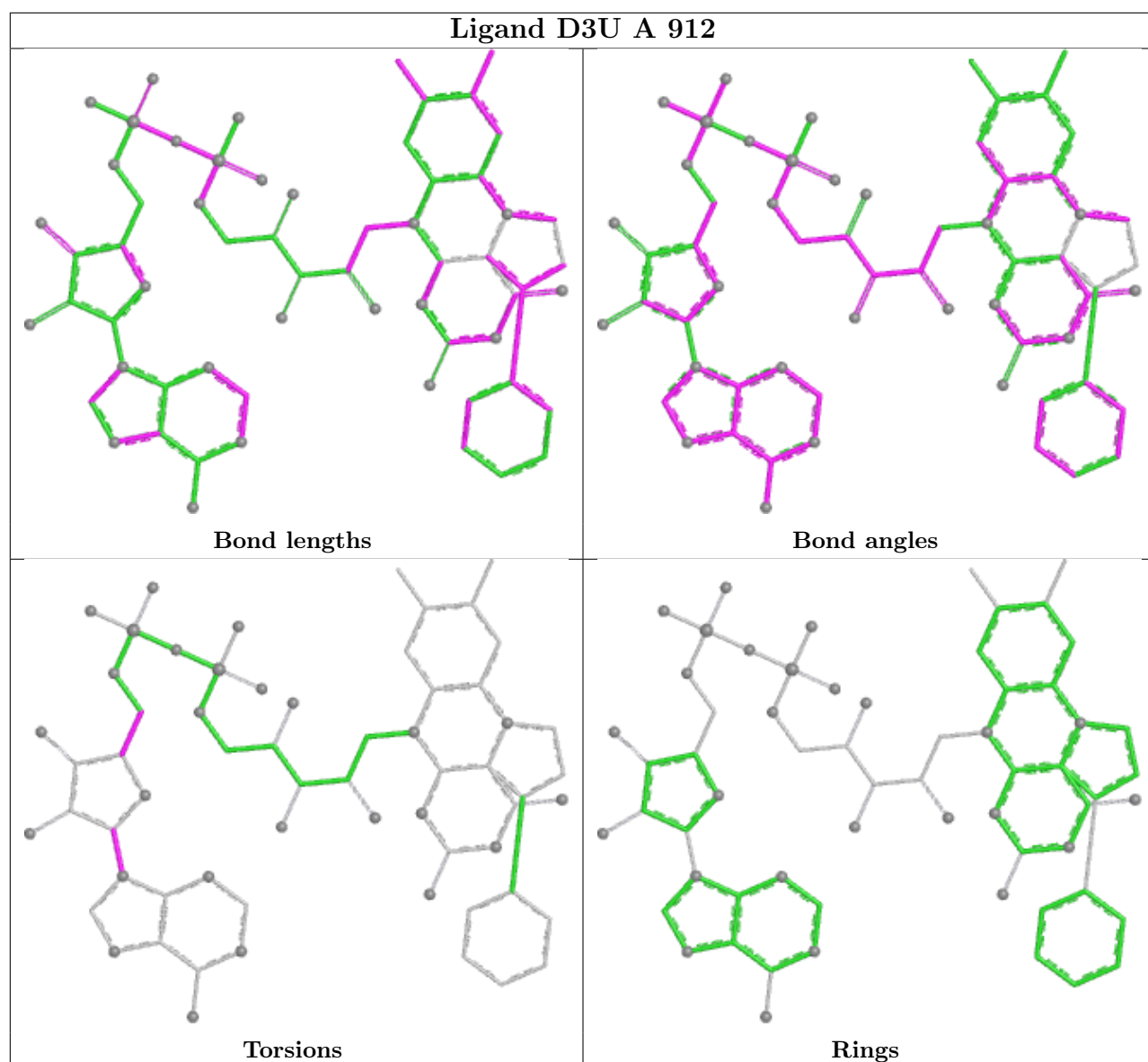
7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	DTT	1	0
5	A	903	ACT	1	0
3	A	901[A]	CW0	1	0
6	A	906	MLA	2	0
8	A	912	D3U	1	0
7	A	910	GOL	1	0
7	A	911	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 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 CW0 A 901 (A)





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	661/662 (99%)	-0.16	8 (1%) 76 70	68, 105, 150, 199	0
2	B	133/140 (95%)	0.19	1 (0%) 82 77	96, 140, 170, 208	0
All	All	794/802 (99%)	-0.10	9 (1%) 78 72	68, 112, 158, 208	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	833	MET	4.7
1	A	744	LYS	4.7
1	A	832	ALA	3.9
1	A	173	GLY	3.5
1	A	271	LYS	2.6
2	B	440	GLU	2.6
1	A	668	ARG	2.3
1	A	469	LYS	2.0
1	A	347	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

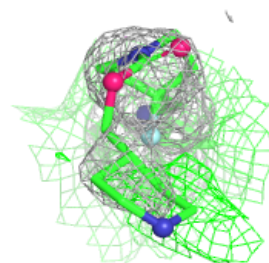
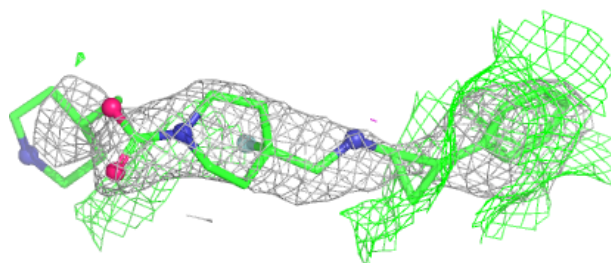
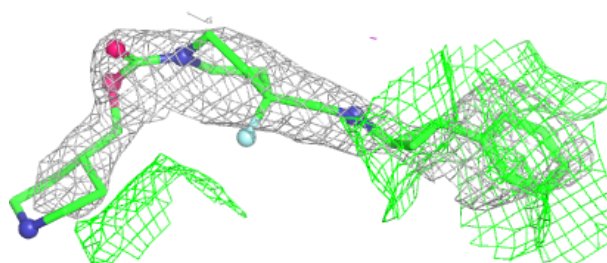
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	911	6/6	0.73	0.19	145,176,184,189	0
6	MLA	A	907	7/7	0.74	0.11	149,174,180,180	0
10	PEG	A	926	7/7	0.78	0.19	146,167,179,182	0
9	EDO	A	913	4/4	0.79	0.29	117,120,129,137	0
10	PEG	A	927	7/7	0.79	0.32	146,164,179,195	0
5	ACT	A	904	4/4	0.82	0.19	129,140,148,152	0
9	EDO	A	919	4/4	0.82	0.27	138,141,151,151	0
9	EDO	A	924	4/4	0.83	0.27	133,135,137,140	0
9	EDO	A	915	4/4	0.83	0.17	147,151,152,155	0
4	DTT	A	902	8/8	0.83	0.23	159,196,217,226	0
9	EDO	A	922	4/4	0.84	0.15	141,147,150,151	0
9	EDO	A	916	4/4	0.85	0.24	135,135,139,140	0
10	PEG	A	925	7/7	0.85	0.22	146,155,166,166	0
11	CL	A	928	1/1	0.85	0.24	143,143,143,143	0
9	EDO	A	917	4/4	0.87	0.17	113,139,140,145	0
3	CW0	A	901[A]	28/28	0.88	0.33	132,168,191,195	0
9	EDO	A	923	4/4	0.89	0.26	122,128,134,138	0
9	EDO	A	920	4/4	0.89	0.27	118,128,141,147	0
6	MLA	A	906	7/7	0.91	0.14	96,109,127,139	0
6	MLA	A	905	7/7	0.91	0.14	120,124,131,133	0
9	EDO	A	914	4/4	0.91	0.29	112,128,132,147	0
11	CL	A	929	1/1	0.91	0.16	140,140,140,140	0
9	EDO	A	918	4/4	0.92	0.24	146,148,157,163	0
9	EDO	A	921	4/4	0.92	0.32	131,133,137,139	0
5	ACT	A	903	4/4	0.93	0.19	85,88,94,104	0
7	GOL	A	909	6/6	0.93	0.18	118,139,153,162	0
7	GOL	A	908	6/6	0.94	0.18	104,118,144,145	0
7	GOL	A	910	6/6	0.94	0.22	115,139,150,158	6
8	D3U	A	912	62/62	0.98	0.08	53,88,111,114	0

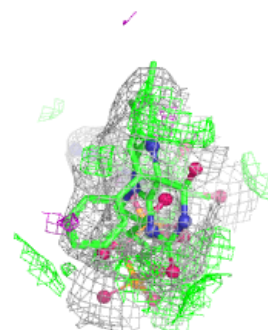
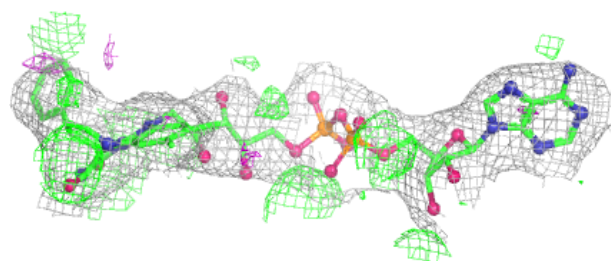
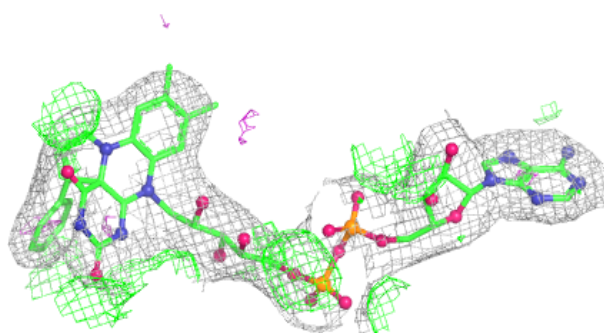
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CW0 A 901 (A):

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

**Electron density around D3U A 912:**

$2mF_o-DF_c$ (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.