



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:19 PM UTC

PDB ID : 6Q2M / pdb_00006q2m
Title : Crystal structure of Photinus pyralis Luciferase Pps6 mutant in complex with DLSA
Authors : Patel, K.D.; Gulick, A.M.
Deposited on : 2019-08-08
Resolution : 2.75 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

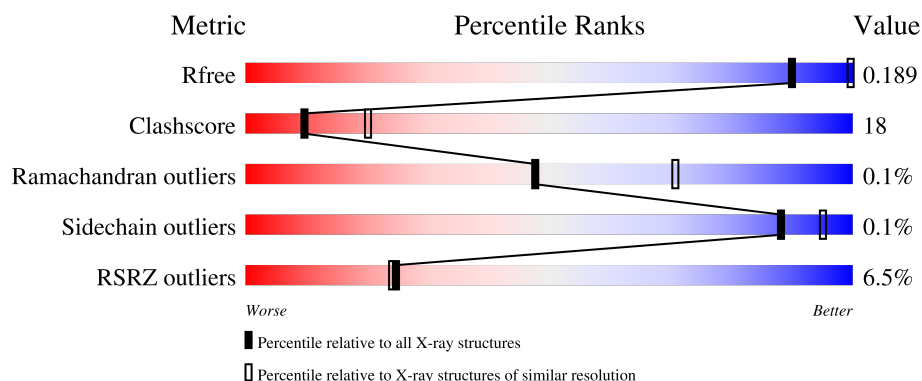
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	555	4% 77% 21% •
1	B	555	10% 70% 21% • 8%
1	C	555	3% 51% 27% 21%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	620	-	-	X	-
5	SLU	A	620	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11970 atoms, of which 2 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 Luciferin 4-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	1	0
			4171	2686	701	766	18			
1	B	512	Total	C	N	O	S	0	0	0
			3766	2411	640	698	17			
1	C	438	Total	C	N	O	S	0	0	0
			3352	2164	560	610	18			

There are 33 discrepancies between the modelled and reference sequences:

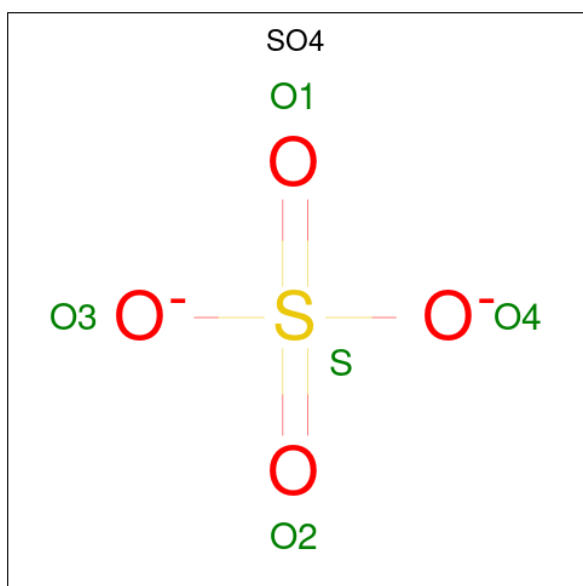
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P08659
A	-3	PRO	-	expression tag	UNP P08659
A	-2	LEU	-	expression tag	UNP P08659
A	-1	GLY	-	expression tag	UNP P08659
A	0	SER	-	expression tag	UNP P08659
A	214	ASN	THR	engineered mutation	UNP P08659
A	222	CYS	ALA	engineered mutation	UNP P08659
A	255	PHE	TYR	engineered mutation	UNP P08659
A	276	THR	SER	engineered mutation	UNP P08659
A	332	ASN	HIS	engineered mutation	UNP P08659
A	354	ASN	GLU	engineered mutation	UNP P08659
B	-4	GLY	-	expression tag	UNP P08659
B	-3	PRO	-	expression tag	UNP P08659
B	-2	LEU	-	expression tag	UNP P08659
B	-1	GLY	-	expression tag	UNP P08659
B	0	SER	-	expression tag	UNP P08659
B	214	ASN	THR	engineered mutation	UNP P08659
B	222	CYS	ALA	engineered mutation	UNP P08659
B	255	PHE	TYR	engineered mutation	UNP P08659
B	276	THR	SER	engineered mutation	UNP P08659
B	332	ASN	HIS	engineered mutation	UNP P08659
B	354	ASN	GLU	engineered mutation	UNP P08659
C	-4	GLY	-	expression tag	UNP P08659

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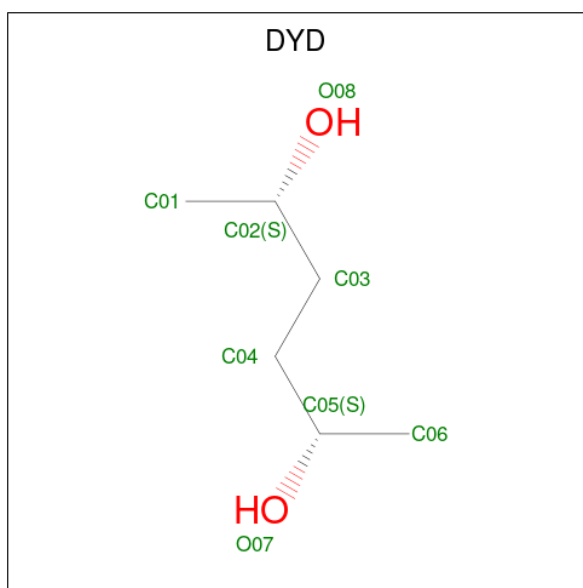
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	PRO	-	expression tag	UNP P08659
C	-2	LEU	-	expression tag	UNP P08659
C	-1	GLY	-	expression tag	UNP P08659
C	0	SER	-	expression tag	UNP P08659
C	214	ASN	THR	engineered mutation	UNP P08659
C	222	CYS	ALA	engineered mutation	UNP P08659
C	255	PHE	TYR	engineered mutation	UNP P08659
C	276	THR	SER	engineered mutation	UNP P08659
C	332	ASN	HIS	engineered mutation	UNP P08659
C	354	ASN	GLU	engineered mutation	UNP P08659

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



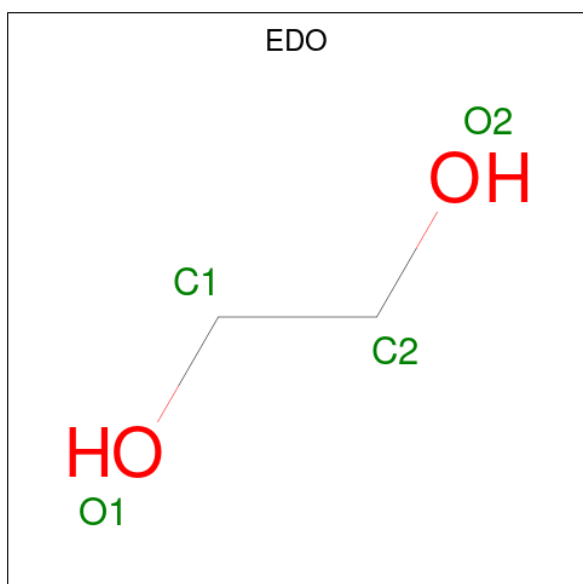
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is (2S,5S)-hexane-2,5-diol (CCD ID: DYD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



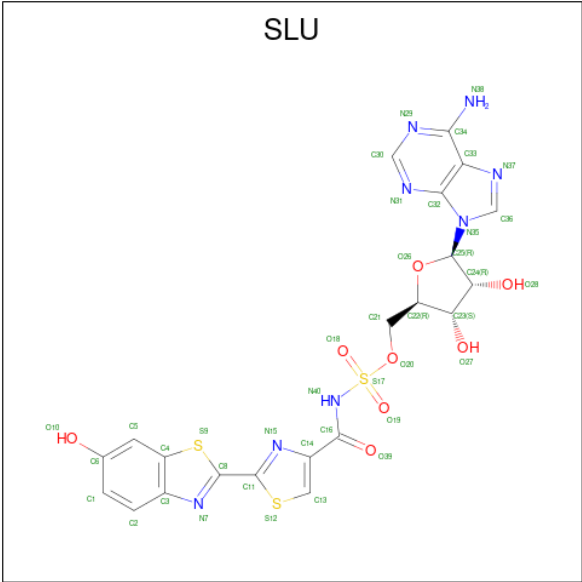
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

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

- Molecule 5 is 5'-O-[N-(DEHYDROLUCIFERYL)-SULFAMOYL] ADENOSINE (CCD ID: SLU) (formula: C₂₁H₁₈N₈O₈S₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			40	21	8	8	3		
5	B	1	Total	C	N	O	S	0	0
			40	21	8	8	3		
5	C	1	Total	C	N	O	S	0	0
			40	21	8	8	3		

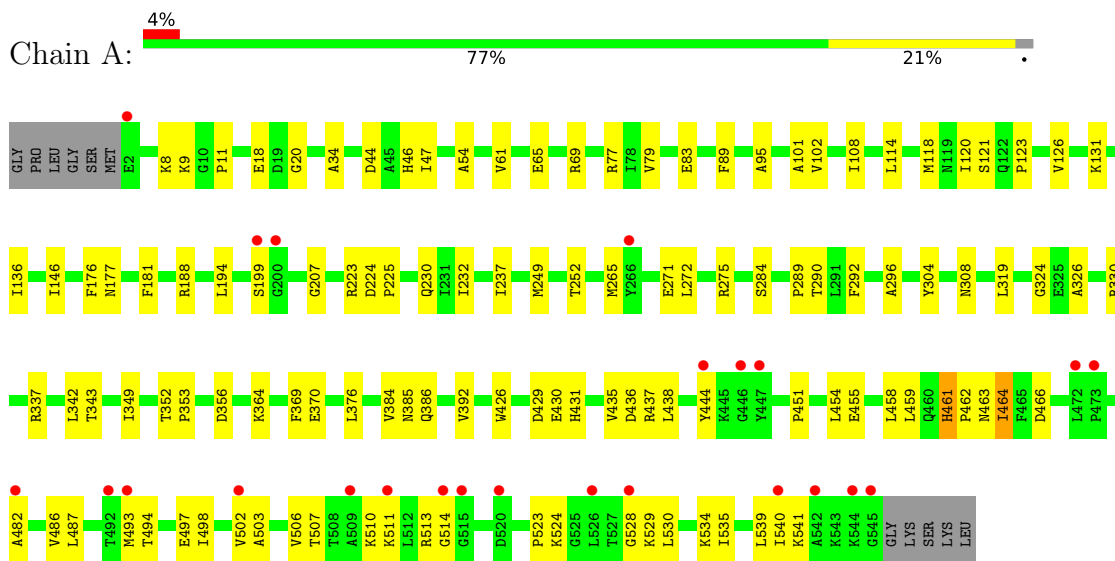
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	B	57	Total	O	0	0
			57	57		
6	C	71	Total	O	0	0
			71	71		

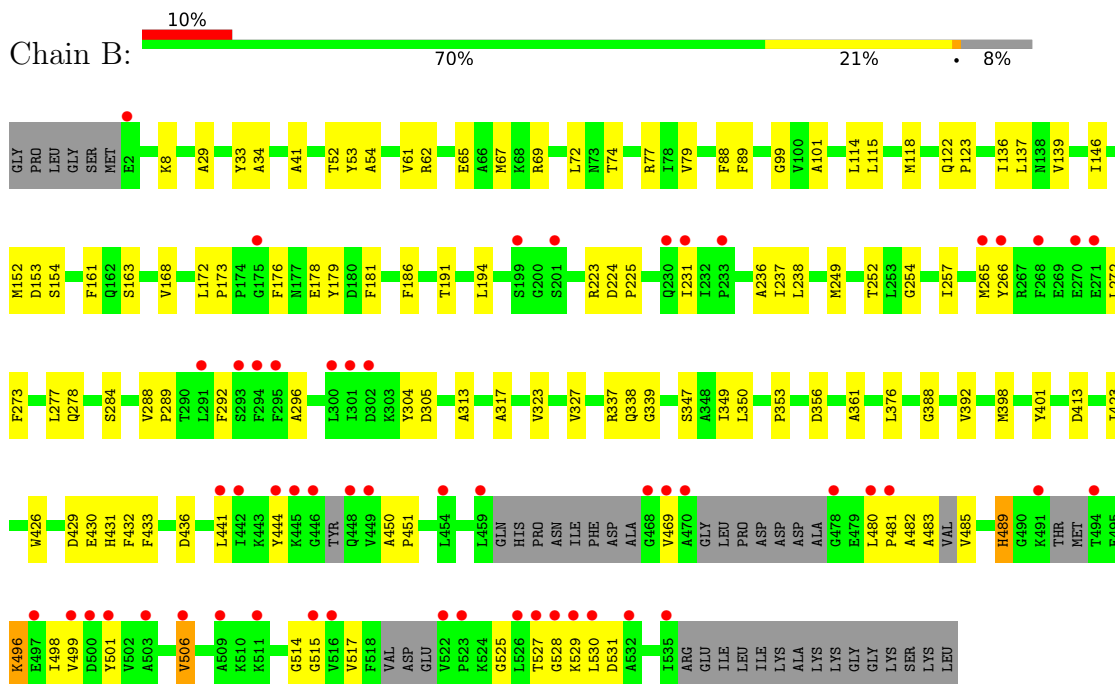
3 Residue-property plots

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.

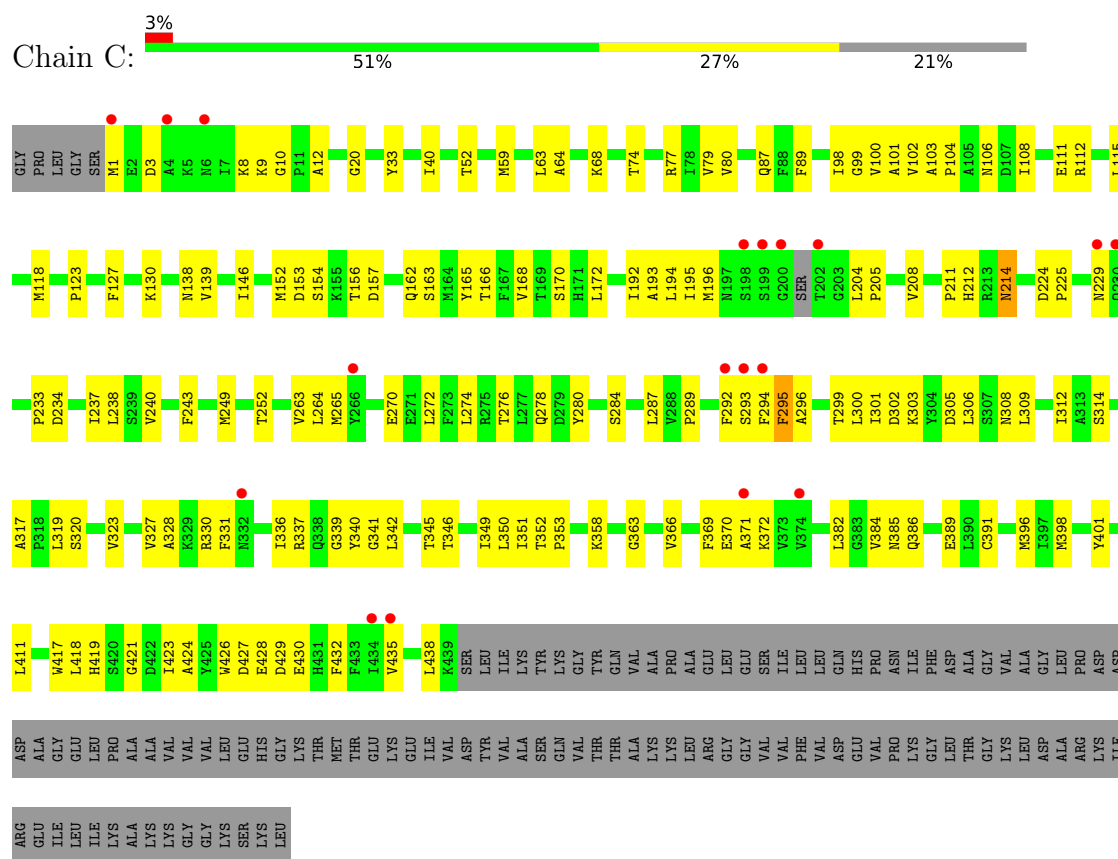
• Molecule 1: Luciferin 4-monooxygenase



• Molecule 1: Luciferin 4-monooxygenase



● Molecule 1: Luciferin 4-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.27Å 95.45Å 152.02Å 90.00° 101.56° 90.00°	Depositor
Resolution (Å)	44.70 – 2.75 44.70 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.9 (44.70-2.75) 90.4 (44.70-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.194 , 0.218 (Not available) , 0.189	Depositor DCC
R_{free} test set	1998 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11970	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: DYD, SLU, EDO, SO4

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	0.44	2/4267 (0.0%)	0.64	3/5790 (0.1%)
1	B	0.34	0/3844	0.58	4/5225 (0.1%)
1	C	0.41	0/3432	0.58	5/4665 (0.1%)
All	All	0.40	2/11543 (0.0%)	0.60	12/15680 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	ILE	C-O	-5.75	1.18	1.24
1	A	437	ARG	C-O	-5.39	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	HIS	CA-C-N	16.42	136.59	119.19
1	A	461	HIS	C-N-CA	16.42	136.59	119.19
1	C	10	GLY	CA-C-N	9.76	129.58	120.21
1	C	10	GLY	C-N-CA	9.76	129.58	120.21
1	C	12	ALA	CA-C-N	6.62	126.38	119.76
1	C	12	ALA	C-N-CA	6.62	126.38	119.76
1	B	496	LYS	N-CA-C	6.05	120.13	112.87
1	B	506	VAL	N-CA-C	5.99	121.80	109.34
1	B	444	TYR	N-CA-C	-5.58	105.11	111.07
1	B	489	HIS	N-CA-C	5.57	118.52	110.28
1	C	295	PHE	N-CA-C	5.40	118.20	109.83
1	A	199	SER	N-CA-C	5.20	117.31	109.41

There are no chirality outliers.

There are no planarity outliers.

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	4171	0	4149	114	0
1	B	3766	0	3563	105	0
1	C	3352	0	3280	182	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	1	0
3	A	16	0	0	3	0
3	C	16	0	0	0	0
4	A	64	1	96	7	0
4	B	28	1	42	4	0
4	C	64	0	96	13	0
5	A	40	0	16	2	0
5	B	40	0	18	5	0
5	C	40	0	17	1	0
6	A	213	0	0	8	0
6	B	57	0	0	3	0
6	C	71	0	0	7	0
All	All	11968	2	11277	406	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 18.

All (406) 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:461:HIS:CD2	1:A:462:PRO:HD2	1.57	1.38
4:B:607:EDO:H12	5:B:611:SLU:H1	1.20	1.15
1:A:352:THR:HG22	6:A:870:HOH:O	1.50	1.12
1:B:237:ILE:HD12	1:B:284:SER:HB3	1.23	1.09
1:C:301:ILE:HD11	1:C:330:ARG:HE	1.10	1.08
1:A:461:HIS:CB	1:A:464:ILE:HD12	1.83	1.07
1:A:461:HIS:HB3	1:A:464:ILE:HD12	1.09	1.07
1:C:237:ILE:HG12	1:C:284:SER:HB3	1.37	1.07
1:A:461:HIS:CD2	1:A:462:PRO:CD	2.37	1.06
1:C:294:PHE:O	1:C:295:PHE:HD1	1.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LEU:HB3	1:C:196:MET:HE3	1.39	1.02
1:C:214:ASN:HD22	1:C:214:ASN:N	1.54	1.02
1:B:483:ALA:HB2	1:B:514:GLY:HA3	1.46	0.98
1:C:294:PHE:O	1:C:295:PHE:CD1	2.16	0.98
1:A:461:HIS:HB3	1:A:464:ILE:CD1	1.93	0.97
1:A:455:GLU:O	1:A:459:LEU:HD13	1.64	0.97
1:C:59:MET:HE3	1:C:63:LEU:HD21	1.44	0.96
1:B:223:ARG:HA	1:B:231:ILE:HD11	1.48	0.95
1:B:525:GLY:HA3	1:B:530:LEU:HB2	1.48	0.95
1:C:165:TYR:HE2	4:C:620:EDO:H11	1.34	0.92
1:B:288:VAL:HB	1:B:528:GLY:HA2	1.51	0.92
1:B:496:LYS:CD	1:B:498:ILE:CB	2.48	0.91
1:C:118:MET:HE2	1:C:146:ILE:HD11	1.52	0.89
1:C:301:ILE:HD11	1:C:330:ARG:NE	1.89	0.88
1:A:353:PRO:HG2	1:A:356:ASP:HB3	1.54	0.88
1:C:214:ASN:HD22	1:C:214:ASN:H	1.23	0.86
1:B:69:ARG:HH22	1:B:173:PRO:HG3	1.39	0.86
1:C:382:LEU:HD23	1:C:386:GLN:HB3	1.56	0.86
1:A:461:HIS:HD2	1:A:462:PRO:HD2	1.07	0.85
1:C:296:ALA:HB2	1:C:327:VAL:CG2	2.06	0.85
1:C:127:PHE:HB3	1:C:152:MET:HE2	1.57	0.84
1:B:496:LYS:HD3	1:B:498:ILE:CB	2.09	0.83
1:C:80:VAL:HG13	1:C:152:MET:HE1	1.61	0.83
1:A:494:THR:OG1	1:A:497:GLU:HG2	1.78	0.82
1:C:59:MET:HE3	1:C:63:LEU:CD2	2.09	0.81
1:A:65:GLU:HG3	1:A:176:PHE:CE1	2.15	0.81
1:B:496:LYS:HD2	1:B:498:ILE:CB	2.08	0.81
1:C:214:ASN:N	1:C:214:ASN:ND2	2.27	0.81
1:C:369:PHE:HZ	1:C:396:MET:HB2	1.46	0.81
1:A:540:ILE:HD12	1:A:541:LYS:N	1.96	0.80
1:B:237:ILE:CD1	1:B:284:SER:HB3	2.10	0.80
1:C:296:ALA:HB2	1:C:327:VAL:HG22	1.62	0.80
1:C:214:ASN:H	1:C:214:ASN:ND2	1.79	0.79
1:C:300:LEU:HD12	1:C:303:LYS:HE3	1.65	0.78
1:A:463:ASN:HD22	1:A:493:MET:HE2	1.49	0.78
1:C:115:LEU:HD13	1:C:139:VAL:HG13	1.65	0.77
1:B:69:ARG:NH2	1:B:173:PRO:HG3	1.98	0.77
1:C:270:GLU:HG3	1:C:295:PHE:HZ	1.50	0.76
1:B:483:ALA:HB1	1:B:515:GLY:O	1.86	0.75
1:B:65:GLU:HG3	1:B:176:PHE:CE1	2.21	0.74
1:C:369:PHE:CZ	1:C:396:MET:HB2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:VAL:CB	1:B:517:VAL:O	2.34	0.74
1:A:77[B]:ARG:NH1	1:A:121:SER:O	2.20	0.74
1:B:254:GLY:O	1:B:257:ILE:HG22	1.86	0.74
1:C:1:MET:HG2	1:C:3:ASP:H	1.51	0.74
1:B:115:LEU:HD13	1:B:139:VAL:HG13	1.70	0.73
1:A:503:ALA:HB2	1:A:511:LYS:HE2	1.70	0.73
1:C:391:CYS:SG	1:C:419:HIS:ND1	2.59	0.73
1:B:223:ARG:CA	1:B:231:ILE:HD11	2.17	0.72
1:C:127:PHE:C	1:C:152:MET:HE3	2.14	0.72
1:B:429:ASP:OD2	1:C:112:ARG:NH2	2.22	0.71
1:B:114:LEU:HD21	1:B:136:ILE:HD13	1.73	0.71
1:C:8:LYS:HE2	1:C:426:TRP:CZ3	2.26	0.71
1:C:127:PHE:CB	1:C:152:MET:HE2	2.20	0.71
1:C:270:GLU:HG3	1:C:295:PHE:CZ	2.25	0.71
1:C:240:VAL:HG23	6:C:767:HOH:O	1.92	0.70
1:A:529:LYS:HE3	5:A:620:SLU:O26	1.91	0.70
1:C:8:LYS:CE	1:C:426:TRP:CZ3	2.73	0.70
1:C:265:MET:HE3	1:C:272:LEU:HD23	1.74	0.70
1:A:364:LYS:NZ	1:A:429:ASP:O	2.24	0.70
1:A:493:MET:HG3	1:A:498:ILE:HG13	1.74	0.70
1:C:165:TYR:HE2	4:C:620:EDO:C1	2.05	0.70
1:B:361:ALA:HB2	1:B:433:PHE:CE1	2.28	0.69
1:C:389:GLU:OE2	1:C:419:HIS:HB3	1.92	0.69
1:C:384:VAL:HG22	1:C:426:TRP:CZ3	2.28	0.69
1:A:65:GLU:HG3	1:A:176:PHE:CZ	2.29	0.68
1:A:376:LEU:HD22	1:A:438:LEU:HD11	1.77	0.67
1:A:436:ASP:OD2	1:A:451:PRO:HD2	1.95	0.67
1:C:265:MET:HB2	6:C:767:HOH:O	1.95	0.67
1:C:339:GLY:O	5:C:621:SLU:N38	2.28	0.67
1:B:65:GLU:HG3	1:B:176:PHE:CZ	2.30	0.67
1:A:77[A]:ARG:HG3	1:A:101:ALA:HB3	1.78	0.66
1:C:301:ILE:CG1	1:C:330:ARG:HH21	2.08	0.66
1:C:118:MET:CE	1:C:146:ILE:HD11	2.23	0.66
1:C:162:GLN:HG2	1:C:166:THR:CG2	2.26	0.66
1:C:292:PHE:HE2	1:C:336:ILE:HG21	1.60	0.66
1:C:77:ARG:HG3	1:C:101:ALA:HB3	1.78	0.66
1:C:80:VAL:HG13	1:C:152:MET:CE	2.25	0.66
1:C:104:PRO:HG2	1:C:196:MET:HE1	1.76	0.66
1:B:349:ILE:HD12	1:B:350:LEU:HG	1.77	0.66
1:C:80:VAL:CG1	1:C:152:MET:HE1	2.26	0.65
1:C:294:PHE:O	1:C:294:PHE:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HH21	4:B:604:EDO:H12	1.60	0.65
1:C:165:TYR:CE2	4:C:620:EDO:H11	2.26	0.65
1:C:292:PHE:CE2	1:C:336:ILE:HG21	2.32	0.65
1:C:111:GLU:OE2	1:C:138:ASN:ND2	2.29	0.65
1:A:342:LEU:HD23	4:A:618:EDO:H22	1.80	0.64
1:B:530:LEU:HD13	1:B:531:ASP:N	2.11	0.64
1:B:483:ALA:HB2	1:B:514:GLY:CA	2.23	0.64
1:B:436:ASP:OD2	1:B:450:ALA:HB1	1.98	0.64
1:A:461:HIS:CG	1:A:464:ILE:HD12	2.32	0.64
1:B:353:PRO:HG2	1:B:356:ASP:HB3	1.80	0.64
1:A:455:GLU:O	1:A:459:LEU:CD1	2.43	0.64
1:A:79:VAL:HG23	1:A:123:PRO:HB3	1.80	0.64
1:C:278:GLN:HG3	1:C:305:ASP:O	1.98	0.63
1:C:64:ALA:HB1	1:C:98:ILE:HG23	1.80	0.63
1:C:162:GLN:HG2	1:C:166:THR:HG21	1.80	0.63
1:C:296:ALA:CB	1:C:327:VAL:HG22	2.28	0.63
1:B:349:ILE:HD13	1:B:392:VAL:HG11	1.79	0.63
1:A:118:MET:HE1	1:A:126:VAL:HG21	1.81	0.62
1:A:326:ALA:O	1:A:330:ARG:HG3	1.99	0.62
1:B:525:GLY:CA	1:B:530:LEU:HB2	2.27	0.62
1:C:194:LEU:HD22	1:C:196:MET:CE	2.30	0.62
1:C:292:PHE:CD2	1:C:319:LEU:HD11	2.35	0.62
1:C:238:LEU:HD12	1:C:263:VAL:O	2.00	0.62
1:B:289:PRO:HA	1:B:292:PHE:CD2	2.34	0.61
4:B:607:EDO:C1	5:B:611:SLU:H1	2.13	0.61
1:A:386:GLN:HA	4:A:609:EDO:H21	1.83	0.61
1:A:461:HIS:CG	1:A:462:PRO:CD	2.82	0.61
1:C:115:LEU:CD1	1:C:139:VAL:HG13	2.30	0.61
1:A:296:ALA:O	1:A:330:ARG:NH1	2.31	0.61
1:A:18:GLU:HG2	6:A:826:HOH:O	2.00	0.60
1:C:243:PHE:HZ	1:C:264:LEU:HD21	1.67	0.60
1:C:301:ILE:HD12	1:C:331:PHE:CZ	2.36	0.60
1:C:384:VAL:HG12	1:C:385:ASN:OD1	2.01	0.60
1:C:168:VAL:HG13	1:C:172:LEU:HD22	1.83	0.60
1:A:454:LEU:O	1:A:458:LEU:HG	2.02	0.60
1:A:118:MET:HE2	1:A:146:ILE:HD11	1.82	0.60
1:C:194:LEU:HD22	1:C:196:MET:HE1	1.84	0.60
1:A:461:HIS:O	4:A:616:EDO:H21	2.02	0.59
1:A:461:HIS:CB	1:A:464:ILE:CD1	2.65	0.59
1:C:194:LEU:HD13	1:C:249:MET:HG2	1.84	0.59
1:C:240:VAL:CG2	6:C:767:HOH:O	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD12	1:B:173:PRO:HD2	1.82	0.59
1:B:525:GLY:HA3	1:B:530:LEU:CB	2.28	0.59
1:C:193:ALA:HB2	1:C:212:HIS:CD2	2.37	0.59
1:C:87:GLN:HE21	4:C:620:EDO:H21	1.68	0.59
1:A:69:ARG:NH2	6:A:702:HOH:O	2.33	0.58
1:B:77:ARG:HH21	1:B:122:GLN:CB	2.16	0.58
1:C:104:PRO:CG	1:C:196:MET:HE1	2.33	0.58
1:B:77:ARG:HH21	1:B:122:GLN:HB2	1.68	0.58
1:B:278:GLN:NE2	1:B:304:TYR:HD1	2.01	0.58
1:A:177:ASN:HB2	4:A:613:EDO:H12	1.86	0.58
1:C:294:PHE:C	1:C:295:PHE:CD1	2.82	0.57
1:B:469:VAL:HG13	1:B:482:ALA:HB3	1.86	0.57
1:C:87:GLN:CG	4:C:620:EDO:H21	2.35	0.57
1:C:165:TYR:CE2	4:C:620:EDO:C1	2.84	0.57
1:C:358:LYS:HZ2	1:C:429:ASP:HB2	1.70	0.57
1:C:229:ASN:HD21	1:C:337:ARG:NH1	2.03	0.56
1:C:208:VAL:HG13	1:C:398:MET:SD	2.45	0.56
1:B:289:PRO:HA	1:B:292:PHE:HD2	1.71	0.56
1:C:292:PHE:CZ	1:C:314:SER:HB2	2.41	0.56
1:C:398:MET:HE2	1:C:411:LEU:HD23	1.88	0.56
1:A:18:GLU:OE2	1:A:223:ARG:NH2	2.38	0.56
1:B:172:LEU:CD1	1:B:173:PRO:HD2	2.36	0.56
1:C:108:ILE:O	1:C:108:ILE:HD12	2.05	0.56
4:A:611:EDO:H22	6:A:878:HOH:O	2.06	0.56
1:C:398:MET:HE1	1:C:401:TYR:CE2	2.41	0.56
1:A:376:LEU:HD22	1:A:438:LEU:CD1	2.36	0.55
1:B:489:HIS:O	1:B:489:HIS:ND1	2.40	0.55
1:B:79:VAL:HG21	1:B:118:MET:HG2	1.87	0.55
1:C:306:LEU:HD12	1:C:331:PHE:HE1	1.71	0.55
1:B:67:MET:HB3	1:B:72:LEU:HD12	1.88	0.55
5:B:611:SLU:H36	5:B:611:SLU:H212	1.89	0.55
1:A:194:LEU:HD22	1:A:249:MET:HG2	1.87	0.55
1:C:349:ILE:HD12	1:C:350:LEU:N	2.22	0.55
1:C:300:LEU:HD12	1:C:303:LYS:CE	2.37	0.55
1:C:341:GLY:C	1:C:342:LEU:HD12	2.31	0.55
1:A:290:THR:HG23	1:A:528:GLY:HA3	1.89	0.55
1:A:493:MET:HG3	1:A:498:ILE:CG1	2.36	0.54
1:C:79:VAL:HG21	1:C:118:MET:HG2	1.88	0.54
1:C:224:ASP:OD1	1:C:225:PRO:HD2	2.06	0.54
4:C:619:EDO:H12	6:C:765:HOH:O	2.07	0.54
1:C:204:LEU:HD12	1:C:205:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:PRO:HB2	1:A:534:LYS:HD3	1.88	0.54
1:B:496:LYS:HG3	1:B:498:ILE:H	1.73	0.53
1:C:358:LYS:NZ	1:C:427:ASP:OD2	2.35	0.53
1:A:224:ASP:OD1	1:A:225:PRO:HD2	2.08	0.53
1:A:524:LYS:HG2	1:A:530:LEU:HD23	1.90	0.53
1:C:33:TYR:HE1	4:C:618:EDO:H22	1.74	0.53
1:C:130:LYS:HE3	1:C:153:ASP:O	2.08	0.53
1:C:274:LEU:HD11	1:C:301:ILE:HG22	1.91	0.53
1:A:289:PRO:HB3	1:A:319:LEU:HD13	1.91	0.52
1:A:507:THR:H	1:A:510:LYS:HE3	1.73	0.52
1:C:87:GLN:HG3	4:C:620:EDO:H21	1.91	0.52
1:A:535:ILE:O	1:A:539:LEU:HG	2.09	0.52
1:C:194:LEU:CB	1:C:196:MET:HE3	2.27	0.52
1:A:289:PRO:HA	1:A:292:PHE:CD1	2.44	0.52
1:A:194:LEU:CD2	1:A:249:MET:HE3	2.39	0.52
1:C:301:ILE:HG12	1:C:330:ARG:HH21	1.75	0.52
1:A:466:ASP:HB3	1:A:486:VAL:HG12	1.92	0.52
1:C:352:THR:HG22	1:C:363:GLY:N	2.24	0.52
1:A:271:GLU:OE2	1:A:275:ARG:HG3	2.09	0.52
1:C:127:PHE:O	1:C:152:MET:HE3	2.10	0.52
1:C:162:GLN:NE2	1:C:166:THR:HG22	2.25	0.52
1:C:8:LYS:HE3	1:C:426:TRP:CZ3	2.45	0.51
1:A:120:ILE:HG21	1:A:207:GLY:HA3	1.92	0.51
1:B:313:ALA:HA	1:B:337:ARG:O	2.10	0.51
1:C:102:VAL:HB	1:C:194:LEU:HD23	1.91	0.51
1:C:79:VAL:HG23	1:C:123:PRO:HB3	1.93	0.51
1:A:466:ASP:HB3	1:A:486:VAL:CG1	2.41	0.51
1:B:265:MET:HE3	1:B:272:LEU:CD2	2.41	0.51
1:C:358:LYS:NZ	1:C:429:ASP:HB2	2.25	0.51
1:A:108:ILE:C	1:A:108:ILE:HD12	2.36	0.51
1:A:461:HIS:CG	1:A:462:PRO:HD3	2.45	0.51
1:B:65:GLU:HG2	1:B:181:PHE:CE1	2.46	0.50
1:B:339:GLY:HA3	5:B:611:SLU:C5	2.41	0.50
1:A:46:HIS:CE1	1:A:272:LEU:HD21	2.46	0.50
1:A:89:PHE:CE2	1:A:252:THR:HG21	2.45	0.50
1:B:62:ARG:HB3	1:B:168:VAL:HG11	1.93	0.50
1:C:79:VAL:CG2	1:C:123:PRO:HG3	2.40	0.50
1:C:391:CYS:HA	1:C:418:LEU:O	2.11	0.50
1:C:8:LYS:HE3	1:C:426:TRP:CE3	2.46	0.50
1:C:33:TYR:CE1	4:C:618:EDO:H22	2.47	0.50
1:B:172:LEU:HG	1:B:173:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:HIS:CD2	1:A:462:PRO:HD3	2.43	0.49
1:B:118:MET:HE2	1:B:146:ILE:HD11	1.93	0.49
1:C:8:LYS:HE2	1:C:426:TRP:CH2	2.46	0.49
1:B:34:ALA:HB1	1:B:54:ALA:HA	1.94	0.49
1:C:9:LYS:HG2	1:C:370:GLU:HG2	1.94	0.49
1:A:230:GLN:O	1:A:232:ILE:HD12	2.13	0.49
1:C:296:ALA:CB	1:C:327:VAL:CG2	2.85	0.49
1:B:388:GLY:O	1:B:423:ILE:HA	2.13	0.49
1:C:20:GLY:H	4:C:605:EDO:H11	1.76	0.49
1:A:466:ASP:OD2	1:A:524:LYS:HE3	2.12	0.49
1:A:523:PRO:CB	1:A:534:LYS:HD3	2.43	0.49
1:B:137:LEU:HD21	1:B:161:PHE:CZ	2.48	0.49
1:B:223:ARG:CB	1:B:231:ILE:HD11	2.43	0.49
1:C:79:VAL:HG23	1:C:123:PRO:HG3	1.95	0.49
1:C:192:ILE:HA	1:C:211:PRO:HA	1.95	0.49
1:C:384:VAL:HG22	1:C:426:TRP:CH2	2.47	0.49
1:B:361:ALA:HB2	1:B:433:PHE:HE1	1.73	0.49
1:C:372:LYS:HE2	1:C:417:TRP:CD2	2.48	0.49
1:A:493:MET:CG	1:A:498:ILE:CG1	2.91	0.49
1:B:288:VAL:HB	1:B:528:GLY:CA	2.35	0.49
1:C:87:GLN:HE21	4:C:620:EDO:C2	2.26	0.49
1:C:417:TRP:NE1	2:C:602:SO4:O3	2.41	0.49
1:A:343:THR:N	5:A:620:SLU:H40	2.11	0.48
1:B:179:TYR:HB3	4:B:608:EDO:H22	1.95	0.48
1:A:507:THR:OG1	1:A:510:LYS:HE2	2.14	0.48
1:C:276:THR:HG23	1:C:280:TYR:CD2	2.48	0.48
1:A:230:GLN:HB3	1:A:232:ILE:HD11	1.95	0.48
1:C:345:THR:O	1:C:346:THR:HB	2.12	0.48
1:A:461:HIS:NE2	1:A:493:MET:CE	2.76	0.48
1:C:349:ILE:O	1:C:366:VAL:HG13	2.13	0.48
1:A:44:ASP:OD2	1:A:47:ILE:HG12	2.14	0.48
1:B:69:ARG:HH12	1:B:173:PRO:HB3	1.79	0.48
1:B:79:VAL:HG23	1:B:123:PRO:HB3	1.95	0.48
1:B:436:ASP:OD2	1:B:451:PRO:HD2	2.13	0.47
1:B:499:VAL:C	1:B:501:TYR:H	2.22	0.47
1:A:83:GLU:OE1	1:A:131:LYS:HE3	2.14	0.47
1:A:194:LEU:HD21	1:A:249:MET:SD	2.53	0.47
1:B:441:LEU:CD2	1:B:450:ALA:HA	2.43	0.47
1:A:230:GLN:C	1:A:232:ILE:HD12	2.39	0.47
1:B:77:ARG:HG3	1:B:101:ALA:HB3	1.94	0.47
1:C:424:ALA:HA	1:C:435:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:HG2	1:A:181:PHE:CE1	2.50	0.47
1:A:20:GLY:N	3:A:602:DYD:O07	2.45	0.47
1:A:131:LYS:NZ	6:A:703:HOH:O	2.35	0.47
1:C:289:PRO:HB3	1:C:319:LEU:HD13	1.97	0.47
1:C:289:PRO:HG3	1:C:317:ALA:HB3	1.97	0.47
1:A:271:GLU:OE2	1:A:304:TYR:OH	2.32	0.47
1:A:461:HIS:NE2	1:A:493:MET:HE1	2.29	0.47
1:B:480:LEU:H	1:B:481:PRO:HD2	1.79	0.47
1:C:292:PHE:CE2	1:C:314:SER:HB2	2.49	0.47
1:C:349:ILE:HD12	1:C:349:ILE:C	2.39	0.47
1:A:337:ARG:HG3	1:A:352:THR:OG1	2.14	0.47
1:B:489:HIS:ND1	1:B:489:HIS:C	2.72	0.47
1:C:157:ASP:OD1	1:C:162:GLN:HA	2.15	0.47
1:C:292:PHE:HD2	1:C:319:LEU:HD11	1.78	0.47
1:A:349:ILE:HD13	1:A:392:VAL:HG11	1.97	0.47
1:B:432:PHE:C	1:B:433:PHE:HD1	2.22	0.47
1:C:154:SER:OG	1:C:156:THR:O	2.28	0.47
1:B:426:TRP:HA	1:B:431:HIS:O	2.15	0.46
1:C:162:GLN:HG2	1:C:166:THR:HG22	1.98	0.46
1:A:429:ASP:O	1:A:430:GLU:HB2	2.14	0.46
1:B:172:LEU:CG	1:B:173:PRO:HD2	2.46	0.46
1:C:287:LEU:O	1:C:314:SER:HA	2.15	0.46
1:A:290:THR:CG2	1:A:528:GLY:HA3	2.45	0.46
1:B:194:LEU:HD22	1:B:249:MET:HG2	1.97	0.46
1:B:278:GLN:HG3	1:B:305:ASP:O	2.15	0.46
1:B:41:ALA:HA	1:B:53:TYR:CE2	2.51	0.46
1:A:444:TYR:CE1	1:A:513:ARG:HD3	2.51	0.46
4:A:612:EDO:H11	6:A:866:HOH:O	2.16	0.46
1:B:289:PRO:HD2	1:B:528:GLY:HA2	1.98	0.46
1:A:8:LYS:CD	1:A:430:GLU:HG2	2.46	0.46
1:B:237:ILE:HA	1:B:284:SER:O	2.15	0.46
1:C:89:PHE:CE2	1:C:252:THR:HG21	2.51	0.46
1:C:423:ILE:O	1:C:435:VAL:HB	2.15	0.46
1:C:104:PRO:CD	1:C:196:MET:HE1	2.46	0.45
1:C:59:MET:O	1:C:63:LEU:HD23	2.17	0.45
1:C:74:THR:HG22	1:C:99:GLY:O	2.17	0.45
1:C:106:ASN:OD1	1:C:108:ILE:HG13	2.17	0.45
1:C:289:PRO:CG	1:C:317:ALA:HB3	2.46	0.45
1:C:294:PHE:C	1:C:295:PHE:HD1	2.14	0.45
1:B:223:ARG:HG2	1:B:231:ILE:CD1	2.46	0.45
1:B:527:THR:HG23	1:B:527:THR:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:O	1:C:302:ASP:HB2	2.16	0.45
1:A:482:ALA:HB2	1:A:514:GLY:HA3	1.99	0.45
1:A:114:LEU:HD21	1:A:136:ILE:HD13	1.99	0.45
1:B:194:LEU:CD2	1:B:249:MET:HE3	2.47	0.45
1:B:236:ALA:O	1:B:237:ILE:HD13	2.16	0.45
1:C:243:PHE:HZ	1:C:264:LEU:CD2	2.27	0.45
1:C:351:ILE:C	1:C:363:GLY:HA3	2.42	0.45
1:C:194:LEU:HD22	1:C:196:MET:HE3	1.99	0.45
1:B:52:THR:HB	6:B:710:HOH:O	2.17	0.45
1:C:323:VAL:O	1:C:327:VAL:HG23	2.17	0.45
1:C:98:ILE:HG13	1:C:100:VAL:HG23	1.97	0.44
1:B:224:ASP:OD1	1:B:225:PRO:HD2	2.17	0.44
1:A:188:ARG:HG2	3:A:602:DYD:C03	2.46	0.44
1:C:296:ALA:HB2	1:C:327:VAL:HG23	1.93	0.44
1:C:371:ALA:HB1	1:C:432:PHE:HE2	1.83	0.44
1:B:88:PHE:HA	1:B:152:MET:HE1	1.99	0.44
1:C:79:VAL:HG23	1:C:123:PRO:CB	2.47	0.44
1:C:104:PRO:CD	1:C:196:MET:CE	2.96	0.44
1:C:204:LEU:HG	1:C:205:PRO:HD2	1.99	0.44
1:A:65:GLU:HG2	1:A:181:PHE:CD1	2.52	0.44
1:B:398:MET:HE1	1:B:401:TYR:CE2	2.53	0.44
1:C:429:ASP:O	1:C:430:GLU:HB2	2.17	0.44
1:C:308:ASN:HB2	6:C:733:HOH:O	2.18	0.44
1:A:34:ALA:HB1	1:A:54:ALA:HA	1.98	0.44
1:A:451:PRO:O	1:A:455:GLU:HG3	2.17	0.44
1:C:127:PHE:HB3	1:C:152:MET:CE	2.39	0.44
1:C:421:GLY:O	1:C:438:LEU:HB2	2.18	0.44
1:A:324:GLY:HA3	4:A:607:EDO:H11	2.00	0.43
1:A:20:GLY:CA	3:A:602:DYD:O07	2.66	0.43
1:C:351:ILE:O	1:C:353:PRO:HD3	2.19	0.43
1:C:211:PRO:HG2	1:C:214:ASN:HD21	1.83	0.43
1:B:429:ASP:O	1:B:430:GLU:HB2	2.18	0.43
1:C:295:PHE:HB3	6:C:720:HOH:O	2.18	0.43
1:A:11:PRO:HD3	6:A:744:HOH:O	2.18	0.43
1:A:308:ASN:HB2	6:A:787:HOH:O	2.17	0.43
1:A:356:ASP:OD2	1:A:364:LYS:HE2	2.17	0.43
1:C:204:LEU:HD12	1:C:205:PRO:CD	2.48	0.43
1:A:461:HIS:HA	1:A:462:PRO:HD3	1.28	0.43
1:A:493:MET:SD	1:A:497:GLU:HG3	2.58	0.43
1:B:65:GLU:O	1:B:69:ARG:HG2	2.18	0.43
1:C:68:LYS:HE3	6:C:768:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLN:NE2	1:C:170:SER:OG	2.47	0.43
1:A:444:TYR:OH	1:A:513:ARG:CD	2.66	0.43
1:A:461:HIS:HD2	1:A:463:ASN:H	1.67	0.43
1:A:118:MET:HE3	1:A:123:PRO:HG3	2.01	0.43
1:A:486:VAL:HG13	1:A:486:VAL:O	2.19	0.43
1:C:8:LYS:HD2	1:C:430:GLU:OE2	2.19	0.43
1:B:489:HIS:O	1:B:489:HIS:CG	2.71	0.43
1:C:287:LEU:HD12	1:C:312:ILE:HG23	2.01	0.43
1:C:293:SER:N	1:C:323:VAL:HG11	2.33	0.43
1:B:317:ALA:CB	1:B:529:LYS:H	2.32	0.43
1:A:426:TRP:HA	1:A:431:HIS:O	2.19	0.42
1:A:435:VAL:O	1:A:436:ASP:HB2	2.17	0.42
1:A:487:LEU:HD21	1:A:493:MET:HB3	2.01	0.42
1:B:347:SER:HA	5:B:611:SLU:S12	2.58	0.42
1:C:292:PHE:HB3	1:C:323:VAL:HG12	2.00	0.42
1:B:74:THR:HA	1:B:99:GLY:O	2.18	0.42
1:C:118:MET:CE	1:C:146:ILE:CD1	2.96	0.42
1:C:233:PRO:O	1:C:234:ASP:HB2	2.19	0.42
1:C:301:ILE:HD12	1:C:331:PHE:HZ	1.83	0.42
1:B:273:PHE:CE2	1:B:277:LEU:HD11	2.54	0.42
1:C:320:SER:HB3	1:C:323:VAL:HB	2.01	0.42
1:B:186:PHE:CE2	1:B:191:THR:HG21	2.54	0.42
1:C:229:ASN:ND2	1:C:337:ARG:HH12	2.16	0.42
1:C:340:TYR:HB3	1:C:350:LEU:HB2	2.01	0.42
1:A:9:LYS:HG2	1:A:370:GLU:HG2	2.01	0.42
1:B:323:VAL:O	1:B:327:VAL:HG23	2.20	0.42
1:B:62:ARG:NE	1:B:178:GLU:OE2	2.49	0.42
1:C:309:LEU:HD21	1:C:312:ILE:HD11	2.02	0.42
1:B:376:LEU:HD13	6:B:730:HOH:O	2.19	0.42
1:C:243:PHE:CZ	1:C:264:LEU:HD21	2.51	0.42
1:A:8:LYS:HD3	1:A:430:GLU:HG2	2.01	0.42
1:A:237:ILE:HD12	1:A:284:SER:HB3	2.01	0.41
1:C:428:GLU:OE1	1:C:428:GLU:N	2.50	0.41
1:B:89:PHE:CE2	1:B:252:THR:HG21	2.56	0.41
1:C:243:PHE:CZ	1:C:264:LEU:CD2	3.02	0.41
1:C:294:PHE:HD2	1:C:294:PHE:C	2.28	0.41
1:A:61:VAL:HG13	1:A:181:PHE:CG	2.55	0.41
1:B:153:ASP:OD1	1:B:153:ASP:N	2.48	0.41
1:C:79:VAL:HA	1:C:103:ALA:O	2.21	0.41
1:B:292:PHE:O	1:B:296:ALA:N	2.53	0.41
1:C:294:PHE:C	1:C:294:PHE:CD2	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ALA:HB2	1:C:336:ILE:CD1	2.50	0.41
1:A:265:MET:HE3	1:A:272:LEU:HG	2.03	0.41
1:A:349:ILE:HG21	1:A:369:PHE:CE1	2.56	0.41
1:B:266:TYR:CD1	1:B:266:TYR:N	2.88	0.41
1:C:40:ILE:HA	1:C:52:THR:HA	2.01	0.41
1:A:95:ALA:HB3	1:A:102:VAL:CG2	2.51	0.41
1:C:1:MET:HG2	1:C:3:ASP:N	2.27	0.41
1:C:77:ARG:HD2	4:C:610:EDO:H22	2.03	0.41
1:C:154:SER:O	1:C:163:SER:HB2	2.21	0.41
1:B:223:ARG:HG2	1:B:231:ILE:HD11	2.02	0.41
1:B:29:ALA:O	1:B:33:TYR:CD2	2.74	0.41
1:A:108:ILE:HD12	1:A:108:ILE:O	2.21	0.40
1:B:8:LYS:HE2	1:B:8:LYS:HA	2.02	0.40
1:B:265:MET:HE3	1:B:272:LEU:HD23	2.03	0.40
1:A:384:VAL:HG22	1:A:385:ASN:OD1	2.21	0.40
1:B:349:ILE:CD1	1:B:392:VAL:HG11	2.50	0.40
1:C:168:VAL:O	1:C:172:LEU:HB2	2.22	0.40
1:C:195:ILE:HA	1:C:208:VAL:O	2.21	0.40
1:C:274:LEU:CD1	1:C:301:ILE:HG22	2.49	0.40
1:A:502:VAL:O	1:A:506:VAL:HG22	2.22	0.40
1:B:61:VAL:HG13	1:B:181:PHE:CG	2.56	0.40
1:B:154:SER:O	1:B:163:SER:HB2	2.22	0.40
1:B:265:MET:CE	1:B:272:LEU:HG	2.52	0.40
1:B:413:ASP:OD1	1:B:413:ASP:C	2.64	0.40
1:C:157:ASP:OD1	1:C:166:THR:HG21	2.21	0.40
1:B:238:LEU:HD23	1:B:277:LEU:HD21	2.04	0.40
1:B:338:GLN:NE2	6:B:712:HOH:O	2.55	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	543/555 (98%)	532 (98%)	11 (2%)	0	100	100
1	B	498/555 (90%)	475 (95%)	22 (4%)	1 (0%)	43	64
1	C	434/555 (78%)	414 (95%)	20 (5%)	0	100	100
All	All	1475/1665 (89%)	1421 (96%)	53 (4%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	506	VAL

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	441/467 (94%)	441 (100%)	0	100	100
1	B	370/467 (79%)	370 (100%)	0	100	100
1	C	352/467 (75%)	351 (100%)	1 (0%)	86	93
All	All	1163/1401 (83%)	1162 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	147	GLN
1	A	308	ASN
1	A	431	HIS
1	A	461	HIS
1	A	463	ASN

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Mol	Chain	Res	Type
1	A	489	HIS
1	B	162	GLN
1	B	244	HIS
1	C	46	HIS
1	C	76	HIS
1	C	87	GLN
1	C	134	GLN
1	C	212	HIS
1	C	214	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

52 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	$\# Z > 2$
4	EDO	A	613	-	3,3,3	0.17	0	2,2,2	0.81	0
4	EDO	C	611	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	C	617	-	3,3,3	0.12	0	2,2,2	0.73	0
4	EDO	C	610	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	B	606	-	3,3,3	0.45	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	604	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	C	614	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	C	620	-	3,3,3	0.37	0	2,2,2	0.32	0
4	EDO	A	607	-	3,3,3	0.47	0	2,2,2	0.27	0
4	EDO	A	616	-	3,3,3	0.26	0	2,2,2	0.43	0
4	EDO	A	610	-	3,3,3	0.28	0	2,2,2	0.68	0
4	EDO	A	609	-	3,3,3	0.31	0	2,2,2	0.49	0
4	EDO	C	605	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	B	607	-	3,3,3	0.13	0	2,2,2	0.38	0
4	EDO	C	619	-	3,3,3	0.41	0	2,2,2	0.83	0
4	EDO	B	610	-	3,3,3	0.19	0	2,2,2	0.70	0
4	EDO	B	605	-	3,3,3	0.44	0	2,2,2	0.31	0
3	DYD	C	603	-	7,7,7	0.44	0	8,8,8	1.89	2 (25%)
4	EDO	A	608	-	3,3,3	0.25	0	2,2,2	0.44	0
5	SLU	A	620	-	45,45,45	5.36	27 (60%)	64,68,68	6.53	32 (50%)
4	EDO	C	618	-	3,3,3	0.30	0	2,2,2	0.44	0
3	DYD	A	603	-	7,7,7	0.50	0	8,8,8	1.62	1 (12%)
4	EDO	C	613	-	3,3,3	0.46	0	2,2,2	0.22	0
4	EDO	C	607	-	3,3,3	0.43	0	2,2,2	0.35	0
2	SO4	A	601	-	4,4,4	0.29	0	6,6,6	0.17	0
4	EDO	A	619	-	3,3,3	0.29	0	2,2,2	0.63	0
5	SLU	C	621	-	45,45,45	5.34	25 (55%)	64,68,68	4.49	24 (37%)
4	EDO	A	611	-	3,3,3	0.27	0	2,2,2	0.87	0
4	EDO	C	616	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	A	618	-	3,3,3	0.36	0	2,2,2	0.56	0
2	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.06	0
4	EDO	A	606	-	3,3,3	0.50	0	2,2,2	0.17	0
5	SLU	B	611	-	45,45,45	2.25	13 (28%)	64,68,68	3.70	26 (40%)
4	EDO	C	609	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	C	612	-	3,3,3	0.43	0	2,2,2	0.29	0
2	SO4	C	601	-	4,4,4	0.27	0	6,6,6	0.07	0
4	EDO	C	608	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	A	615	-	3,3,3	0.15	0	2,2,2	0.26	0
2	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.06	0
4	EDO	A	614	-	3,3,3	0.36	0	2,2,2	0.34	0
4	EDO	B	609	-	3,3,3	0.21	0	2,2,2	0.50	0
2	SO4	C	602	-	4,4,4	0.26	0	6,6,6	0.09	0
4	EDO	A	617	-	3,3,3	0.19	0	2,2,2	0.47	0
2	SO4	B	601	-	4,4,4	0.24	0	6,6,6	0.13	0
3	DYD	A	602	-	7,7,7	0.42	0	8,8,8	1.87	2 (25%)
3	DYD	C	604	-	7,7,7	0.44	0	8,8,8	1.57	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	608	-	3,3,3	0.30	0	2,2,2	0.50	0
4	EDO	A	612	-	3,3,3	0.32	0	2,2,2	0.65	0
4	EDO	A	605	-	3,3,3	0.39	0	2,2,2	0.46	0
4	EDO	C	615	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	A	604	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	C	606	-	3,3,3	0.46	0	2,2,2	0.28	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
4	EDO	A	613	-	-	0/1/1/1	-
4	EDO	C	611	-	-	0/1/1/1	-
4	EDO	C	617	-	-	0/1/1/1	-
4	EDO	C	610	-	-	1/1/1/1	-
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	B	604	-	-	1/1/1/1	-
4	EDO	C	614	-	-	1/1/1/1	-
4	EDO	C	620	-	-	0/1/1/1	-
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	A	616	-	-	1/1/1/1	-
4	EDO	A	610	-	-	0/1/1/1	-
4	EDO	A	609	-	-	1/1/1/1	-
4	EDO	C	605	-	-	0/1/1/1	-
4	EDO	B	607	-	-	0/1/1/1	-
4	EDO	C	619	-	-	0/1/1/1	-
4	EDO	B	610	-	-	0/1/1/1	-
4	EDO	B	605	-	-	0/1/1/1	-
3	DYD	C	603	-	-	2/5/5/5	-
4	EDO	A	608	-	-	1/1/1/1	-
5	SLU	A	620	-	-	8/22/39/39	0/6/6/6
4	EDO	C	618	-	-	0/1/1/1	-
3	DYD	A	603	-	-	1/5/5/5	-
4	EDO	C	613	-	-	1/1/1/1	-
4	EDO	C	607	-	-	0/1/1/1	-
4	EDO	A	619	-	-	0/1/1/1	-
5	SLU	C	621	-	-	4/22/39/39	0/6/6/6
4	EDO	A	611	-	-	0/1/1/1	-
4	EDO	C	616	-	-	0/1/1/1	-
4	EDO	A	618	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	606	-	-	0/1/1/1	-
5	SLU	B	611	-	-	7/22/39/39	0/6/6/6
4	EDO	C	609	-	-	0/1/1/1	-
4	EDO	C	612	-	-	0/1/1/1	-
4	EDO	C	608	-	-	0/1/1/1	-
4	EDO	A	615	-	-	1/1/1/1	-
4	EDO	A	614	-	-	0/1/1/1	-
4	EDO	B	609	-	-	1/1/1/1	-
4	EDO	A	617	-	-	1/1/1/1	-
3	DYD	C	604	-	-	1/5/5/5	-
3	DYD	A	602	-	-	2/5/5/5	-
4	EDO	B	608	-	-	0/1/1/1	-
4	EDO	A	612	-	-	1/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	C	615	-	-	1/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	C	606	-	-	1/1/1/1	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	620	SLU	C8-S9	-19.55	1.48	1.75
5	C	621	SLU	C8-S9	-17.57	1.51	1.75
5	C	621	SLU	C11-S12	-16.16	1.46	1.73
5	C	621	SLU	C4-S9	-14.97	1.44	1.74
5	A	620	SLU	C11-S12	-14.12	1.49	1.73
5	A	620	SLU	C4-S9	-13.72	1.47	1.74
5	A	620	SLU	C13-S12	-11.72	1.43	1.71
5	B	611	SLU	C16-N40	7.49	1.47	1.38
5	C	621	SLU	C14-C16	-7.21	1.35	1.48
5	C	621	SLU	C13-S12	-7.12	1.54	1.71
5	C	621	SLU	O20-S17	-6.96	1.45	1.60
5	C	621	SLU	C8-C11	-6.64	1.34	1.46
5	A	620	SLU	C3-N7	6.43	1.52	1.39
5	A	620	SLU	O19-S17	-5.55	1.37	1.42
5	C	621	SLU	C33-N37	-5.41	1.29	1.39
5	C	621	SLU	C3-C4	-5.10	1.32	1.40
5	A	620	SLU	C36-N35	-5.04	1.29	1.37
5	C	621	SLU	C2-C3	-4.91	1.32	1.40
5	A	620	SLU	O39-C16	-4.83	1.14	1.23
5	C	621	SLU	C33-C32	-4.82	1.30	1.39
5	A	620	SLU	S17-N40	4.75	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	621	SLU	S17-N40	-4.73	1.51	1.59
5	A	620	SLU	C33-C32	-4.65	1.30	1.39
5	A	620	SLU	C14-N15	4.64	1.48	1.38
5	C	621	SLU	C36-N35	-4.56	1.29	1.37
5	A	620	SLU	O18-S17	-4.45	1.38	1.42
5	B	611	SLU	C34-N38	4.39	1.45	1.34
5	B	611	SLU	C8-C11	-4.37	1.38	1.46
5	C	621	SLU	C3-N7	-4.36	1.31	1.39
5	A	620	SLU	O27-C23	-4.35	1.32	1.43
5	C	621	SLU	C16-N40	-4.34	1.34	1.38
5	B	611	SLU	O20-S17	-4.31	1.51	1.60
5	C	621	SLU	C5-C4	-4.30	1.32	1.39
5	B	611	SLU	C3-N7	-4.27	1.31	1.39
5	A	620	SLU	C24-C25	-4.25	1.40	1.53
5	A	620	SLU	C8-C11	-4.19	1.39	1.46
5	C	621	SLU	C33-C34	-3.67	1.30	1.41
5	A	620	SLU	C32-N35	-3.64	1.30	1.37
5	C	621	SLU	C32-N35	-3.57	1.30	1.37
5	A	620	SLU	C33-N37	-3.52	1.32	1.39
5	B	611	SLU	C14-N15	-3.43	1.31	1.38
5	B	611	SLU	S17-N40	3.36	1.65	1.59
5	A	620	SLU	C2-C3	-3.26	1.34	1.40
5	B	611	SLU	C33-N37	-3.11	1.33	1.39
5	B	611	SLU	O19-S17	2.93	1.45	1.42
5	A	620	SLU	C5-C4	-2.91	1.34	1.39
5	A	620	SLU	C13-C14	2.85	1.41	1.36
5	C	621	SLU	C14-N15	-2.74	1.32	1.38
5	A	620	SLU	O20-C21	-2.72	1.36	1.46
5	C	621	SLU	O18-S17	2.63	1.44	1.42
5	A	620	SLU	C34-N29	-2.60	1.28	1.35
5	A	620	SLU	C24-C23	-2.59	1.46	1.53
5	A	620	SLU	C8-N7	2.49	1.37	1.30
5	C	621	SLU	C24-C25	-2.48	1.45	1.53
5	A	620	SLU	C5-C6	-2.42	1.35	1.39
5	C	621	SLU	C23-C22	-2.40	1.46	1.53
5	A	620	SLU	C16-N40	2.40	1.41	1.38
5	B	611	SLU	C24-C23	-2.34	1.47	1.53
5	C	621	SLU	O26-C22	-2.20	1.40	1.45
5	B	611	SLU	C23-C22	-2.18	1.47	1.53
5	C	621	SLU	C30-N31	2.18	1.37	1.33
5	C	621	SLU	C24-C23	-2.10	1.47	1.53
5	B	611	SLU	O18-S17	2.06	1.44	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	611	SLU	O28-C24	-2.05	1.37	1.43
5	A	620	SLU	C23-C22	-2.00	1.47	1.53

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	620	SLU	C13-S12-C11	25.77	109.60	89.21
5	A	620	SLU	C4-S9-C8	24.07	104.86	88.92
5	C	621	SLU	C4-S9-C8	20.11	102.24	88.92
5	A	620	SLU	O19-S17-O18	-18.84	92.63	120.85
5	A	620	SLU	C11-C8-S9	18.42	136.00	119.98
5	C	621	SLU	C11-C8-S9	13.53	131.75	119.98
5	C	621	SLU	C13-S12-C11	13.12	99.59	89.21
5	B	611	SLU	O19-S17-O18	-12.86	101.59	120.85
5	C	621	SLU	O19-S17-O18	-12.37	102.32	120.85
5	A	620	SLU	C8-C11-S12	10.94	137.41	121.14
5	B	611	SLU	C4-S9-C8	10.40	95.81	88.92
5	A	620	SLU	C11-C8-N7	-9.50	112.62	123.35
5	B	611	SLU	S9-C8-N7	-9.05	104.60	116.17
5	B	611	SLU	C13-S12-C11	8.16	95.67	89.21
5	C	621	SLU	S9-C8-N7	-8.05	105.88	116.17
5	A	620	SLU	C25-N35-C36	-7.79	109.80	127.09
5	B	611	SLU	S12-C11-N15	-7.26	105.25	114.49
5	A	620	SLU	C8-C11-N15	-7.18	114.50	123.51
5	C	621	SLU	N29-C30-N31	-6.93	118.10	128.58
5	B	611	SLU	C14-C13-S12	-6.86	102.31	110.24
5	B	611	SLU	C11-C8-N7	6.27	130.43	123.35
5	A	620	SLU	O20-S17-N40	6.03	121.30	105.69
5	A	620	SLU	N29-C30-N31	-5.88	119.68	128.58
5	B	611	SLU	C11-C8-S9	5.73	124.96	119.98
5	B	611	SLU	C8-C11-S12	5.61	129.49	121.14
5	B	611	SLU	C33-C32-N31	-5.34	119.37	126.72
5	A	620	SLU	C32-N35-C25	5.27	138.96	126.63
5	C	621	SLU	C33-C32-N31	-5.26	119.47	126.72
5	A	620	SLU	C14-C13-S12	-5.25	104.18	110.24
5	A	620	SLU	C32-N35-C36	5.24	111.24	105.74
5	A	620	SLU	S12-C11-N15	-5.10	107.99	114.49
5	B	611	SLU	C3-N7-C8	5.02	121.04	109.84
5	C	621	SLU	C21-O20-S17	4.95	127.35	116.97
5	A	620	SLU	N35-C36-N37	-4.87	107.02	113.94
5	A	620	SLU	C33-C32-N31	-4.86	120.03	126.72
5	A	620	SLU	O20-C21-C22	-4.71	99.17	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	611	SLU	C3-C4-S9	-4.58	102.97	109.75
5	A	620	SLU	N31-C32-N35	4.40	134.65	127.17
5	A	620	SLU	C21-O20-S17	4.28	125.96	116.97
5	A	620	SLU	C5-C4-C3	-4.25	118.83	121.99
5	B	611	SLU	C14-N15-C11	4.14	117.21	110.10
5	B	611	SLU	N29-C30-N31	-4.08	122.40	128.58
3	A	603	DYD	C03-C04-C05	-4.07	107.47	113.10
3	A	602	DYD	C04-C03-C02	-4.07	107.48	113.10
3	C	603	DYD	C03-C04-C05	-4.06	107.49	113.10
5	B	611	SLU	C33-N37-C36	4.02	109.78	103.45
5	C	621	SLU	S12-C11-N15	-4.02	109.38	114.49
5	A	620	SLU	C4-C3-N7	-4.01	108.21	115.20
5	C	621	SLU	C13-C14-N15	-4.00	109.93	115.43
5	A	620	SLU	S9-C8-N7	-3.94	111.14	116.17
5	C	621	SLU	O20-S17-N40	3.91	115.82	105.69
5	B	611	SLU	N31-C32-N35	3.89	133.78	127.17
3	C	604	DYD	C03-C04-C05	-3.88	107.73	113.10
5	A	620	SLU	C21-C22-C23	-3.86	101.30	115.21
5	A	620	SLU	C13-C14-C16	3.67	130.02	123.92
5	B	611	SLU	C32-C33-N37	-3.60	106.46	110.58
5	C	621	SLU	C30-N31-C32	3.53	120.46	111.83
5	A	620	SLU	C30-N31-C32	3.52	120.42	111.83
5	B	611	SLU	C30-N31-C32	3.49	120.35	111.83
5	B	611	SLU	C5-C4-S9	3.46	134.72	126.07
5	C	621	SLU	C34-C33-C32	3.46	121.90	117.18
3	C	603	DYD	C04-C03-C02	-3.45	108.33	113.10
5	C	621	SLU	C33-C34-N38	-3.31	115.08	123.29
3	A	602	DYD	C03-C04-C05	-3.22	108.64	113.10
5	C	621	SLU	N31-C32-N35	3.21	132.62	127.17
5	A	620	SLU	O26-C25-N35	3.15	114.14	108.09
5	C	621	SLU	N35-C36-N37	-3.13	109.50	113.94
5	A	620	SLU	O10-C6-C1	-3.02	111.59	120.00
5	B	611	SLU	C13-C14-N15	2.99	119.55	115.43
5	A	620	SLU	C13-C14-N15	-2.91	111.43	115.43
5	B	611	SLU	O20-S17-O19	2.88	114.21	105.48
5	A	620	SLU	O26-C22-C23	-2.86	99.48	105.15
5	A	620	SLU	C33-N37-C36	2.81	107.87	103.45
5	A	620	SLU	O10-C6-C5	2.81	127.19	119.85
5	B	611	SLU	N35-C36-N37	-2.76	110.02	113.94
5	B	611	SLU	O20-S17-N40	2.48	112.11	105.69
5	C	621	SLU	C5-C4-S9	2.45	132.19	126.07
5	C	621	SLU	C8-C11-N15	2.40	126.52	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	611	SLU	O26-C22-C23	2.39	109.91	105.15
5	C	621	SLU	C33-N37-C36	2.38	107.19	103.45
5	C	621	SLU	C1-C6-C5	-2.35	117.61	120.19
5	C	621	SLU	C6-C5-C4	2.32	121.81	118.60
5	B	611	SLU	C13-C14-C16	-2.29	120.11	123.92
5	C	621	SLU	C5-C4-C3	-2.23	120.33	121.99
5	A	620	SLU	C5-C4-S9	2.20	131.57	126.07
5	C	621	SLU	C25-N35-C36	-2.16	122.29	127.09
5	B	611	SLU	C2-C3-C4	-2.06	116.64	119.59
5	C	621	SLU	N38-C34-N29	2.05	122.95	118.38

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	DYD	C03-C04-C05-C06
3	A	602	DYD	C03-C04-C05-O07
5	A	620	SLU	C13-C14-C16-O39
5	A	620	SLU	C13-C14-C16-N40
5	A	620	SLU	C21-O20-S17-N40
5	B	611	SLU	C13-C14-C16-O39
5	B	611	SLU	C13-C14-C16-N40
5	B	611	SLU	C16-N40-S17-O18
5	C	621	SLU	C13-C14-C16-O39
5	C	621	SLU	C13-C14-C16-N40
5	A	620	SLU	N15-C14-C16-N40
4	B	604	EDO	O1-C1-C2-O2
5	A	620	SLU	N15-C14-C16-O39
5	A	620	SLU	C21-O20-S17-O18
5	A	620	SLU	C21-O20-S17-O19
3	C	603	DYD	C01-C02-C03-C04
4	A	607	EDO	O1-C1-C2-O2
4	A	609	EDO	O1-C1-C2-O2
4	A	612	EDO	O1-C1-C2-O2
4	A	618	EDO	O1-C1-C2-O2
5	B	611	SLU	N15-C14-C16-O39
5	B	611	SLU	N15-C14-C16-N40
5	C	621	SLU	N15-C14-C16-O39
5	C	621	SLU	N15-C14-C16-N40
4	B	609	EDO	O1-C1-C2-O2
5	B	611	SLU	C21-O20-S17-N40
3	C	603	DYD	O08-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
4	A	617	EDO	O1-C1-C2-O2
4	C	606	EDO	O1-C1-C2-O2
3	A	603	DYD	O08-C02-C03-C04
4	A	615	EDO	O1-C1-C2-O2
4	A	616	EDO	O1-C1-C2-O2
5	B	611	SLU	C21-O20-S17-O19
4	A	608	EDO	O1-C1-C2-O2
4	C	615	EDO	O1-C1-C2-O2
3	C	604	DYD	C02-C03-C04-C05
4	C	613	EDO	O1-C1-C2-O2
4	C	614	EDO	O1-C1-C2-O2
5	A	620	SLU	O20-C21-C22-O26
4	C	610	EDO	O1-C1-C2-O2

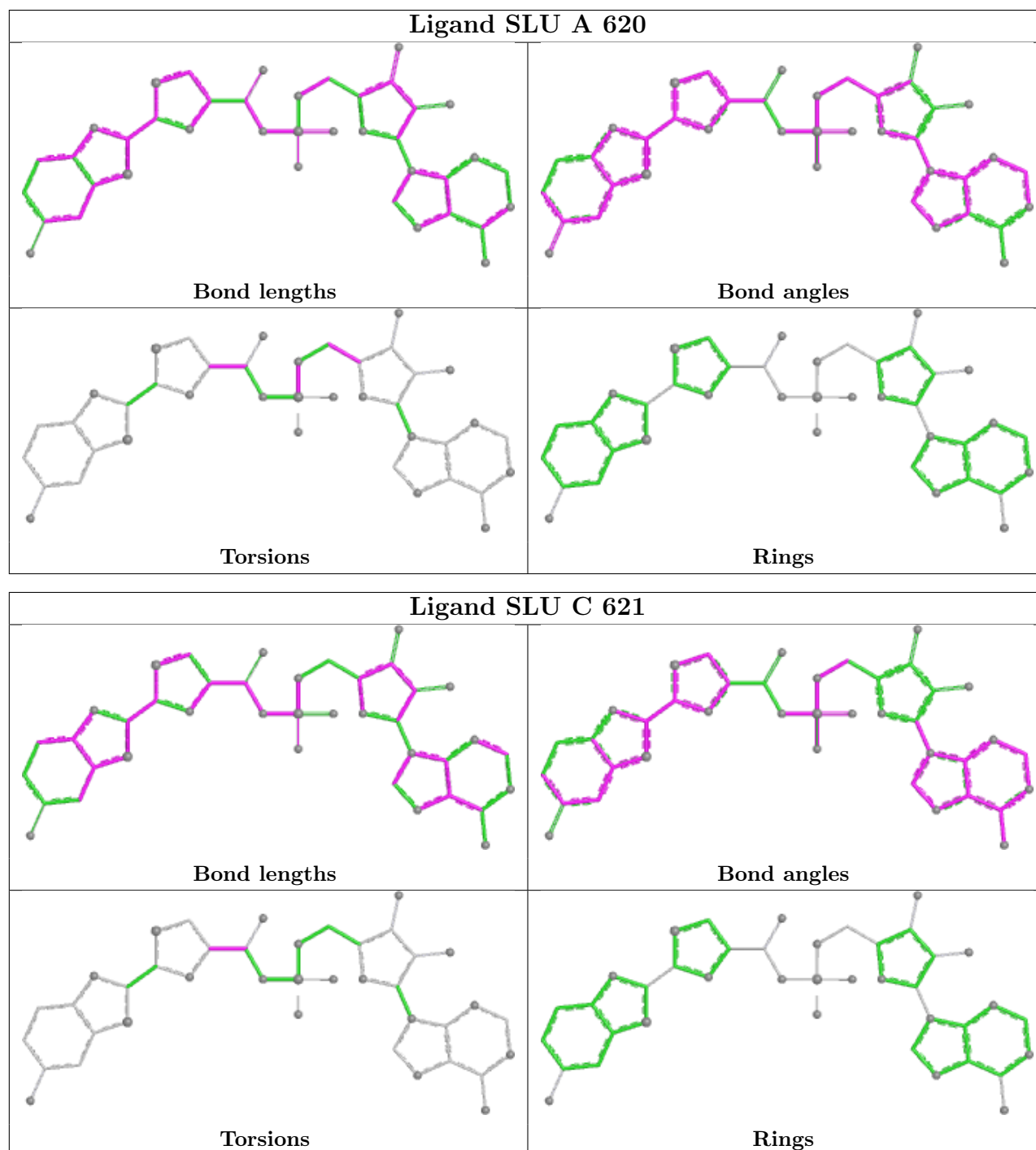
There are no ring outliers.

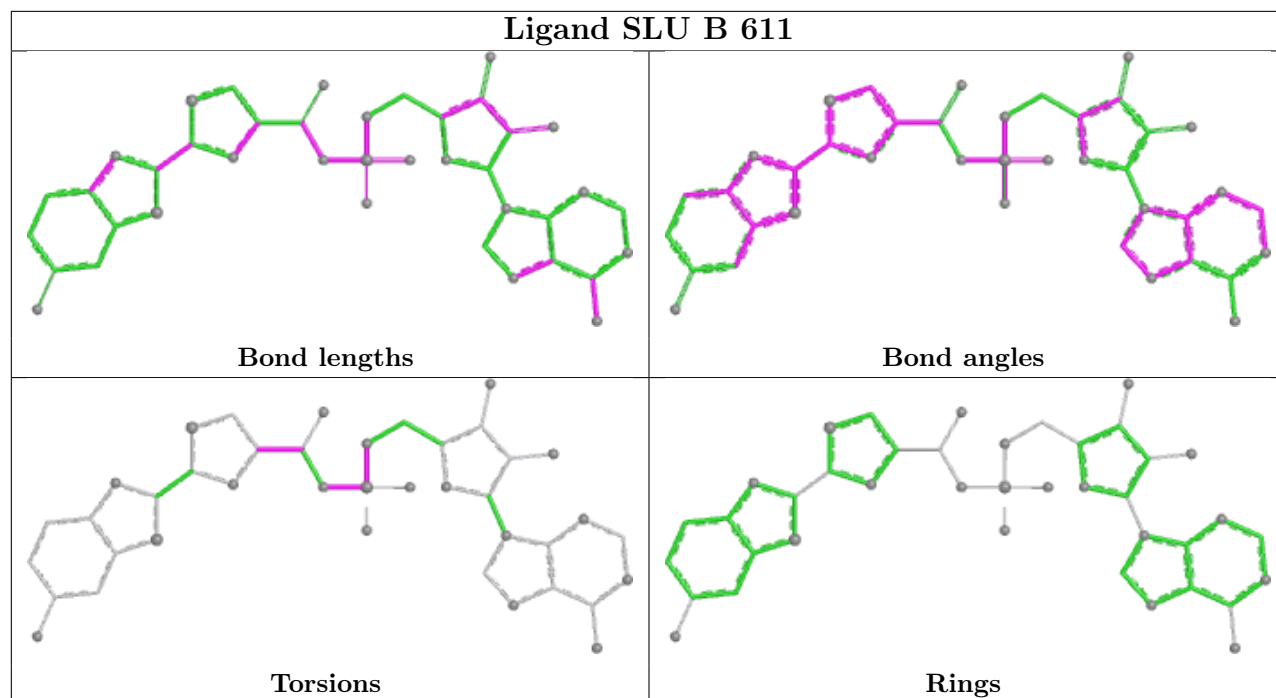
20 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	613	EDO	1	0
4	C	610	EDO	1	0
4	B	604	EDO	1	0
4	C	620	EDO	8	0
4	A	607	EDO	1	0
4	A	616	EDO	1	0
4	A	609	EDO	1	0
4	C	605	EDO	1	0
4	B	607	EDO	2	0
4	C	619	EDO	1	0
5	A	620	SLU	2	0
4	C	618	EDO	2	0
5	C	621	SLU	1	0
4	A	611	EDO	1	0
4	A	618	EDO	1	0
5	B	611	SLU	5	0
2	C	602	SO4	1	0
3	A	602	DYD	3	0
4	B	608	EDO	1	0
4	A	612	EDO	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	544/555 (98%)	-0.05	24 (4%)	39	38	13, 34, 87, 108	1 (0%)
1	B	512/555 (92%)	0.48	55 (10%)	11	10	33, 52, 108, 128	0
1	C	438/555 (78%)	0.31	18 (4%)	41	39	25, 49, 80, 101	0
All	All	1494/1665 (89%)	0.24	97 (6%)	25	24	13, 46, 96, 128	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	PHE	4.2
1	B	444	TYR	4.0
1	B	526	LEU	4.0
1	C	374	VAL	4.0
1	B	491	LYS	3.8
1	B	481	PRO	3.8
1	B	500	ASP	3.8
1	A	502	VAL	3.8
1	B	230	GLN	3.7
1	B	233	PRO	3.7
1	B	522	VAL	3.7
1	A	515	GLY	3.6
1	C	200	GLY	3.6
1	B	480	LEU	3.6
1	B	494	THR	3.5
1	B	295	PHE	3.5
1	B	499	VAL	3.5
1	C	199	SER	3.4
1	B	302	ASP	3.4
1	B	293	SER	3.4
1	B	199	SER	3.3
1	C	435	VAL	3.3
1	B	527	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	266	TYR	3.3
1	B	468	GLY	3.3
1	A	200	GLY	3.2
1	A	447	TYR	3.2
1	A	544	LYS	3.1
1	B	449	VAL	3.1
1	B	523	PRO	3.1
1	B	470	ALA	3.1
1	B	271	GLU	3.1
1	B	445	LYS	3.0
1	B	497	GLU	3.0
1	B	231	ILE	3.0
1	B	448	GLN	3.0
1	B	516	VAL	3.0
1	B	446	GLY	2.9
1	C	202	THR	2.9
1	B	2	GLU	2.9
1	B	535	ILE	2.9
1	B	532	ALA	2.9
1	B	201	SER	2.8
1	B	270	GLU	2.8
1	A	520	ASP	2.8
1	C	229	ASN	2.8
1	B	515	GLY	2.8
1	B	503	ALA	2.8
1	A	526	LEU	2.7
1	A	545	GLY	2.7
1	A	444	TYR	2.7
1	B	501	TYR	2.7
1	B	442	ILE	2.7
1	B	528	GLY	2.7
1	B	268	PHE	2.7
1	A	511	LYS	2.7
1	B	511	LYS	2.6
1	C	293	SER	2.6
1	B	441	LEU	2.6
1	C	266	TYR	2.6
1	C	371	ALA	2.6
1	A	199	SER	2.5
1	A	2	GLU	2.5
1	A	493	MET	2.5
1	A	540	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	446	GLY	2.5
1	B	266	TYR	2.5
1	A	473	PRO	2.4
1	B	506	VAL	2.4
1	C	4	ALA	2.4
1	C	292	PHE	2.4
1	A	472	LEU	2.3
1	C	294	PHE	2.3
1	B	509	ALA	2.3
1	A	492	THR	2.3
1	B	530	LEU	2.3
1	A	482	ALA	2.3
1	C	434	ILE	2.2
1	B	265	MET	2.2
1	B	300	LEU	2.2
1	A	528	GLY	2.2
1	C	230	GLN	2.2
1	B	291	LEU	2.2
1	A	509	ALA	2.2
1	C	6	ASN	2.2
1	B	175	GLY	2.2
1	B	478	GLY	2.2
1	A	542	ALA	2.1
1	C	198	SER	2.1
1	B	454	LEU	2.1
1	B	469	VAL	2.1
1	B	529	LYS	2.1
1	C	1	MET	2.1
1	B	459	LEU	2.1
1	C	332	ASN	2.1
1	A	514	GLY	2.1
1	B	301	ILE	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 ⓘ

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
4	EDO	B	606	4/4	0.51	0.24	66,76,81,82	0
2	SO4	C	602	5/5	0.53	0.22	92,102,114,120	0
4	EDO	A	616	4/4	0.57	0.21	67,75,76,77	0
3	DYD	C	603	8/8	0.59	0.23	48,58,65,65	0
4	EDO	C	616	4/4	0.59	0.26	60,67,72,81	0
4	EDO	B	608	4/4	0.64	0.16	65,69,70,73	0
4	EDO	B	605	4/4	0.65	0.21	69,75,83,87	0
4	EDO	C	612	4/4	0.66	0.22	66,67,68,74	0
4	EDO	A	606	4/4	0.69	0.19	43,50,51,54	0
4	EDO	A	608	4/4	0.70	0.18	57,63,67,69	0
4	EDO	C	615	4/4	0.70	0.18	56,59,64,69	0
4	EDO	A	610	4/4	0.70	0.22	54,57,70,74	0
3	DYD	A	602	8/8	0.71	0.24	46,52,59,59	0
4	EDO	C	614	4/4	0.71	0.18	65,69,74,75	0
4	EDO	C	607	4/4	0.73	0.14	64,69,73,80	0
3	DYD	A	603	8/8	0.74	0.18	36,44,48,52	0
4	EDO	C	605	4/4	0.75	0.15	44,57,65,71	0
4	EDO	B	607	4/4	0.76	0.20	44,45,51,52	0
4	EDO	B	609	4/4	0.76	0.16	57,58,61,64	0
4	EDO	B	610	4/4	0.76	0.15	51,61,61,62	0
4	EDO	C	618	4/4	0.76	0.22	35,44,54,55	4
3	DYD	C	604	8/8	0.77	0.24	62,77,88,88	0
2	SO4	A	601	5/5	0.77	0.20	86,97,110,121	0
4	EDO	A	612	4/4	0.78	0.15	53,59,60,63	0
4	EDO	C	617	4/4	0.78	0.23	45,45,57,62	4
4	EDO	C	613	4/4	0.78	0.16	54,55,57,61	0
4	EDO	B	604	4/4	0.79	0.18	56,57,64,67	0
4	EDO	A	614	4/4	0.80	0.21	39,53,55,63	0
4	EDO	C	608	4/4	0.81	0.15	52,58,59,72	0
4	EDO	C	611	4/4	0.81	0.18	45,50,55,56	0
2	SO4	C	601	5/5	0.81	0.14	68,71,95,105	0
4	EDO	A	604	4/4	0.82	0.22	45,50,53,54	0
4	EDO	A	613	4/4	0.82	0.23	47,48,53,64	0
2	SO4	B	603	5/5	0.83	0.24	69,86,100,111	0
4	EDO	C	610	4/4	0.83	0.18	62,62,72,72	0
4	EDO	A	609	4/4	0.84	0.14	40,41,51,52	4
4	EDO	C	620	4/4	0.84	0.18	45,48,49,56	0

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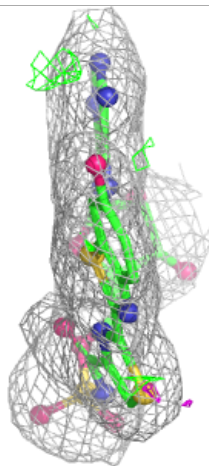
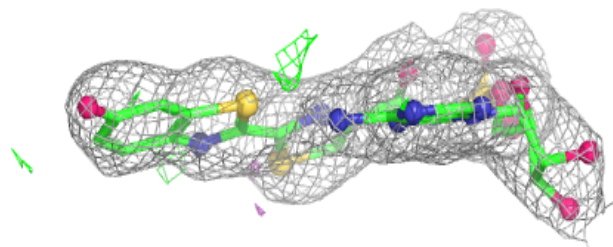
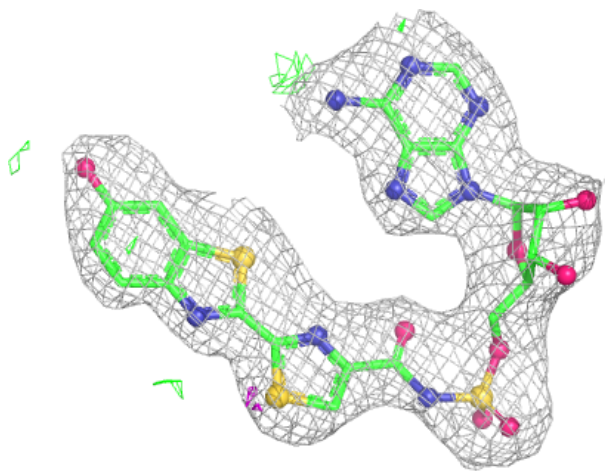
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	611	4/4	0.85	0.22	44,45,48,50	0
4	EDO	C	606	4/4	0.86	0.14	47,50,51,62	0
4	EDO	C	609	4/4	0.86	0.19	40,46,46,50	0
4	EDO	A	607	4/4	0.87	0.16	38,39,42,56	0
4	EDO	A	618	4/4	0.87	0.15	37,51,51,57	0
2	SO4	B	601	5/5	0.88	0.26	63,85,97,100	0
4	EDO	C	619	4/4	0.89	0.13	33,41,42,43	0
4	EDO	A	615	4/4	0.89	0.12	44,46,52,55	0
4	EDO	A	619	4/4	0.90	0.15	45,45,49,62	0
2	SO4	B	602	5/5	0.90	0.19	63,65,76,77	0
4	EDO	A	617	4/4	0.92	0.11	42,48,52,53	0
4	EDO	A	605	4/4	0.93	0.12	32,32,36,48	0
5	SLU	B	611	40/40	0.94	0.09	33,40,47,52	0
5	SLU	C	621	40/40	0.95	0.07	41,49,59,62	0
5	SLU	A	620	40/40	0.97	0.07	23,29,37,40	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.

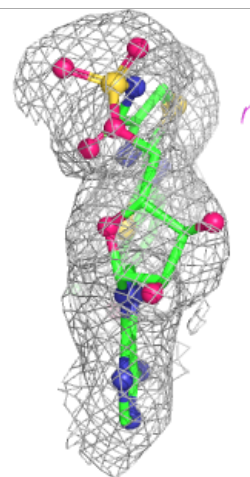
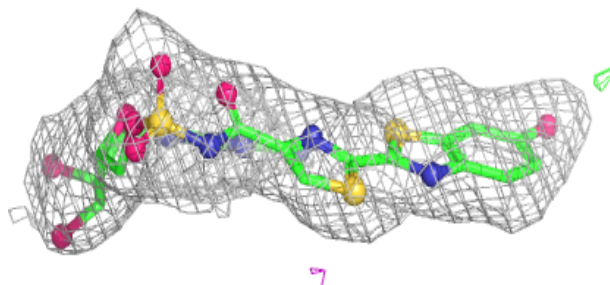
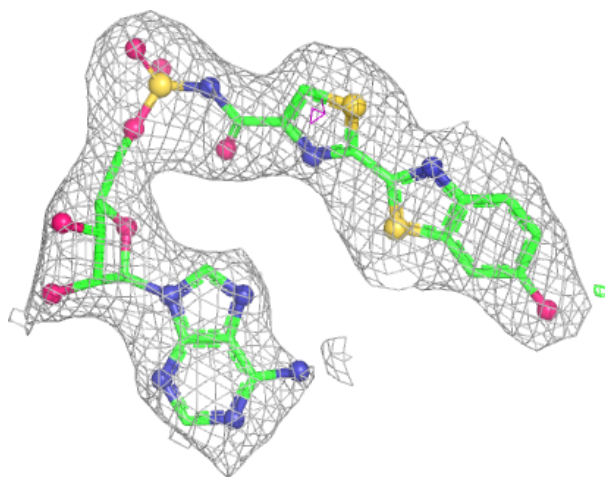
Electron density around SLU B 611:

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



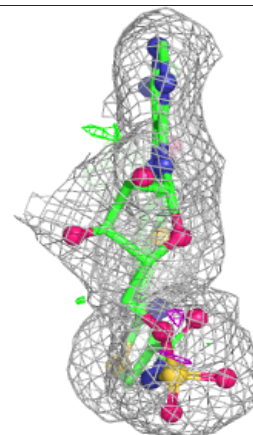
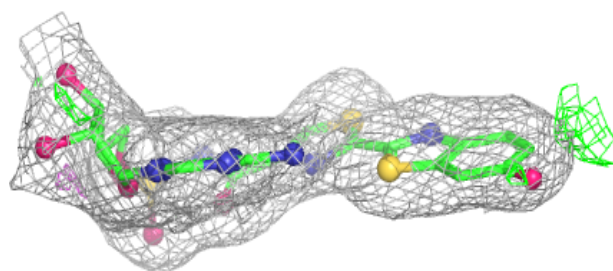
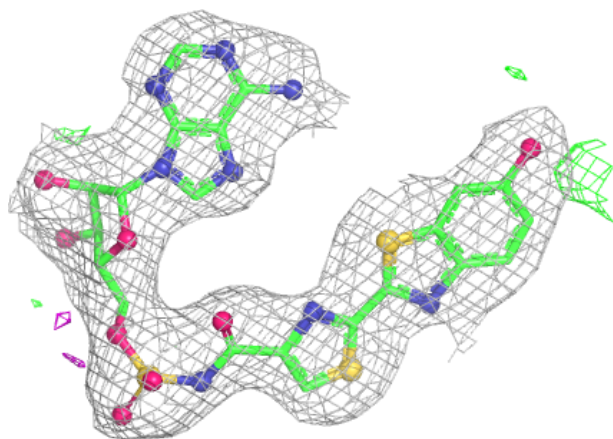
Electron density around SLU C 621:

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



Electron density around SLU A 620:

$2mF_o-DF_c$ (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.