



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 3OE1 / pdb_00003oe1
Title : Pyruvate decarboxylase variant Glu473Asp from *Z. mobilis* in complex with reaction intermediate 2-lactyl-ThDP
Authors : Meyer, D.; Neumann, P.; Parthier, C.; Tittmann, K.
Deposited on : 2010-08-12
Resolution : 1.99 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

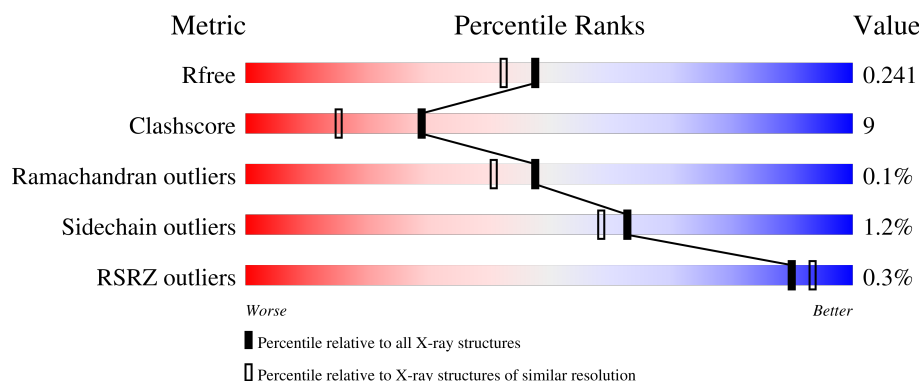
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	568	83% 16% .
1	B	568	% 84% 14% ..
1	C	568	79% 20% ..
1	D	568	79% 18% .

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
3	TDL	A	611	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18375 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 Pyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	1	1	0
			4277	2722	728	809	18			
1	B	560	Total	C	N	O	S	0	0	0
			4226	2688	720	800	18			
1	C	565	Total	C	N	O	S	0	0	0
			4265	2713	727	807	18			
1	D	555	Total	C	N	O	S	0	1	0
			4207	2676	716	796	19			

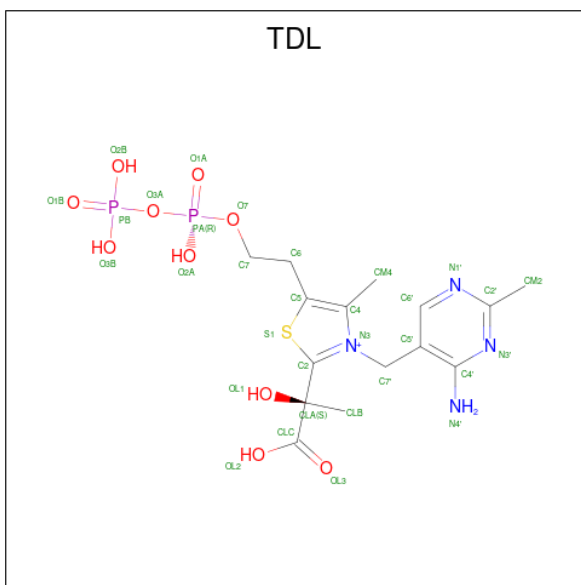
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	473	ASP	GLU	engineered mutation	UNP P06672
B	473	ASP	GLU	engineered mutation	UNP P06672
C	473	ASP	GLU	engineered mutation	UNP P06672
D	473	ASP	GLU	engineered mutation	UNP P06672

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

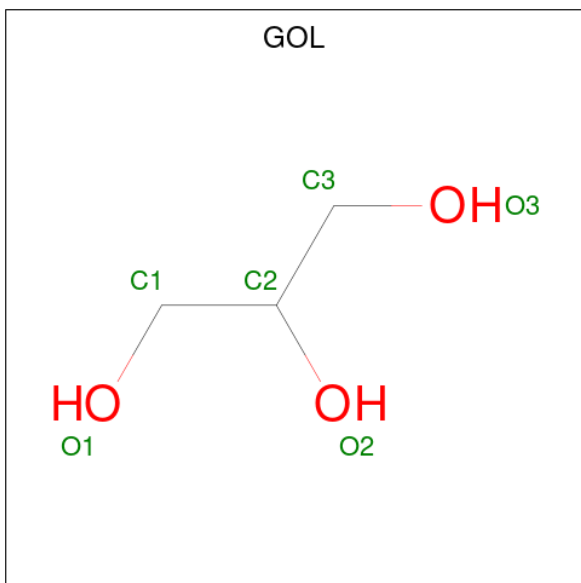
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-HYDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (CCD ID: TDL) (formula: C₁₅H₂₃N₄O₁₀P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0
3	B	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0
3	C	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0
3	D	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



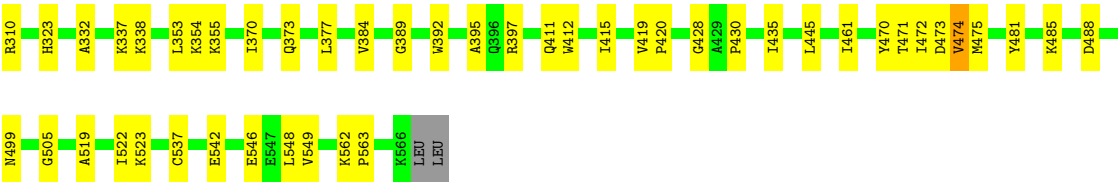
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

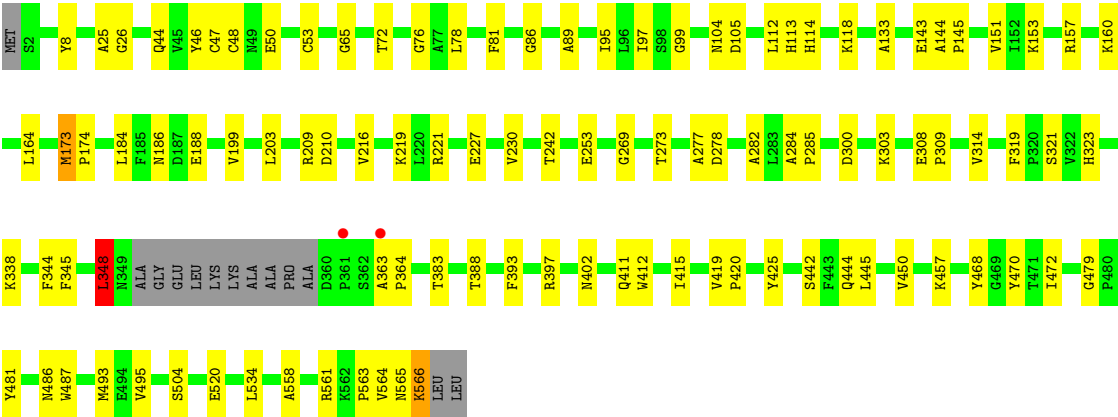
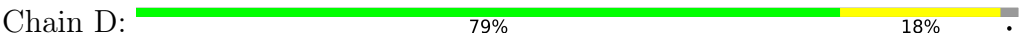
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	346	Total	O	0	0
			346	346		
5	B	307	Total	O	0	0
			307	307		
5	C	297	Total	O	0	0
			297	297		
5	D	306	Total	O	0	0
			306	306		

- Molecule 1: Pyruvate decarboxylase





• Molecule 1: Pyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.49Å 165.36Å 95.87Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	19.58 – 1.99 19.58 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.58-1.99) 88.1 (19.58-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.194 , 0.246 0.191 , 0.241	Depositor DCC
R_{free} test set	6428 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.126 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18375	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/4370	0.71	0/5942
1	B	0.32	0/4317	0.74	5/5871 (0.1%)
1	C	0.32	0/4357	0.71	0/5924
1	D	0.33	0/4297	0.73	4/5841 (0.1%)
All	All	0.33	0/17341	0.72	9/23578 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	ASP	CA-C-N	6.77	126.45	119.82
1	B	360	ASP	C-N-CA	6.77	126.45	119.82
1	D	348	LEU	N-CA-C	-5.88	104.56	110.97
1	B	348	LEU	N-CA-C	5.86	118.54	111.40
1	D	99	GLY	N-CA-C	-5.79	105.13	112.54
1	D	173	MET	CA-C-N	5.22	125.12	119.85
1	D	173	MET	C-N-CA	5.22	125.12	119.85
1	B	357	ALA	CA-C-N	5.13	125.05	119.76
1	B	357	ALA	C-N-CA	5.13	125.05	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4277	0	4242	71	0
1	B	4226	0	4187	66	0
1	C	4265	0	4234	91	0
1	D	4207	0	4168	85	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	19	9	0
3	B	32	0	19	7	0
3	C	32	0	19	7	0
3	D	32	0	19	7	0
4	D	12	0	16	2	0
5	A	346	0	0	7	0
5	B	307	0	0	6	0
5	C	297	0	0	9	0
5	D	306	0	0	8	0
All	All	18375	0	16923	295	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 9.

All (295) 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:C:12:ARG:HH11	1:C:15:GLN:HE22	1.03	0.95
1:D:344:PHE:CE2	1:D:348:LEU:HD11	2.04	0.91
1:D:558:ALA:O	1:D:561:ARG:HG3	1.73	0.88
1:A:292:THR:HG23	1:A:295:TRP:H	1.36	0.87
3:B:611:TDL:OL1	3:B:611:TDL:N4'	2.09	0.85
1:A:34:ASP:OD2	1:B:477:HIS:HE1	1.63	0.82
1:C:302:LYS:H	1:C:302:LYS:HD2	1.48	0.78
1:A:388:THR:HG21	3:A:611:TDL:HLB2	1.64	0.77
1:C:12:ARG:HH11	1:C:15:GLN:NE2	1.83	0.77
1:C:415:ILE:HD13	3:C:611:TDL:HM42	1.66	0.77
1:C:471:THR:HA	1:C:474:VAL:HG12	1.68	0.75
1:C:102:ASN:HD22	1:C:104:ASN:H	1.36	0.74
3:C:611:TDL:N4'	3:C:611:TDL:OL1	2.17	0.74
1:A:493:MET:HE3	1:A:534:LEU:HD13	1.69	0.74
1:B:44:GLN:HG3	5:B:1263:HOH:O	1.88	0.74
1:B:470:TYR:CD1	3:B:611:TDL:H62	2.25	0.72
1:B:119:THR:HG21	1:D:143:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:NH1	1:C:15:GLN:HE22	1.83	0.71
1:C:475:MET:HE2	1:C:549:VAL:HG22	1.74	0.70
1:D:314:VAL:HG12	5:D:864:HOH:O	1.91	0.70
1:A:237:GLY:HA2	1:A:256:HIS:CE1	2.26	0.69
1:A:288:ASN:O	1:A:292:THR:HG22	1.92	0.69
1:B:74:SER:H	1:B:124:GLN:HE22	1.39	0.69
1:D:419:VAL:HB	1:D:420:PRO:HD3	1.74	0.69
3:D:611:TDL:OL1	3:D:611:TDL:N4'	2.25	0.69
1:C:170:ILE:HA	1:C:173:MET:HG3	1.74	0.69
1:B:16:ILE:HG13	1:B:18:LEU:HD13	1.76	0.68
1:D:89:ALA:HB1	1:D:411:GLN:HG3	1.74	0.68
1:D:227:GLU:O	1:D:230:VAL:HG22	1.94	0.67
1:C:563:PRO:HG2	1:D:173:MET:HE1	1.77	0.67
1:C:216:VAL:HB	1:C:242:THR:HG22	1.76	0.66
5:B:969:HOH:O	1:D:566:LYS:HB3	1.96	0.66
1:C:377:LEU:HD11	1:C:522:ILE:HD13	1.78	0.66
1:B:306:LEU:HD22	1:B:308:GLU:HG3	1.78	0.65
1:C:323:HIS:HD2	5:C:1223:HOH:O	1.78	0.65
1:A:89:ALA:HB1	1:A:411:GLN:HG3	1.78	0.65
1:B:74:SER:N	1:B:124:GLN:HE22	1.94	0.65
1:A:12:ARG:HD2	1:A:184:LEU:HD11	1.78	0.64
1:A:34:ASP:OD2	1:B:477:HIS:CE1	2.49	0.64
1:C:84:ILE:HG13	1:C:96:LEU:HD22	1.78	0.64
1:C:471:THR:HA	1:C:474:VAL:CG1	2.29	0.63
1:C:415:ILE:CD1	3:C:611:TDL:HM42	2.28	0.62
1:D:188:GLU:O	1:D:323:HIS:HE1	1.81	0.62
1:A:27:ASP:HA	1:A:30:LEU:HG	1.81	0.62
1:D:319:PHE:HD2	5:D:864:HOH:O	1.83	0.62
1:B:459:PRO:HB3	1:B:529:THR:HA	1.82	0.62
1:D:344:PHE:O	1:D:348:LEU:HD12	1.99	0.62
1:C:44:GLN:HG2	1:C:46:TYR:CE1	2.36	0.61
1:A:276:GLU:HG3	1:A:344:PHE:CZ	2.35	0.61
1:B:237:GLY:HA2	1:B:256:HIS:CE1	2.36	0.61
1:C:377:LEU:HD21	1:C:522:ILE:HG21	1.82	0.60
1:A:84:ILE:HG13	1:A:96:LEU:HD22	1.84	0.59
1:D:65:GLY:HA2	4:D:569:GOL:H2	1.84	0.59
1:A:292:THR:HG21	1:A:295:TRP:CE3	2.37	0.59
1:C:102:ASN:ND2	1:C:104:ASN:H	1.99	0.59
1:D:144:ALA:HB3	1:D:145:PRO:HD3	1.84	0.59
1:C:472:ILE:HA	1:C:548:LEU:HD21	1.83	0.59
1:D:363:ALA:HB1	1:D:364:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:GLN:O	1:C:377:LEU:HG	2.03	0.59
1:D:253:GLU:HB2	1:D:402:ASN:ND2	2.18	0.59
1:A:196:ASN:O	1:A:200:GLU:HG3	2.03	0.59
1:C:232:PHE:HA	1:C:332:ALA:HB2	1.85	0.59
1:A:415:ILE:CD1	3:A:611:TDL:HM42	2.33	0.58
1:A:292:THR:HG23	1:A:295:TRP:N	2.14	0.58
1:C:272:LYS:O	1:C:276:GLU:HG2	2.03	0.58
1:D:345:PHE:HA	1:D:348:LEU:CD1	2.33	0.58
1:A:388:THR:CG2	3:A:611:TDL:HLB2	2.31	0.58
1:B:419:VAL:HB	1:B:420:PRO:HD3	1.86	0.57
1:D:221:ARG:HD2	4:D:569:GOL:H12	1.87	0.57
1:D:415:ILE:HD13	3:D:611:TDL:HM42	1.85	0.57
1:B:362:SER:O	1:B:362:SER:OG	2.23	0.57
3:A:611:TDL:OL1	3:A:611:TDL:H7'1	2.05	0.57
1:D:344:PHE:CD2	1:D:348:LEU:HD11	2.40	0.57
1:B:86:GLY:HA2	1:B:412:TRP:CG	2.41	0.56
1:D:72:THR:HG22	5:D:577:HOH:O	2.05	0.56
1:C:470:TYR:CD1	3:C:611:TDL:H62	2.41	0.56
1:D:345:PHE:HA	1:D:348:LEU:HD13	1.87	0.56
1:B:2:SER:HB3	5:B:947:HOH:O	2.06	0.55
1:A:419:VAL:HB	1:A:420:PRO:HD3	1.88	0.55
1:C:188:GLU:O	1:C:323:HIS:HE1	1.89	0.55
1:B:144:ALA:HB3	1:B:145:PRO:HD3	1.87	0.55
1:B:113:HIS:O	1:B:114:HIS:HB2	2.06	0.55
1:B:408:TYR:HB3	1:B:410:MET:HG3	1.87	0.55
1:B:415:ILE:HD13	3:B:611:TDL:HM43	1.88	0.55
1:D:564:VAL:HG12	1:D:565:ASN:H	1.72	0.55
1:B:361:PRO:HB3	1:B:516:GLY:N	2.22	0.54
1:B:470:TYR:HB3	3:B:611:TDL:H61	1.89	0.54
1:A:170:ILE:HA	1:A:173:MET:HG3	1.88	0.54
1:C:353:LEU:HB3	5:C:1087:HOH:O	2.06	0.54
1:A:188:GLU:O	1:A:323:HIS:HE1	1.89	0.54
1:C:485:LYS:HE2	1:D:504:SER:O	2.06	0.54
1:D:415:ILE:CD1	3:D:611:TDL:HM42	2.37	0.54
1:D:219:LYS:HB2	1:D:284:ALA:HB1	1.88	0.54
1:D:308:GLU:HB3	1:D:309:PRO:HD2	1.89	0.54
1:B:348:LEU:O	1:B:349:ASN:HB2	2.08	0.54
1:C:123:TYR:O	1:C:127:MET:HG3	2.08	0.53
1:A:219:LYS:HB2	1:A:284:ALA:HB1	1.90	0.53
1:D:86:GLY:HA2	1:D:412:TRP:CG	2.44	0.53
1:C:546:GLU:HG2	5:C:976:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASP:HA	1:C:30:LEU:HG	1.91	0.53
1:C:263:GLY:O	1:C:266:SER:HB2	2.09	0.53
1:D:415:ILE:HB	1:D:442:SER:OG	2.08	0.53
1:C:260:THR:HB	1:C:267:TYR:CD1	2.44	0.53
1:D:472:ILE:HG21	3:D:611:TDL:S1	2.49	0.53
1:A:415:ILE:HD13	3:A:611:TDL:HM42	1.91	0.53
3:A:611:TDL:OL1	3:A:611:TDL:N4'	2.39	0.53
1:A:144:ALA:HB3	1:A:145:PRO:HD3	1.91	0.52
1:D:383:THR:HG21	1:D:425:TYR:CZ	2.44	0.52
1:B:415:ILE:HD13	3:B:611:TDL:CM4	2.39	0.52
1:B:308:GLU:HB3	1:B:309:PRO:HD2	1.92	0.52
1:B:566:LYS:HD3	1:C:104:ASN:O	2.10	0.52
1:C:211:LYS:HB2	1:C:278:ASP:H	1.74	0.52
1:B:450:VAL:HG11	1:B:493:MET:HE1	1.92	0.52
1:A:379:THR:HB	1:A:380:PRO:HD2	1.91	0.52
1:C:310:ARG:HD2	5:C:1227:HOH:O	2.10	0.52
1:C:499:ASN:HD21	1:C:505:GLY:H	1.58	0.51
1:A:213:ALA:HB1	1:A:274:MET:HE1	1.90	0.51
1:B:358:PRO:HD3	5:B:650:HOH:O	2.09	0.51
1:B:433:ARG:HG2	1:B:435:ILE:CD1	2.40	0.51
1:C:250:PHE:CG	1:C:251:PRO:HD2	2.45	0.51
1:D:209:ARG:HB3	1:D:278:ASP:HB3	1.93	0.51
1:D:277:ALA:O	1:D:303:LYS:HE2	2.11	0.51
1:D:273:THR:HG21	1:D:345:PHE:HB2	1.92	0.51
1:C:88:TYR:CE2	1:C:160:LYS:HG2	2.46	0.50
1:A:423:PHE:O	1:A:427:VAL:HG23	2.10	0.50
1:C:261:SER:HA	1:C:266:SER:OG	2.12	0.50
1:A:481:TYR:HB2	1:B:25:ALA:HB2	1.92	0.50
1:B:219:LYS:HB2	1:B:284:ALA:HB1	1.94	0.50
1:B:216:VAL:HG13	1:B:220:LEU:HD22	1.93	0.50
1:B:566:LYS:HD3	1:C:108:ALA:HB2	1.92	0.50
1:A:440:ASP:HB2	1:A:489:TYR:OH	2.12	0.50
1:C:473:ASP:OD1	3:C:611:TDL:OL2	2.30	0.50
1:A:200:GLU:HG2	5:A:1049:HOH:O	2.12	0.50
1:A:113:HIS:O	1:A:114:HIS:HB2	2.11	0.50
1:C:370:ILE:HD11	1:C:537:CYS:HB3	1.94	0.50
1:C:470:TYR:HB3	3:C:611:TDL:H61	1.93	0.49
1:D:78:LEU:O	1:D:81:PHE:HB2	2.12	0.49
1:C:252:GLU:HG2	1:C:257:TYR:CE2	2.46	0.49
1:D:520:GLU:HG2	5:D:668:HOH:O	2.11	0.49
1:C:16:ILE:HG13	1:C:18:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:PHE:O	1:D:397:ARG:HG3	2.13	0.49
1:D:472:ILE:CG2	3:D:611:TDL:S1	3.01	0.49
1:B:151:VAL:HG21	1:B:164:LEU:HG	1.95	0.48
1:D:564:VAL:HG12	1:D:565:ASN:N	2.27	0.48
5:A:717:HOH:O	1:B:113:HIS:HB2	2.12	0.48
1:C:237:GLY:HA2	1:C:256:HIS:CE1	2.49	0.48
1:D:210:ASP:O	1:D:338:LYS:HB3	2.13	0.48
1:C:236:LEU:HB3	5:C:1135:HOH:O	2.14	0.48
1:D:44:GLN:HG2	1:D:46:TYR:CE1	2.48	0.48
1:B:44:GLN:HG2	1:B:46:TYR:CE1	2.48	0.48
1:B:119:THR:HG22	5:B:648:HOH:O	2.14	0.48
1:D:269:GLY:O	1:D:273:THR:HG23	2.13	0.48
1:C:89:ALA:HB1	1:C:411:GLN:HG3	1.96	0.48
1:B:440:ASP:HB2	1:B:489:TYR:OH	2.14	0.47
1:C:103:ASN:HD21	1:D:563:PRO:HG3	1.79	0.47
1:B:89:ALA:HB1	1:B:411:GLN:HG3	1.96	0.47
1:D:113:HIS:O	1:D:114:HIS:HB2	2.13	0.47
1:D:285:PRO:HD2	1:D:308:GLU:OE2	2.14	0.47
1:C:26:GLY:HA2	3:D:611:TDL:H7'2	1.96	0.47
1:D:151:VAL:HG21	1:D:164:LEU:HG	1.96	0.47
3:A:611:TDL:H4'1	3:A:611:TDL:CLA	2.27	0.47
1:B:264:GLU:OE2	1:B:550:LYS:HB3	2.14	0.47
1:B:300:ASP:OD1	1:B:302:LYS:HE3	2.15	0.47
1:A:308:GLU:HB3	1:A:309:PRO:HD2	1.97	0.47
1:A:50:GLU:HG2	1:A:76:GLY:HA2	1.97	0.46
1:B:549:VAL:O	1:B:553:LYS:HG3	2.15	0.46
1:D:86:GLY:HA2	1:D:412:TRP:CD2	2.50	0.46
1:A:310:ARG:HD2	5:A:613:HOH:O	2.14	0.46
1:C:25:ALA:HB2	1:D:481:TYR:HB2	1.97	0.46
1:A:300:ASP:OD1	1:A:301:PRO:HD2	2.15	0.46
1:B:31:VAL:O	1:B:34:ASP:HB2	2.15	0.46
1:C:216:VAL:HG13	1:C:220:LEU:HD22	1.97	0.46
1:C:519:ALA:O	1:C:523:LYS:HG3	2.15	0.46
1:D:314:VAL:N	5:D:864:HOH:O	2.49	0.46
1:A:188:GLU:CD	1:D:186:ASN:HD22	2.23	0.46
1:A:425:TYR:HB3	5:A:592:HOH:O	2.14	0.46
1:C:389:GLY:O	1:C:392:TRP:HB2	2.15	0.46
1:D:105:ASP:HB3	1:D:112:LEU:HD11	1.98	0.46
1:C:48:CYS:O	1:D:445:LEU:HG	2.16	0.46
1:A:113:HIS:HD2	1:B:289:ASP:OD2	1.99	0.46
1:C:353:LEU:HD23	1:C:355:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:HIS:HD2	5:D:642:HOH:O	1.97	0.46
1:C:13:LEU:HG	1:C:18:LEU:HD22	1.97	0.45
3:B:611:TDL:H4'1	3:B:611:TDL:CLA	2.24	0.45
1:D:450:VAL:HG11	1:D:493[A]:MET:HE1	1.98	0.45
1:A:470:TYR:HB3	3:A:611:TDL:H61	1.98	0.45
1:B:479:GLY:HA3	1:B:481:TYR:CZ	2.51	0.45
1:C:144:ALA:HB3	1:C:145:PRO:HD3	1.98	0.45
1:C:188:GLU:O	1:C:323:HIS:CE1	2.70	0.45
1:A:93:PRO:HG3	1:A:159:LYS:HA	1.98	0.45
1:A:300:ASP:OD1	1:A:302:LYS:HG2	2.17	0.45
1:C:102:ASN:HD21	1:C:104:ASN:ND2	2.14	0.45
1:D:300:ASP:HB3	1:D:303:LYS:CD	2.46	0.45
1:A:237:GLY:HA2	1:A:256:HIS:HE1	1.80	0.45
1:B:308:GLU:HB3	1:B:309:PRO:CD	2.47	0.45
1:D:273:THR:HG21	1:D:345:PHE:HD1	1.81	0.45
1:D:50:GLU:HG2	1:D:76:GLY:CA	2.47	0.45
1:D:273:THR:HG22	1:D:344:PHE:CD2	2.52	0.45
1:B:470:TYR:O	1:B:474:VAL:HG23	2.18	0.44
1:A:86:GLY:HA2	1:A:412:TRP:CG	2.53	0.44
1:A:123:TYR:O	1:A:127:MET:HG3	2.17	0.44
1:C:488:ASP:HB3	1:D:495:VAL:HA	1.99	0.44
1:D:216:VAL:HB	1:D:242:THR:HG22	1.98	0.44
1:D:444:GLN:HG2	1:D:487:TRP:CH2	2.52	0.44
1:C:159:LYS:O	1:C:160:LYS:HD2	2.17	0.44
1:A:114:HIS:HA	1:B:412:TRP:O	2.18	0.44
1:A:151:VAL:HG21	1:A:164:LEU:HG	2.00	0.44
1:C:435:ILE:HD13	1:C:461:ILE:HB	1.99	0.44
1:A:202:THR:O	1:A:206:ILE:HG12	2.17	0.44
1:C:337:LYS:C	1:C:338:LYS:HD2	2.43	0.44
1:C:86:GLY:HA2	1:C:412:TRP:CG	2.52	0.44
1:C:481:TYR:HB3	1:D:46:TYR:CE1	2.53	0.44
3:C:611:TDL:H7'2	1:D:26:GLY:HA2	2.00	0.44
1:B:417:TRP:O	1:B:420:PRO:HD2	2.18	0.44
1:C:542:GLU:HB2	5:C:1160:HOH:O	2.18	0.43
1:D:470:TYR:CD1	3:D:611:TDL:H62	2.53	0.43
1:A:160:LYS:HE2	5:A:863:HOH:O	2.18	0.43
1:B:253:GLU:H	1:B:402:ASN:HD21	1.65	0.43
1:D:8:TYR:CE1	1:D:145:PRO:HA	2.53	0.43
1:A:188:GLU:O	1:A:323:HIS:CE1	2.71	0.43
1:D:388:THR:HB	1:D:415:ILE:HG22	1.99	0.43
1:C:353:LEU:HD11	1:C:397:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:TYR:CE1	1:D:486:ASN:HB2	2.54	0.43
1:D:565:ASN:OD1	1:D:566:LYS:HB2	2.18	0.43
1:A:25:ALA:HB2	1:B:481:TYR:HB2	2.00	0.43
1:A:216:VAL:HB	1:A:242:THR:HG22	2.00	0.43
1:A:412:TRP:O	1:B:114:HIS:HA	2.19	0.43
1:C:120:ASP:HB3	5:C:605:HOH:O	2.19	0.43
1:A:244:ALA:HB2	1:A:262:TRP:CD2	2.53	0.43
1:D:493[A]:MET:HE2	1:D:493[A]:MET:HA	1.99	0.43
1:C:445:LEU:HG	1:D:48:CYS:O	2.19	0.43
1:D:47:CYS:SG	1:D:53:CYS:HA	2.59	0.43
1:A:16:ILE:HG13	1:A:18:LEU:HD13	2.01	0.43
1:B:566:LYS:CD	1:C:108:ALA:HB2	2.49	0.43
1:C:290:TYR:CZ	1:D:113:HIS:CD2	3.07	0.42
1:C:428:GLY:C	1:C:430:PRO:HD3	2.44	0.42
1:D:199:VAL:O	1:D:203:LEU:HG	2.19	0.42
1:B:13:LEU:O	1:B:16:ILE:HG12	2.19	0.42
1:B:74:SER:HB3	1:B:114:HIS:O	2.19	0.42
1:B:86:GLY:HA2	1:B:412:TRP:CD2	2.54	0.42
1:B:400:LEU:HA	1:B:401:PRO:HD2	1.90	0.42
1:A:186:ASN:HD22	1:D:321:SER:HB3	1.84	0.42
1:C:338:LYS:HD2	1:C:338:LYS:N	2.34	0.42
1:A:115:ALA:HB3	5:A:858:HOH:O	2.20	0.42
1:C:115:ALA:HB3	5:C:607:HOH:O	2.18	0.42
1:D:300:ASP:HB3	1:D:303:LYS:HD2	2.01	0.42
1:A:415:ILE:HD11	3:A:611:TDL:HM42	2.02	0.42
1:B:22:PHE:HA	1:B:45:VAL:O	2.19	0.42
1:A:50:GLU:HG2	1:A:76:GLY:CA	2.50	0.42
1:B:272:LYS:O	1:B:275:LYS:HG2	2.19	0.42
1:C:247:LYS:HE2	1:C:395:ALA:O	2.19	0.42
1:D:95:ILE:HG22	1:D:97:ILE:HD11	2.02	0.42
1:A:298:ILE:HG23	1:A:299:PRO:HD2	2.01	0.42
1:C:13:LEU:O	1:C:18:LEU:HB2	2.20	0.42
1:D:89:ALA:HB1	1:D:411:GLN:CG	2.44	0.42
1:D:173:MET:HA	1:D:174:PRO:HD3	1.85	0.42
1:A:566:LYS:HB3	1:D:104:ASN:O	2.20	0.41
1:C:84:ILE:HD11	1:C:96:LEU:HB2	2.02	0.41
1:C:282:ALA:HB1	1:C:285:PRO:HG3	2.02	0.41
1:C:481:TYR:HB2	1:D:25:ALA:HB2	2.02	0.41
1:D:308:GLU:HB3	1:D:309:PRO:CD	2.50	0.41
1:A:100:ALA:HB1	1:A:101:PRO:HD2	2.01	0.41
1:C:9:LEU:HD21	1:C:97:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:THR:CA	1:C:474:VAL:HG12	2.46	0.41
1:B:410:MET:HE2	5:B:1256:HOH:O	2.19	0.41
1:C:298:ILE:HA	1:C:299:PRO:HD3	1.93	0.41
1:C:562:LYS:HA	5:D:988:HOH:O	2.20	0.41
1:C:55:PHE:CE1	1:C:83:ALA:HA	2.56	0.41
1:D:479:GLY:HA3	1:D:481:TYR:CZ	2.55	0.41
1:C:419:VAL:HB	1:C:420:PRO:CD	2.51	0.41
1:D:282:ALA:HB1	1:D:285:PRO:HG3	2.02	0.41
1:A:231:LYS:HA	5:A:688:HOH:O	2.20	0.41
1:C:233:ALA:HB1	1:C:240:VAL:HG21	2.03	0.41
1:A:199:VAL:O	1:A:203:LEU:HG	2.20	0.41
1:B:300:ASP:OD2	1:B:302:LYS:HG2	2.20	0.41
1:B:493:MET:HA	1:B:493:MET:HE2	2.01	0.41
1:A:276:GLU:HG3	1:A:344:PHE:CE2	2.56	0.41
1:C:109:GLY:HA3	5:C:1148:HOH:O	2.21	0.41
1:C:294:GLY:O	1:C:295:TRP:HB2	2.20	0.41
1:A:246:ALA:O	1:A:249:PHE:HB2	2.21	0.41
1:A:452:GLN:HA	1:A:452:GLN:OE1	2.21	0.41
1:A:464:LEU:HD13	1:A:464:LEU:C	2.46	0.41
1:B:12:ARG:HD2	1:B:184:LEU:HD11	2.02	0.41
1:B:415:ILE:HG23	3:B:611:TDL:N4'	2.36	0.41
1:B:437:MET:HE2	1:B:437:MET:HB3	1.85	0.41
1:C:102:ASN:HD22	1:C:104:ASN:N	2.12	0.41
1:C:384:VAL:HG22	1:C:435:ILE:HB	2.02	0.41
1:A:92:LEU:HA	1:A:93:PRO:HD3	1.87	0.41
1:D:157:ARG:HD3	5:D:1077:HOH:O	2.21	0.41
1:A:48:CYS:O	1:B:445:LEU:HG	2.21	0.40
1:D:133:ALA:HB2	1:D:160:LYS:HB2	2.03	0.40
1:A:209:ARG:HB3	1:A:278:ASP:HB2	2.02	0.40
1:A:479:GLY:HA3	1:A:481:TYR:CZ	2.57	0.40
1:B:387:GLU:HG2	1:B:438:VAL:HG23	2.04	0.40
1:A:74:SER:HB3	1:A:114:HIS:O	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	564/568 (99%)	554 (98%)	10 (2%)	0	100	100
1	B	556/568 (98%)	536 (96%)	18 (3%)	2 (0%)	30	20
1	C	563/568 (99%)	551 (98%)	12 (2%)	0	100	100
1	D	552/568 (97%)	540 (98%)	12 (2%)	0	100	100
All	All	2235/2272 (98%)	2181 (98%)	52 (2%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	503	ASP
1	B	262	TRP

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	435/437 (100%)	431 (99%)	4 (1%)	70	67
1	B	430/437 (98%)	426 (99%)	4 (1%)	70	67
1	C	434/437 (99%)	428 (99%)	6 (1%)	59	54
1	D	430/437 (98%)	423 (98%)	7 (2%)	55	50
All	All	1729/1748 (99%)	1708 (99%)	21 (1%)	63	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	399	LYS
1	A	464	LEU
1	A	471	THR

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Mol	Chain	Res	Type
1	B	302	LYS
1	B	306	LEU
1	B	362	SER
1	B	449	GLU
1	C	13	LEU
1	C	264	GLU
1	C	266	SER
1	C	275	LYS
1	C	354	LYS
1	C	474	VAL
1	D	118	LYS
1	D	153	LYS
1	D	184	LEU
1	D	348	LEU
1	D	457	LYS
1	D	534	LEU
1	D	566	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	186	ASN
1	A	256	HIS
1	A	315	ASN
1	A	323	HIS
1	A	381	ASN
1	A	396	GLN
1	A	434	ASN
1	A	466	ASN
1	A	486	ASN
1	B	124	GLN
1	B	256	HIS
1	B	402	ASN
1	B	477	HIS
1	B	528	ASN
1	C	15	GLN
1	C	102	ASN
1	C	256	HIS
1	C	323	HIS
1	C	396	GLN
1	C	499	ASN

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Mol	Chain	Res	Type
1	C	565	ASN
1	D	186	ASN
1	D	196	ASN
1	D	256	HIS
1	D	323	HIS
1	D	396	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
3	TDL	A	611	2	28,33,33	1.15	4 (14%)	34,51,51	1.42	5 (14%)
3	TDL	D	611	2	28,33,33	1.10	4 (14%)	34,51,51	1.45	6 (17%)
4	GOL	D	570	-	5,5,5	0.36	0	5,5,5	0.37	0
3	TDL	C	611	2	28,33,33	1.13	4 (14%)	34,51,51	1.42	6 (17%)
3	TDL	B	611	2	28,33,33	1.16	4 (14%)	34,51,51	1.41	4 (11%)
4	GOL	D	569	-	5,5,5	0.41	0	5,5,5	0.32	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
3	TDL	A	611	2	-	6/26/29/29	0/2/2/2
3	TDL	D	611	2	-	6/26/29/29	0/2/2/2
4	GOL	D	570	-	-	3/4/4/4	-
3	TDL	C	611	2	-	8/26/29/29	0/2/2/2
3	TDL	B	611	2	-	9/26/29/29	0/2/2/2
4	GOL	D	569	-	-	4/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	TDL	PA-O3A	2.88	1.62	1.59
3	C	611	TDL	PA-O3A	2.84	1.62	1.59
3	B	611	TDL	PA-O3A	2.82	1.62	1.59
3	B	611	TDL	C5-C4	2.77	1.41	1.35
3	C	611	TDL	C5-C4	2.68	1.40	1.35
3	D	611	TDL	C5-C4	2.58	1.40	1.35
3	A	611	TDL	C5-C4	2.57	1.40	1.35
3	D	611	TDL	C5'-C4'	-2.46	1.38	1.42
3	D	611	TDL	C4-N3	-2.38	1.37	1.40
3	B	611	TDL	C4-N3	-2.38	1.37	1.40
3	A	611	TDL	C4-N3	-2.36	1.37	1.40
3	C	611	TDL	C5'-C4'	-2.17	1.39	1.42
3	A	611	TDL	C5'-C4'	-2.16	1.39	1.42
3	B	611	TDL	C5'-C4'	-2.10	1.39	1.42
3	C	611	TDL	C4-N3	-2.09	1.37	1.40
3	D	611	TDL	PA-O3A	2.06	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	611	TDL	N1'-C2'-N3'	-3.28	120.08	125.53
3	C	611	TDL	C6'-N1'-C2'	3.19	121.32	116.07
3	C	611	TDL	N1'-C2'-N3'	-3.15	120.28	125.53
3	A	611	TDL	C6'-N1'-C2'	3.15	121.25	116.07
3	B	611	TDL	CM2-C2'-N1'	3.13	120.54	117.20
3	B	611	TDL	N1'-C2'-N3'	-3.01	120.52	125.53
3	D	611	TDL	N1'-C2'-N3'	-2.87	120.76	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	611	TDL	C6'-N1'-C2'	2.82	120.71	116.07
3	D	611	TDL	C6'-N1'-C2'	2.73	120.55	116.07
3	C	611	TDL	CM2-C2'-N1'	2.65	120.02	117.20
3	A	611	TDL	CM2-C2'-N1'	2.64	120.01	117.20
3	D	611	TDL	C6'-C5'-C4'	2.44	118.55	115.55
3	C	611	TDL	CM4-C4-C5	-2.40	121.61	127.75
3	C	611	TDL	C5'-C6'-N1'	-2.36	119.99	123.83
3	D	611	TDL	C5'-C6'-N1'	-2.36	119.99	123.83
3	D	611	TDL	CM2-C2'-N1'	2.33	119.68	117.20
3	A	611	TDL	C5'-C6'-N1'	-2.24	120.18	123.83
3	B	611	TDL	C5'-C6'-N1'	-2.22	120.21	123.83
3	D	611	TDL	CM4-C4-C5	-2.17	122.19	127.75
3	C	611	TDL	O3B-PB-O2B	2.05	115.48	107.80
3	A	611	TDL	CM4-C4-C5	-2.01	122.61	127.75

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	611	TDL	OL1-CLA-CLC-OL2
3	B	611	TDL	PA-O3A-PB-O3B
3	B	611	TDL	S1-C2-CLA-OL1
3	B	611	TDL	C2-CLA-CLC-OL2
3	B	611	TDL	C2-CLA-CLC-OL3
3	B	611	TDL	OL1-CLA-CLC-OL2
3	B	611	TDL	OL1-CLA-CLC-OL3
3	C	611	TDL	PA-O3A-PB-O3B
3	C	611	TDL	S1-C2-CLA-OL1
3	C	611	TDL	C2-CLA-CLC-OL2
3	C	611	TDL	C2-CLA-CLC-OL3
3	C	611	TDL	OL1-CLA-CLC-OL2
3	C	611	TDL	OL1-CLA-CLC-OL3
3	D	611	TDL	C2-CLA-CLC-OL2
3	D	611	TDL	OL1-CLA-CLC-OL2
4	D	569	GOL	O1-C1-C2-C3
4	D	569	GOL	C1-C2-C3-O3
4	D	569	GOL	O2-C2-C3-O3
4	D	570	GOL	C1-C2-C3-O3
4	D	569	GOL	O1-C1-C2-O2
4	D	570	GOL	O2-C2-C3-O3
3	D	611	TDL	C2-CLA-CLC-OL3
3	D	611	TDL	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	B	611	TDL	C4'-C5'-C7'-N3
3	B	611	TDL	PA-O3A-PB-O1B
3	D	611	TDL	PB-O3A-PA-O1A
3	B	611	TDL	C6'-C5'-C7'-N3
3	A	611	TDL	PA-O3A-PB-O1B
3	A	611	TDL	PB-O3A-PA-O1A
3	A	611	TDL	S1-C2-CLA-OL1
3	D	611	TDL	S1-C2-CLA-OL1
3	C	611	TDL	PA-O3A-PB-O1B
3	C	611	TDL	PA-O3A-PB-O2B
4	D	570	GOL	O1-C1-C2-O2
3	A	611	TDL	OL1-CLA-CLC-OL3
3	A	611	TDL	PB-O3A-PA-O2A

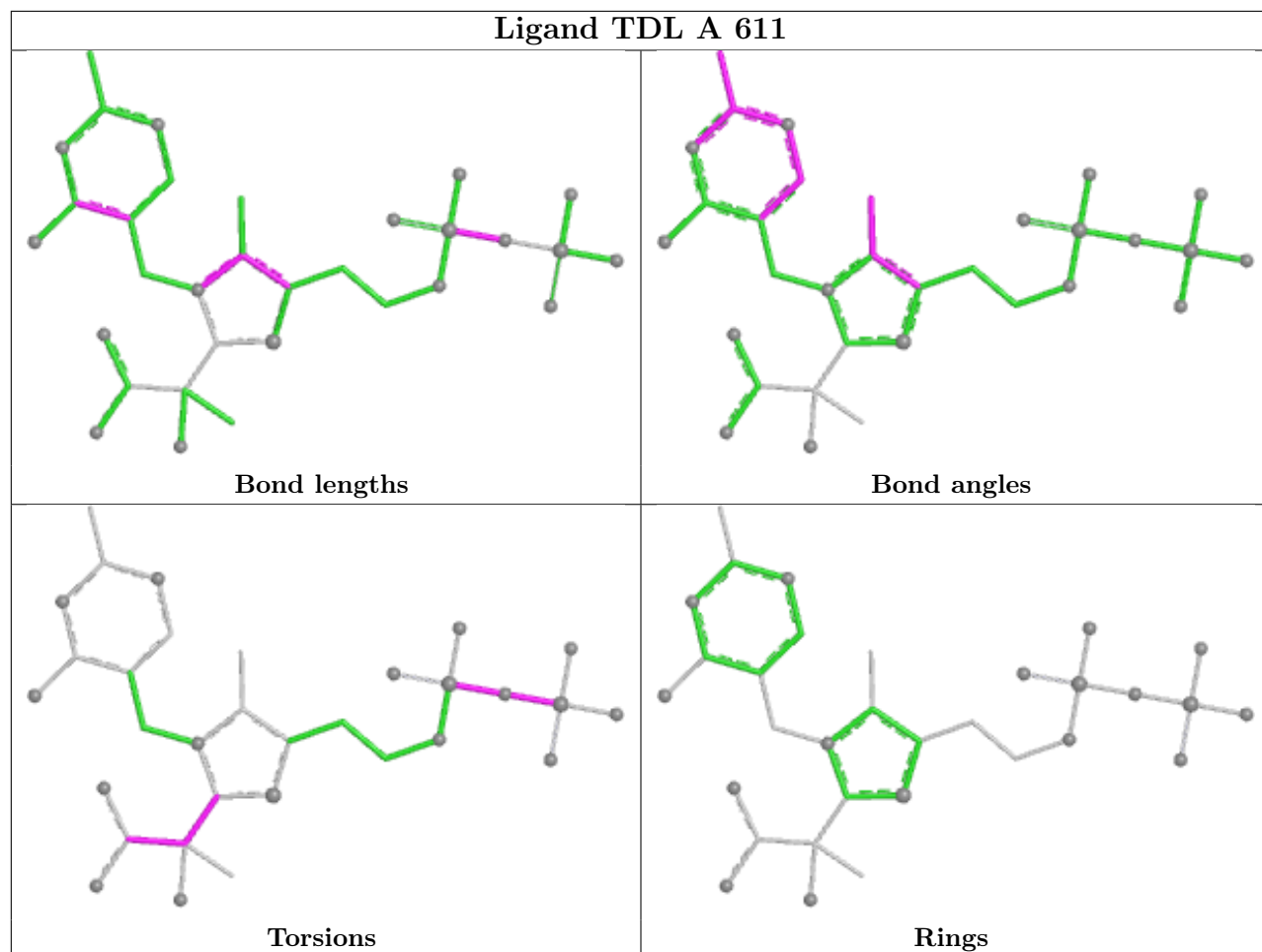
There are no ring outliers.

5 monomers are involved in 32 short contacts:

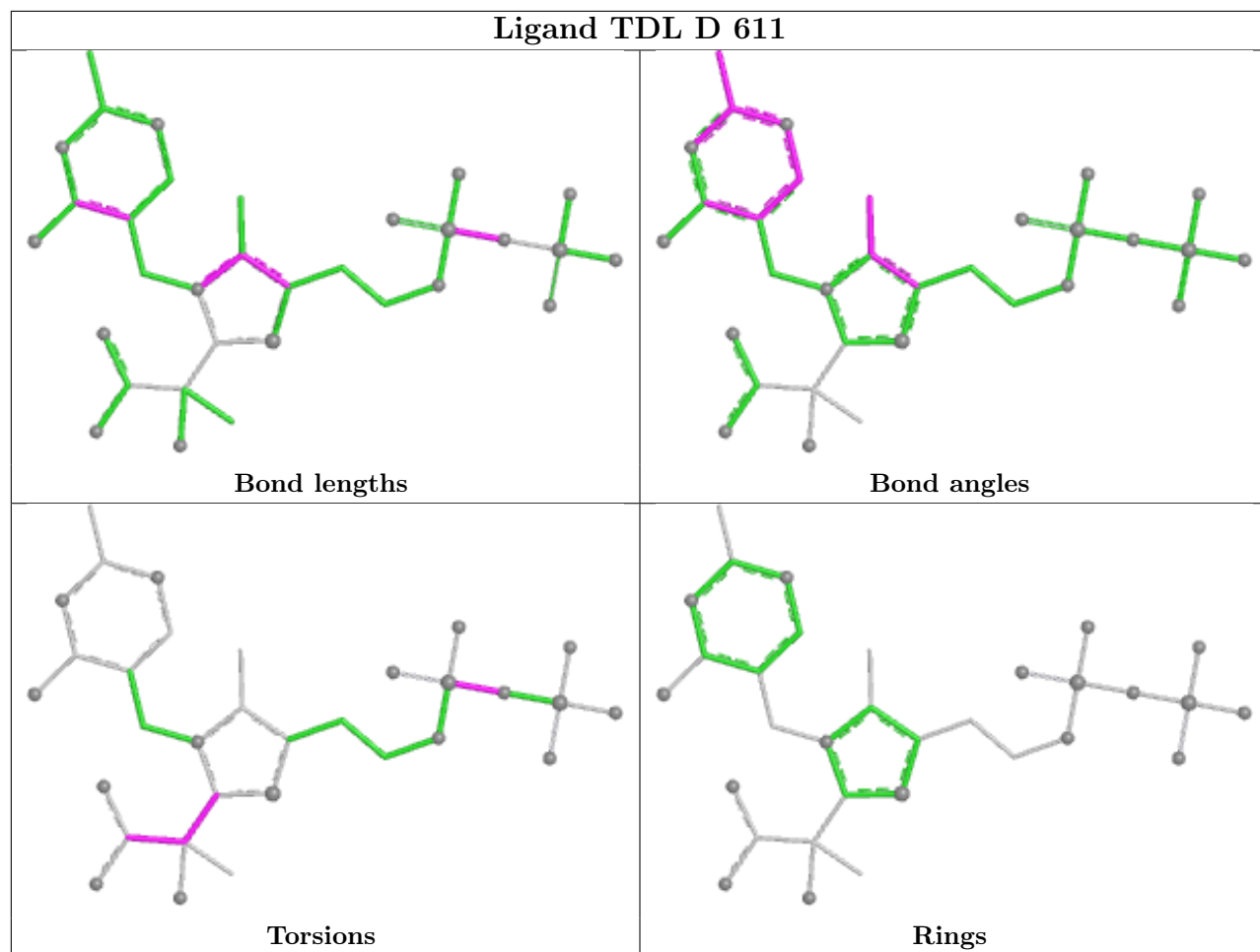
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	611	TDL	9	0
3	D	611	TDL	7	0
3	C	611	TDL	7	0
3	B	611	TDL	7	0
4	D	569	GOL	2	0

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.

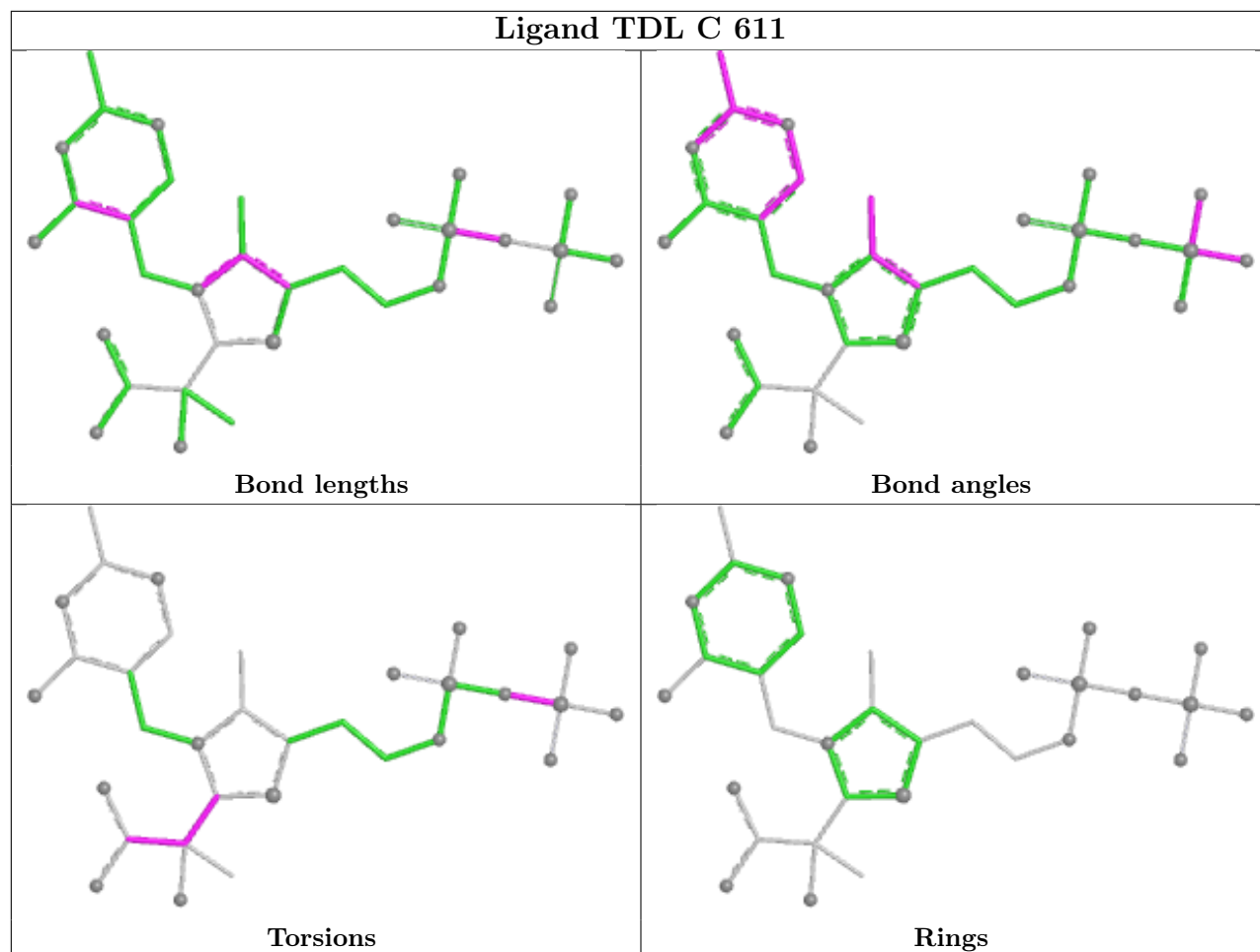
Ligand TDL A 611

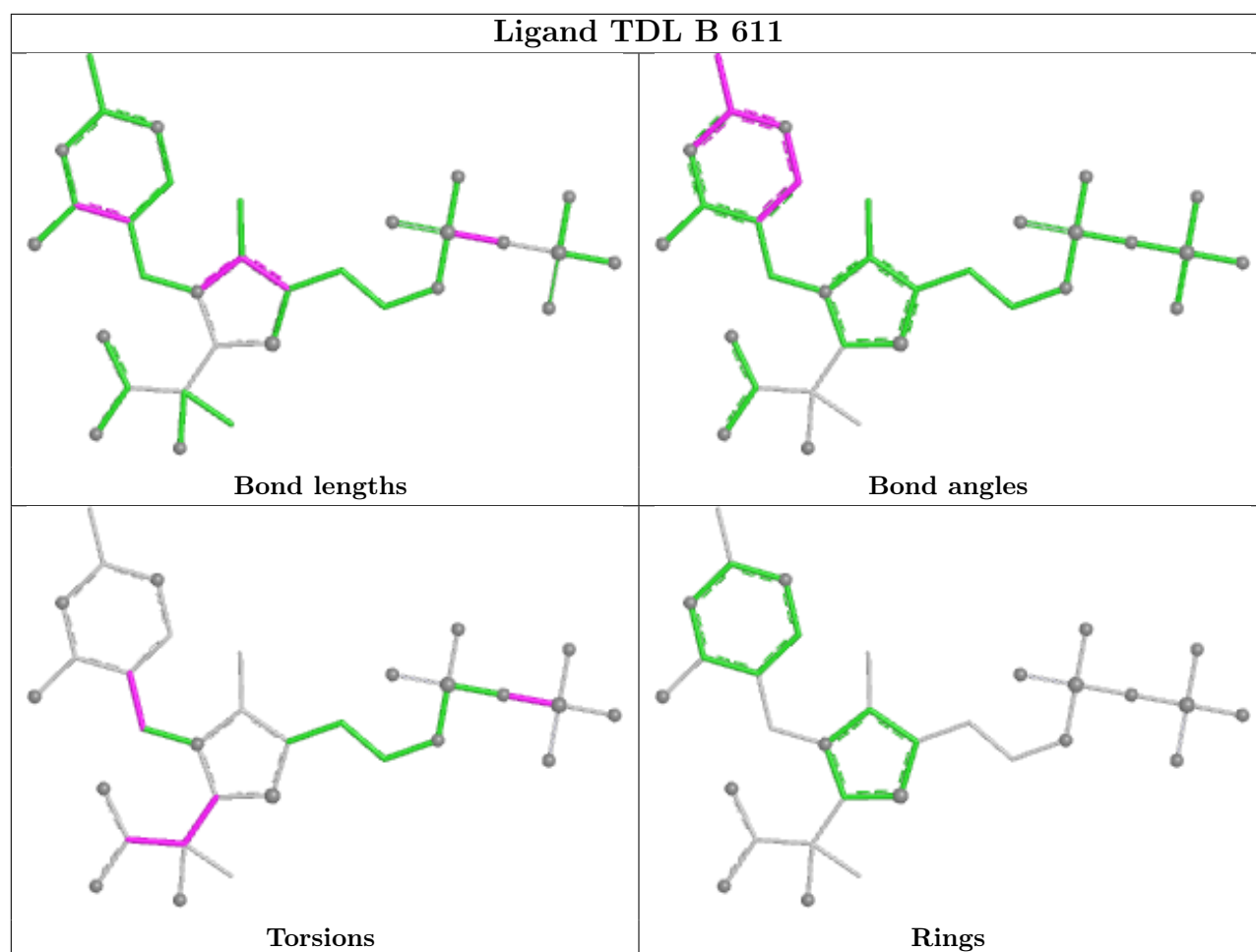


Ligand TDL D 611



Ligand TDL C 611





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	565/568 (99%)	-1.44	0 100 100	9, 22, 36, 50	53 (9%)
1	B	560/568 (98%)	-1.37	4 (0%) 84 89	3, 23, 35, 49	83 (14%)
1	C	565/568 (99%)	-1.32	0 100 100	9, 26, 43, 58	95 (16%)
1	D	555/568 (97%)	-1.39	2 (0%) 88 92	12, 23, 36, 53	56 (10%)
All	All	2245/2272 (98%)	-1.38	6 (0%) 90 93	3, 23, 38, 58	287 (12%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	ALA	4.1
1	B	356	ALA	3.6
1	B	358	PRO	2.8
1	D	361	PRO	2.4
1	B	359	ALA	2.2
1	D	363	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

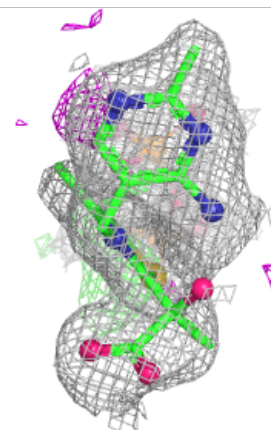
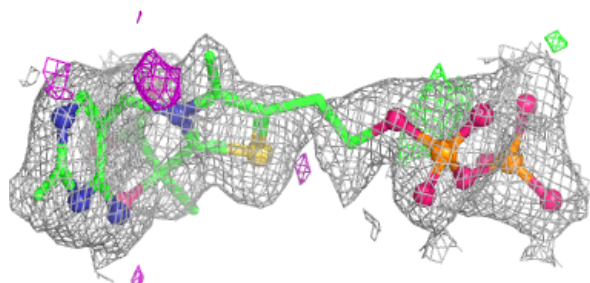
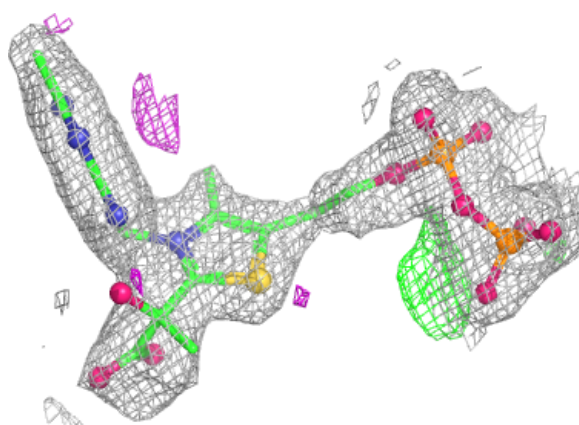
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	601	1/1	0.99	0.03	23,23,23,23	0
2	MG	B	601	1/1	0.99	0.03	26,26,26,26	0
2	MG	D	601	1/1	0.99	0.02	26,26,26,26	0
4	GOL	D	569	6/6	0.99	0.04	35,40,42,43	0
4	GOL	D	570	6/6	0.99	0.03	37,39,42,47	0
3	TDL	B	611	32/32	1.00	0.03	10,23,40,45	0
3	TDL	C	611	32/32	1.00	0.03	12,30,44,48	0
3	TDL	D	611	32/32	1.00	0.03	8,23,42,46	0
2	MG	C	601	1/1	1.00	0.05	24,24,24,24	0
3	TDL	A	611	32/32	1.00	0.02	10,23,46,49	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.

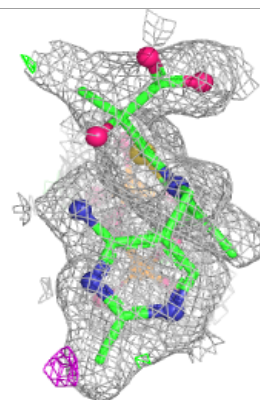
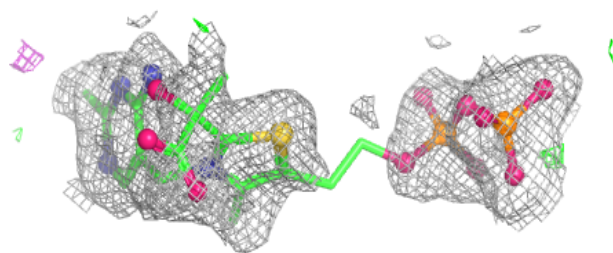
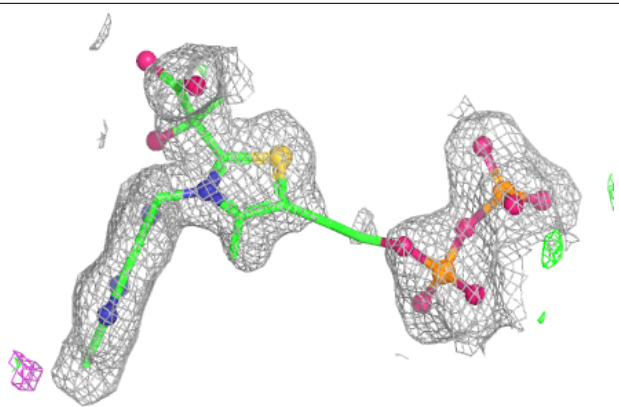
Electron density around TDL B 611:

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

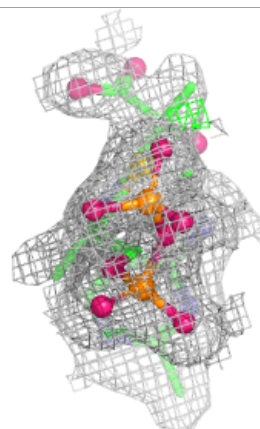
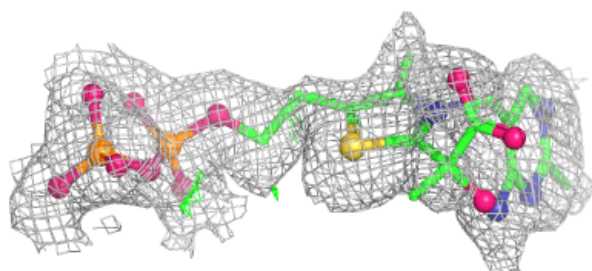
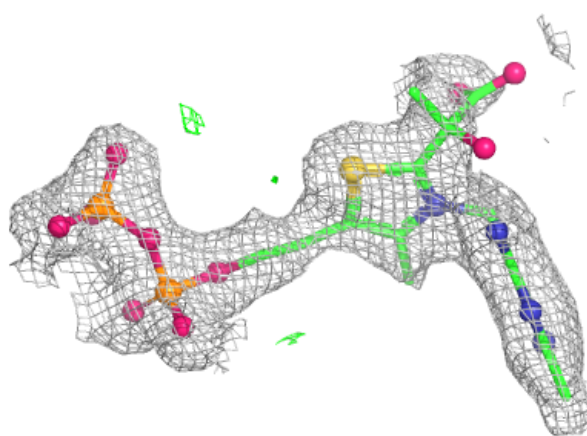


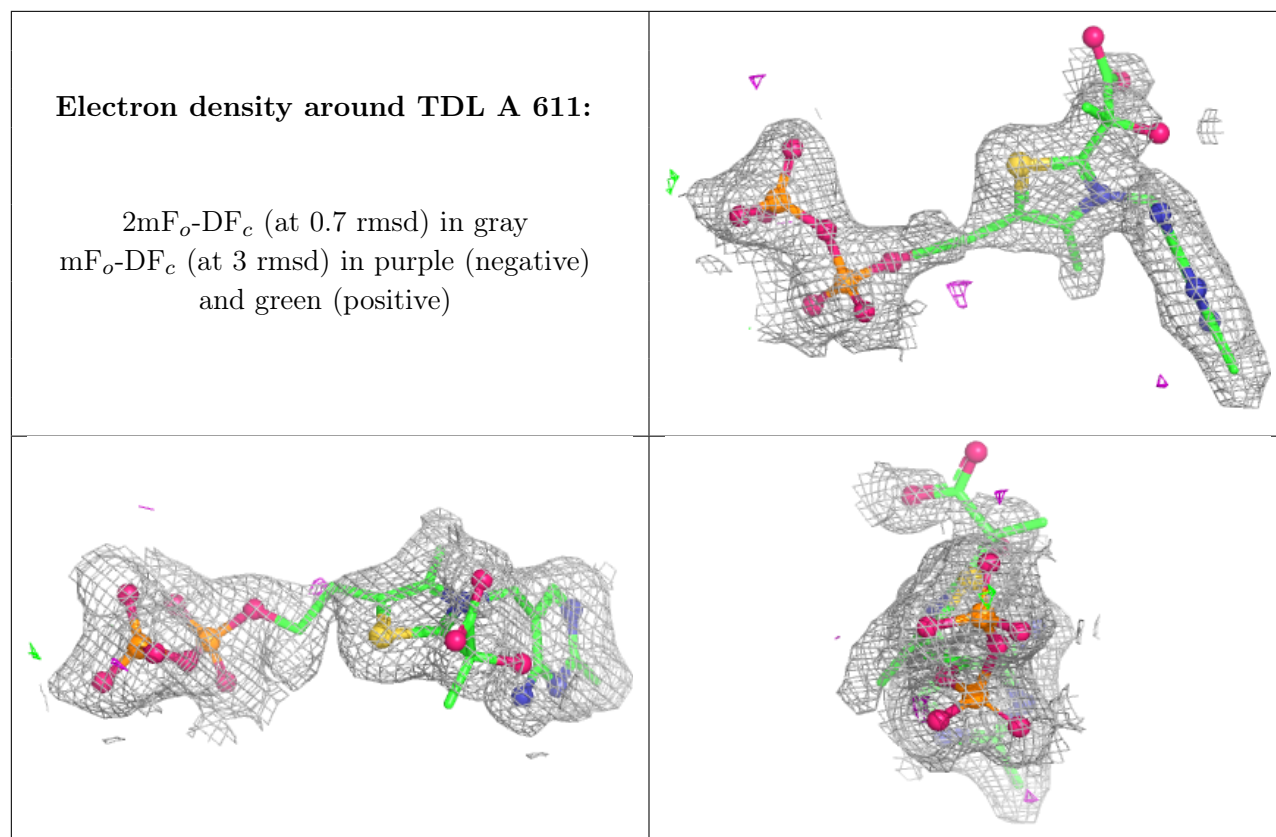
Electron density around TDL C 611:

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

**Electron density around TDL D 611:**

$2mF_o-DF_c$ (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.