



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:08 PM UTC

PDB ID : 4K9N / pdb_00004k9n
Title : Crystal Structure of the Ala460Ile mutant of Benzoylformate Decarboxylase from *Pseudomonas putida*
Authors : Brodtkin, H.R.; McLeish, M.J.
Deposited on : 2013-04-20
Resolution : 1.70 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

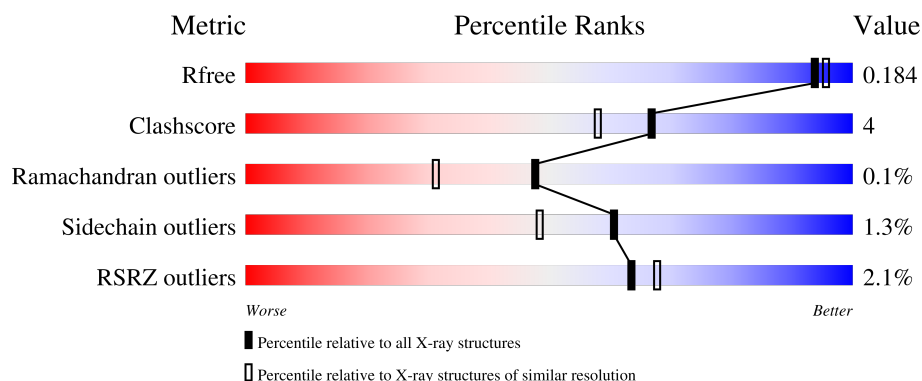
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	530	0% 92% 7% .
1	B	530	2% 92% 6% ..
1	C	530	3% 92% 5% ..
1	D	530	3% 91% 7% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17652 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 Benzoylformate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	6	0
			3969	2516	683	748	22			
1	B	524	Total	C	N	O	S	0	7	0
			3970	2516	683	750	21			
1	C	524	Total	C	N	O	S	0	7	0
			3972	2517	683	751	21			
1	D	524	Total	C	N	O	S	0	6	0
			3970	2516	683	750	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ILE	ALA	engineered mutation	UNP P20906
A	526	HIS	-	expression tag	UNP P20906
A	527	HIS	-	expression tag	UNP P20906
A	528	HIS	-	expression tag	UNP P20906
A	529	HIS	-	expression tag	UNP P20906
A	530	HIS	-	expression tag	UNP P20906
A	531	HIS	-	expression tag	UNP P20906
B	460	ILE	ALA	engineered mutation	UNP P20906
B	526	HIS	-	expression tag	UNP P20906
B	527	HIS	-	expression tag	UNP P20906
B	528	HIS	-	expression tag	UNP P20906
B	529	HIS	-	expression tag	UNP P20906
B	530	HIS	-	expression tag	UNP P20906
B	531	HIS	-	expression tag	UNP P20906
C	460	ILE	ALA	engineered mutation	UNP P20906
C	526	HIS	-	expression tag	UNP P20906
C	527	HIS	-	expression tag	UNP P20906
C	528	HIS	-	expression tag	UNP P20906
C	529	HIS	-	expression tag	UNP P20906
C	530	HIS	-	expression tag	UNP P20906
C	531	HIS	-	expression tag	UNP P20906

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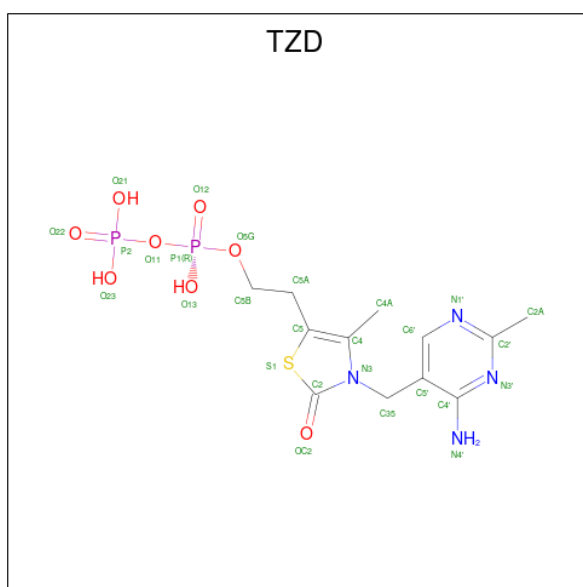
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Chain	Residue	Modelled	Actual	Comment	Reference
D	460	ILE	ALA	engineered mutation	UNP P20906
D	526	HIS	-	expression tag	UNP P20906
D	527	HIS	-	expression tag	UNP P20906
D	528	HIS	-	expression tag	UNP P20906
D	529	HIS	-	expression tag	UNP P20906
D	530	HIS	-	expression tag	UNP P20906
D	531	HIS	-	expression tag	UNP P20906

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

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

- Molecule 3 is 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TZD) (formula: $C_{12}H_{18}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	
			27	12	4	8	2	1	0
3	B	1	Total	C	N	O	P	S	
			27	12	4	8	2	1	0
3	C	1	Total	C	N	O	P	S	
			27	12	4	8	2	1	0
3	D	1	Total	C	N	O	P	S	
			27	12	4	8	2	1	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

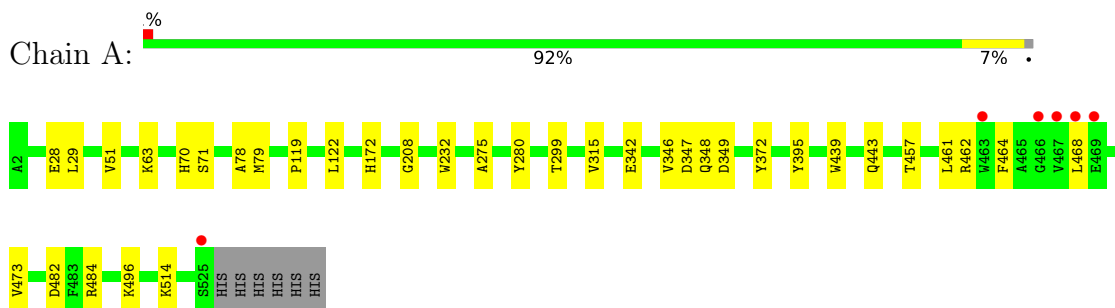
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	477	Total	O		
			477	477	0	0
5	B	458	Total	O		
			458	458	0	0
5	C	375	Total	O		
			375	375	0	0
5	D	341	Total	O		
			341	341	0	0

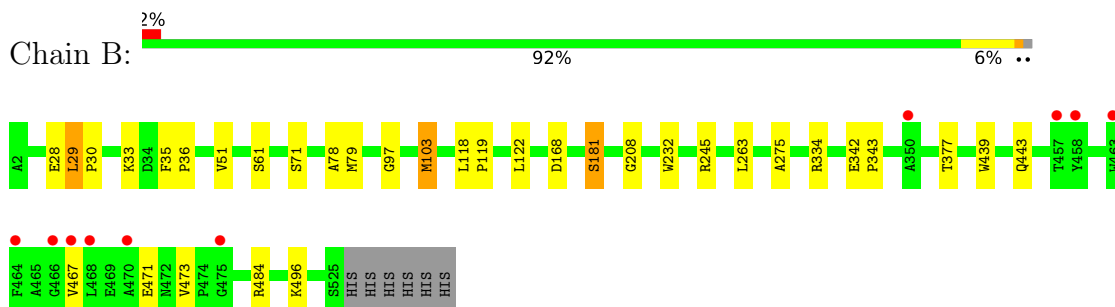
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

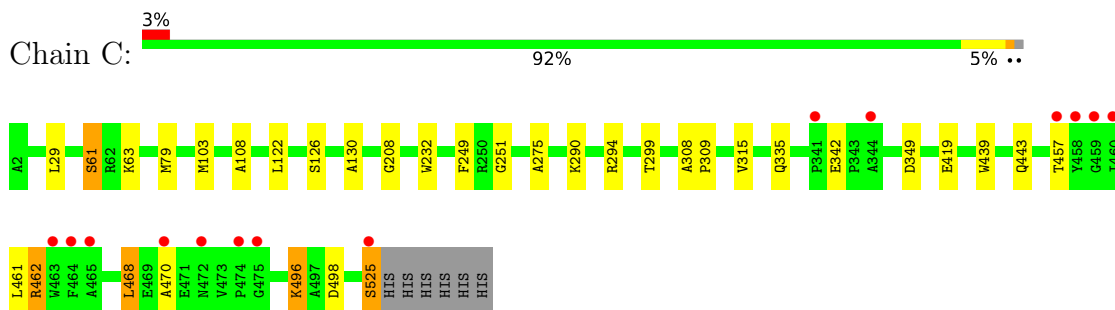
- Molecule 1: Benzoylformate decarboxylase



- Molecule 1: Benzoylformate decarboxylase

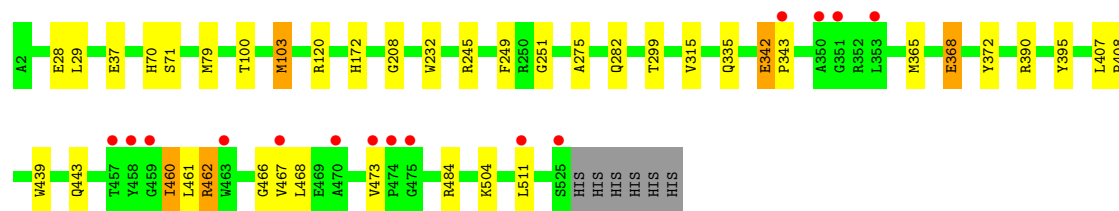


- Molecule 1: Benzoylformate decarboxylase



- Molecule 1: Benzoylformate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.64Å 163.50Å 175.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.72 – 1.70 38.72 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.1 (38.72-1.70) 89.2 (38.72-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.165 , 0.185 0.164 , 0.184	Depositor DCC
R_{free} test set	2004 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	1.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17652	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 2.61% 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: GOL, MG, TZD

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	0.61	0/4084	0.75	0/5581
1	B	0.58	0/4088	0.76	2/5587 (0.0%)
1	C	0.58	0/4090	0.77	2/5590 (0.0%)
1	D	0.52	0/4085	0.73	0/5583
All	All	0.57	0/16347	0.75	4/22341 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	5
1	D	0	2
All	All	0	11

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	LYS	CA-C-N	-5.50	114.11	119.78
1	C	290	LYS	C-N-CA	-5.50	114.11	119.78
1	B	71	SER	CB-CA-C	-5.42	109.34	115.79
1	B	377	THR	N-CA-C	5.30	117.80	111.71

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232[A]	TRP	Mainchain
1	A	232[B]	TRP	Mainchain
1	B	181[B]	SER	Mainchain
1	B	61[B]	SER	Mainchain
1	C	126	SER	Mainchain
1	C	232[A]	TRP	Mainchain
1	C	232[B]	TRP	Mainchain
1	C	61[A]	SER	Mainchain
1	C	61[B]	SER	Mainchain
1	D	232[A]	TRP	Mainchain
1	D	232[B]	TRP	Mainchain

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	3969	0	3916	40	0
1	B	3970	0	3917	33	0
1	C	3972	0	3916	31	2
1	D	3970	0	3913	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	15	1	0
3	B	27	0	15	0	0
3	C	27	0	15	1	0
3	D	27	0	15	1	0
4	C	6	0	8	1	0
5	A	477	0	0	11	0
5	B	458	0	0	6	3
5	C	375	0	0	3	0
5	D	341	0	0	5	1
All	All	17652	0	15730	118	3

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 4.

All (118) 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:B:79[B]:MET:HE1	1:D:79[B]:MET:HE1	1.26	1.09
1:A:79[B]:MET:HE1	1:C:79[B]:MET:CE	1.84	1.05
1:A:79[B]:MET:HE1	1:C:79[B]:MET:HE1	1.06	1.03
1:A:79[B]:MET:CE	1:C:79[B]:MET:HE1	1.91	0.99
1:B:79[B]:MET:CE	1:D:79[B]:MET:HE1	1.98	0.92
1:A:63:LYS:NZ	5:A:1096:HOH:O	2.01	0.87
1:B:79[B]:MET:HE1	1:D:79[B]:MET:CE	2.05	0.87
1:A:342:GLU:HG2	5:A:1033:HOH:O	1.76	0.85
1:A:79[B]:MET:CE	1:C:79[B]:MET:CE	2.51	0.85
1:B:79[B]:MET:SD	1:D:79[B]:MET:CE	2.66	0.83
1:B:79[B]:MET:CE	1:D:79[B]:MET:CE	2.61	0.78
1:A:79[B]:MET:CE	1:C:79[B]:MET:SD	2.74	0.75
1:A:342:GLU:OE2	5:A:1033:HOH:O	2.03	0.74
1:D:439:TRP:CZ2	1:D:443:GLN:HG3	2.24	0.71
1:A:342:GLU:CG	5:A:1033:HOH:O	2.36	0.71
1:D:511:LEU:O	5:D:1032:HOH:O	2.08	0.71
1:A:484:ARG:HD3	5:A:1135:HOH:O	1.90	0.70
1:B:79[B]:MET:SD	1:D:79[B]:MET:HE2	2.32	0.70
1:B:79[B]:MET:CE	1:D:79[B]:MET:SD	2.79	0.70
1:C:457:THR:OG1	1:C:462:ARG:HD2	1.93	0.69
1:A:79[B]:MET:SD	1:C:79[B]:MET:CE	2.83	0.67
1:B:439:TRP:CZ2	1:B:443:GLN:HG3	2.29	0.66
1:A:468:LEU:HD21	5:C:1051:HOH:O	1.96	0.66
1:D:120:ARG:NH1	5:D:958:HOH:O	2.24	0.66
1:B:484:ARG:HD3	5:B:948:HOH:O	1.96	0.66
1:D:172:HIS:HD2	5:D:1028:HOH:O	1.81	0.64
1:A:79[B]:MET:HE2	1:C:79[B]:MET:SD	2.38	0.64
1:C:439:TRP:CZ2	1:C:443:GLN:HG3	2.32	0.63
1:A:342:GLU:CD	5:A:1033:HOH:O	2.41	0.62
1:C:79[A]:MET:HE3	1:C:122:LEU:HD12	1.82	0.61
1:A:439:TRP:CZ2	1:A:443:GLN:HG3	2.36	0.60
1:D:439:TRP:CE2	1:D:443:GLN:HG3	2.36	0.59
1:D:484:ARG:HD3	5:D:882:HOH:O	2.02	0.58
1:C:130:ALA:HA	4:C:603:GOL:H31	1.85	0.58
1:B:79[B]:MET:SD	1:D:79[B]:MET:HE1	2.41	0.57
1:A:347:ASP:HA	5:A:988:HOH:O	2.05	0.57
1:B:439:TRP:CE2	1:B:443:GLN:HG3	2.40	0.57
1:A:63:LYS:HE3	5:A:854:HOH:O	2.05	0.56
1:A:484:ARG:HD2	1:A:496:LYS:HD2	1.87	0.56
1:A:79[B]:MET:SD	1:C:79[B]:MET:HE2	2.45	0.56
1:B:181[B]:SER:HB2	5:B:1057:HOH:O	2.04	0.56
1:A:348:GLN:O	5:A:943:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:VAL:HG11	1:C:29:LEU:HD22	1.88	0.56
1:C:61[B]:SER:HB3	1:C:63:LYS:HG2	1.87	0.56
1:B:208:GLY:HA3	1:B:275:ALA:HB2	1.87	0.55
1:A:172:HIS:HD2	5:A:1002:HOH:O	1.89	0.55
1:D:100:THR:CG2	1:D:103[B]:MET:HG3	2.37	0.55
1:A:461:LEU:HD11	3:A:603:TZD:H4A2	1.89	0.55
1:C:461:LEU:HD11	3:C:602:TZD:H4A2	1.90	0.54
1:D:208:GLY:HA3	1:D:275:ALA:HB2	1.89	0.54
1:C:457:THR:OG1	1:C:462:ARG:CD	2.56	0.54
1:B:79[B]:MET:HE2	1:D:79[B]:MET:SD	2.48	0.53
1:A:208:GLY:HA3	1:A:275:ALA:HB2	1.91	0.53
1:B:103[A]:MET:HE1	1:D:282:GLN:O	2.09	0.53
1:B:168:ASP:OD2	5:B:1077:HOH:O	2.19	0.52
1:D:461:LEU:HD11	3:D:602:TZD:H4A2	1.92	0.52
1:A:79[A]:MET:HE3	1:A:122:LEU:HD12	1.91	0.51
1:C:103[B]:MET:HE3	1:C:108:ALA:HB2	1.92	0.51
1:B:28:GLU:OE2	1:B:97:GLY:HA3	2.10	0.51
1:D:368:GLU:HG2	1:D:390:ARG:CZ	2.39	0.51
1:A:280:TYR:CB	1:C:103[B]:MET:HE1	2.41	0.50
1:A:28:GLU:OE2	1:A:70:HIS:HA	2.12	0.49
1:B:33:LYS:HA	1:D:473:VAL:HG22	1.95	0.49
1:C:249:PHE:CE2	1:C:251:GLY:HA2	2.47	0.48
1:C:208:GLY:HA3	1:C:275:ALA:HB2	1.95	0.48
1:C:335:GLN:HB2	5:C:1030:HOH:O	2.13	0.48
1:B:245:ARG:NH1	5:B:808:HOH:O	2.28	0.47
1:A:79[A]:MET:CE	1:A:119:PRO:HA	2.45	0.47
1:A:439:TRP:CE2	1:A:443:GLN:HG3	2.49	0.47
1:B:473:VAL:HG11	1:D:29:LEU:HD22	1.97	0.46
1:A:484:ARG:HD2	1:A:496:LYS:CD	2.45	0.46
1:C:439:TRP:CE2	1:C:443:GLN:HG3	2.51	0.45
1:D:100:THR:HG23	1:D:103[B]:MET:HG3	1.98	0.45
1:D:249:PHE:CE2	1:D:251:GLY:HA2	2.52	0.45
1:D:342:GLU:HG3	1:D:343:PRO:HD2	1.98	0.45
1:B:232[B]:TRP:HZ3	5:B:1110:HOH:O	2.00	0.44
1:D:368:GLU:CG	1:D:390:ARG:NH1	2.81	0.44
1:A:280:TYR:HB2	1:C:103[B]:MET:HE1	1.99	0.44
1:D:299:THR:O	1:D:315:VAL:HA	2.18	0.44
1:D:466:GLY:C	1:D:468:LEU:N	2.75	0.44
1:B:79[A]:MET:HE3	1:B:122:LEU:HD12	2.00	0.44
1:D:462:ARG:CG	1:D:462:ARG:HH11	2.31	0.43
1:A:346:VAL:HG22	5:A:916:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HB3	1:B:119:PRO:HD3	2.00	0.43
1:C:79[A]:MET:CE	1:C:122:LEU:HD12	2.48	0.43
1:D:365:MET:HE1	1:D:504:LYS:HG2	1.99	0.43
1:B:79[B]:MET:HE1	1:D:79[B]:MET:SD	2.56	0.43
1:D:28:GLU:OE2	1:D:70:HIS:HA	2.18	0.43
1:D:245:ARG:NH1	5:D:819:HOH:O	2.44	0.43
1:A:28:GLU:CD	1:A:70:HIS:HA	2.44	0.42
1:B:484:ARG:HD2	1:B:496:LYS:HB3	2.01	0.42
1:A:464:PHE:HE2	5:C:1052:HOH:O	2.02	0.42
1:A:299:THR:O	1:A:315:VAL:HA	2.20	0.42
1:A:372:TYR:O	1:A:395:TYR:HA	2.20	0.42
1:C:496:LYS:HE3	1:C:498:ASP:OD2	2.20	0.42
1:D:372:TYR:O	1:D:395:TYR:HA	2.20	0.42
1:B:29:LEU:CB	1:B:30:PRO:HD3	2.50	0.42
1:A:51:VAL:HG21	1:A:78:ALA:HB1	2.01	0.41
1:C:308:ALA:HA	1:C:309:PRO:HD3	1.95	0.41
1:D:407:LEU:HB3	1:D:408:PRO:CD	2.50	0.41
1:D:460:ILE:HD12	1:D:460:ILE:HA	1.83	0.41
1:B:29:LEU:HB2	1:B:30:PRO:HD3	2.01	0.41
1:A:457:THR:OG1	1:A:462:ARG:HD2	2.21	0.41
1:C:525:SER:O	1:C:525:SER:OG	2.34	0.41
1:B:334:ARG:NE	5:B:1060:HOH:O	2.51	0.41
1:B:79[B]:MET:SD	1:D:79[B]:MET:SD	3.18	0.41
1:C:299:THR:O	1:C:315:VAL:HA	2.21	0.41
1:C:439:TRP:CH2	1:C:443:GLN:HG3	2.56	0.41
1:D:368:GLU:HG2	1:D:390:ARG:NH1	2.35	0.41
1:D:468:LEU:HD23	1:D:468:LEU:HA	1.86	0.41
1:B:35:PHE:HA	1:B:36:PRO:HD3	1.95	0.41
1:A:349:ASP:C	1:A:349:ASP:OD1	2.64	0.41
1:B:51:VAL:HG21	1:B:78:ALA:HB1	2.03	0.41
1:C:468:LEU:C	1:C:470:ALA:N	2.77	0.40
1:B:29:LEU:HA	1:B:29:LEU:HD22	1.75	0.40
1:C:349:ASP:OD1	1:C:349:ASP:C	2.64	0.40
1:A:482:ASP:OD1	1:A:482:ASP:C	2.63	0.40
1:B:342:GLU:HG3	1:B:343:PRO:HD2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:GLU:OE1	5:B:1126:HOH:O[2_375]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:GLU:CG	5:B:1126:HOH:O[2_375]	2.17	0.03
5:B:1120:HOH:O	5:D:872:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/530 (100%)	522 (99%)	5 (1%)	1 (0%)	43	28
1	B	529/530 (100%)	522 (99%)	7 (1%)	0	100	100
1	C	529/530 (100%)	521 (98%)	8 (2%)	0	100	100
1	D	528/530 (100%)	518 (98%)	9 (2%)	1 (0%)	43	28
All	All	2114/2120 (100%)	2083 (98%)	29 (1%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	D	71	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/417 (100%)	415 (100%)	2 (0%)	81	76
1	B	418/417 (100%)	412 (99%)	6 (1%)	59	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	418/417 (100%)	412 (99%)	6 (1%)	59	46
1	D	417/417 (100%)	408 (98%)	9 (2%)	45	29
All	All	1670/1668 (100%)	1647 (99%)	23 (1%)	61	46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	514	LYS
1	B	29	LEU
1	B	103[A]	MET
1	B	103[B]	MET
1	B	263	LEU
1	B	467	VAL
1	B	471	GLU
1	C	294	ARG
1	C	342	GLU
1	C	462	ARG
1	C	468	LEU
1	C	496	LYS
1	C	525	SER
1	D	37	GLU
1	D	103[A]	MET
1	D	103[B]	MET
1	D	335	GLN
1	D	342	GLU
1	D	368	GLU
1	D	460	ILE
1	D	462	ARG
1	D	467	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	59	GLN
1	A	151	GLN
1	A	172	HIS
1	A	215	ASN
1	B	23	ASN

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Mol	Chain	Res	Type
1	B	151	GLN
1	B	172	HIS
1	B	215	ASN
1	C	59	GLN
1	C	151	GLN
1	C	172	HIS
1	C	327	ASN
1	D	59	GLN
1	D	151	GLN
1	D	172	HIS
1	D	391	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](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	TZD	D	602	2	27,28,28	2.09	6 (22%)	37,42,42	2.52	9 (24%)
4	GOL	C	603	-	5,5,5	0.24	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TZD	B	603	2	27,28,28	2.07	6 (22%)	37,42,42	2.53	9 (24%)
3	TZD	A	603	2	27,28,28	2.09	6 (22%)	37,42,42	2.54	8 (21%)
3	TZD	C	602	2	27,28,28	2.08	6 (22%)	37,42,42	2.48	8 (21%)

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	TZD	D	602	2	-	0/17/17/17	0/2/2/2
4	GOL	C	603	-	-	2/4/4/4	-
3	TZD	B	603	2	-	1/17/17/17	0/2/2/2
3	TZD	A	603	2	-	1/17/17/17	0/2/2/2
3	TZD	C	602	2	-	0/17/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	TZD	C5-C4	7.13	1.50	1.35
3	C	602	TZD	C5-C4	7.10	1.49	1.35
3	A	603	TZD	C5-C4	7.06	1.49	1.35
3	B	603	TZD	C5-C4	7.02	1.49	1.35
3	D	602	TZD	OC2-C2	4.77	1.28	1.21
3	A	603	TZD	OC2-C2	4.75	1.28	1.21
3	C	602	TZD	OC2-C2	4.74	1.28	1.21
3	B	603	TZD	OC2-C2	4.72	1.28	1.21
3	D	602	TZD	C5'-C4'	3.51	1.48	1.42
3	A	603	TZD	C5'-C4'	3.49	1.48	1.42
3	B	603	TZD	C5'-C4'	3.46	1.48	1.42
3	C	602	TZD	C5'-C4'	3.45	1.48	1.42
3	A	603	TZD	C2-S1	-3.26	1.73	1.77
3	C	602	TZD	C2-S1	-3.22	1.73	1.77
3	B	603	TZD	C2-S1	-3.13	1.74	1.77
3	D	602	TZD	C2-S1	-3.13	1.74	1.77
3	D	602	TZD	C2-N3	-2.61	1.34	1.38
3	B	603	TZD	C2-N3	-2.60	1.34	1.38
3	A	603	TZD	C2-N3	-2.58	1.34	1.38
3	C	602	TZD	C2-N3	-2.55	1.34	1.38
3	A	603	TZD	C4-N3	-2.30	1.35	1.39
3	B	603	TZD	C4-N3	-2.23	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	TZD	C4-N3	-2.17	1.35	1.39
3	D	602	TZD	C4-N3	-2.15	1.35	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	TZD	C5-S1-C2	-9.29	87.18	91.64
3	A	603	TZD	C5-S1-C2	-9.28	87.18	91.64
3	D	602	TZD	C5-S1-C2	-9.07	87.28	91.64
3	C	602	TZD	C5-S1-C2	-8.94	87.35	91.64
3	D	602	TZD	S1-C2-N3	7.54	118.36	110.22
3	B	603	TZD	S1-C2-N3	7.54	118.36	110.22
3	A	603	TZD	S1-C2-N3	7.54	118.36	110.22
3	C	602	TZD	S1-C2-N3	7.46	118.27	110.22
3	D	602	TZD	OC2-C2-N3	-3.96	120.72	125.37
3	A	603	TZD	OC2-C2-N3	-3.91	120.78	125.37
3	B	603	TZD	OC2-C2-N3	-3.79	120.93	125.37
3	C	602	TZD	OC2-C2-N3	-3.70	121.03	125.37
3	A	603	TZD	C6'-N1'-C2'	3.63	122.04	116.07
3	D	602	TZD	C6'-N1'-C2'	3.62	122.02	116.07
3	B	603	TZD	C6'-N1'-C2'	3.61	122.00	116.07
3	C	602	TZD	C6'-N1'-C2'	3.59	121.96	116.07
3	C	602	TZD	OC2-C2-S1	-3.23	120.70	125.00
3	B	603	TZD	OC2-C2-S1	-3.23	120.71	125.00
3	A	603	TZD	OC2-C2-S1	-3.11	120.86	125.00
3	D	602	TZD	OC2-C2-S1	-3.07	120.91	125.00
3	D	602	TZD	N4'-C4'-N3'	2.83	120.84	117.03
3	A	603	TZD	N4'-C4'-N3'	2.74	120.72	117.03
3	B	603	TZD	N4'-C4'-N3'	2.73	120.71	117.03
3	C	602	TZD	N4'-C4'-N3'	2.70	120.68	117.03
3	D	602	TZD	C5'-C6'-N1'	-2.62	119.57	123.83
3	C	602	TZD	C5'-C6'-N1'	-2.62	119.58	123.83
3	A	603	TZD	C5'-C6'-N1'	-2.60	119.60	123.83
3	B	603	TZD	C5'-C6'-N1'	-2.59	119.61	123.83
3	A	603	TZD	N1'-C2'-N3'	-2.37	121.59	125.53
3	B	603	TZD	N1'-C2'-N3'	-2.35	121.63	125.53
3	D	602	TZD	N1'-C2'-N3'	-2.34	121.64	125.53
3	C	602	TZD	N1'-C2'-N3'	-2.27	121.75	125.53
3	B	603	TZD	C5'-C4'-N3'	-2.01	118.37	121.31
3	D	602	TZD	C5'-C4'-N3'	-2.01	118.37	121.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

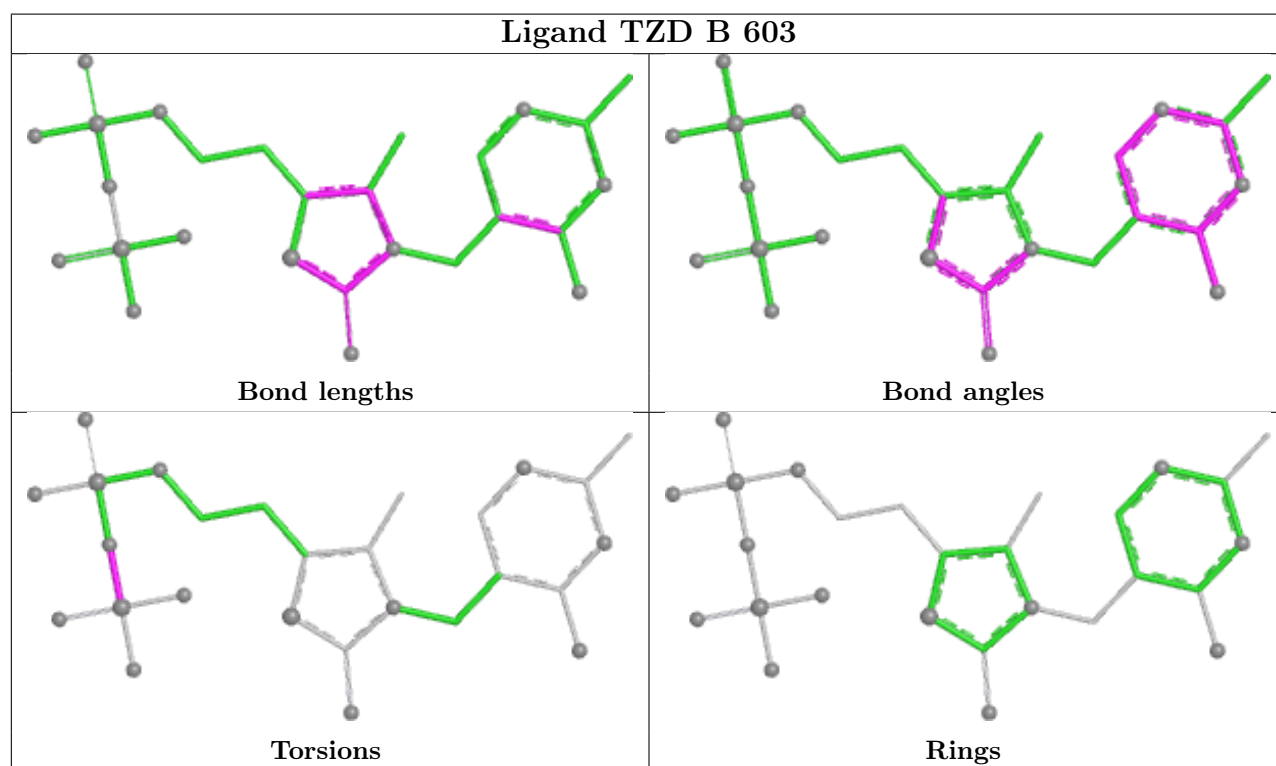
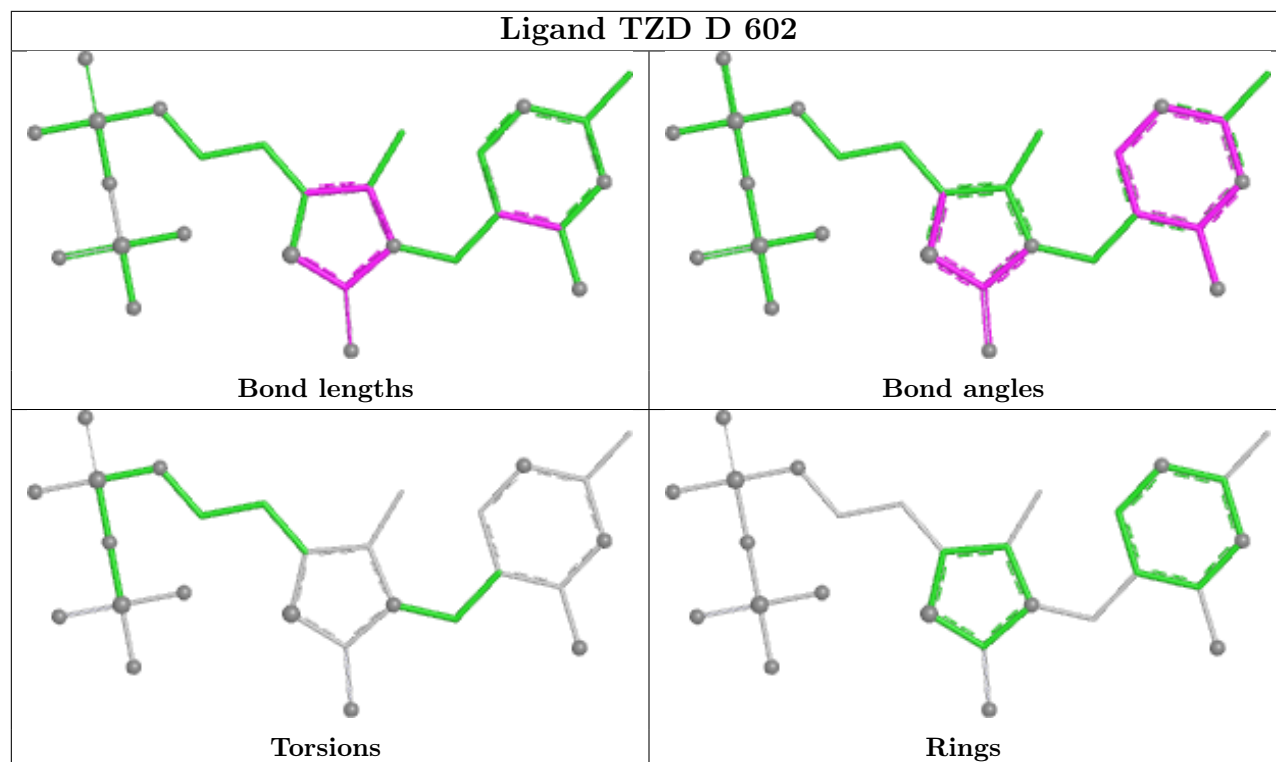
Mol	Chain	Res	Type	Atoms
4	C	603	GOL	C1-C2-C3-O3
4	C	603	GOL	O2-C2-C3-O3
3	A	603	TZD	P1-O11-P2-O22
3	B	603	TZD	P1-O11-P2-O22

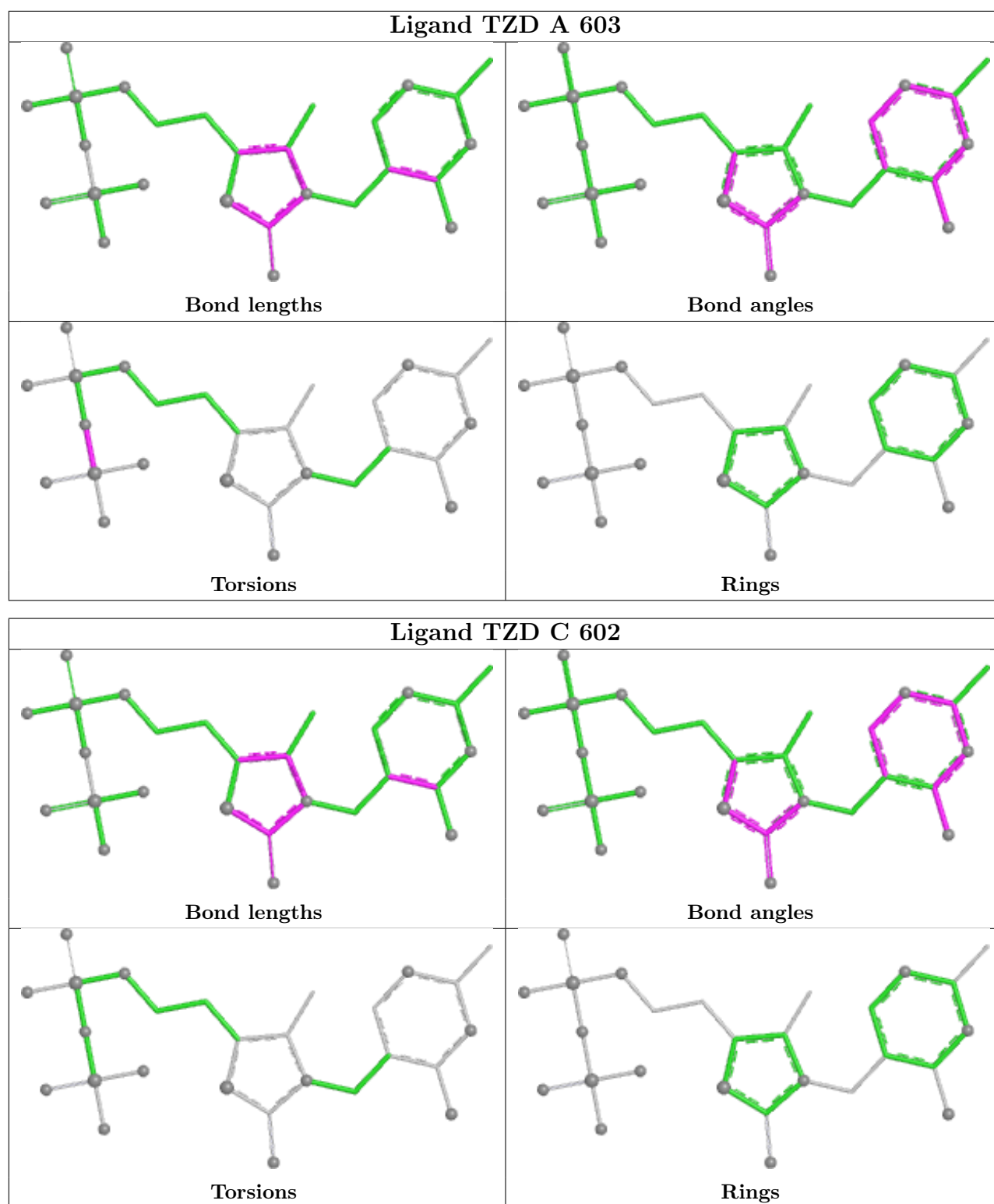
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	TZD	1	0
4	C	603	GOL	1	0
3	A	603	TZD	1	0
3	C	602	TZD	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 ⓘ

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	524/530 (98%)	-0.17	6 (1%) 78 81	12, 21, 32, 63	12 (2%)
1	B	524/530 (98%)	-0.10	10 (1%) 66 71	13, 22, 37, 64	9 (1%)
1	C	524/530 (98%)	0.01	14 (2%) 56 60	12, 23, 40, 61	10 (1%)
1	D	524/530 (98%)	0.22	15 (2%) 53 58	13, 27, 48, 66	9 (1%)
All	All	2096/2120 (98%)	-0.01	45 (2%) 63 68	12, 23, 42, 66	40 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	VAL	4.8
1	B	470	ALA	4.2
1	B	475	GLY	3.7
1	D	470	ALA	3.6
1	A	525	SER	3.5
1	A	463	TRP	3.5
1	C	470	ALA	3.4
1	D	459	GLY	3.3
1	C	459	GLY	3.2
1	C	475	GLY	3.0
1	C	344	ALA	3.0
1	B	466	GLY	2.9
1	C	463	TRP	2.9
1	D	511	LEU	2.8
1	D	350	ALA	2.7
1	D	525	SER	2.7
1	B	468	LEU	2.7
1	D	473	VAL	2.7
1	D	474	PRO	2.6
1	C	458	TYR	2.6
1	C	460	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	466	GLY	2.6
1	B	464	PHE	2.6
1	D	343	PRO	2.5
1	D	457	THR	2.5
1	C	464	PHE	2.5
1	D	467	VAL	2.5
1	A	468	LEU	2.4
1	C	472	ASN	2.4
1	B	463	TRP	2.4
1	C	525	SER	2.3
1	D	475	GLY	2.3
1	C	474	PRO	2.3
1	B	457	THR	2.3
1	B	467	VAL	2.3
1	D	463	TRP	2.2
1	C	457	THR	2.2
1	D	353	LEU	2.2
1	B	458	TYR	2.2
1	D	458	TYR	2.2
1	C	465	ALA	2.1
1	D	351	GLY	2.1
1	B	350	ALA	2.0
1	C	341	PRO	2.0
1	A	469	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

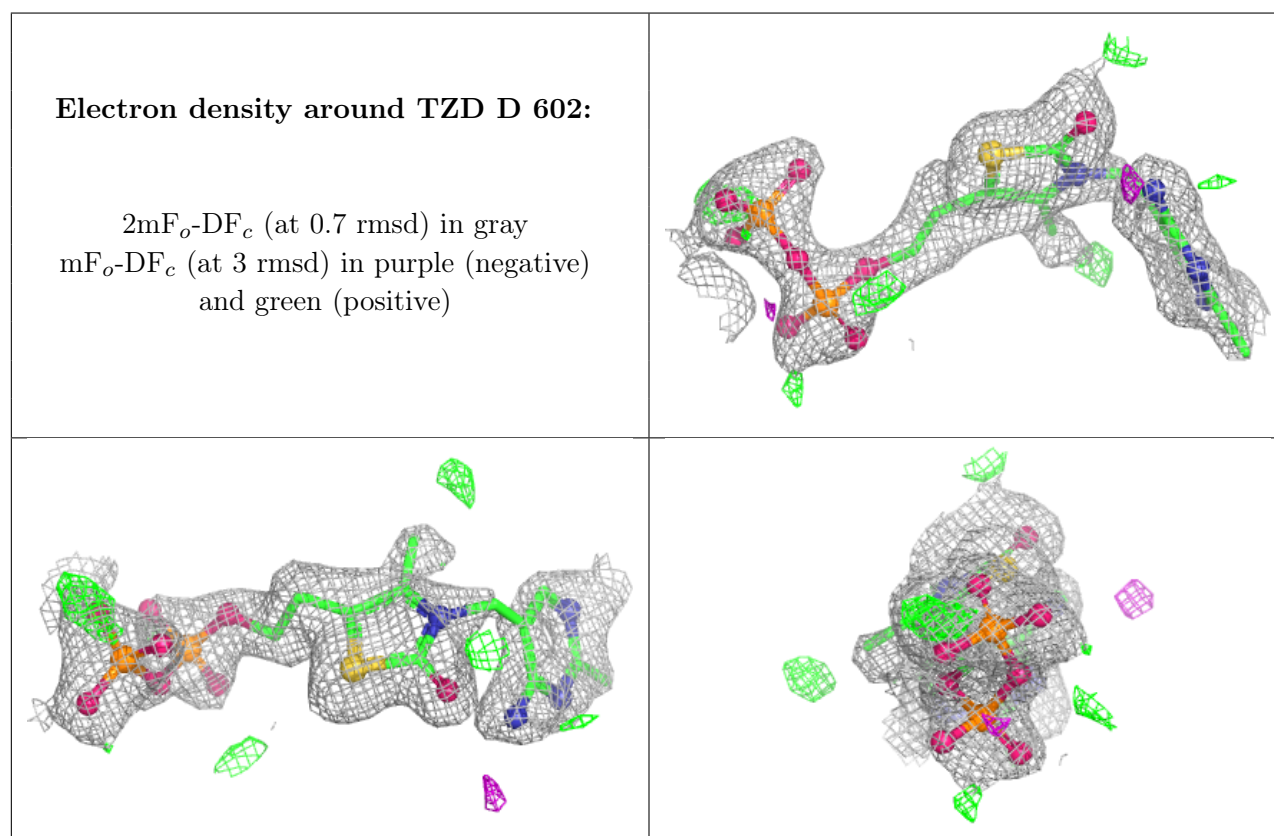
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

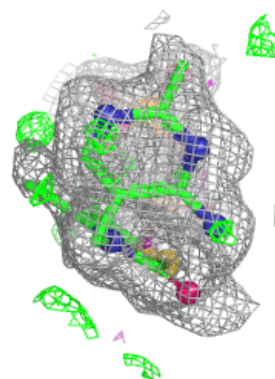
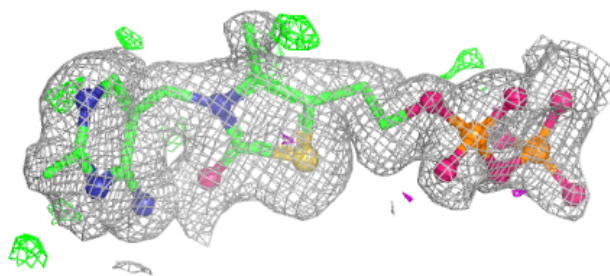
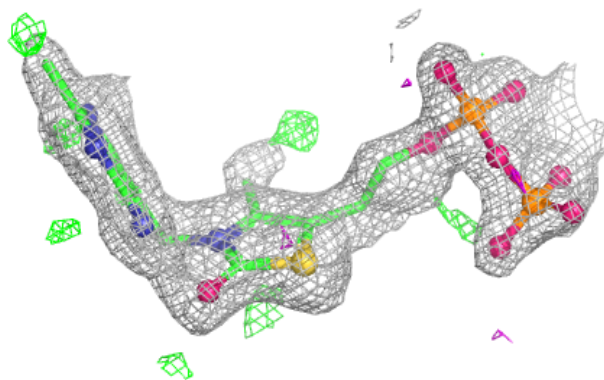
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	603	6/6	0.83	0.13	27,34,36,44	3
3	TZD	D	602	27/27	0.92	0.11	23,31,35,39	26
3	TZD	C	602	27/27	0.94	0.09	21,28,32,33	27
3	TZD	A	603	27/27	0.95	0.08	20,24,29,33	27
3	TZD	B	603	27/27	0.96	0.08	23,26,31,34	27
2	MG	B	601	1/1	0.96	0.07	23,23,23,23	0
2	MG	A	601	1/1	0.98	0.07	19,19,19,19	0
2	MG	B	602	1/1	0.99	0.11	15,15,15,15	0
2	MG	C	601	1/1	0.99	0.04	23,23,23,23	0
2	MG	D	601	1/1	0.99	0.04	28,28,28,28	0
2	MG	A	602	1/1	0.99	0.10	14,14,14,14	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.

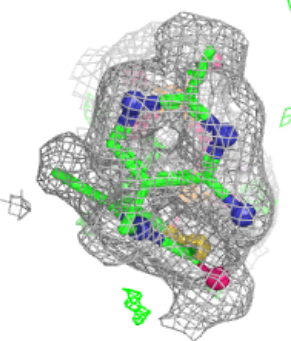
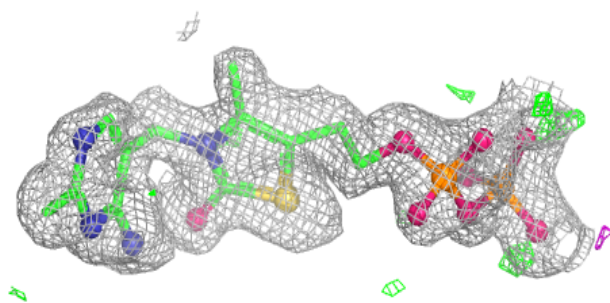
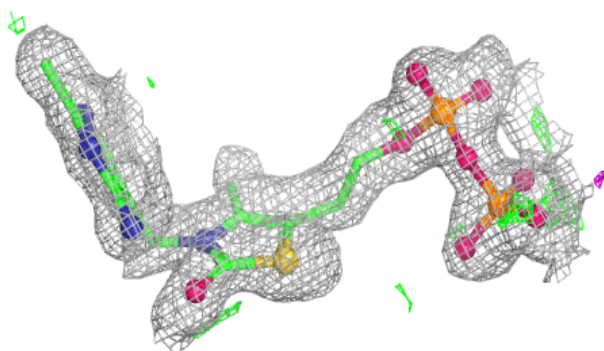


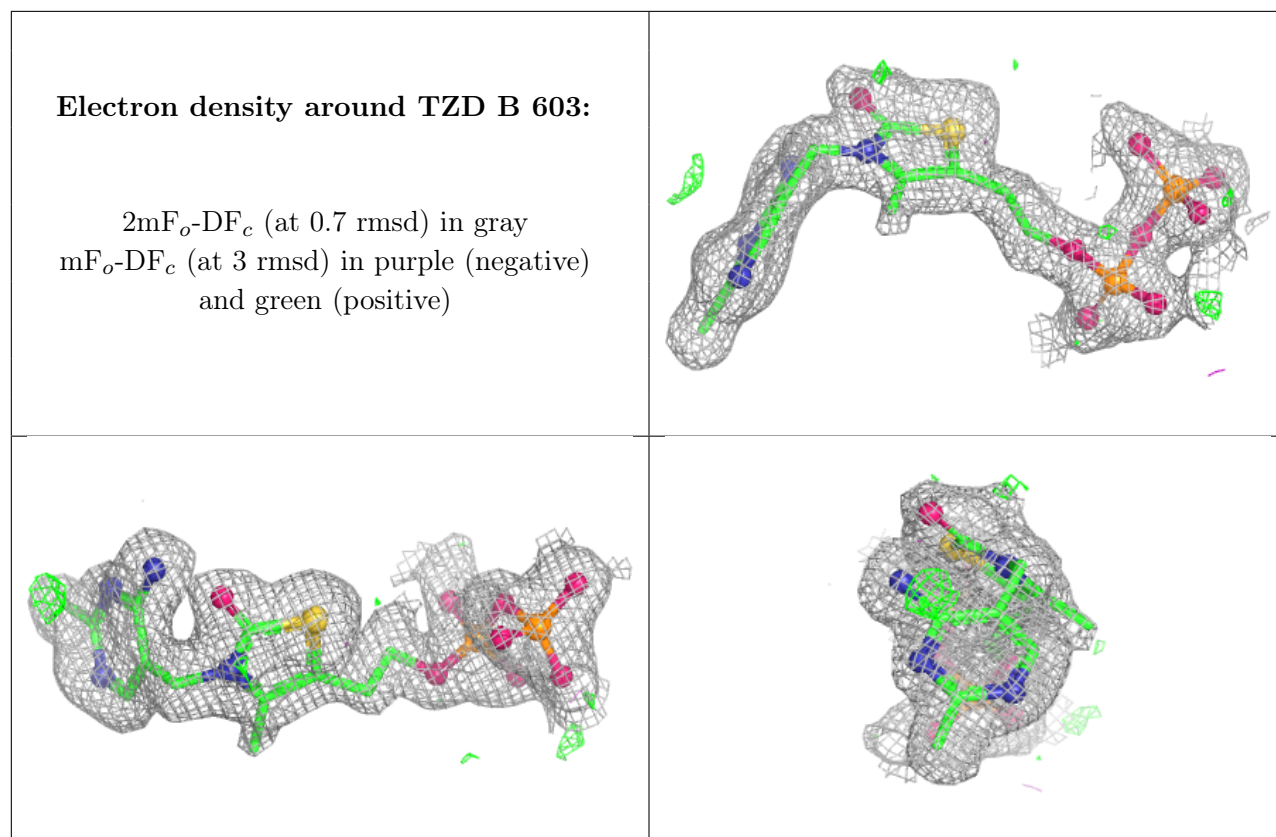
Electron density around TZD C 602:

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

**Electron density around TZD A 603:**

$2mF_o-DF_c$ (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.