



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:29 am BST

PDB ID : 4K9N
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

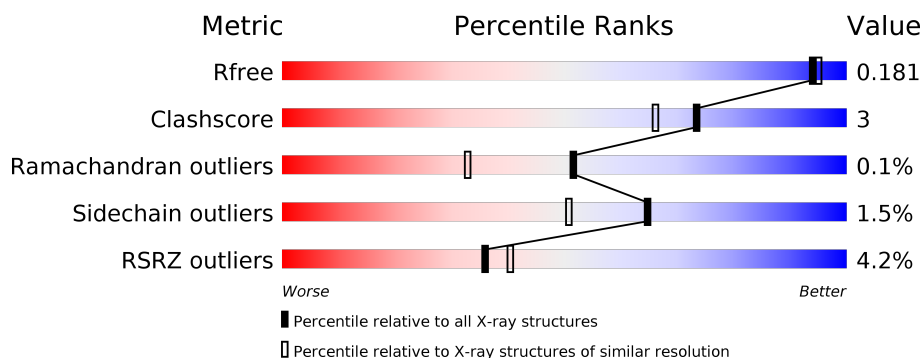
1 Overall quality at a glance

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 on 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	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> <div>•</div> </div>
1	B	530	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> <div>••</div> </div>
1	C	530	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> <div>••</div> </div>
1	D	530	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> <div>••</div> </div>

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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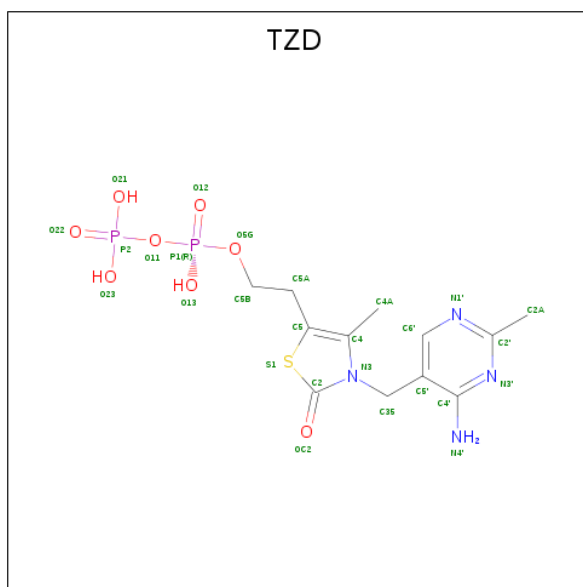
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Chain	Residue	Modelled	Actual	Comment	Reference
D	460	ILE	ALA	ENGINEERED MUTATION	UNP P20906
D	526	HIS	-	EXPRESSION TAG	UNP P20906
D	527	HIS	-	EXPRESSION TAG	UNP P20906
D	528	HIS	-	EXPRESSION TAG	UNP P20906
D	529	HIS	-	EXPRESSION TAG	UNP P20906
D	530	HIS	-	EXPRESSION TAG	UNP P20906
D	531	HIS	-	EXPRESSION TAG	UNP P20906

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	D	1	Total Mg 1 1	0	0
2	C	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 (three-letter code: TZD) (formula: C₁₂H₁₈N₄O₈P₂S).



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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

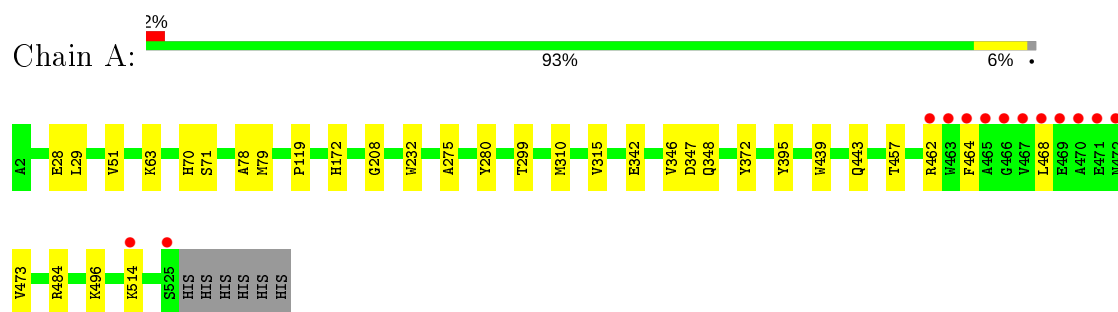
- Molecule 5 is water.

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

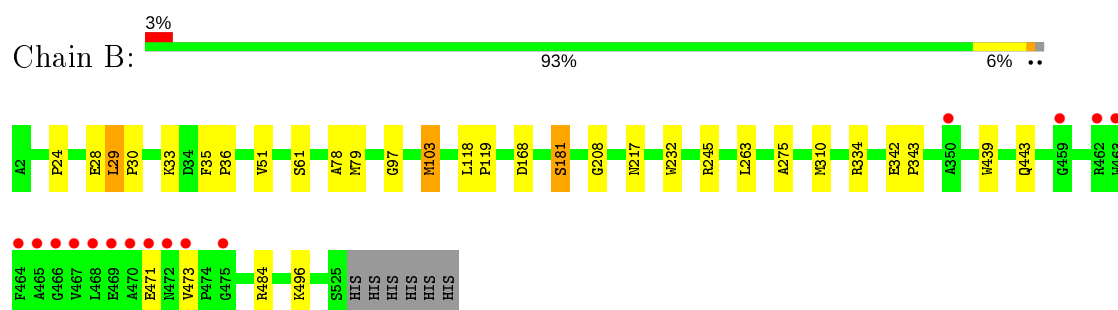
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

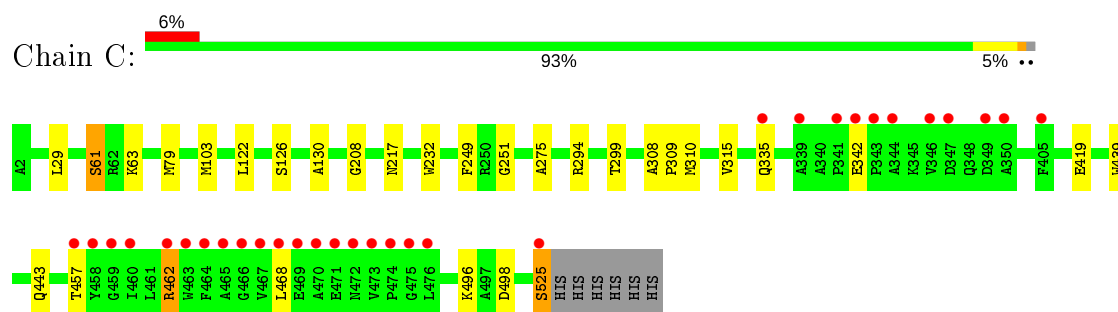
- Molecule 1: Benzoylformate decarboxylase



- Molecule 1: Benzoylformate decarboxylase

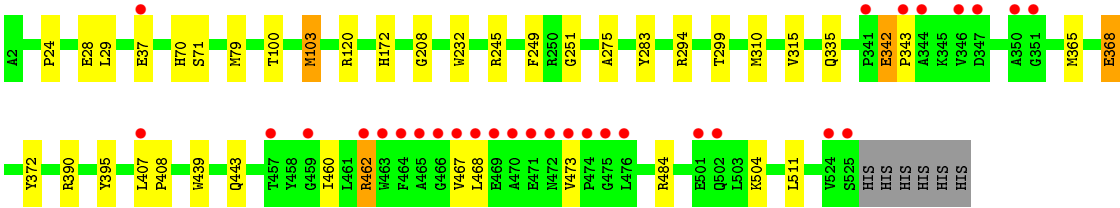


- Molecule 1: Benzoylformate decarboxylase



- 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	70.64 Å 163.50 Å 175.50 Å 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 1.70 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.165 , 0.185 0.162 , 0.181	Depositor DCC
R_{free} test set	2004 reflections (1.01%)	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)	0.37 , 45.6	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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/4084	0.59	0/5581
1	B	0.47	0/4088	0.59	0/5587
1	C	0.47	0/4090	0.59	0/5590
1	D	0.40	0/4085	0.55	0/5583
All	All	0.45	0/16347	0.58	0/22341

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.

There are no bond angle outliers.

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

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Mol	Chain	Res	Type	Group
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	34	0
1	B	3970	0	3917	31	0
1	C	3972	0	3916	25	2
1	D	3970	0	3913	36	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	0	0
3	B	27	0	15	1	0
3	C	27	0	15	0	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	104	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 3.

All (104) 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:79[B]:MET:HE1	1:C:79[B]:MET:HE1	1.07	1.06
1:A:79[B]:MET:HE1	1:C:79[B]:MET:CE	1.88	1.01
1:A:79[B]:MET:CE	1:C:79[B]:MET:HE1	1.90	1.00
1:B:79[B]:MET:HE1	1:D:79[B]:MET:HE1	1.46	0.96
1:A:63:LYS:NZ	5:A:1096:HOH:O	2.01	0.93
1:B:79[B]:MET:SD	1:D:79[B]:MET:HE2	2.07	0.93
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:B:79[B]:MET:HE2	1:D:79[B]:MET:SD	2.28	0.73
1:B:79[B]:MET:HE1	1:D:79[B]:MET:CE	2.19	0.72
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:CE	1:D:79[B]:MET:SD	2.79	0.70
1:A:79[B]:MET:HE2	1:C:79[B]:MET:SD	2.32	0.70
1:B:79[B]:MET:CE	1:D:79[B]:MET:HE1	2.17	0.69
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:C:439:TRP:CZ2	1:C:443:GLN:HG3	2.32	0.63
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:A:347:ASP:HA	5:A:988:HOH:O	2.05	0.57
1:A:342:GLU:CD	5:A:1033:HOH:O	2.41	0.57
1:B:439:TRP:CE2	1:B:443:GLN:HG3	2.40	0.57
1:A:484:ARG:HD2	1:A:496:LYS:HD2	1.87	0.56
1:A:63:LYS:HE3	5:A:854:HOH:O	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLY:HA3	1:B:275:ALA:HB2	1.87	0.55
1:A:79[B]:MET:SD	1:C:79[B]:MET:HE2	2.47	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: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:A:208:GLY:HA3	1:A:275:ALA:HB2	1.91	0.53
1:B:168:ASP:OD2	5:B:1077:HOH:O	2.19	0.52
1:A:280:TYR:HB2	1:C:103[B]:MET:HE3	1.92	0.52
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
3:B:603:TZD:H4A3	1:D:24:PRO:O	2.12	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:D:299:THR:O	1:D:315:VAL:HA	2.18	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
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:B:24:PRO:O	3:D:602:TZD:H4A3	2.18	0.43
1:D:245:ARG:NH1	5:D:819:HOH:O	2.44	0.43
1:D:28:GLU:OE2	1:D:70:HIS:HA	2.18	0.43
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:D:365:MET:HE1	1:D:504:LYS:HG2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:51:VAL:HG21	1:B:78:ALA:HB1	2.03	0.41
1:B:103[A]:MET:HE2	1:D:283:TYR:HA	2.03	0.41
1:B:29:LEU:HA	1:B:29:LEU:HD22	1.75	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
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 ⓘ

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	528/530 (100%)	522 (99%)	5 (1%)	1 (0%)	47	30
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%)	47	30
All	All	2114/2120 (100%)	2083 (98%)	29 (1%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

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

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	417/417 (100%)	414 (99%)	3 (1%)	84	77
1	B	418/417 (100%)	411 (98%)	7 (2%)	60	46
1	C	418/417 (100%)	411 (98%)	7 (2%)	60	46
1	D	417/417 (100%)	407 (98%)	10 (2%)	49	31
All	All	1670/1668 (100%)	1643 (98%)	27 (2%)	65	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	310	MET
1	A	514	LYS
1	B	29	LEU
1	B	103[A]	MET
1	B	103[B]	MET
1	B	217	ASN
1	B	263	LEU
1	B	310	MET

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Mol	Chain	Res	Type
1	B	471	GLU
1	C	217	ASN
1	C	294	ARG
1	C	310	MET
1	C	342	GLU
1	C	462	ARG
1	C	468	LEU
1	C	525	SER
1	D	37	GLU
1	D	103[A]	MET
1	D	103[B]	MET
1	D	294	ARG
1	D	310	MET
1	D	335	GLN
1	D	342	GLU
1	D	368	GLU
1	D	462	ARG
1	D	467	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	C	172	HIS
1	C	391	ASN
1	D	172	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

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	23,28,28	1.41	2 (8%)	28,42,42	2.02	6 (21%)
4	GOL	C	603	-	5,5,5	0.24	0	5,5,5	0.31	0
3	TZD	B	603	2	23,28,28	1.40	2 (8%)	28,42,42	1.98	6 (21%)
3	TZD	A	603	2	23,28,28	1.40	3 (13%)	28,42,42	2.02	6 (21%)
3	TZD	C	602	2	23,28,28	1.40	2 (8%)	28,42,42	2.02	6 (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	-	0/16/17/17	0/2/2/2
4	GOL	C	603	-	-	2/4/4/4	-
3	TZD	B	603	2	-	1/16/17/17	0/2/2/2
3	TZD	A	603	2	-	1/16/17/17	0/2/2/2
3	TZD	C	602	2	-	0/16/17/17	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	TZD	OC2-C2	4.62	1.28	1.21
3	A	603	TZD	OC2-C2	4.59	1.28	1.21
3	C	602	TZD	OC2-C2	4.58	1.28	1.21
3	B	603	TZD	OC2-C2	4.57	1.28	1.21
3	D	602	TZD	C5'-C4'	3.35	1.48	1.42
3	A	603	TZD	C5'-C4'	3.33	1.48	1.42
3	B	603	TZD	C5'-C4'	3.30	1.48	1.42
3	C	602	TZD	C5'-C4'	3.30	1.48	1.42
3	A	603	TZD	C4-N3	-2.02	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	TZD	C5A-C5-C4	6.63	132.76	127.43
3	A	603	TZD	C5A-C5-C4	6.63	132.75	127.43
3	C	602	TZD	C5A-C5-C4	6.63	132.75	127.43
3	B	603	TZD	C5A-C5-C4	6.28	132.47	127.43
3	A	603	TZD	C6'-N1'-C2'	3.57	122.04	115.96
3	D	602	TZD	C6'-N1'-C2'	3.56	122.02	115.96
3	B	603	TZD	C6'-N1'-C2'	3.55	122.00	115.96
3	C	602	TZD	C6'-N1'-C2'	3.53	121.96	115.96
3	C	602	TZD	P1-O11-P2	-3.09	122.23	132.83
3	A	603	TZD	P1-O11-P2	-2.92	122.82	132.83
3	D	602	TZD	P1-O11-P2	-2.81	123.17	132.83
3	B	603	TZD	P1-O11-P2	-2.76	123.34	132.83
3	D	602	TZD	N4'-C4'-N3'	2.69	120.84	117.03
3	A	603	TZD	N4'-C4'-N3'	2.61	120.72	117.03
3	B	603	TZD	N4'-C4'-N3'	2.60	120.71	117.03
3	C	602	TZD	N4'-C4'-N3'	2.58	120.68	117.03
3	D	602	TZD	C5'-C6'-N1'	-2.55	119.57	123.82
3	C	602	TZD	C5'-C6'-N1'	-2.55	119.58	123.82
3	A	603	TZD	C5'-C6'-N1'	-2.53	119.60	123.82
3	B	603	TZD	C5'-C6'-N1'	-2.52	119.61	123.82
3	A	603	TZD	N1'-C2'-N3'	-2.29	121.59	125.54
3	B	603	TZD	N1'-C2'-N3'	-2.27	121.63	125.54
3	D	602	TZD	N1'-C2'-N3'	-2.27	121.64	125.54
3	C	602	TZD	N1'-C2'-N3'	-2.20	121.75	125.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

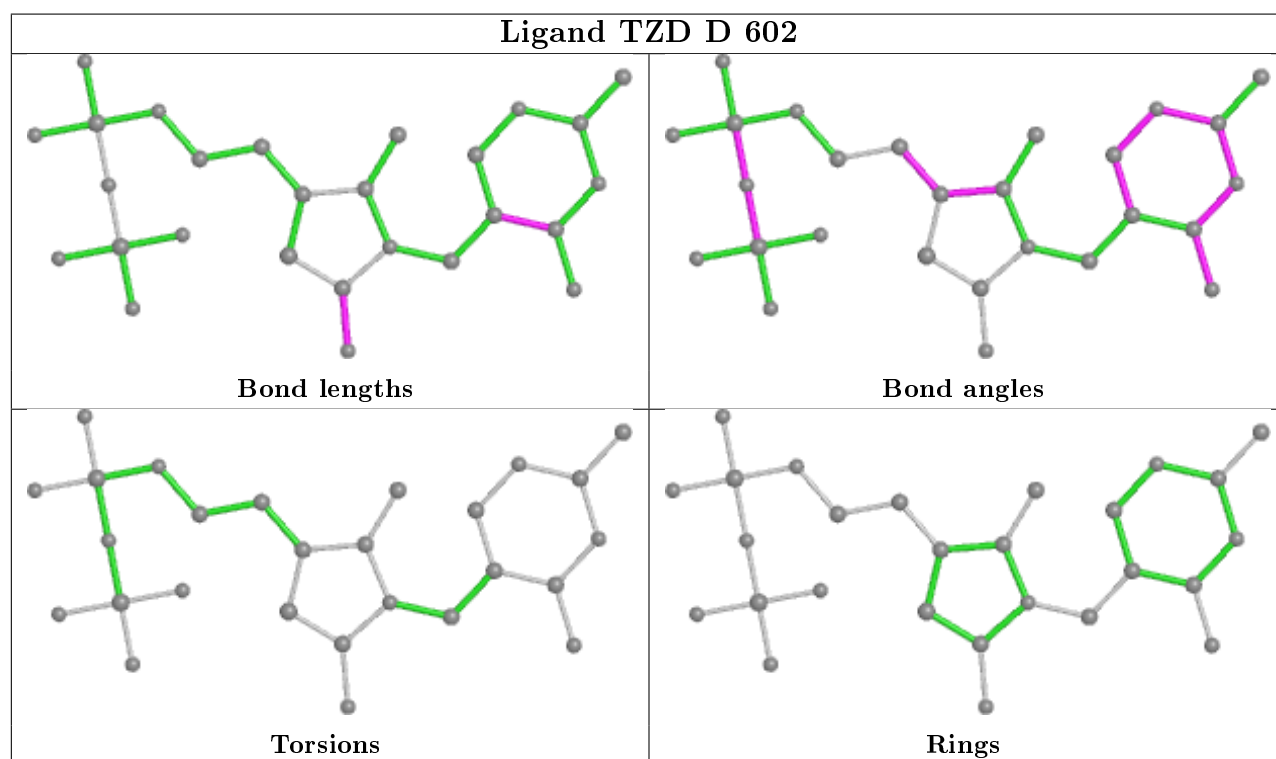
Mol	Chain	Res	Type	Atoms
4	C	603	GOL	C1-C2-C3-O3
4	C	603	GOL	O2-C2-C3-O3
3	B	603	TZD	P1-O11-P2-O22
3	A	603	TZD	P1-O11-P2-O22

There are no ring outliers.

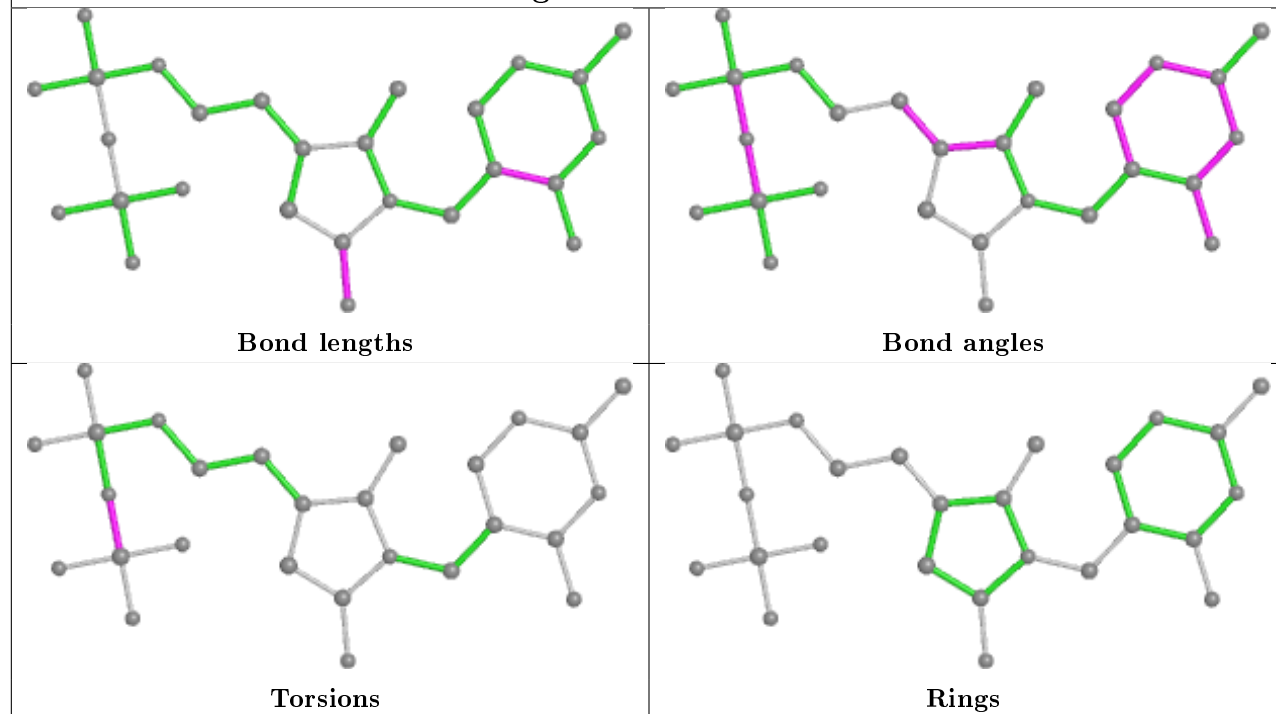
3 monomers are involved in 3 short contacts:

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

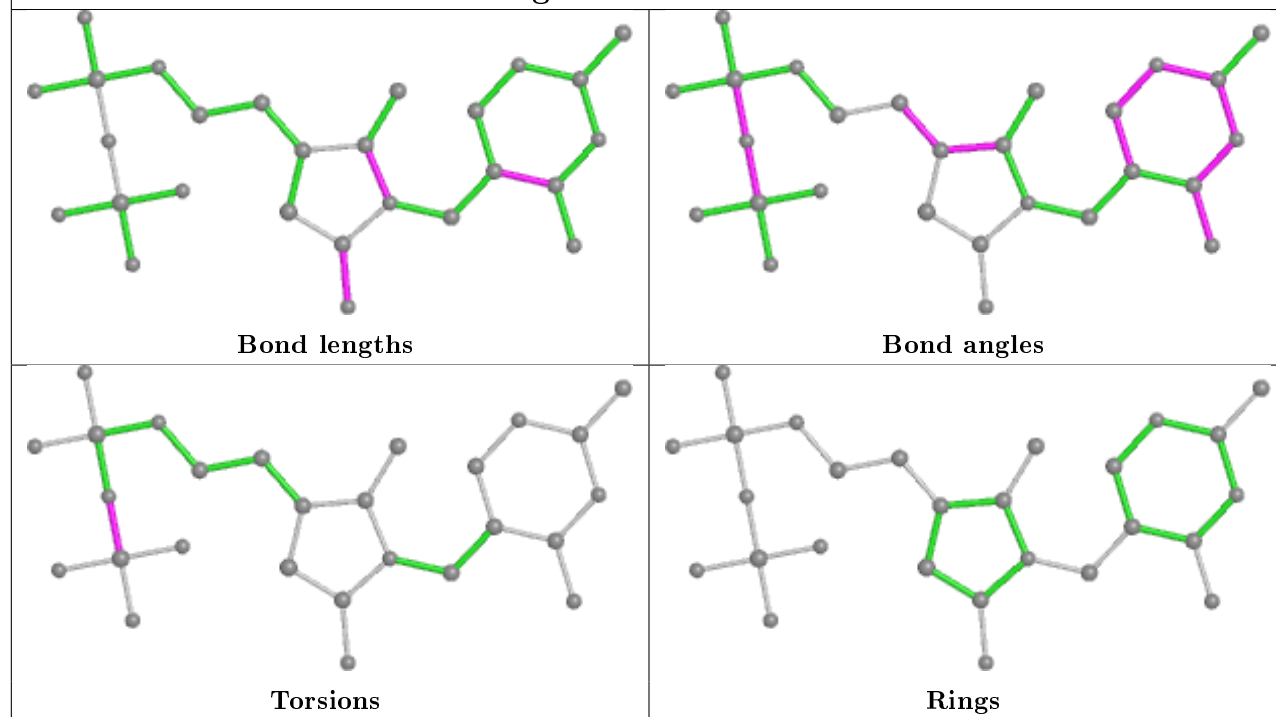
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

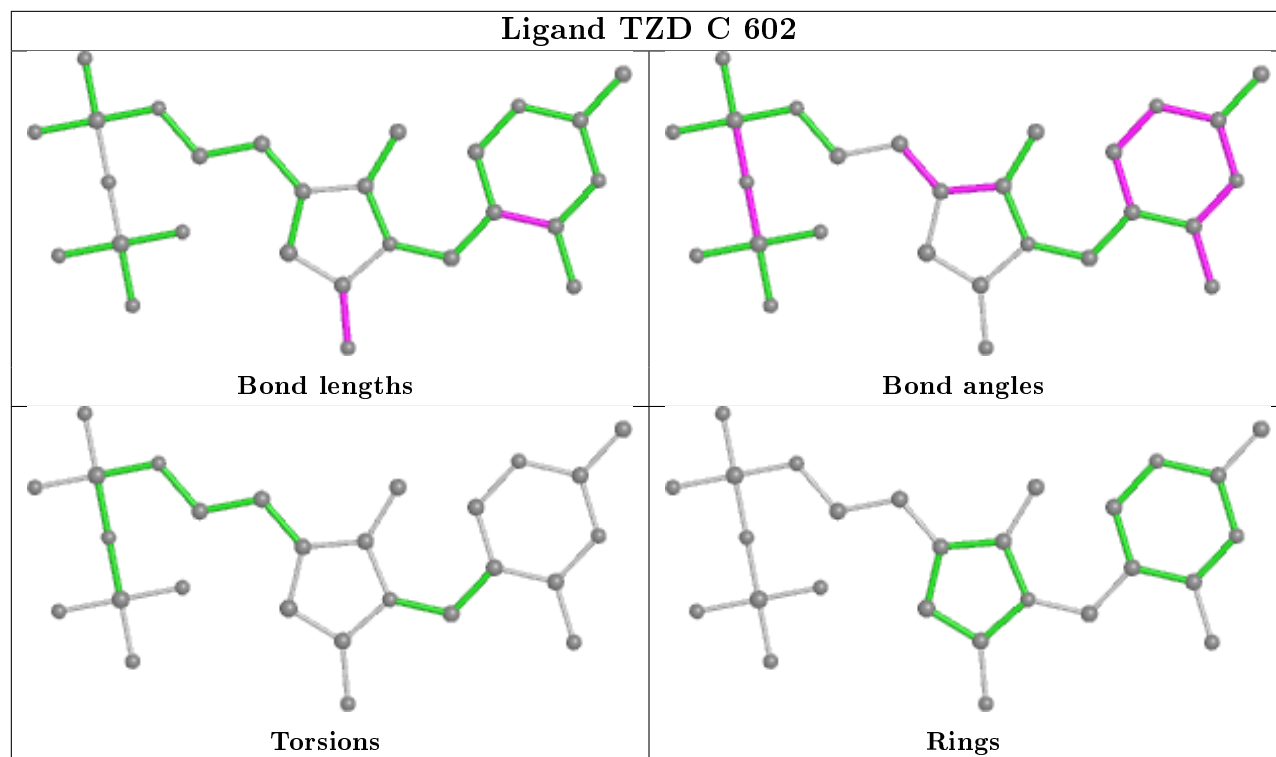


Ligand TZD B 603



Ligand TZD A 603





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	524/530 (98%)	-0.23	13 (2%) 57 61	15, 21, 33, 63	6 (1%)
1	B	524/530 (98%)	-0.24	15 (2%) 51 56	16, 22, 37, 64	2 (0%)
1	C	524/530 (98%)	0.03	31 (5%) 22 24	16, 23, 41, 61	3 (0%)
1	D	524/530 (98%)	0.10	30 (5%) 23 26	18, 27, 49, 69	3 (0%)
All	All	2096/2120 (98%)	-0.09	89 (4%) 36 40	15, 23, 42, 69	14 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	TRP	6.8
1	D	470	ALA	6.7
1	A	467	VAL	6.3
1	D	467	VAL	6.0
1	D	463	TRP	5.8
1	C	470	ALA	5.7
1	C	463	TRP	5.6
1	D	468	LEU	5.5
1	B	470	ALA	5.3
1	A	468	LEU	5.2
1	B	468	LEU	5.0
1	C	464	PHE	4.9
1	D	469	GLU	4.9
1	D	472	ASN	4.9
1	C	467	VAL	4.6
1	C	472	ASN	4.6
1	C	460	ILE	4.5
1	B	467	VAL	4.5
1	C	468	LEU	4.4
1	D	459	GLY	4.2
1	D	466	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	469	GLU	4.1
1	C	465	ALA	4.1
1	D	471	GLU	4.0
1	C	346	VAL	4.0
1	D	350	ALA	4.0
1	A	464	PHE	4.0
1	C	525	SER	3.8
1	C	466	GLY	3.7
1	D	343	PRO	3.7
1	D	465	ALA	3.7
1	D	464	PHE	3.6
1	A	469	GLU	3.6
1	C	473	VAL	3.6
1	D	524	VAL	3.6
1	D	473	VAL	3.6
1	A	466	GLY	3.5
1	A	470	ALA	3.5
1	C	471	GLU	3.5
1	B	466	GLY	3.5
1	D	346	VAL	3.4
1	B	464	PHE	3.4
1	B	465	ALA	3.3
1	C	350	ALA	3.3
1	C	347	ASP	3.2
1	C	459	GLY	3.2
1	D	525	SER	3.2
1	C	469	GLU	3.1
1	D	351	GLY	3.1
1	B	475	GLY	3.0
1	A	514	LYS	3.0
1	C	341	PRO	2.9
1	B	463	TRP	2.9
1	B	462	ARG	2.9
1	B	472	ASN	2.9
1	D	462	ARG	2.8
1	D	474	PRO	2.7
1	D	475	GLY	2.7
1	B	473	VAL	2.6
1	D	37	GLU	2.6
1	C	462	ARG	2.6
1	C	475	GLY	2.6
1	D	347	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	471	GLU	2.6
1	D	344	ALA	2.5
1	D	341	PRO	2.5
1	C	343	PRO	2.4
1	C	474	PRO	2.4
1	C	342	GLU	2.4
1	B	350	ALA	2.4
1	D	501	GLU	2.4
1	C	458	TYR	2.4
1	D	502	GLN	2.3
1	A	462	ARG	2.3
1	D	457	THR	2.2
1	D	476	LEU	2.2
1	C	349	ASP	2.2
1	C	339	ALA	2.2
1	A	472	ASN	2.2
1	A	471	GLU	2.2
1	C	335	GLN	2.1
1	A	525	SER	2.1
1	C	457	THR	2.1
1	C	405	PHE	2.1
1	B	459	GLY	2.1
1	C	476	LEU	2.1
1	A	465	ALA	2.0
1	C	344	ALA	2.0
1	D	407	LEU	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 [\(i\)](#)

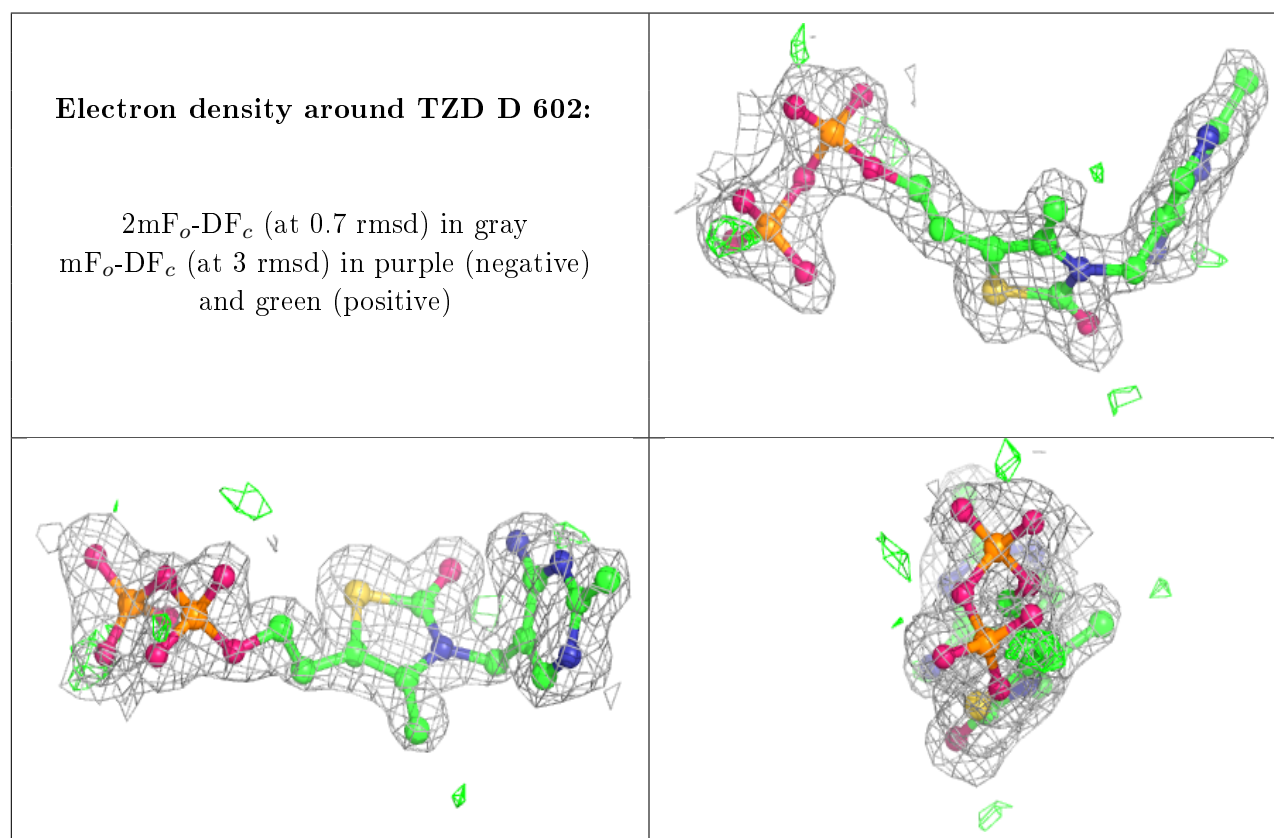
There are no carbohydrates in this entry.

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.

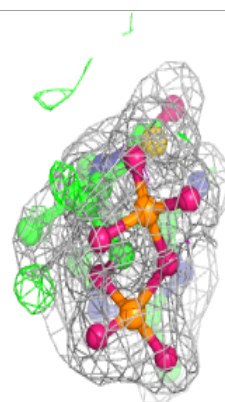
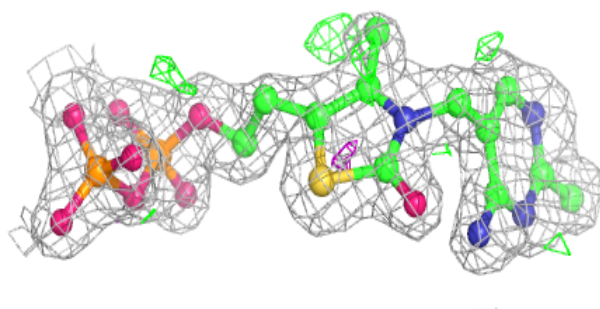
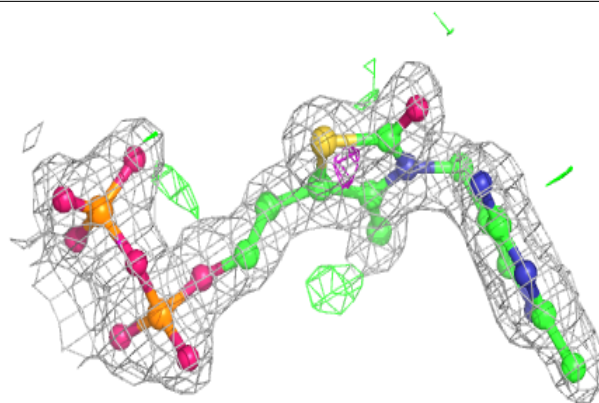
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	C	603	6/6	0.87	0.12	27,34,36,44	3
3	TZD	D	602	27/27	0.93	0.12	23,31,35,39	26
3	TZD	C	602	27/27	0.94	0.10	21,28,32,33	27
3	TZD	B	603	27/27	0.95	0.10	23,26,31,34	27
2	MG	B	601	1/1	0.96	0.07	23,23,23,23	0
3	TZD	A	603	27/27	0.96	0.10	20,24,29,33	27
2	MG	A	601	1/1	0.99	0.08	19,19,19,19	0
2	MG	A	602	1/1	0.99	0.16	14,14,14,14	0
2	MG	C	601	1/1	0.99	0.06	23,23,23,23	0
2	MG	D	601	1/1	0.99	0.05	28,28,28,28	0
2	MG	B	602	1/1	0.99	0.16	15,15,15,15	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.

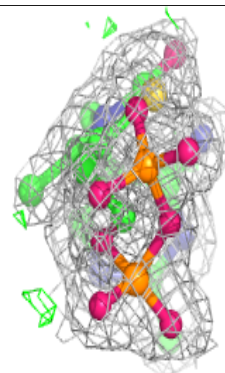
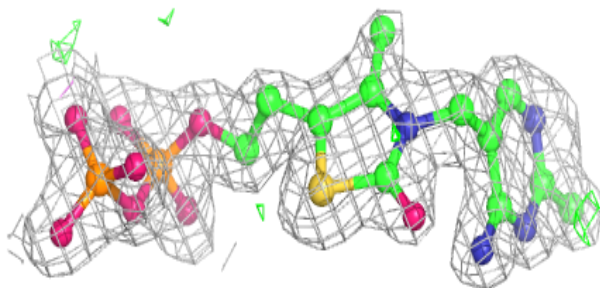
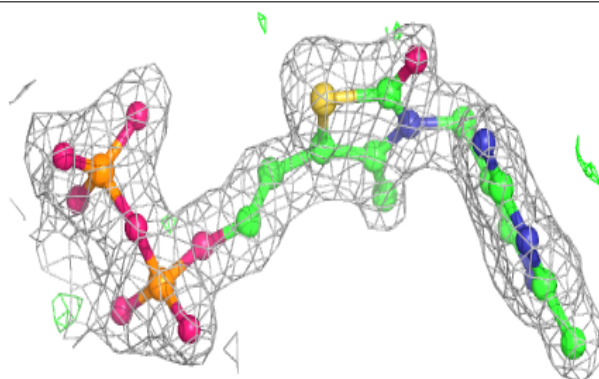


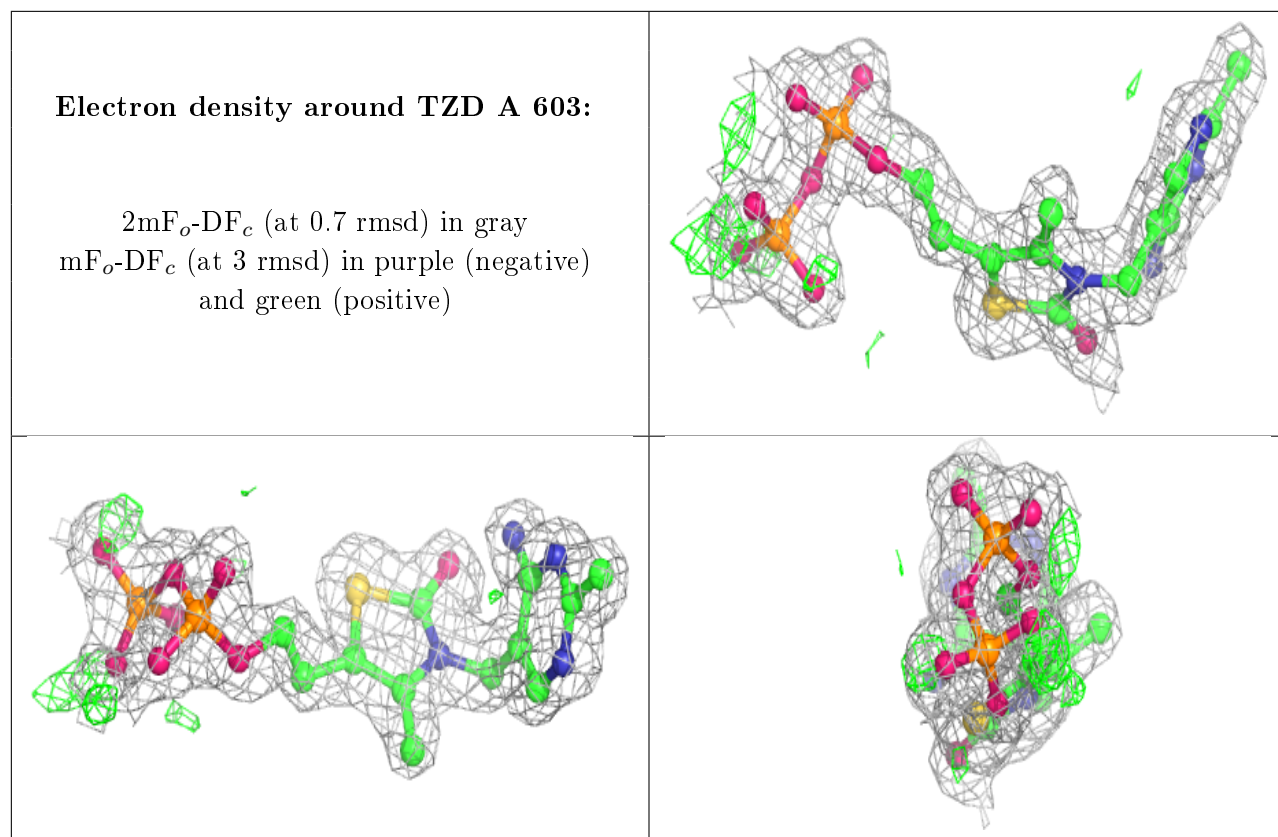
Electron density around TZD C 602:

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

**Electron density around TZD B 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.