Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2024 – 06:15 PM JST

PDB ID	:	8XRU
Title	:	The crystal structure of a GH3 enzyme CcBgl3B with glycerol
Authors	:	Su, J.Y.
Deposited on	:	2024-01-08
Resolution	:	2.02 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:

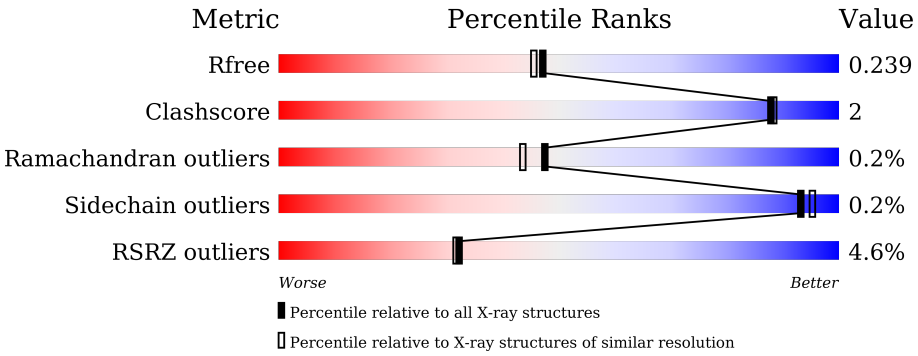
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	768	2% 92% 6%
1	B	768	% 94%
1	C	768	7% 21% 76%

2 Entry composition

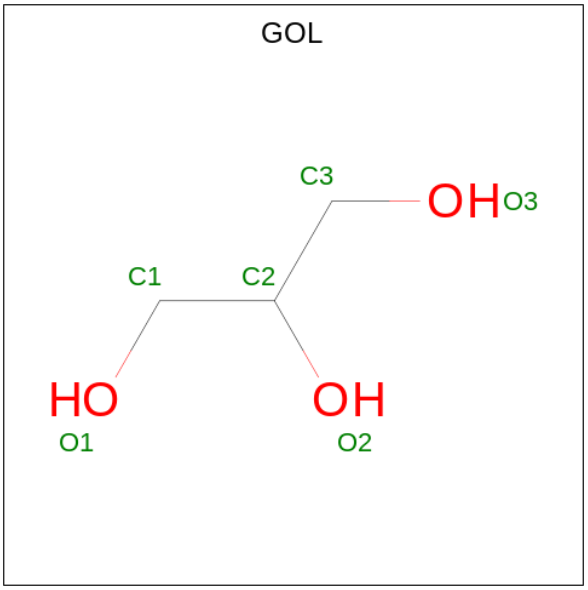
There are 4 unique types of molecules in this entry. The entry contains 14015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GH3 enzyme CcBgl3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5623	3538	999	1071	15			
1	B	747	Total	C	N	O	S	0	0	0
			5593	3522	995	1061	15			
1	C	184	Total	C	N	O		0	0	0
			1260	791	230	239				

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

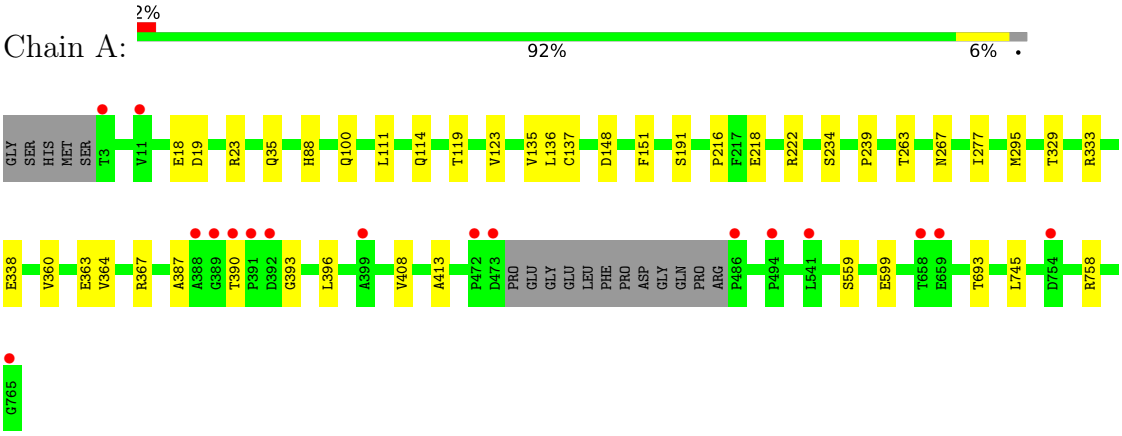
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	700	Total O 700 700	0	0
4	B	755	Total O 755 755	0	0
4	C	58	Total O 58 58	0	0

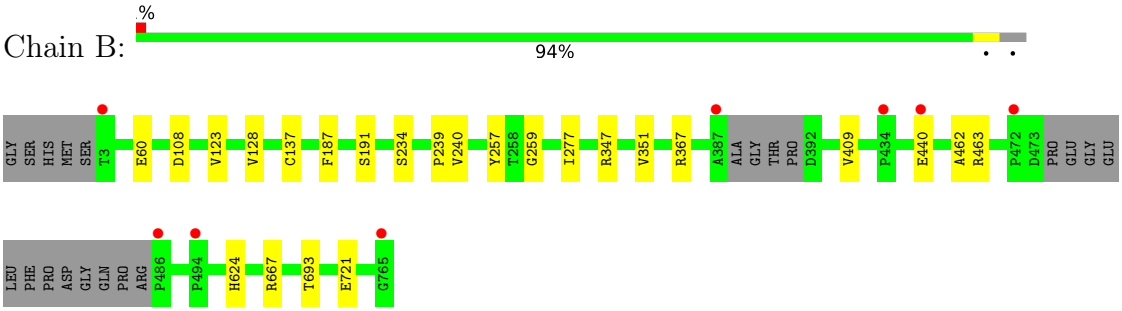
3 Residue-property plots (i)

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.

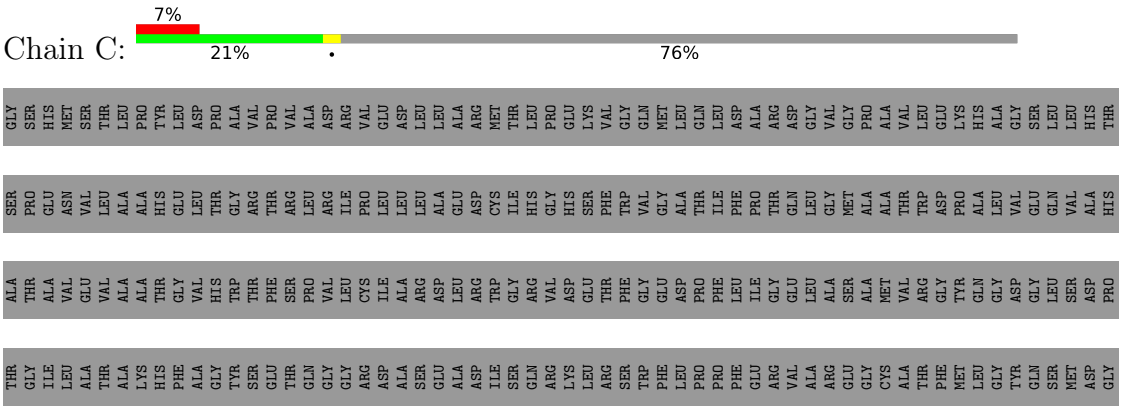
• Molecule 1: GH3 enzyme CcBgl3B

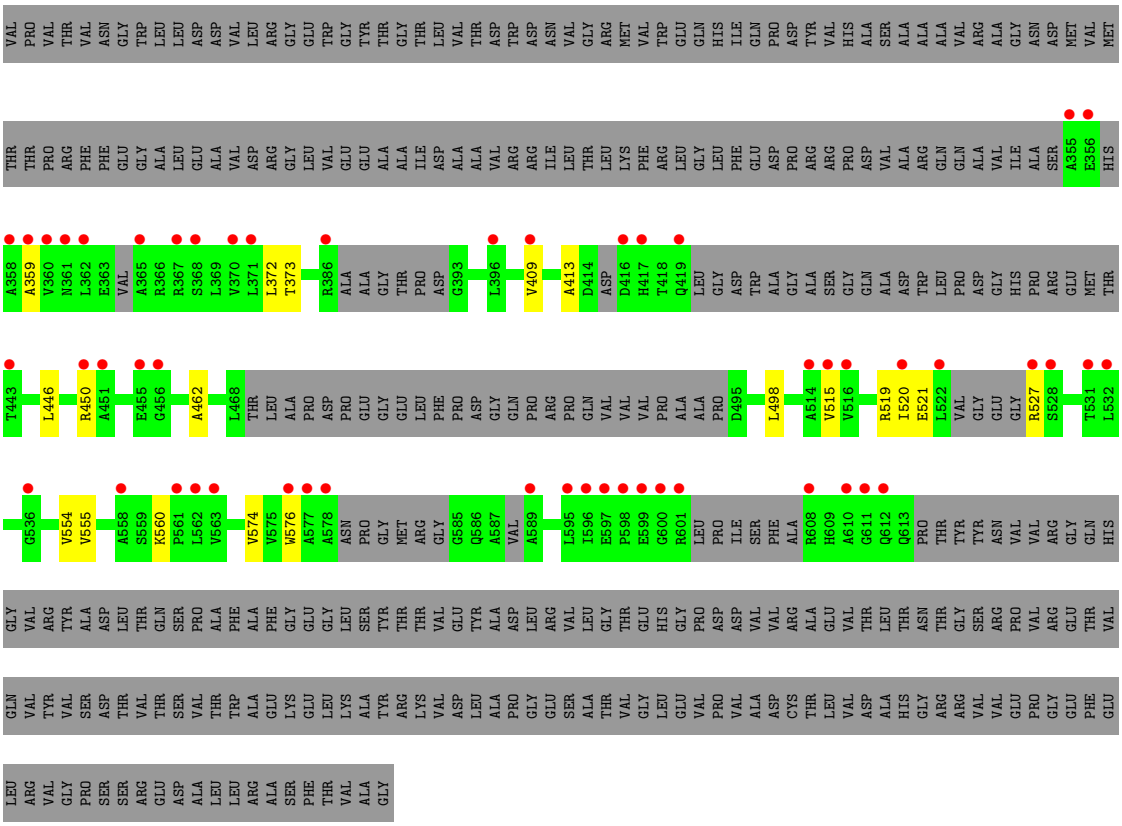


• Molecule 1: GH3 enzyme CcBgl3B



• Molecule 1: GH3 enzyme CcBgl3B




VAL PRO VAL THR VAL ASN GLY TRP LEU LEU ASP ASP VAL LEU ARG GLY GLU TRP GLY TYR THR GLY THR LEU VAL THR ASP TRP ASP ASN VAL GLY ARG MET VAL TRP GLU GLN HIS ILE GLN PRO ASP TYR VAL HIS ALA SER ALA ALA ALA VAL ARG ALA GLY ASN ASP MET VAL MET
THR THR PRO ARG PHE PHE GLU GLY ALA LEU GLU GLU ALA VAL ASP ARG GLY LEU VAL GLU GLU ALA ALA ILE ASP ALA ALA VAL ARG ARG ILE LEU THR LEU LYS PHE ARG LEU GLY LEU PHE GLU ASP PRO ARG ARG PRO ASP VAL ALA ARG GLN GLN ALA VAL ILE ALA SER A355 E356 HIS
A358 A359 V360 N361 L362 E363 VAL A365 R366 R367 S368 L369 V370 L371 L372 T373 R386 ALA ALA GLY THR PRO ASP G393 L396 V409 A413 D414 ASP D416 H417 T418 Q419 LEU GLY ASP TRP ALA GLY ALA SER GLY GLN ALA ASP TRP LEU PRO ASP GLY HIS PRO ARG GLU MET THR
T443 L446 R450 A451 E455 G456 A462 L468 THR LEU ALA PRO ASP PRO GLU GLY GLU LEU PHE PRO ASP GLY GLN PRO ARG PRO GLN VAL VAL PRO ALA ALA PRO D495 L498 A514 V515 V516 R519 I520 E521 L522 VAL GLY GLU GLY R527 S528 T531 L532
G536 V554 V555 A558 S559 K560 P561 L562 V563 V574 V575 W576 A577 A578 ASN PRO GLY MET ARG GLY G585 Q586 A587 VAL A589 L596 I596 E597 P598 E599 G600 R601 LEU PRO ILE SER PHE ALA R608 H609 A610 G611 Q612 Q613 PRO THR TYR TYR ASN VAL VAL ARG GLY GLN HIS
GLY VAL ARG TYR ALA ASP LEU THR GLN SER PRO ALA PHE ALA PHE GLY GLU GLY LEU SER TYR THR THR VAL GLU TYR ALA ASP LEU ARG VAL LEU GLY THR GLU HIS GLY PRO ASP ASP VAL VAL ARG ALA GLU VAL THR LEU THR ASN THR GLY SER ARG PRO VAL ARG GLU THR VAL
GLN VAL TYR VAL SER ASP THR VAL THR SER VAL THR TRP ALA GLU LYS GLU LEU LYS ALA TYR ARG LYS VAL ASP LEU ALA PRO GLY GLU SER ALA THR VAL GLY LEU GLU VAL PRO VAL ALA ASP CYS THR LEU VAL ASP ALA HIS GLY ARG ARG VAL VAL GLU PRO GLY GLU PHE GLU
LEU ARG VAL GLY PRO SER SER ARG GLU ASP ALA LEU LEU ARG ALA SER PHE THR VAL ALA GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.99Å 182.05Å 145.28Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	19.85 – 2.02 19.85 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.85-2.02) 98.9 (19.85-2.02)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.02Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.205 , 0.235 0.209 , 0.239	Depositor DCC
R_{free} test set	1998 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.854	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14015	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CA

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	0.40	0/5746	0.58	0/7859
1	B	0.38	0/5714	0.57	0/7812
1	C	0.37	0/1269	0.62	0/1730
All	All	0.39	0/12729	0.58	0/17401

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5623	0	5538	27	0
1	B	5593	0	5511	13	0
1	C	1260	0	1240	12	0
2	A	12	0	16	0	0
2	B	12	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	700	0	0	1	0
4	B	755	0	0	2	0
4	C	58	0	0	0	0
All	All	14015	0	12321	50	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 2.

All (50) 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:100:GLN:HG3	1:A:151:PHE:CE1	2.22	0.75
1:A:338:GLU:OE1	1:A:338:GLU:N	2.31	0.64
1:C:554:VAL:HB	1:C:574:VAL:HG12	1.80	0.63
1:C:446:LEU:HD11	1:C:450:ARG:HE	1.64	0.63
1:C:519:ARG:HG2	1:C:520:ILE:H	1.64	0.62
1:A:137:CYS:HB3	1:A:191:SER:HB3	1.86	0.57
1:A:367:ARG:NE	1:A:599:GLU:OE2	2.35	0.56
1:A:100:GLN:NE2	1:A:135:VAL:O	2.39	0.56
1:B:137:CYS:HB3	1:B:191:SER:HB3	1.86	0.56
1:A:329:THR:O	1:A:333:ARG:HG3	2.07	0.54
1:B:463:ARG:NH1	4:B:912:HOH:O	2.40	0.54
1:A:100:GLN:HG3	1:A:151:PHE:CD1	2.43	0.53
1:A:88:HIS:CD2	1:A:123:VAL:HA	2.42	0.53
1:A:693:THR:O	1:B:277:ILE:HA	2.09	0.53
1:C:372:LEU:HD11	1:C:576:TRP:CB	2.39	0.53
1:C:521:GLU:O	1:C:527:ARG:HD3	2.10	0.52
1:A:363:GLU:O	1:A:367:ARG:HG2	2.10	0.51
1:B:347:ARG:O	1:B:351:VAL:HG22	2.12	0.50
1:A:360:VAL:O	1:A:364:VAL:HG23	2.13	0.49
1:A:277:ILE:HA	1:B:693:THR:O	2.12	0.49
1:A:19:ASP:O	1:A:23:ARG:HG3	2.13	0.49
1:A:408:VAL:HG12	1:A:413:ALA:HB1	1.94	0.48
1:C:515:VAL:HA	1:C:555:VAL:O	2.13	0.48
1:A:136:LEU:HD23	1:A:216:PRO:HB2	1.95	0.47
1:A:390:THR:HG22	1:A:393:GLY:H	1.79	0.47
1:A:218:GLU:O	1:A:222:ARG:HG3	2.15	0.47
1:A:148:ASP:HB3	1:A:559:SER:HB2	1.98	0.46
1:B:108:ASP:OD2	1:B:367:ARG:NH2	2.49	0.46
1:A:234:SER:HA	1:A:239:PRO:HA	1.98	0.45
1:C:413:ALA:HA	1:C:515:VAL:HG11	1.98	0.45
1:B:60:GLU:HG3	4:B:1370:HOH:O	2.15	0.45
1:C:372:LEU:N	1:C:372:LEU:HD12	2.31	0.45
1:B:257:TYR:CZ	1:B:259:GLY:HA3	2.51	0.44
1:B:123:VAL:HG13	1:B:128:VAL:HB	1.98	0.44
1:B:187:PHE:O	1:B:240:VAL:HG11	2.17	0.44
1:B:667:ARG:NH1	1:B:721:GLU:OE2	2.50	0.43
1:A:18:GLU:OE2	4:A:901:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:SER:HA	1:B:239:PRO:HA	2.01	0.43
1:A:119:THR:O	1:A:123:VAL:HG23	2.19	0.43
1:A:263:THR:HB	1:A:267:ASN:HB2	2.00	0.42
1:A:367:ARG:HE	1:A:599:GLU:CD	2.22	0.42
1:A:745:LEU:O	1:A:758:ARG:HA	2.18	0.42
1:C:409:VAL:HA	1:C:462:ALA:O	2.20	0.42
1:A:35:GLN:HB2	1:A:295:MET:HE2	2.02	0.41
1:C:515:VAL:HB	1:C:555:VAL:HB	2.03	0.41
1:C:372:LEU:HD11	1:C:576:TRP:HB2	2.02	0.41
1:C:373:THR:OG1	1:C:574:VAL:HG22	2.20	0.41
1:A:111:LEU:HA	1:A:114:GLN:HE21	1.86	0.41
1:A:387:ALA:HA	1:A:396:LEU:HD11	2.03	0.41
1:B:409:VAL:HA	1:B:462:ALA:O	2.21	0.40

There are no symmetry-related clashes.

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	747/768 (97%)	730 (98%)	17 (2%)	0	100 100
1	B	741/768 (96%)	725 (98%)	15 (2%)	1 (0%)	51 48
1	C	162/768 (21%)	153 (94%)	7 (4%)	2 (1%)	13 6
All	All	1650/2304 (72%)	1608 (98%)	39 (2%)	3 (0%)	47 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	440	GLU
1	C	560	LYS
1	C	359	ALA

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	573/589 (97%)	573 (100%)	0	100 100
1	B	569/589 (97%)	568 (100%)	1 (0%)	93 95
1	C	115/589 (20%)	114 (99%)	1 (1%)	78 82
All	All	1257/1767 (71%)	1255 (100%)	2 (0%)	93 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	624	HIS
1	C	498	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	349	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	GOL	A	801	-	5,5,5	0.45	0	5,5,5	0.99	0
2	GOL	A	802	-	5,5,5	0.75	0	5,5,5	0.90	0
2	GOL	B	801	-	5,5,5	0.41	0	5,5,5	1.09	0
2	GOL	B	802	-	5,5,5	0.60	0	5,5,5	0.46	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
2	GOL	A	801	-	-	3/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	B	801	-	-	4/4/4/4	-
2	GOL	B	802	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	C1-C2-C3-O3
2	B	801	GOL	C1-C2-C3-O3
2	B	802	GOL	O1-C1-C2-C3
2	B	802	GOL	C1-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	B	802	GOL	O1-C1-C2-O2
2	B	801	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	802	GOL	O2-C2-C3-O3
2	B	801	GOL	O2-C2-C3-O3
2	B	801	GOL	O1-C1-C2-C3
2	A	801	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	751/768 (97%)	-0.32	17 (2%) 60 59	23, 31, 49, 82	0
1	B	747/768 (97%)	-0.38	8 (1%) 80 80	23, 31, 44, 70	0
1	C	184/768 (23%)	1.35	52 (28%) 0 0	43, 66, 86, 101	0
All	All	1682/2304 (73%)	-0.17	77 (4%) 32 32	23, 32, 69, 101	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	598	PRO	5.0
1	C	576	TRP	4.8
1	C	612	GLN	4.7
1	C	532	LEU	4.6
1	C	520	ILE	4.6
1	B	765	GLY	4.6
1	C	443	THR	4.4
1	C	589	ALA	4.4
1	C	417	HIS	4.3
1	A	3	THR	4.3
1	C	601	ARG	4.2
1	A	658	THR	4.2
1	A	472	PRO	4.2
1	C	360	VAL	4.2
1	C	600	GLY	4.1
1	C	368	SER	4.0
1	C	355	ALA	4.0
1	A	389	GLY	4.0
1	A	765	GLY	3.9
1	C	367	ARG	3.9
1	B	472	PRO	3.9
1	C	361	ASN	3.9
1	A	392	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	473	ASP	3.7
1	A	486	PRO	3.7
1	A	494	PRO	3.7
1	C	558	ALA	3.7
1	C	419	GLN	3.5
1	C	416	ASP	3.5
1	C	516	VAL	3.5
1	A	388	ALA	3.5
1	C	597	GLU	3.4
1	A	391	PRO	3.4
1	C	608	ARG	3.2
1	B	387	ALA	3.2
1	C	599	GLU	3.2
1	C	362	LEU	3.1
1	A	390	THR	3.1
1	C	522	LEU	3.1
1	C	358	ALA	3.1
1	C	595	LEU	3.1
1	C	370	VAL	3.0
1	B	486	PRO	3.0
1	B	494	PRO	3.0
1	C	528	SER	3.0
1	A	399	ALA	2.8
1	C	514	ALA	2.8
1	C	611	GLY	2.8
1	C	371	LEU	2.7
1	C	356	GLU	2.7
1	A	11	VAL	2.7
1	C	455	GLU	2.7
1	B	434	PRO	2.6
1	C	456	GLY	2.6
1	C	563	VAL	2.5
1	C	451	ALA	2.5
1	C	396	LEU	2.4
1	B	440	GLU	2.4
1	C	578	ALA	2.4
1	C	386	ARG	2.4
1	C	450	ARG	2.3
1	C	527	ARG	2.3
1	C	365	ALA	2.3
1	A	754	ASP	2.3
1	A	659	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	610	ALA	2.3
1	C	515	VAL	2.3
1	C	561	PRO	2.3
1	C	359	ALA	2.2
1	C	577	ALA	2.2
1	C	531	THR	2.2
1	C	536	GLY	2.1
1	C	596	ILE	2.1
1	C	409	VAL	2.1
1	B	3	THR	2.1
1	C	562	LEU	2.0
1	A	541	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 monosaccharides in this entry.

6.4 Ligands (i)

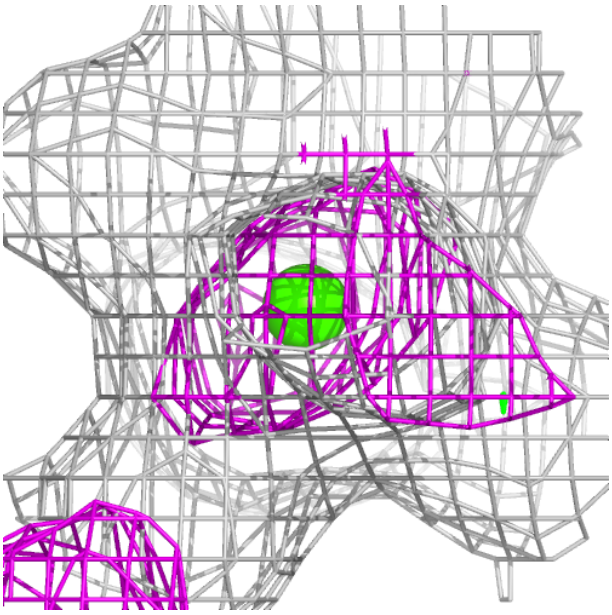
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

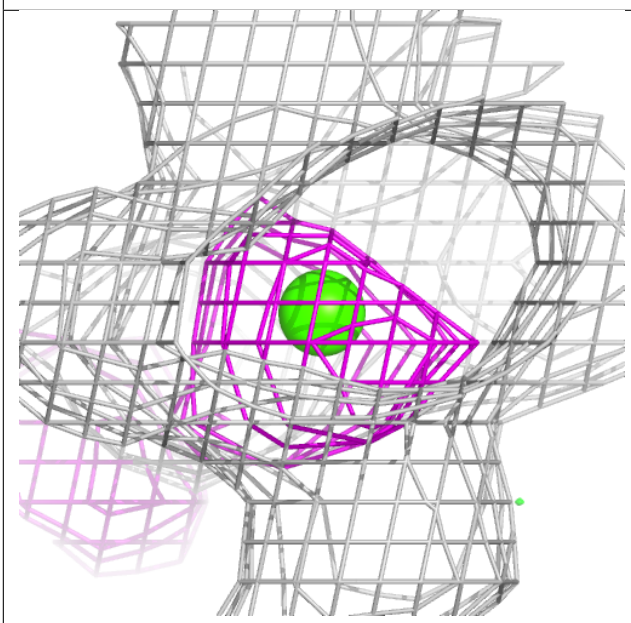
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	801	6/6	0.83	0.17	32,33,37,40	0
2	GOL	B	801	6/6	0.83	0.17	30,35,37,42	0
2	GOL	A	802	6/6	0.84	0.23	35,38,43,54	0
2	GOL	B	802	6/6	0.84	0.24	38,40,41,43	0
3	CA	A	803	1/1	0.98	0.08	44,44,44,44	0
3	CA	B	803	1/1	0.99	0.03	44,44,44,44	0

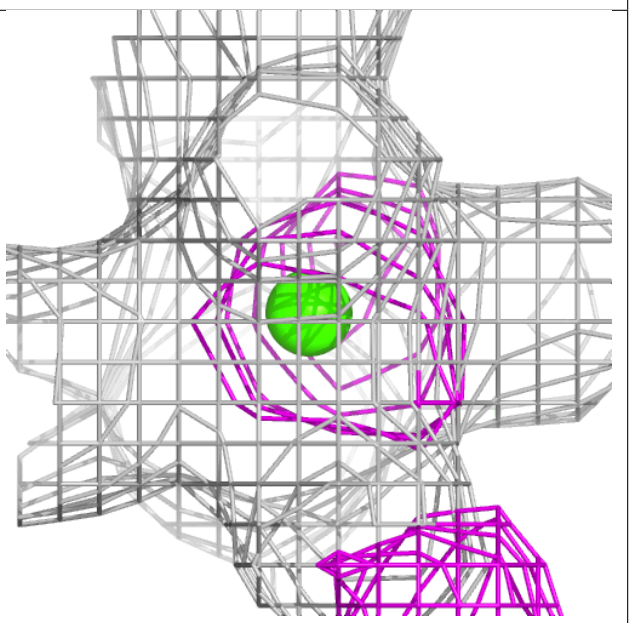
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CA A 803:

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

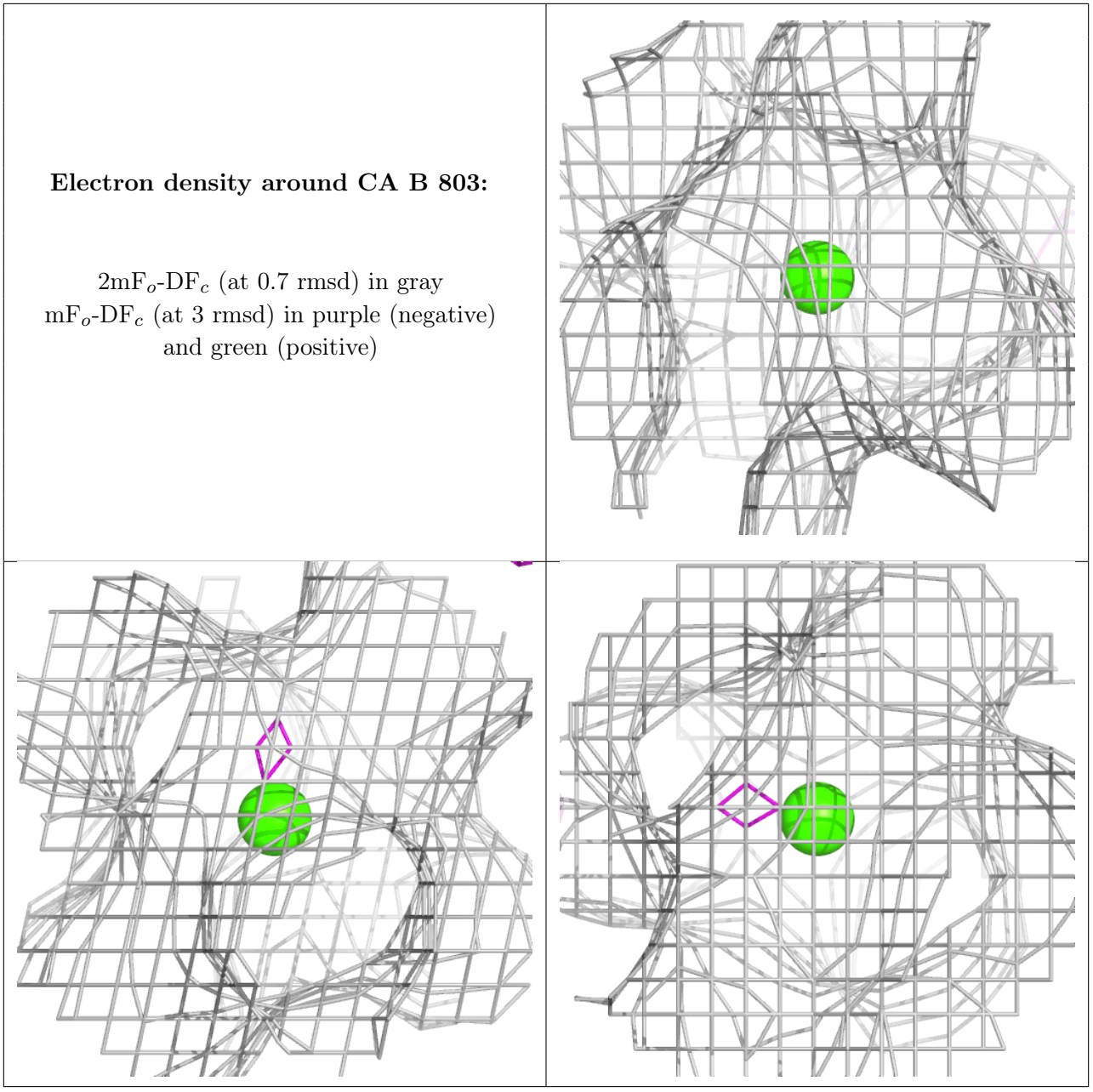






Electron density around CA B 803:

$2mF_o$-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

There are no such residues in this entry.