



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:38 pm BST

PDB ID : 4Q3R  
Title : Crystal structure of Schistosoma mansoni arginase in complex with inhibitor ABHDP  
Authors : Hai, Y.; Edwards, J.E.; Van Zandt, M.C.; Hoffmann, K.F.; Christianson, D.W.  
Deposited on : 2014-04-12  
Resolution : 2.17 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](mailto: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.

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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

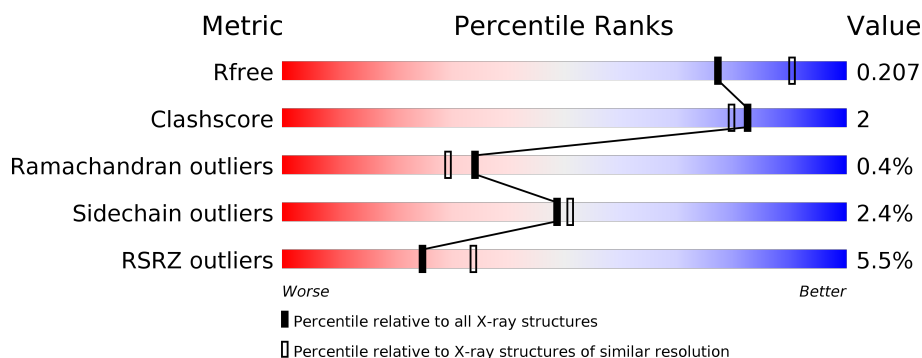
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>83%</span> <span>• • 13%</span> </div> </div>
1	B	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 82%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>82%</span> <span>• 14%</span> </div> </div>
2	C	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 82%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>82%</span> <span>• • 14%</span> </div> </div>
2	D	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 1%, yellow 1%, green 70%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>16%</span> <span>70%</span> <span>10% • 18%</span> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10942 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 Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	3	0
			2605	1639	457	494	15			
1	B	333	Total	C	N	O	S	0	2	0
			2566	1619	446	486	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
A	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
A	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
A	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
A	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
A	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
A	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
A	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
A	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	0	MET	-	EXPRESSION TAG	UNP Q6WVP6
B	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
B	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
B	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
B	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
B	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
B	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
B	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
B	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
B	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	0	MET	-	EXPRESSION TAG	UNP Q6WVP6

- Molecule 2 is a protein called Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	333	Total	C	N	O	S	0	1	0
			2558	1612	446	484	16			
2	D	314	Total	C	N	O	S	0	0	0
			2405	1522	414	456	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
C	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
C	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
C	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
C	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
C	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
C	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
C	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	0	MET	-	EXPRESSION TAG	UNP Q6WVP6
D	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
D	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
D	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
D	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
D	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
D	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	0	MET	-	EXPRESSION TAG	UNP Q6WVP6

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0
3	D	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0

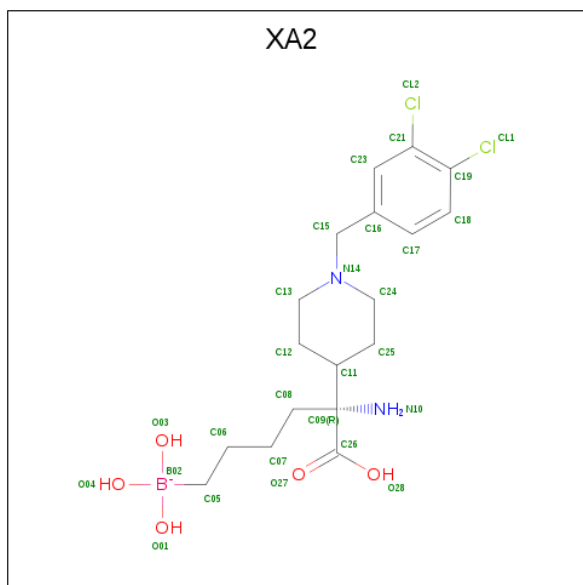
- Molecule 4 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total Cs 4 4	0	0
4	A	3	Total Cs 3 3	0	0
4	D	1	Total Cs 1 1	0	0
4	C	3	Total Cs 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Cl 2 2	0	0
5	A	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is (R)-2-amino-6-borono-2-(1-(3,4-dichlorobenzyl)piperidin-4-yl)hexanoic acid (three-letter code: XA2) (formula: C<sub>18</sub>H<sub>28</sub>BCl<sub>2</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 28	B 1	C 18	Cl 2	N 2	O 5	0	0
6	B	1	Total 28	B 1	C 18	Cl 2	N 2	O 5	0	0

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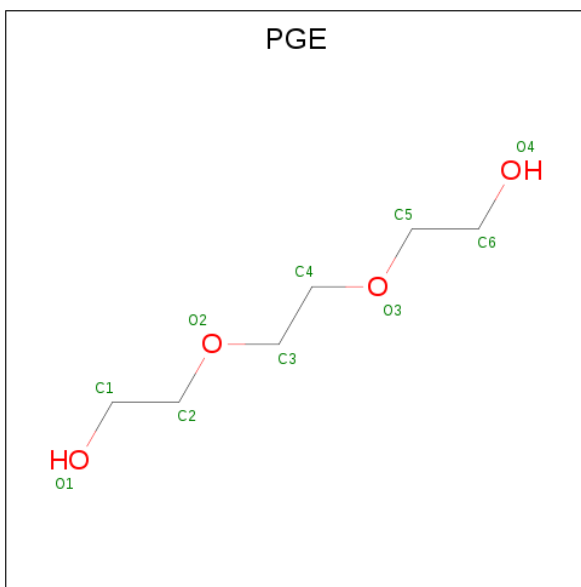
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	B	C	Cl	N	O	
			28	1	18	2	2	5	
6	D	1	Total	B	C	Cl	N	O	
			28	1	18	2	2	5	

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is water.

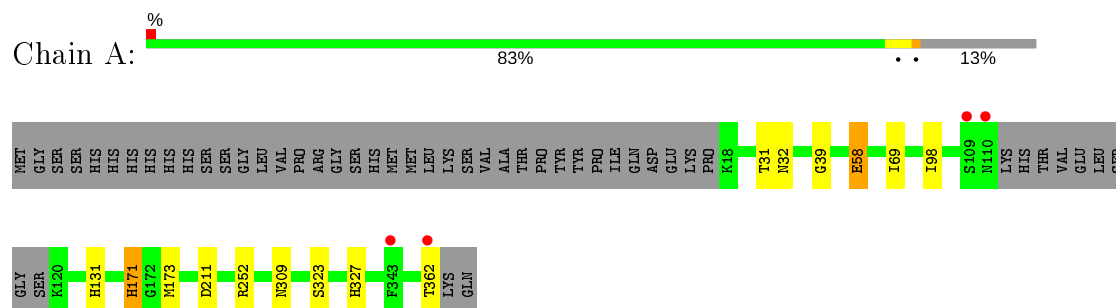
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	244	Total	O	0	0
			244	244		
9	B	237	Total	O	0	0
			237	237		
9	C	130	Total	O	0	0
			130	130		
9	D	16	Total	O	0	0
			16	16		



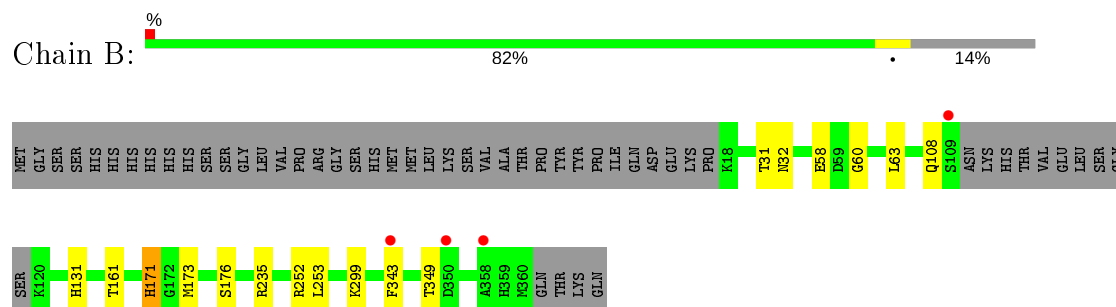
### 3 Residue-property plots [i](#)

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.

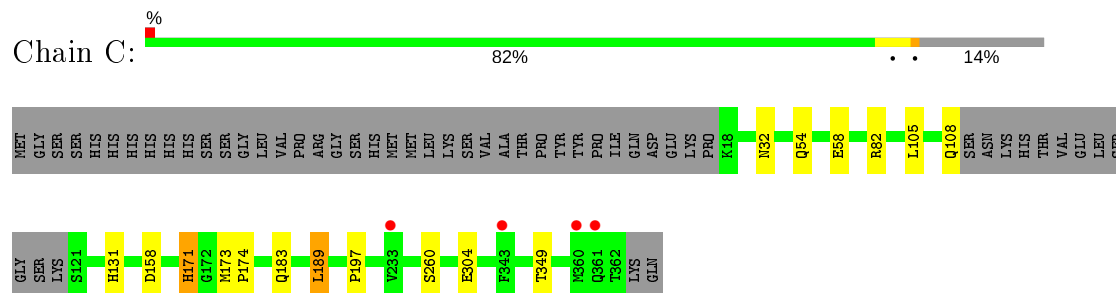
- Molecule 1: Arginase



- Molecule 1: Arginase

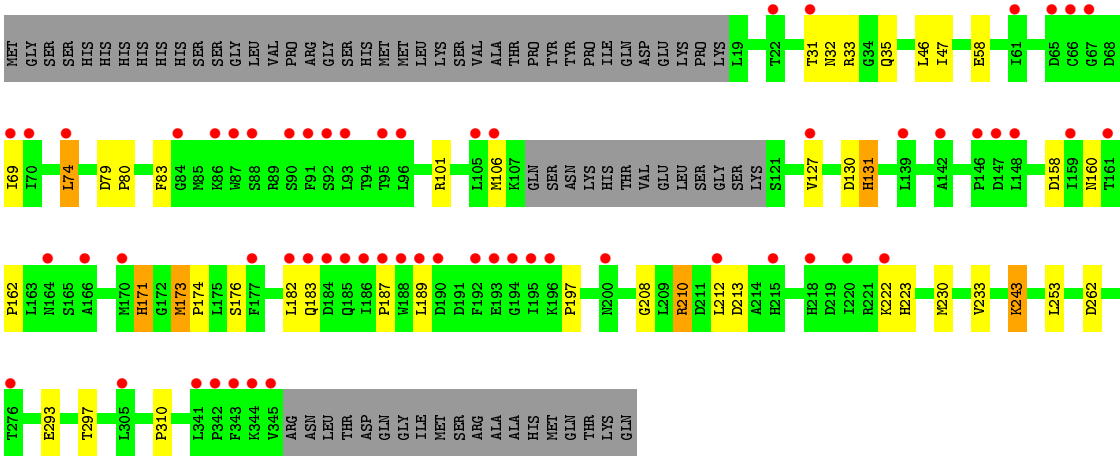


- Molecule 2: Arginase



- Molecule 2: Arginase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.49 Å   177.49 Å   177.49 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.23 – 2.17 49.23 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.23-2.17) 98.3 (49.23-2.17)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.16 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.174 , 0.206 0.176 , 0.207	Depositor DCC
$R_{free}$ test set	4812 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CSO, PGE, CL, XA2, MN, CS

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	0.46	0/2647	0.57	0/3583
1	B	0.44	0/2611	0.56	0/3536
2	C	0.37	0/2608	0.53	0/3535
2	D	0.32	1/2451 (0.0%)	0.48	1/3326 (0.0%)
All	All	0.40	1/10317 (0.0%)	0.54	1/13980 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	80	PRO	N-CD	5.43	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	79	ASP	C-N-CD	5.56	140.08	128.40

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	2605	0	2621	10	0
1	B	2566	0	2587	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2558	0	2573	10	0
2	D	2405	0	2416	21	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
6	A	28	0	25	3	0
6	B	28	0	25	2	0
6	C	28	0	25	3	0
6	D	28	0	26	2	0
7	A	12	0	16	0	0
7	B	12	0	16	0	0
7	C	12	0	16	0	0
8	A	10	0	14	5	0
9	A	244	0	0	2	0
9	B	237	0	0	2	0
9	C	130	0	0	1	0
9	D	16	0	0	0	0
All	All	10942	0	10360	51	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 (51) 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)
8:A:410:PGE:H5	1:B:299:LYS:HD3	1.74	0.70
1:A:252:ARG:HB3	8:A:410:PGE:H62	1.75	0.69
2:D:243:LYS:NZ	2:D:293:GLU:OE1	2.28	0.67
2:D:69:ILE:HD11	2:D:101:ARG:HG2	1.76	0.65
2:D:230:MET:HE1	2:D:233:VAL:HG21	1.79	0.64
8:A:410:PGE:H4	1:B:253:LEU:O	2.04	0.57
2:D:208:GLY:HA2	2:D:230:MET:HE3	1.86	0.56
2:D:33:ARG:NH2	2:D:74:LEU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:HIS:CE1	2:D:262:ASP:HB2	2.42	0.55
2:D:253:LEU:HD22	2:D:297:THR:HG23	1.89	0.54
1:A:171:HIS:CE1	6:A:407:XA2:H5	2.44	0.52
1:B:171:HIS:CE1	6:B:409:XA2:H5	2.45	0.52
2:C:183:GLN:HG3	2:C:197:PRO:HG3	1.91	0.51
2:D:160:ASN:O	2:D:176:SER:OG	2.27	0.51
2:D:46:LEU:HD22	2:D:310:PRO:HG3	1.93	0.51
2:D:173:MET:N	2:D:174:PRO:HD3	2.27	0.50
1:A:69:ILE:HD13	1:A:98:ILE:HA	1.93	0.50
1:A:323:SER:O	1:A:327:HIS:HD2	1.94	0.49
2:D:158:ASP:HB3	2:D:174:PRO:HD2	1.95	0.49
1:A:211:ASP:OD2	9:A:633:HOH:O	2.20	0.49
1:A:362:THR:OG1	1:A:362:THR:O	2.29	0.48
2:D:208:GLY:HA2	2:D:230:MET:CE	2.43	0.48
2:C:82:ARG:HD2	9:C:596:HOH:O	2.14	0.47
1:A:171:HIS:CG	6:A:407:XA2:H5	2.49	0.47
8:A:410:PGE:H12	1:B:252:ARG:O	2.15	0.47
2:C:105:LEU:O	2:C:108:GLN:HG2	2.16	0.46
1:A:39:GLY:HA3	1:A:309:ASN:OD1	2.17	0.45
2:D:210:ARG:HD3	2:D:230:MET:HG3	1.97	0.45
1:B:235:ARG:NH2	9:B:555:HOH:O	2.45	0.45
1:B:171:HIS:CG	6:B:409:XA2:H5	2.51	0.45
2:D:83:PHE:HE2	2:D:189:LEU:HD21	1.82	0.45
2:C:171:HIS:CE1	6:C:407:XA2:H5	2.53	0.44
2:D:31:THR:HG22	2:D:130:ASP:OD2	2.17	0.44
8:A:410:PGE:H12	1:B:252:ARG:HB3	1.98	0.44
2:D:183:GLN:HG3	2:D:197:PRO:HG3	2.00	0.43
2:D:171:HIS:CG	6:D:404:XA2:H5	2.53	0.43
1:A:58[B]:GLU:HG3	9:A:634:HOH:O	2.19	0.43
2:C:260:SER:HA	2:C:304:GLU:HG2	2.00	0.43
1:A:171:HIS:ND1	6:A:407:XA2:H5	2.34	0.42
1:B:58[B]:GLU:HG3	9:B:611:HOH:O	2.19	0.42
2:D:213:ASP:OD1	6:D:404:XA2:H22	2.18	0.42
2:D:222:LYS:HE3	2:D:223:HIS:NE2	2.35	0.42
2:D:47:ILE:HD12	2:D:127:VAL:HG11	2.01	0.42
1:B:60:GLY:HA3	1:B:343:PHE:CZ	2.54	0.42
2:C:82:ARG:NH2	2:C:189:LEU:HG	2.35	0.41
2:C:54:GLN:O	2:C:58:GLU:HG2	2.20	0.41
2:C:171:HIS:CD2	6:C:407:XA2:H5	2.55	0.41
2:C:171:HIS:CG	6:C:407:XA2:H5	2.55	0.41
1:B:161:THR:HG22	1:B:176:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ASP:HB3	2:C:174:PRO:HD2	2.03	0.41
2:D:162:PRO:HG2	2:D:187:PRO:HD2	2.03	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	334/385 (87%)	328 (98%)	5 (2%)	1 (0%)	41	37
1	B	330/385 (86%)	324 (98%)	5 (2%)	1 (0%)	41	37
2	C	330/385 (86%)	321 (97%)	8 (2%)	1 (0%)	41	37
2	D	310/385 (80%)	302 (97%)	6 (2%)	2 (1%)	25	18
All	All	1304/1540 (85%)	1275 (98%)	24 (2%)	5 (0%)	34	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	210	ARG
1	A	173	MET
1	B	173	MET
2	D	173	MET
2	C	173	MET

### 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	285/326 (87%)	279 (98%)	6 (2%)	53	57
1	B	281/326 (86%)	274 (98%)	7 (2%)	47	49
2	C	281/327 (86%)	276 (98%)	5 (2%)	59	63
2	D	264/327 (81%)	254 (96%)	10 (4%)	33	31
All	All	1111/1306 (85%)	1083 (98%)	28 (2%)	49	49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	32	ASN
1	A	58[A]	GLU
1	A	58[B]	GLU
1	A	131	HIS
1	A	171	HIS
1	B	31	THR
1	B	32	ASN
1	B	63	LEU
1	B	108	GLN
1	B	131	HIS
1	B	171	HIS
1	B	349	THR
2	C	32	ASN
2	C	131	HIS
2	C	171	HIS
2	C	189	LEU
2	C	349	THR
2	D	32	ASN
2	D	35	GLN
2	D	58	GLU
2	D	74	LEU
2	D	106	MET
2	D	131	HIS
2	D	171	HIS
2	D	182	LEU
2	D	212	LEU
2	D	243	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	351	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSO	A	336	1	3,6,7	0.76	0	0,6,8	0.00	-
1	CSO	B	336	1	3,6,7	0.64	0	0,6,8	0.00	-

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
1	CSO	A	336	1	-	0/1/5/7	-
1	CSO	B	336	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 23 are monoatomic - leaving 11 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
8	PGE	A	410	-	9,9,9	0.31	0	8,8,8	0.33	0
7	GOL	A	408	-	5,5,5	0.46	0	5,5,5	0.55	0
6	XA2	C	407	3	21,29,29	1.47	3 (14%)	27,42,42	0.90	0
7	GOL	B	411	-	5,5,5	0.39	0	5,5,5	0.31	0
7	GOL	B	410	-	5,5,5	0.26	0	5,5,5	0.71	0
6	XA2	A	407	3	21,29,29	1.47	1 (4%)	27,42,42	0.90	0
7	GOL	C	408	-	5,5,5	0.32	0	5,5,5	0.30	0
6	XA2	D	404	3	21,29,29	1.45	2 (9%)	27,42,42	0.93	2 (7%)
6	XA2	B	409	3	21,29,29	1.36	1 (4%)	27,42,42	1.00	2 (7%)
7	GOL	A	409	-	5,5,5	0.42	0	5,5,5	0.70	0
7	GOL	C	409	-	5,5,5	0.43	0	5,5,5	0.30	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
8	PGE	A	410	-	-	3/7/7/7	-
7	GOL	A	408	-	-	2/4/4/4	-
6	XA2	C	407	3	-	1/14/35/35	0/2/2/2
7	GOL	B	411	-	-	2/4/4/4	-
7	GOL	B	410	-	-	2/4/4/4	-
6	XA2	A	407	3	-	1/14/35/35	0/2/2/2
7	GOL	C	408	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	XA2	D	404	3	-	4/14/35/35	0/2/2/2
6	XA2	B	409	3	-	1/14/35/35	0/2/2/2
7	GOL	A	409	-	-	2/4/4/4	-
7	GOL	C	409	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	XA2	B02-C05	5.26	1.71	1.57
6	C	407	XA2	B02-C05	5.01	1.71	1.57
6	B	409	XA2	B02-C05	4.79	1.70	1.57
6	D	404	XA2	B02-C05	4.75	1.70	1.57
6	C	407	XA2	C12-C11	-2.16	1.47	1.53
6	D	404	XA2	C12-C11	-2.15	1.47	1.53
6	C	407	XA2	C08-C09	2.08	1.57	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	409	XA2	C07-C06-C05	-2.68	106.42	112.81
6	D	404	XA2	C24-N14-C13	2.32	114.06	108.83
6	D	404	XA2	B02-C05-C06	-2.14	108.06	115.64
6	B	409	XA2	C25-C11-C12	2.02	113.23	109.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	408	GOL	O1-C1-C2-O2
7	A	408	GOL	O1-C1-C2-C3
6	A	407	XA2	B02-C05-C06-C07
7	B	411	GOL	O1-C1-C2-C3
7	C	409	GOL	O1-C1-C2-C3
6	D	404	XA2	C07-C08-C09-N10
6	D	404	XA2	C07-C08-C09-C11
6	D	404	XA2	C07-C08-C09-C26
7	B	410	GOL	O1-C1-C2-C3
8	A	410	PGE	O2-C3-C4-O3
6	C	407	XA2	B02-C05-C06-C07
6	B	409	XA2	B02-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
7	C	409	GOL	O1-C1-C2-O2
7	B	410	GOL	O1-C1-C2-O2
8	A	410	PGE	O1-C1-C2-O2
7	B	411	GOL	O1-C1-C2-O2
8	A	410	PGE	C1-C2-O2-C3
7	A	409	GOL	O1-C1-C2-C3
7	A	409	GOL	O1-C1-C2-O2
6	D	404	XA2	C05-C06-C07-C08

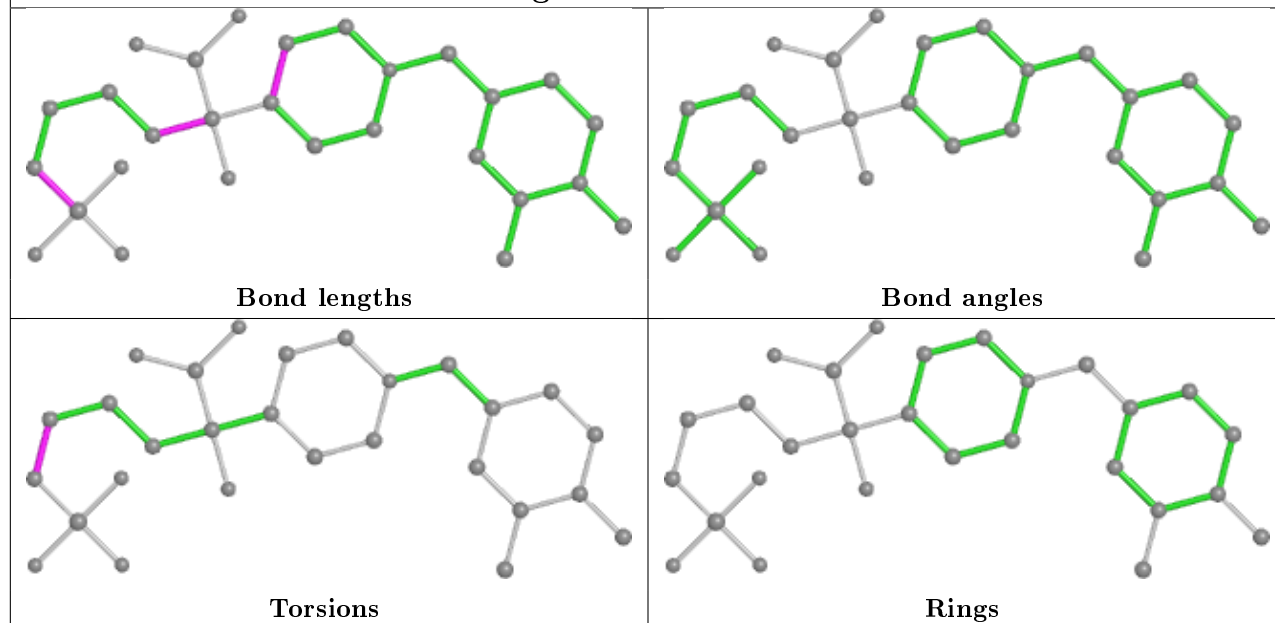
There are no ring outliers.

5 monomers are involved in 15 short contacts:

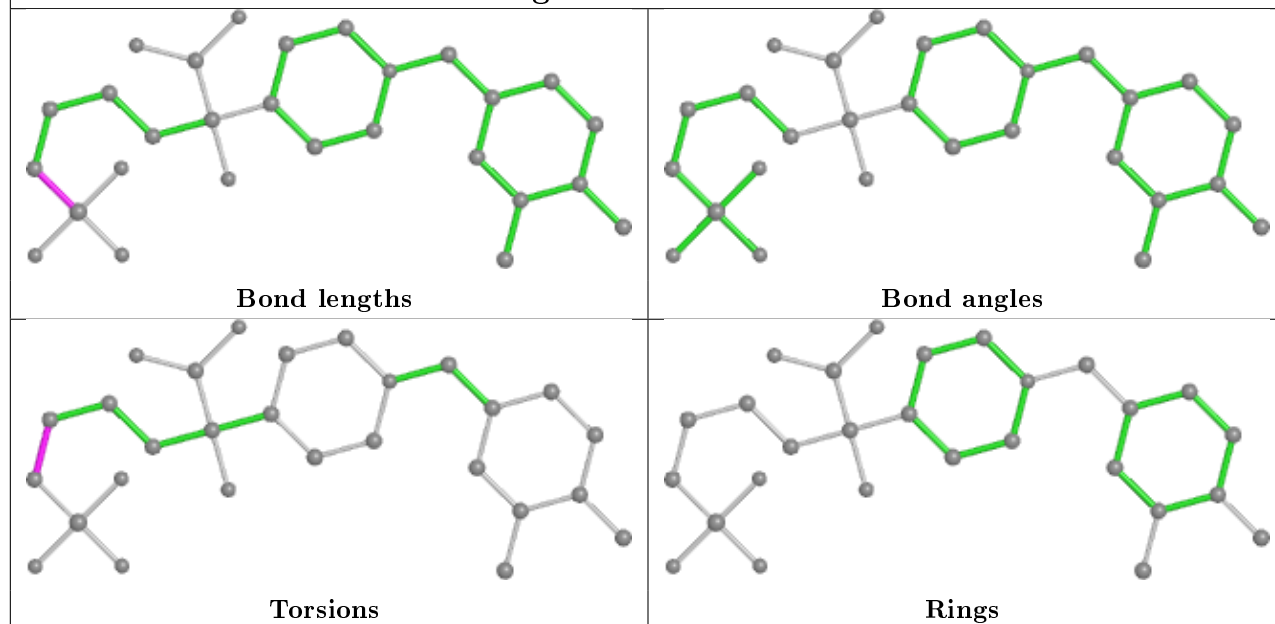
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	410	PGE	5	0
6	C	407	XA2	3	0
6	A	407	XA2	3	0
6	D	404	XA2	2	0
6	B	409	XA2	2	0

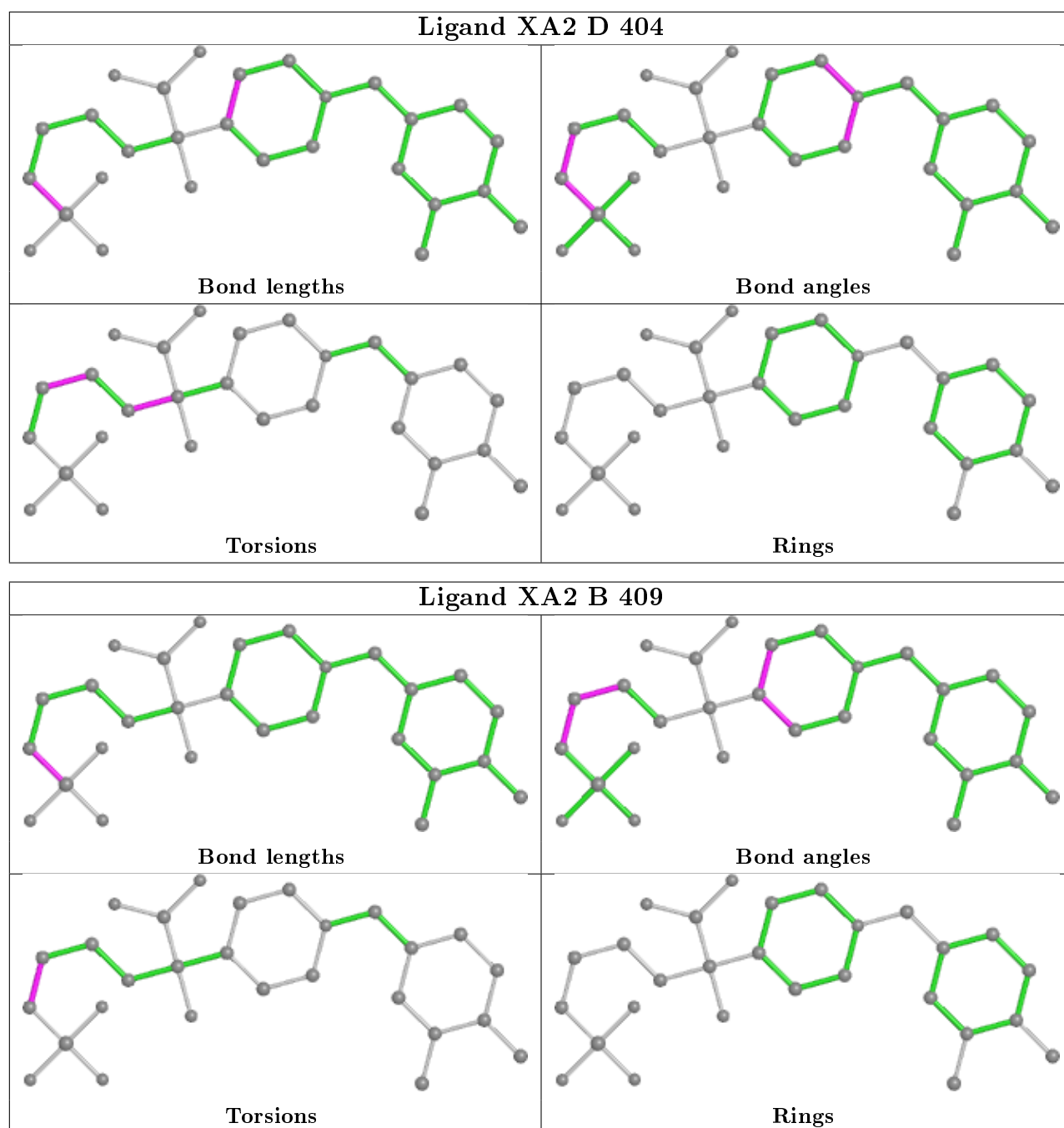
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 XA2 C 407



## Ligand XA2 A 407





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/385 (87%)	-0.23	4 (1%) 79 83	12, 18, 42, 69	0
1	B	332/385 (86%)	-0.05	4 (1%) 79 83	12, 18, 42, 76	0
2	C	333/385 (86%)	-0.23	4 (1%) 79 83	19, 26, 46, 80	1 (0%)
2	D	314/385 (81%)	1.09	60 (19%) 1 1	34, 60, 84, 101	0
All	All	1314/1540 (85%)	0.13	72 (5%) 25 34	12, 25, 72, 101	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	345	VAL	6.7
2	D	343	PHE	6.6
1	B	343	PHE	6.0
2	D	189	LEU	4.9
2	D	184	ASP	4.8
2	D	344	LYS	4.6
2	D	74	LEU	4.4
2	D	188	TRP	4.3
2	D	91	PHE	4.3
2	D	177	PHE	4.1
2	D	192	PHE	4.1
1	B	350	ASP	3.9
1	B	109	SER	3.9
2	D	146	PRO	3.8
2	D	147	ASP	3.8
2	D	69	ILE	3.6
2	D	195	ILE	3.6
1	B	358	ALA	3.6
2	D	187	PRO	3.5
1	A	109	SER	3.5
2	D	341	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	22	THR	3.4
2	D	193	GLU	3.4
2	D	96	LEU	3.4
2	D	70	ILE	3.3
2	D	182	LEU	3.3
2	D	190	ASP	3.2
2	D	105	LEU	3.2
2	C	343	PHE	3.2
2	D	148	LEU	3.2
1	A	343	PHE	3.1
2	D	220	ILE	3.1
2	D	90	SER	3.0
2	D	161	THR	2.9
2	D	342	PRO	2.9
2	D	166	ALA	2.9
1	A	362	THR	2.9
2	D	139	LEU	2.8
2	D	186	ILE	2.8
2	D	87	TRP	2.8
2	D	65	ASP	2.8
2	C	361	GLN	2.8
1	A	110	ASN	2.7
2	D	92	SER	2.6
2	D	183	GLN	2.6
2	D	95	THR	2.6
2	D	164	ASN	2.5
2	D	170	MET	2.5
2	D	159	ILE	2.5
2	D	215	HIS	2.4
2	D	66	CYS	2.4
2	D	106	MET	2.4
2	D	185	GLN	2.3
2	D	222	LYS	2.3
2	D	127	VAL	2.3
2	D	196	LYS	2.2
2	D	86	LYS	2.2
2	D	67	GLY	2.2
2	D	200	ASN	2.2
2	D	276	THR	2.2
2	D	194	GLY	2.2
2	D	305	LEU	2.1
2	D	212	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	31	THR	2.1
2	D	61	ILE	2.1
2	C	360	MET	2.1
2	D	88	SER	2.1
2	D	84	GLY	2.1
2	D	93	LEU	2.0
2	D	218	HIS	2.0
2	D	142	ALA	2.0
2	C	233	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSO	A	336	7/8	0.95	0.09	16,17,27,30	0
1	CSO	B	336	7/8	0.96	0.08	15,18,28,28	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	CS	A	404	1/1	0.45	0.26	135,135,135,135	1
4	CS	B	404	1/1	0.66	0.13	130,130,130,130	0
4	CS	C	406	1/1	0.69	0.13	106,106,106,106	1
6	XA2	D	404	28/28	0.74	0.27	45,65,87,103	0
8	PGE	A	410	10/10	0.78	0.28	51,62,72,82	0
4	CS	B	406	1/1	0.85	0.12	86,86,86,86	1
4	CS	C	404	1/1	0.88	0.10	87,87,87,87	1

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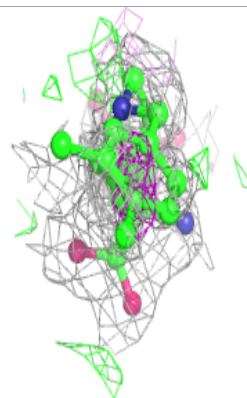
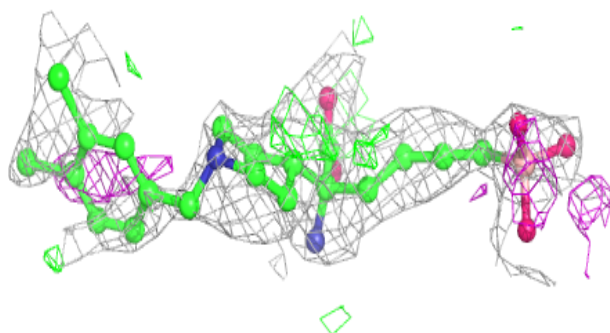
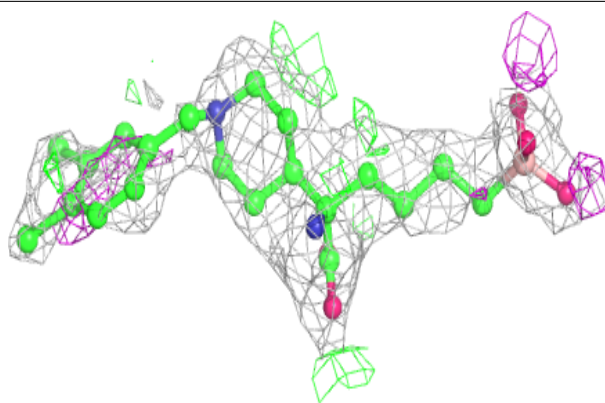
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	XA2	B	409	28/28	0.88	0.16	15,25,55,73	0
5	CL	B	408	1/1	0.89	0.09	61,61,61,61	1
7	GOL	C	408	6/6	0.90	0.13	29,39,45,49	1
6	XA2	C	407	28/28	0.90	0.15	19,30,68,86	0
6	XA2	A	407	28/28	0.90	0.17	16,23,59,74	0
7	GOL	B	410	6/6	0.91	0.16	25,30,36,46	1
7	GOL	B	411	6/6	0.93	0.14	23,29,33,34	1
7	GOL	C	409	6/6	0.95	0.14	32,35,39,44	1
4	CS	A	405	1/1	0.95	0.09	86,86,86,86	1
7	GOL	A	409	6/6	0.95	0.10	24,26,31,40	0
7	GOL	A	408	6/6	0.96	0.14	24,29,41,42	1
5	CL	C	405	1/1	0.96	0.07	54,54,54,54	0
5	CL	A	406	1/1	0.96	0.12	49,49,49,49	1
3	MN	D	402	1/1	0.97	0.04	44,44,44,44	0
5	CL	B	407	1/1	0.97	0.12	47,47,47,47	0
4	CS	D	403	1/1	0.98	0.04	59,59,59,59	1
3	MN	D	401	1/1	0.98	0.05	42,42,42,42	0
4	CS	B	405	1/1	0.98	0.06	58,58,58,58	1
4	CS	C	403	1/1	0.98	0.03	53,53,53,53	0
4	CS	A	403	1/1	0.99	0.07	42,42,42,42	1
3	MN	C	402	1/1	0.99	0.14	25,25,25,25	0
4	CS	B	403	1/1	0.99	0.06	45,45,45,45	0
3	MN	B	401	1/1	1.00	0.10	11,11,11,11	0
3	MN	A	401	1/1	1.00	0.12	15,15,15,15	0
3	MN	C	401	1/1	1.00	0.12	25,25,25,25	0
3	MN	A	402	1/1	1.00	0.12	15,15,15,15	0
3	MN	B	402	1/1	1.00	0.12	11,11,11,11	0

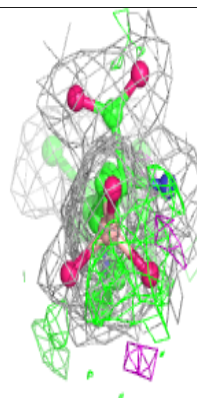
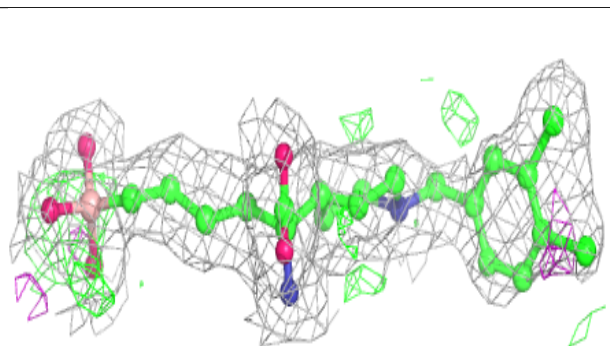
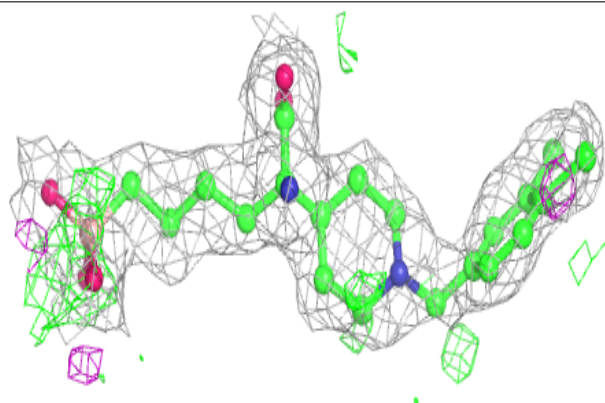
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XA2 D 404:**

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

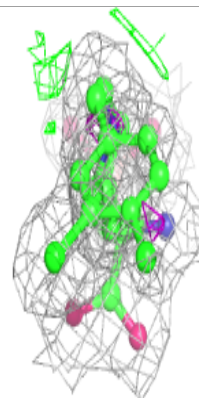
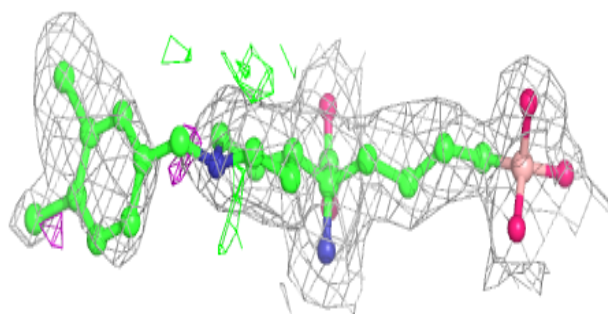
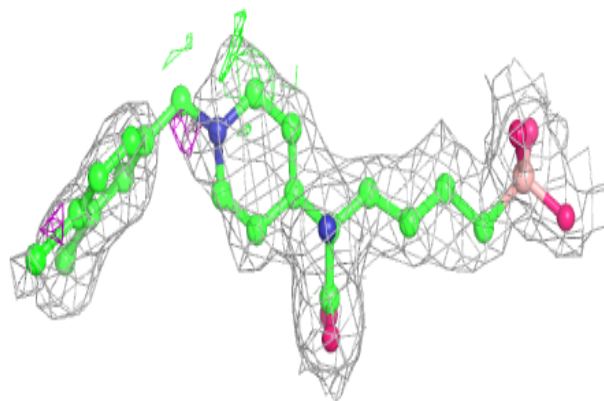
**Electron density around XA2 B 409:**

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

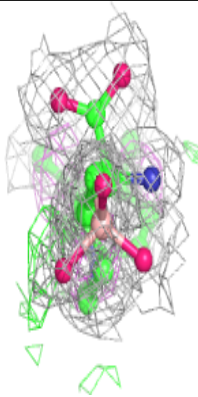
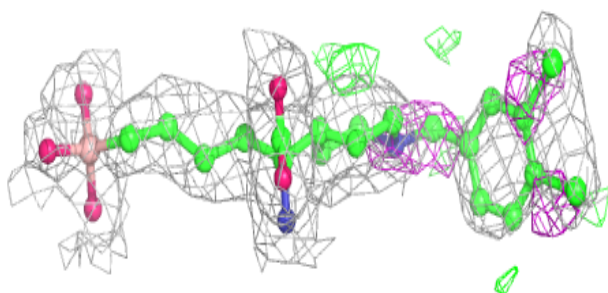
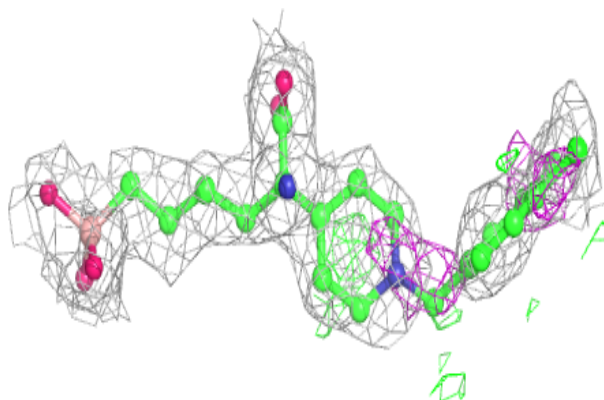


**Electron density around XA2 C 407:**

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

**Electron density around XA2 A 407:**

$2mF_o-DF_c$  (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.