



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 03:39 AM EDT

PDB ID : 8ER4
Title : Co-crystal structure of Chaetomium glucosidase with compound 23
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2022-10-11
Resolution : 2.30 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

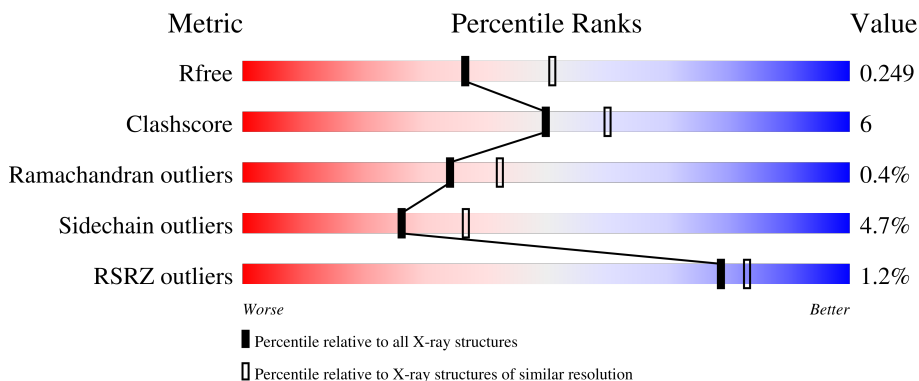
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	819	 2% 79% 13% • 7%
1	B	819	 80% 13% • 6%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 12522 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 Chaetomium alpha glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	765	6024	3862	1020	1129	13	0	2	0
1	B	767	6015	3859	1015	1128	13	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP G0SFD1
A	0	GLY	-	expression tag	UNP G0SFD1
A	1	ILE	-	expression tag	UNP G0SFD1
A	2	LEU	-	expression tag	UNP G0SFD1
A	3	PRO	-	expression tag	UNP G0SFD1
A	4	SER	-	expression tag	UNP G0SFD1
A	5	PRO	-	expression tag	UNP G0SFD1
A	6	GLY	-	expression tag	UNP G0SFD1
A	7	MET	-	expression tag	UNP G0SFD1
A	8	PRO	-	expression tag	UNP G0SFD1
A	9	ALA	-	expression tag	UNP G0SFD1
A	10	LEU	-	expression tag	UNP G0SFD1
A	11	LEU	-	expression tag	UNP G0SFD1
A	12	SER	-	expression tag	UNP G0SFD1
A	13	LEU	-	expression tag	UNP G0SFD1
A	14	VAL	-	expression tag	UNP G0SFD1
A	15	SER	-	expression tag	UNP G0SFD1
A	16	LEU	-	expression tag	UNP G0SFD1
A	17	LEU	-	expression tag	UNP G0SFD1
A	18	SER	-	expression tag	UNP G0SFD1
A	19	VAL	-	expression tag	UNP G0SFD1
A	20	LEU	-	expression tag	UNP G0SFD1
A	21	LEU	-	expression tag	UNP G0SFD1
A	22	MET	-	expression tag	UNP G0SFD1
A	23	GLY	-	expression tag	UNP G0SFD1

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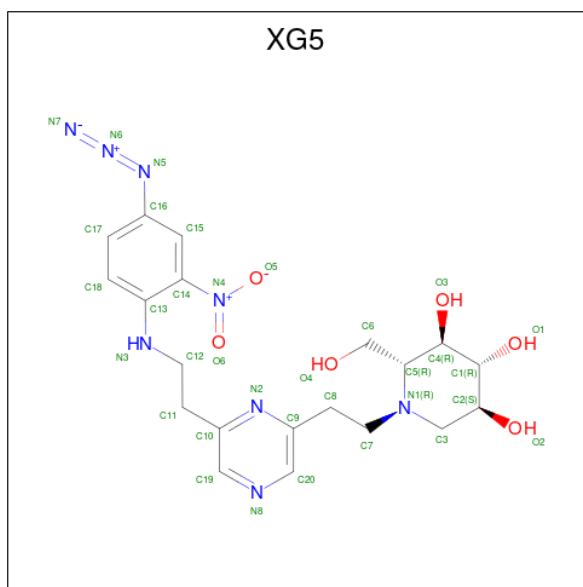
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP G0SFD1
A	811	GLY	-	expression tag	UNP G0SFD1
A	812	HIS	-	expression tag	UNP G0SFD1
A	813	HIS	-	expression tag	UNP G0SFD1
A	814	HIS	-	expression tag	UNP G0SFD1
A	815	HIS	-	expression tag	UNP G0SFD1
A	816	HIS	-	expression tag	UNP G0SFD1
A	817	HIS	-	expression tag	UNP G0SFD1
B	-1	MET	-	initiating methionine	UNP G0SFD1
B	0	GLY	-	expression tag	UNP G0SFD1
B	1	ILE	-	expression tag	UNP G0SFD1
B	2	LEU	-	expression tag	UNP G0SFD1
B	3	PRO	-	expression tag	UNP G0SFD1
B	4	SER	-	expression tag	UNP G0SFD1
B	5	PRO	-	expression tag	UNP G0SFD1
B	6	GLY	-	expression tag	UNP G0SFD1
B	7	MET	-	expression tag	UNP G0SFD1
B	8	PRO	-	expression tag	UNP G0SFD1
B	9	ALA	-	expression tag	UNP G0SFD1
B	10	LEU	-	expression tag	UNP G0SFD1
B	11	LEU	-	expression tag	UNP G0SFD1
B	12	SER	-	expression tag	UNP G0SFD1
B	13	LEU	-	expression tag	UNP G0SFD1
B	14	VAL	-	expression tag	UNP G0SFD1
B	15	SER	-	expression tag	UNP G0SFD1
B	16	LEU	-	expression tag	UNP G0SFD1
B	17	LEU	-	expression tag	UNP G0SFD1
B	18	SER	-	expression tag	UNP G0SFD1
B	19	VAL	-	expression tag	UNP G0SFD1
B	20	LEU	-	expression tag	UNP G0SFD1
B	21	LEU	-	expression tag	UNP G0SFD1
B	22	MET	-	expression tag	UNP G0SFD1
B	23	GLY	-	expression tag	UNP G0SFD1
B	24	CYS	-	expression tag	UNP G0SFD1
B	25	VAL	-	expression tag	UNP G0SFD1
B	26	ALA	-	expression tag	UNP G0SFD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP G0SFD1
B	814	HIS	-	expression tag	UNP G0SFD1
B	815	HIS	-	expression tag	UNP G0SFD1
B	816	HIS	-	expression tag	UNP G0SFD1
B	817	HIS	-	expression tag	UNP G0SFD1

- Molecule 2 is (2R,3R,4R,5S)-1-(2-{6-[2-(4-azido-2-nitroanilino)ethyl]pyrazin-2-yl}ethyl)-2-(hydroxymethyl)piperidine-3,4,5-triol (three-letter code: XG5) (formula: C₂₀H₂₆N₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	N	O	0	0
			34	20	8	6		
2	B	1	Total	C	N	O	0	0
			34	20	8	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



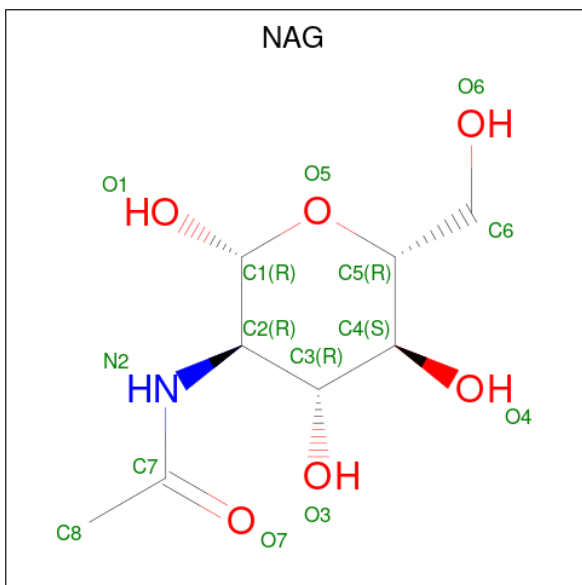
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0

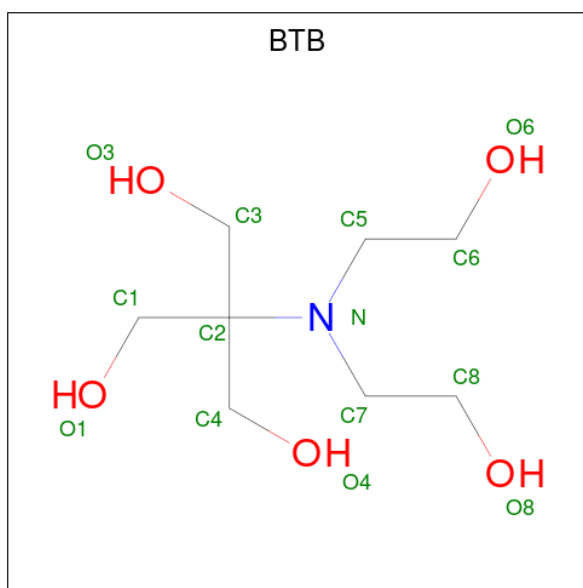
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0

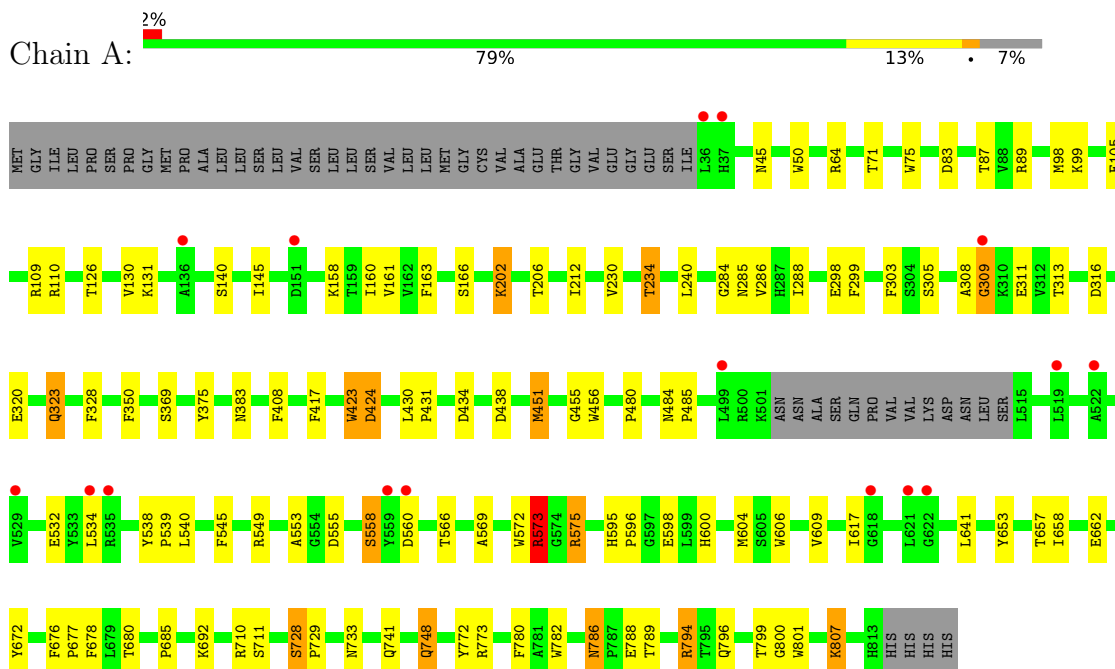
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	176	176	176	0	0
7	B	143	143	143	0	0

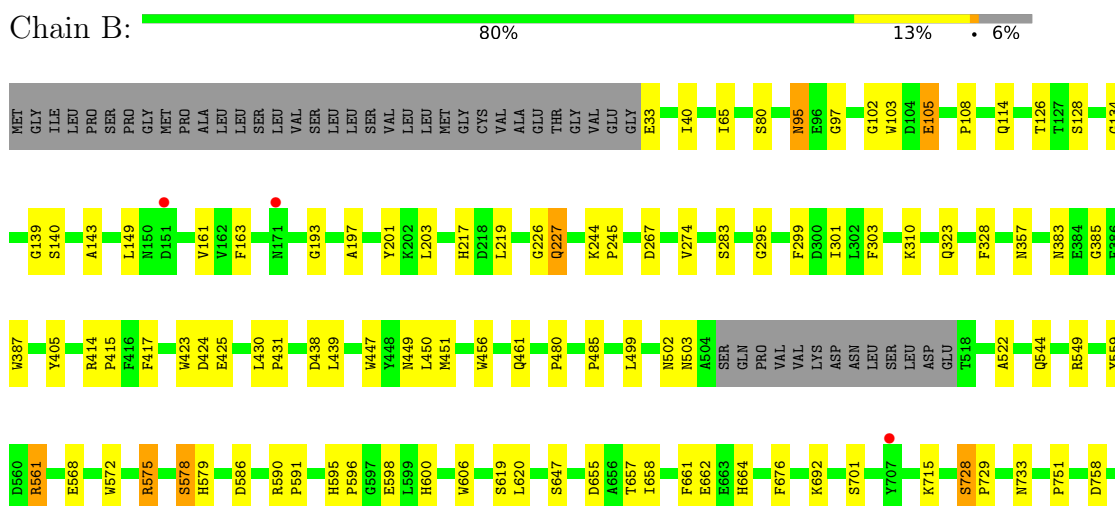
3 Residue-property plots i

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: Chaetomium alpha glucosidase



- Molecule 1: Chaetomium alpha glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.65Å 177.20Å 180.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 2.30 46.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.80-2.30) 99.0 (46.76-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.32Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.198 , 0.246 0.201 , 0.249	Depositor DCC
R_{free} test set	4698 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtrriage
Anisotropy	0.471	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12522	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: NAG, GOL, XG5, BTB, SO4

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	0.73	0/6202	0.87	7/8454 (0.1%)
1	B	0.73	0/6191	0.86	1/8444 (0.0%)
All	All	0.73	0/12393	0.87	8/16898 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	575	ARG	CB-CA-C	9.00	128.40	110.40
1	A	575	ARG	CB-CA-C	7.71	125.82	110.40
1	A	794	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	794	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	573	ARG	CG-CD-NE	-5.46	100.33	111.80
1	A	710	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	794	ARG	CB-CA-C	5.17	120.75	110.40
1	A	158	LYS	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	780	PHE	Peptide
1	B	780	PHE	Peptide

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	6024	0	5615	71	0
1	B	6015	0	5592	64	0
2	A	34	0	0	1	0
2	B	34	0	0	0	0
3	A	6	0	8	1	0
3	B	12	0	16	1	0
4	A	40	0	0	1	0
4	B	10	0	0	0	0
5	B	14	0	13	0	0
6	B	14	0	19	0	0
7	A	176	0	0	3	1
7	B	143	0	0	2	1
All	All	12522	0	11263	136	1

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 6.

All (136) 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:685:PRO:HG3	1:A:748:GLN:HE22	1.22	1.01
1:A:451:MET:HE1	1:A:540:LEU:HB3	1.59	0.83
1:B:114:GLN:NE2	1:B:414:ARG:HH12	1.76	0.83
1:A:451:MET:CE	1:A:540:LEU:HB3	2.11	0.80
1:B:766:ASN:O	1:B:770:THR:HG23	1.81	0.80
1:B:572:TRP:H	1:B:600:HIS:HD2	1.30	0.78
1:A:383:ASN:CB	7:A:1061:HOH:O	2.35	0.74
1:B:786:ASN:HD22	1:B:789:THR:H	1.35	0.74
1:A:685:PRO:CG	1:A:748:GLN:HE22	2.00	0.74
1:A:206:THR:HB	3:A:902:GOL:H32	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:ASN:O	1:B:770:THR:CG2	2.44	0.65
1:B:217:HIS:HD2	1:B:219:LEU:H	1.45	0.64
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.47	0.63
1:B:103:TRP:H	1:B:357:ASN:ND2	1.95	0.63
4:A:909:SO4:O4	7:A:1001:HOH:O	2.15	0.61
1:B:217:HIS:HE1	1:B:267:ASP:O	1.83	0.61
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.83	0.61
1:B:244:LYS:HB3	1:B:245:PRO:HD3	1.84	0.60
1:B:203:LEU:HD11	1:B:301:ILE:CG2	2.33	0.59
1:B:572:TRP:H	1:B:600:HIS:CD2	2.18	0.59
1:A:434:ASP:OD2	1:A:807:LYS:HD3	2.02	0.59
1:A:786:ASN:HD22	1:A:789:THR:H	1.49	0.59
1:B:578:SER:HB2	1:B:579:HIS:CE1	2.39	0.57
1:A:423:TRP:H	1:A:484:ASN:ND2	2.02	0.57
1:A:672:TYR:CZ	1:A:711:SER:HA	2.40	0.57
1:A:532:GLU:HA	1:A:532:GLU:OE1	2.05	0.57
1:A:672:TYR:CE2	1:A:711:SER:HA	2.40	0.57
1:A:786:ASN:ND2	1:A:788:GLU:H	2.02	0.56
1:B:733:ASN:HB3	1:B:801:TRP:CG	2.40	0.56
1:A:424:ASP:OD2	2:A:901:XG5:O4	2.24	0.55
1:B:40:ILE:HD12	1:B:522:ALA:HB1	1.89	0.55
1:A:109:ARG:O	1:A:131:LYS:HE3	2.07	0.55
1:A:234:THR:HG23	7:B:1024:HOH:O	2.05	0.55
1:A:451:MET:SD	1:A:455:GLY:HA2	2.47	0.54
1:A:555:ASP:OD2	1:A:558:SER:HB3	2.06	0.54
1:A:234:THR:HA	1:A:285:ASN:OD1	2.08	0.54
1:B:103:TRP:H	1:B:357:ASN:HD21	1.56	0.54
1:A:430:LEU:HB2	1:A:431:PRO:HD3	1.90	0.53
1:B:786:ASN:OD1	1:B:793:GLN:NE2	2.39	0.53
1:B:114:GLN:HE21	1:B:414:ARG:HH12	1.54	0.53
1:B:95:ASN:HD22	1:B:97:GLY:H	1.55	0.53
1:A:451:MET:HE3	1:A:540:LEU:HB3	1.90	0.52
1:A:140:SER:HB3	1:A:303:PHE:O	2.09	0.52
1:A:786:ASN:ND2	1:A:789:THR:H	2.07	0.52
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.92	0.52
1:A:423:TRP:H	1:A:484:ASN:HD22	1.58	0.51
1:B:128:SER:O	1:B:143:ALA:HA	2.11	0.51
1:B:549:ARG:NH1	1:B:568:GLU:OE2	2.41	0.51
1:A:161:VAL:HG11	1:A:299:PHE:CE1	2.46	0.51
1:A:553:ALA:O	1:A:573:ARG:NH2	2.39	0.51
1:B:385:GLY:HA2	1:B:387:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:HG22	7:A:1036:HOH:O	2.11	0.50
1:B:193:GLY:HA3	1:B:201:TYR:CZ	2.48	0.49
1:A:234:THR:CG2	7:B:1024:HOH:O	2.59	0.49
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.47	0.49
1:B:140:SER:HB3	1:B:303:PHE:O	2.13	0.48
1:A:83:ASP:O	1:A:87:THR:HG23	2.14	0.48
1:A:598:GLU:OE2	1:A:600:HIS:CE1	2.67	0.48
1:B:559:TYR:CE1	1:B:658:ILE:HG13	2.49	0.48
1:B:799:THR:N	1:B:800:GLY:HA3	2.29	0.48
1:B:105:GLU:HG3	1:B:328:PHE:CG	2.49	0.47
1:A:658:ILE:HD13	1:A:662:GLU:HA	1.96	0.47
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.97	0.47
1:B:701:SER:OG	1:B:715:LYS:NZ	2.38	0.47
1:A:658:ILE:CD1	1:A:662:GLU:HA	2.44	0.47
1:A:161:VAL:HG11	1:A:299:PHE:HE1	1.80	0.46
1:B:590:ARG:HB3	1:B:591:PRO:HD2	1.96	0.46
1:B:786:ASN:HB2	1:B:793:GLN:NE2	2.30	0.46
1:A:534:LEU:HD22	1:A:617:ILE:HD13	1.98	0.46
1:A:64:ARG:HD3	1:A:408:PHE:CD1	2.51	0.46
1:A:678:PHE:CE1	1:A:741:GLN:HB3	2.51	0.46
1:A:202:LYS:CE	1:A:311:GLU:OE1	2.63	0.46
1:A:234:THR:HG22	1:A:284:GLY:HA2	1.98	0.46
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.51	0.46
1:A:786:ASN:ND2	1:A:788:GLU:N	2.64	0.46
1:A:595:HIS:CE1	1:A:658:ILE:HG13	2.51	0.45
1:B:658:ILE:HG22	1:B:662:GLU:HA	1.97	0.45
1:B:108:PRO:HG2	1:B:439:LEU:HD22	1.98	0.45
1:A:130:VAL:HG21	1:A:320:GLU:HB3	1.98	0.45
1:A:538:TYR:HB3	1:A:539:PRO:HD3	1.99	0.45
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.31	0.45
1:B:661:PHE:O	1:B:662:GLU:HB2	2.16	0.45
1:A:308:ALA:O	1:A:309:GLY:O	2.35	0.45
1:A:313:THR:O	1:A:316:ASP:HB2	2.17	0.44
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.48	0.44
1:A:64:ARG:HD3	1:A:408:PHE:CE1	2.52	0.44
1:A:75:TRP:HA	1:A:160:ILE:O	2.18	0.44
1:B:103:TRP:N	1:B:357:ASN:HD21	2.16	0.44
1:B:451:MET:CE	1:B:544:GLN:HB2	2.48	0.44
1:A:545:PHE:CZ	1:A:549:ARG:HD2	2.53	0.43
1:B:102:GLY:CA	1:B:357:ASN:HD21	2.31	0.43
1:B:226:GLY:H	1:B:227:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HD13	1:B:461:GLN:NE2	2.33	0.43
1:B:134:GLY:O	1:B:139:GLY:HA2	2.19	0.43
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.19	0.43
1:A:572:TRP:H	1:A:600:HIS:HD2	1.66	0.43
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.54	0.43
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.66	0.43
1:B:217:HIS:CD2	1:B:219:LEU:H	2.31	0.43
1:B:385:GLY:HA2	1:B:387:TRP:CH2	2.54	0.43
1:A:105:GLU:HG2	1:A:328:PHE:CD1	2.54	0.42
1:B:163:PHE:CE1	1:B:301:ILE:HD13	2.54	0.42
1:A:595:HIS:CE1	1:A:658:ILE:CG1	3.02	0.42
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.54	0.42
1:B:405:TYR:CE2	3:B:904:GOL:H32	2.55	0.42
1:B:728:SER:N	1:B:729:PRO:CD	2.82	0.42
1:B:595:HIS:ND1	1:B:596:PRO:HD2	2.33	0.42
1:A:166:SER:HA	1:A:285:ASN:O	2.19	0.42
1:B:226:GLY:H	1:B:227:GLN:HE22	1.67	0.42
1:B:149:LEU:HD11	1:B:295:GLY:HA2	2.01	0.42
1:B:425:GLU:HG2	1:B:447:TRP:NE1	2.34	0.42
1:B:149:LEU:CD1	1:B:295:GLY:HA2	2.50	0.42
1:B:161:VAL:HG11	1:B:299:PHE:HE1	1.84	0.42
1:B:451:MET:HE1	1:B:544:GLN:HB2	2.01	0.42
1:A:799:THR:N	1:A:800:GLY:HA3	2.35	0.41
1:A:485:PRO:HB3	1:A:606:TRP:CE2	2.56	0.41
1:A:641:LEU:HD23	1:A:641:LEU:HA	1.91	0.41
1:B:499:LEU:HD23	1:B:499:LEU:HA	1.82	0.41
1:A:728:SER:OG	1:A:729:PRO:HD3	2.20	0.41
1:A:240:LEU:HD22	1:A:286:VAL:CG2	2.51	0.41
1:A:569:ALA:HA	1:A:604:MET:CE	2.51	0.41
1:B:161:VAL:HG11	1:B:299:PHE:CE1	2.55	0.41
1:B:414:ARG:N	1:B:415:PRO:HD2	2.36	0.41
1:A:89:ARG:NH2	1:A:98:MET:HE2	2.36	0.41
1:A:350:PHE:CE1	1:A:772:TYR:HA	2.56	0.41
1:A:145:ILE:O	1:A:298:GLU:HA	2.21	0.40
1:A:609:VAL:HG23	1:A:680:THR:HB	2.03	0.40
1:A:672:TYR:CE1	1:A:711:SER:HA	2.56	0.40
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.57	0.40
1:A:71:THR:HB	1:A:163:PHE:CZ	2.57	0.40
1:B:591:PRO:HD2	1:B:598:GLU:OE2	2.21	0.40
1:A:230:VAL:HA	1:A:288:ILE:O	2.21	0.40
1:A:782:TRP:CZ3	1:A:796:GLN:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:HD22	1:B:95:ASN:C	2.25	0.40
1:A:50:TRP:O	1:A:131:LYS:NZ	2.40	0.40
1:A:653:TYR:CD2	1:A:677:PRO:HG2	2.56	0.40

All (1) 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)
7:A:1147:HOH:O	7:B:1122:HOH:O[7_454]	1.99	0.21

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	763/819 (93%)	738 (97%)	21 (3%)	4 (0%)	29 35
1	B	763/819 (93%)	740 (97%)	21 (3%)	2 (0%)	41 50
All	All	1526/1638 (93%)	1478 (97%)	42 (3%)	6 (0%)	34 42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	A	728	SER
1	B	728	SER
1	A	560	ASP
1	B	503	ASN
1	A	375	TYR

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	613/707 (87%)	587 (96%)	26 (4%)	30	42
1	B	611/707 (86%)	579 (95%)	32 (5%)	23	32
All	All	1224/1414 (87%)	1166 (95%)	58 (5%)	26	37

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	99	LYS
1	A	202	LYS
1	A	212	ILE
1	A	234	THR
1	A	305	SER
1	A	323	GLN
1	A	369	SER
1	A	417	PHE
1	A	423	TRP
1	A	424	ASP
1	A	438	ASP
1	A	451	MET
1	A	558	SER
1	A	566	THR
1	A	573	ARG
1	A	575	ARG
1	A	596	PRO
1	A	657	THR
1	A	676	PHE
1	A	692	LYS
1	A	748	GLN
1	A	773	ARG
1	A	786	ASN
1	A	794	ARG
1	A	807	LYS
1	B	33	GLU

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Mol	Chain	Res	Type
1	B	80	SER
1	B	95	ASN
1	B	105	GLU
1	B	126	THR
1	B	227	GLN
1	B	274	VAL
1	B	283	SER
1	B	310	LYS
1	B	323	GLN
1	B	383	ASN
1	B	417	PHE
1	B	423	TRP
1	B	424	ASP
1	B	438	ASP
1	B	449	ASN
1	B	502	ASN
1	B	561	ARG
1	B	575	ARG
1	B	578	SER
1	B	586	ASP
1	B	619	SER
1	B	620	LEU
1	B	647	SER
1	B	657	THR
1	B	676	PHE
1	B	692	LYS
1	B	751	PRO
1	B	758	ASP
1	B	770	THR
1	B	788	GLU
1	B	801	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	85	GLN
1	A	120	GLN
1	A	157	GLN
1	A	167	GLN
1	A	231	GLN
1	A	242	GLN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	261	ASN
1	A	323	GLN
1	A	397	HIS
1	A	398	GLN
1	A	461	GLN
1	A	484	ASN
1	A	600	HIS
1	A	639	HIS
1	A	748	GLN
1	A	786	ASN
1	A	793	GLN
1	B	95	ASN
1	B	114	GLN
1	B	120	GLN
1	B	137	HIS
1	B	167	GLN
1	B	217	HIS
1	B	227	GLN
1	B	249	GLN
1	B	323	GLN
1	B	357	ASN
1	B	368	HIS
1	B	383	ASN
1	B	461	GLN
1	B	484	ASN
1	B	600	HIS
1	B	664	HIS
1	B	748	GLN
1	B	786	ASN
1	B	793	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](#)

17 ligands 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
4	SO4	A	907	-	4,4,4	0.48	0	6,6,6	0.28	0
4	SO4	B	906	-	4,4,4	0.54	0	6,6,6	0.21	0
3	GOL	A	902	-	5,5,5	0.15	0	5,5,5	0.33	0
2	XG5	A	901	-	34,36,36	3.44	13 (38%)	40,49,49	1.76	10 (25%)
4	SO4	A	904	-	4,4,4	0.28	0	6,6,6	0.07	0
6	BTB	B	903	-	13,13,13	1.58	3 (23%)	7,16,16	0.87	0
5	NAG	B	902	1	14,14,15	0.76	0	17,19,21	2.18	3 (17%)
4	SO4	A	908	-	4,4,4	0.38	0	6,6,6	0.12	0
4	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	A	909	-	4,4,4	0.37	0	6,6,6	0.14	0
4	SO4	A	910	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	A	906	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	B	907	-	4,4,4	0.20	0	6,6,6	0.21	0
3	GOL	B	904	-	5,5,5	0.30	0	5,5,5	0.57	0
3	GOL	B	905	-	5,5,5	0.09	0	5,5,5	0.28	0
2	XG5	B	901	-	34,36,36	3.55	17 (50%)	40,49,49	2.70	15 (37%)
4	SO4	A	903	-	4,4,4	0.26	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	902	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XG5	A	901	-	-	3/18/40/40	0/3/3/3
6	BTB	B	903	-	-	2/21/21/21	-
5	NAG	B	902	1	-	0/6/23/26	0/1/1/1
3	GOL	B	904	-	-	1/4/4/4	-
3	GOL	B	905	-	-	3/4/4/4	-
2	XG5	B	901	-	-	3/18/40/40	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	XG5	C7-N1	-11.55	1.26	1.47
2	B	901	XG5	C7-N1	-11.07	1.27	1.47
2	B	901	XG5	O6-N4	8.51	1.37	1.22
2	A	901	XG5	O6-N4	8.29	1.36	1.22
2	A	901	XG5	N6-N5	7.21	1.44	1.24
2	B	901	XG5	N6-N5	6.84	1.43	1.24
2	A	901	XG5	C2-C1	-5.72	1.44	1.52
2	B	901	XG5	C2-C1	-5.62	1.44	1.52
2	B	901	XG5	C8-C9	5.19	1.62	1.51
2	A	901	XG5	C20-C9	4.90	1.48	1.39
2	B	901	XG5	C20-C9	4.85	1.47	1.39
6	B	903	BTB	C2-N	4.11	1.56	1.48
2	B	901	XG5	C13-N3	3.71	1.47	1.37
2	B	901	XG5	C6-C5	3.53	1.58	1.52
2	A	901	XG5	C13-N3	3.13	1.46	1.37
2	A	901	XG5	C19-C10	3.07	1.44	1.39
2	A	901	XG5	C15-C14	3.06	1.45	1.39
2	A	901	XG5	O1-C1	2.97	1.50	1.43
2	B	901	XG5	O1-C1	2.79	1.49	1.43
2	B	901	XG5	C14-N4	2.72	1.50	1.45
2	B	901	XG5	C1-C4	-2.58	1.45	1.52
2	A	901	XG5	C13-C14	-2.45	1.37	1.40
2	B	901	XG5	C10-N2	2.44	1.38	1.34
2	B	901	XG5	C18-C17	2.41	1.43	1.38
2	B	901	XG5	C7-C8	2.36	1.58	1.52
6	B	903	BTB	C7-N	2.26	1.51	1.48
2	A	901	XG5	C5-N1	-2.26	1.43	1.48
2	B	901	XG5	C9-N2	2.23	1.38	1.34
2	A	901	XG5	C6-C5	2.18	1.56	1.52
2	B	901	XG5	C19-C10	2.13	1.43	1.39
6	B	903	BTB	C5-N	2.09	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	XG5	C11-C10	2.04	1.55	1.51
2	B	901	XG5	O2-C2	2.03	1.47	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	XG5	C20-C9-N2	-9.09	114.92	120.85
5	B	902	NAG	C1-O5-C5	7.34	122.14	112.19
2	A	901	XG5	C19-C10-N2	-5.54	117.23	120.85
2	B	901	XG5	C9-N2-C10	5.45	124.79	118.16
2	B	901	XG5	C8-C9-N2	5.29	123.83	115.95
2	B	901	XG5	C6-C5-C4	-4.36	106.22	112.90
2	B	901	XG5	C19-C10-N2	-4.21	118.10	120.85
2	B	901	XG5	C11-C10-N2	4.11	122.08	115.95
2	A	901	XG5	C11-C10-N2	4.03	121.94	115.95
2	B	901	XG5	C19-N8-C20	3.99	122.92	117.48
2	B	901	XG5	C16-N5-N6	3.50	122.97	116.02
2	B	901	XG5	O1-C1-C4	-3.49	102.27	110.35
2	A	901	XG5	C3-C2-C1	-3.10	106.70	110.24
2	A	901	XG5	C9-C20-N8	-3.03	118.81	122.72
2	B	901	XG5	C10-C19-N8	-2.80	119.11	122.72
5	B	902	NAG	O3-C3-C2	-2.76	103.77	109.47
2	A	901	XG5	C8-C9-N2	2.71	119.99	115.95
2	B	901	XG5	C8-C7-N1	2.71	119.86	113.74
2	A	901	XG5	C11-C12-N3	2.53	115.99	111.75
2	A	901	XG5	O6-N4-C14	-2.48	114.79	119.03
2	B	901	XG5	C7-C8-C9	2.38	116.14	111.73
2	B	901	XG5	C3-C2-C1	-2.36	107.55	110.24
5	B	902	NAG	C8-C7-N2	-2.25	112.28	116.10
2	A	901	XG5	C9-N2-C10	2.22	120.87	118.16
2	A	901	XG5	C6-C5-C4	-2.22	109.50	112.90
2	A	901	XG5	C16-N5-N6	2.09	120.18	116.02
2	B	901	XG5	C15-C14-C13	-2.00	119.71	121.53
2	B	901	XG5	C9-C20-N8	-2.00	120.14	122.72

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	XG5	C14-C13-N3-C12
2	B	901	XG5	C16-N5-N6-N7
2	B	901	XG5	C18-C13-N3-C12

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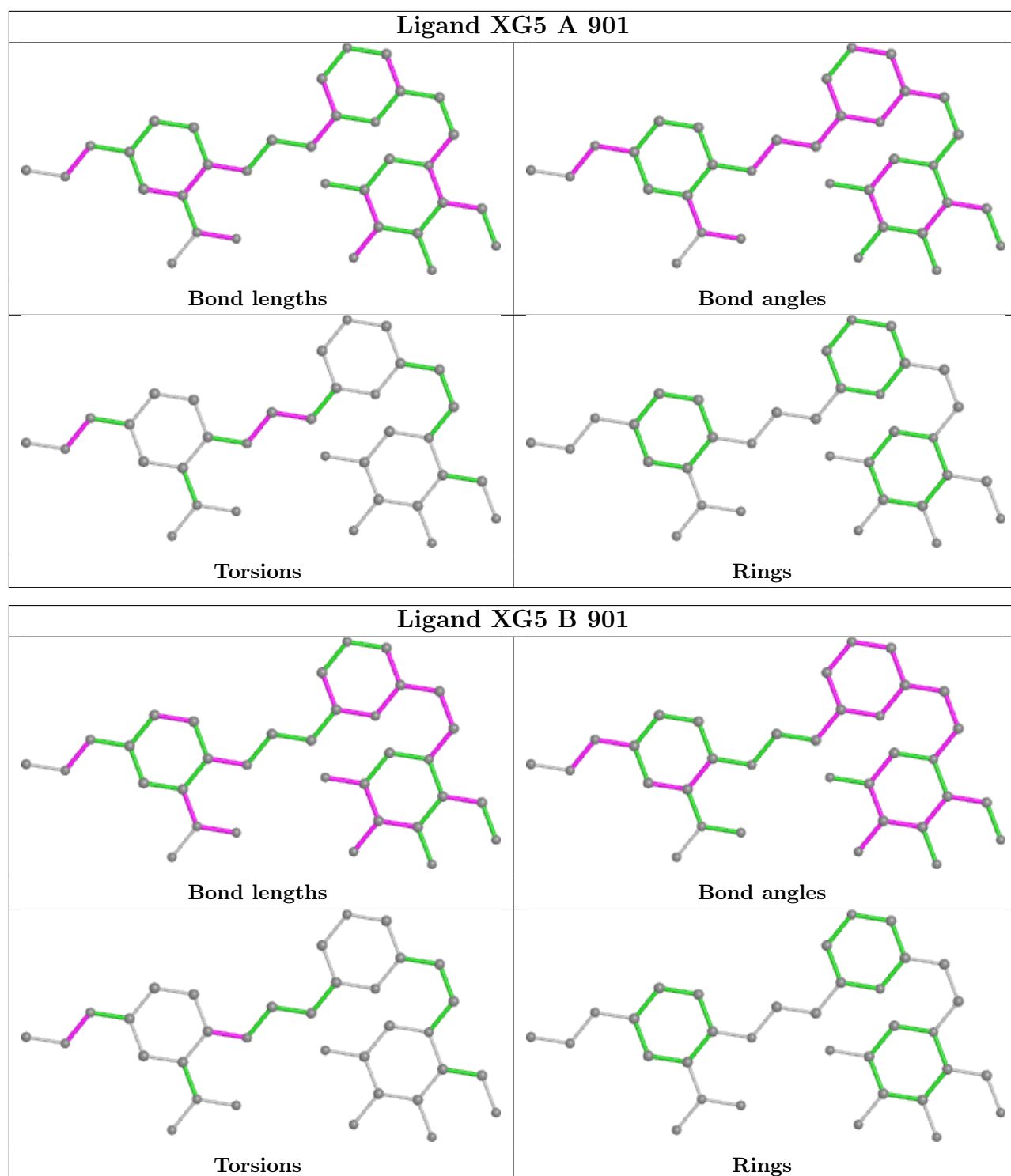
Mol	Chain	Res	Type	Atoms
3	A	902	GOL	O1-C1-C2-O2
3	A	902	GOL	O1-C1-C2-C3
3	B	905	GOL	C1-C2-C3-O3
3	B	905	GOL	O2-C2-C3-O3
6	B	903	BTB	N-C7-C8-O8
2	A	901	XG5	C16-N5-N6-N7
2	A	901	XG5	C11-C12-N3-C13
3	B	905	GOL	O1-C1-C2-O2
6	B	903	BTB	N-C5-C6-O6
2	A	901	XG5	C10-C11-C12-N3
3	A	902	GOL	C1-C2-C3-O3
3	B	904	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GOL	1	0
2	A	901	XG5	1	0
4	A	909	SO4	1	0
3	B	904	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	765/819 (93%)	-0.12	16 (2%) 63 70	29, 44, 71, 102	0
1	B	767/819 (93%)	-0.25	3 (0%) 92 95	30, 45, 66, 101	0
All	All	1532/1638 (93%)	-0.18	19 (1%) 79 83	29, 45, 69, 102	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	HIS	3.6
1	A	560	ASP	3.3
1	A	622	GLY	3.3
1	A	136	ALA	3.2
1	A	621	LEU	3.0
1	A	529	VAL	2.9
1	A	309	GLY	2.9
1	A	36	LEU	2.7
1	A	559	TYR	2.5
1	B	707	TYR	2.4
1	B	171	ASN	2.4
1	A	522	ALA	2.4
1	A	618	GLY	2.3
1	A	534	LEU	2.3
1	A	151	ASP	2.2
1	A	499	LEU	2.1
1	B	151	ASP	2.0
1	A	519	LEU	2.0
1	A	535	ARG	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](#)

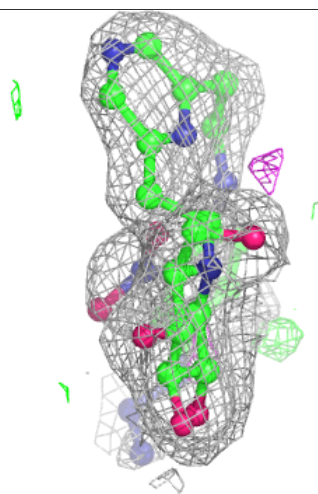
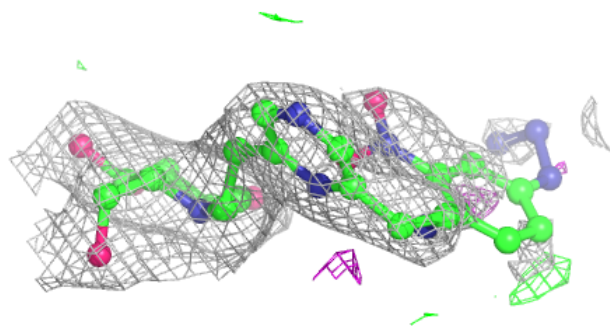
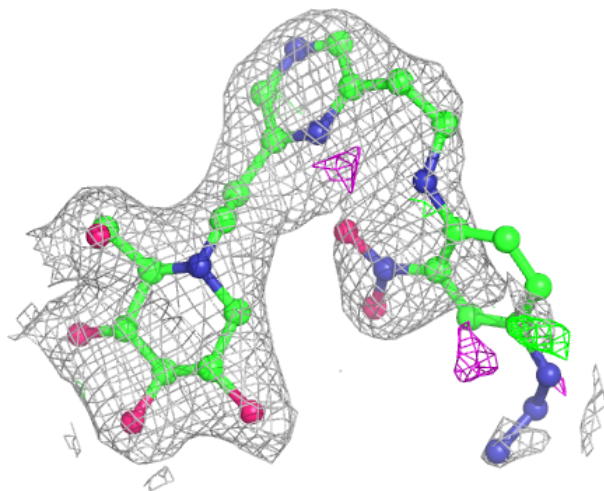
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

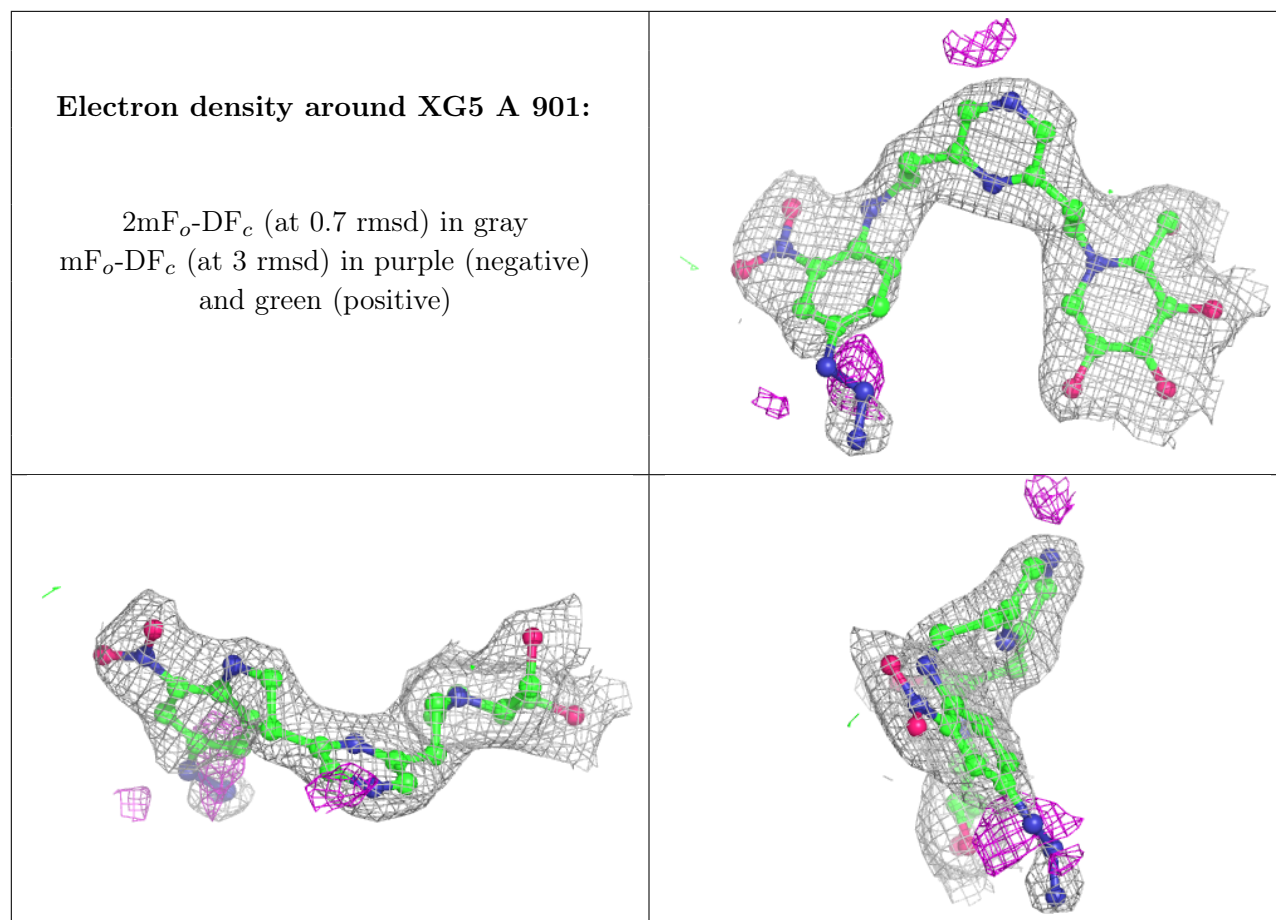
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BTB	B	903	14/14	0.79	0.17	54,76,83,86	0
4	SO4	A	904	5/5	0.85	0.48	88,112,127,132	0
4	SO4	A	910	5/5	0.87	0.20	77,85,105,105	0
4	SO4	A	906	5/5	0.87	0.41	100,112,127,130	0
4	SO4	A	909	5/5	0.88	0.16	107,108,114,119	0
5	NAG	B	902	14/15	0.89	0.26	55,75,89,94	0
3	GOL	B	905	6/6	0.89	0.20	70,75,80,81	0
3	GOL	A	902	6/6	0.91	0.15	53,60,70,72	0
2	XG5	B	901	34/34	0.91	0.18	36,66,120,131	0
3	GOL	B	904	6/6	0.93	0.20	35,53,55,62	0
2	XG5	A	901	34/34	0.94	0.17	30,48,79,82	0
4	SO4	A	905	5/5	0.95	0.17	70,70,81,94	0
4	SO4	A	903	5/5	0.96	0.21	71,80,90,91	0
4	SO4	A	908	5/5	0.97	0.13	60,62,82,83	0
4	SO4	B	907	5/5	0.97	0.14	45,59,71,74	0
4	SO4	B	906	5/5	0.99	0.10	35,38,47,47	0
4	SO4	A	907	5/5	0.99	0.14	39,44,46,49	0

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

Electron density around XG5 B 901:

$2mF_o-DF_c$ (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.