



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 03:27 PM EDT

PDB ID : 8E5U
Title : Co-crystal structure of Chaetomium glucosidase with compound 9
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2022-08-22
Resolution : 2.33 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

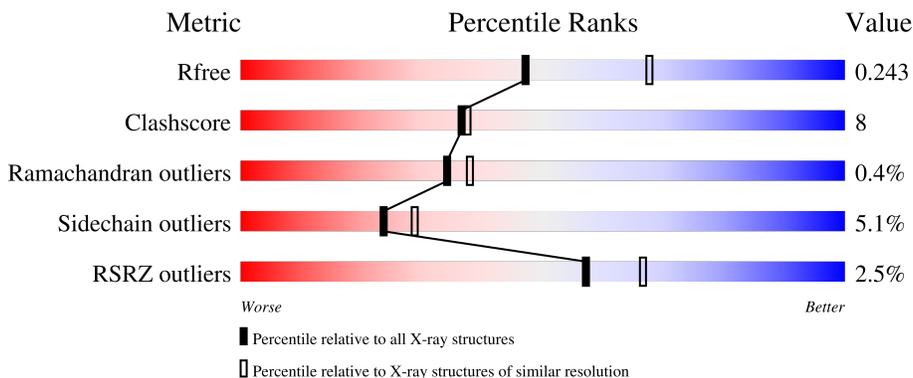
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	 4% 77% 14% • 7%
1	B	819	 % 78% 14% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	907	-	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 12640 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	762	6051	3891	1019	1128	13	0	2	0
1	B	763	6073	3897	1020	1143	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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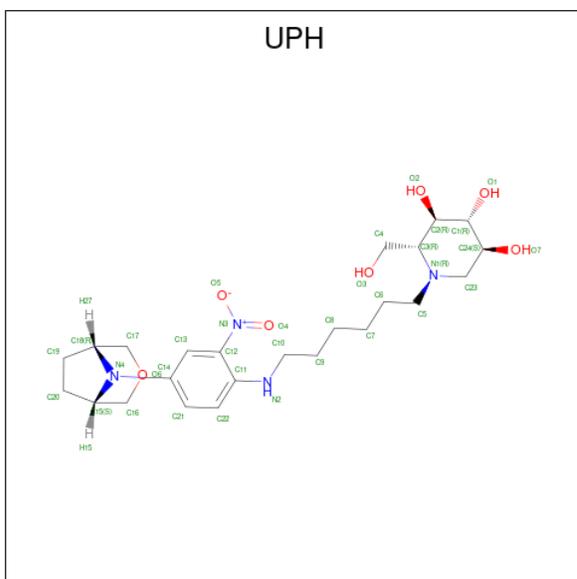
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP 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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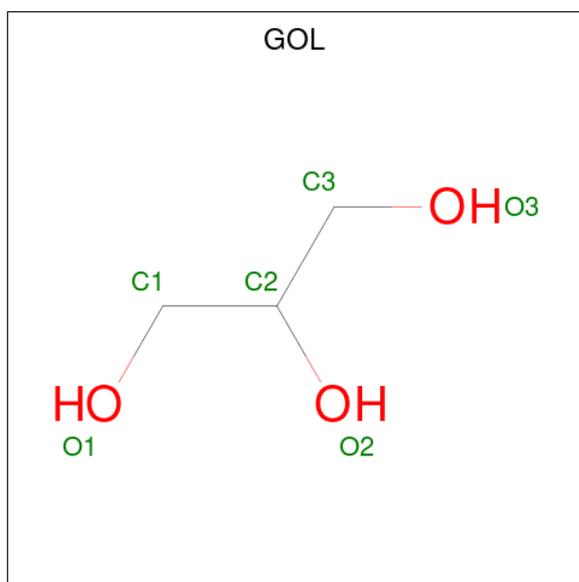
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP 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)-2-(hydroxymethyl)-1-(6-{2-nitro-4-[(1R,5S)-3-oxa-8-azabicyclo[3.2.1]octan-8-yl]anilino}hexyl)piperidine-3,4,5-triol (three-letter code: UPH) (formula: C₂₄H₃₈N₄O₇) (labeled as "Ligand of Interest" by depositor).



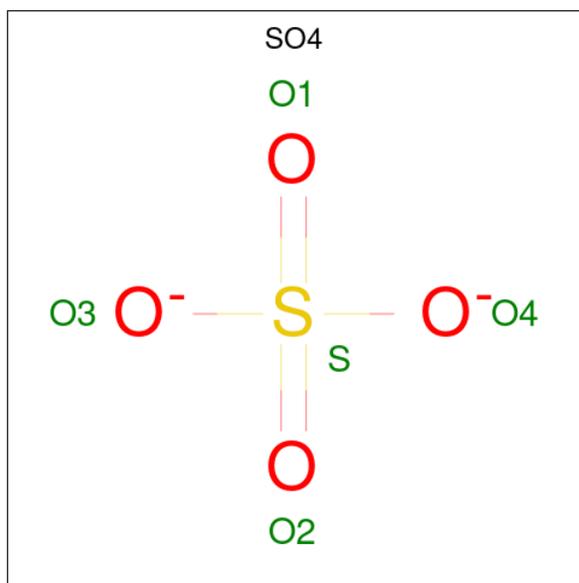
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			35	24	4	7		
2	B	1	Total	C	N	O	0	0
			35	24	4	7		

- 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		

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



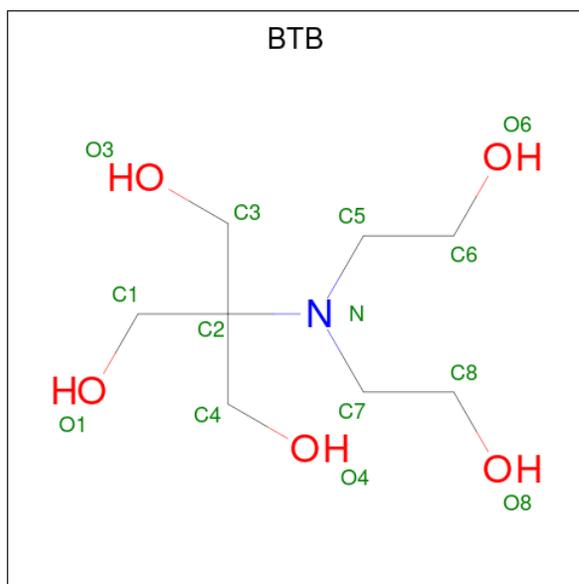
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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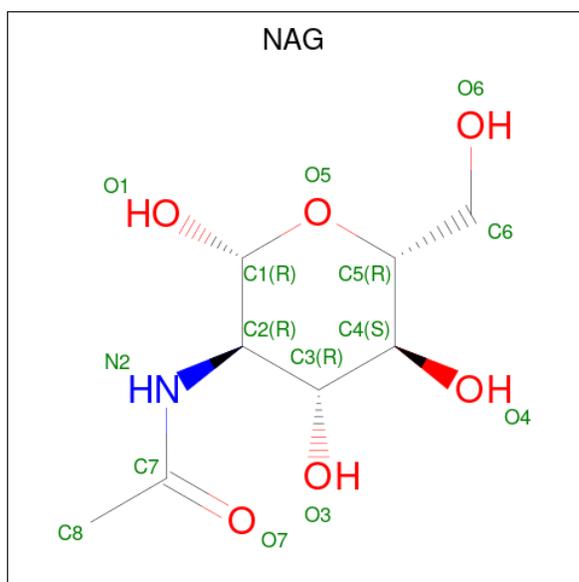
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0

- Molecule 5 is 2-[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		
5	B	1	14	8	1	5	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

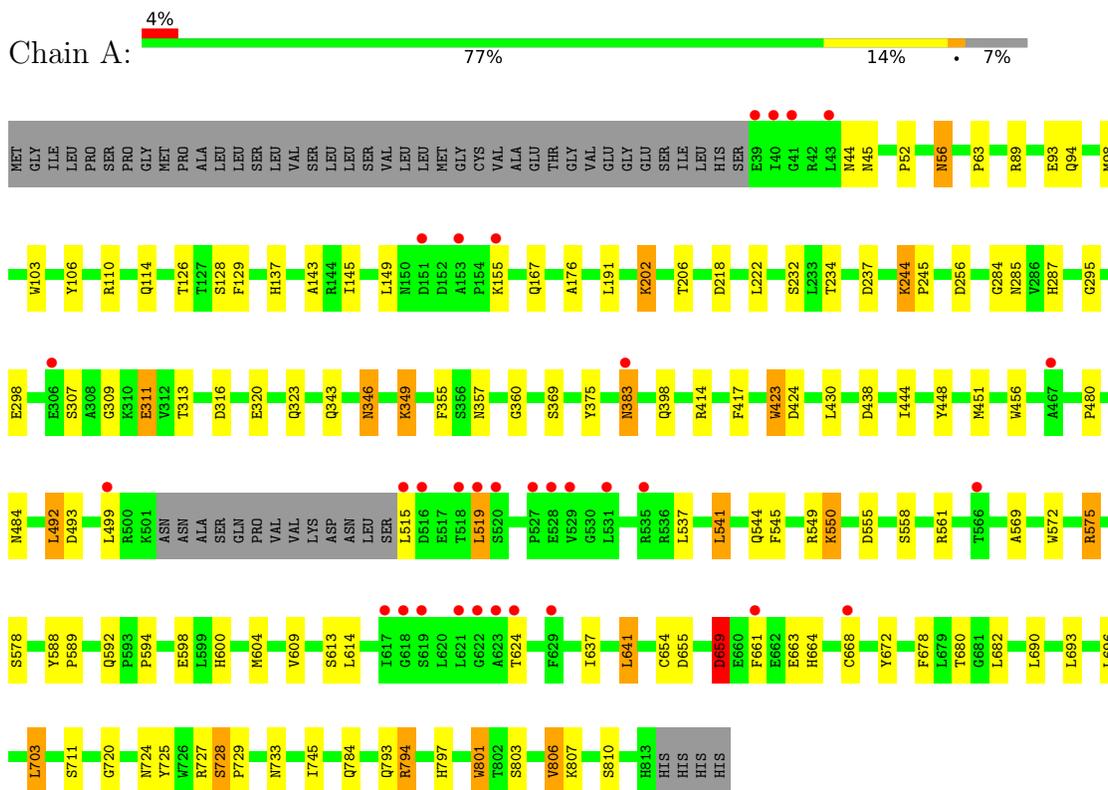
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	168	168	168	0	0
7	B	189	189	189	0	0

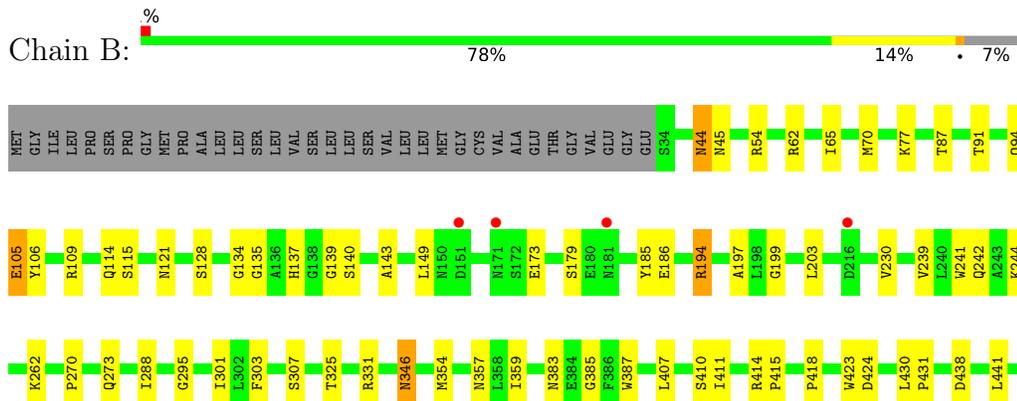
3 Residue-property plots [i](#)

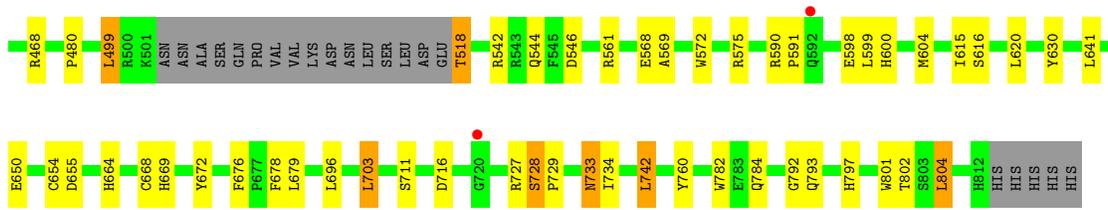
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	135.93Å 179.59Å 180.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 2.33 46.86 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.91-2.33) 98.5 (46.86-2.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.243 0.192 , 0.243	Depositor DCC
R_{free} test set	4528 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtrriage
Anisotropy	0.520	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	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	12640	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: BTB, UPH, GOL, SO4, NAG

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	0.39	0/6232	0.78	2/8485 (0.0%)
1	B	0.41	0/6249	0.81	2/8505 (0.0%)
All	All	0.40	0/12481	0.79	4/16990 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ASN	CB-CA-C	7.19	124.79	110.40
1	A	575	ARG	CB-CA-C	6.61	123.62	110.40
1	A	659	ASP	CB-CA-C	-6.32	97.75	110.40
1	B	105	GLU	CB-CA-C	-5.95	98.51	110.40

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	6051	0	5733	95	0
1	B	6073	0	5737	87	0
2	A	35	0	0	5	0
2	B	35	0	0	4	0
3	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	30	0	0	2	0
4	B	25	0	0	1	0
5	B	14	0	19	1	0
6	B	14	0	13	0	0
7	A	168	0	0	3	0
7	B	189	0	0	4	0
All	All	12640	0	11510	189	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 8.

All (189) 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)
2:B:1003:UPH:C16	2:B:1003:UPH:O6	1.69	1.40
2:A:901:UPH:C16	2:A:901:UPH:O6	1.70	1.38
2:A:901:UPH:O6	2:A:901:UPH:C17	1.72	1.36
2:B:1003:UPH:O6	2:B:1003:UPH:C17	1.72	1.34
1:A:654:CYS:SG	1:A:668:CYS:HB2	1.99	1.02
1:A:659:ASP:HB3	1:A:661:PHE:H	1.30	0.96
1:A:126:THR:HG22	7:A:1064:HOH:O	1.69	0.92
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.06	0.92
5:B:1001:BTB:H82	7:B:1161:HOH:O	1.73	0.87
1:B:561:ARG:HE	1:B:664:HIS:CD2	1.95	0.84
1:B:572:TRP:H	1:B:600:HIS:HD2	1.27	0.83
1:A:346:ASN:H	1:A:346:ASN:HD22	1.24	0.81
1:A:572:TRP:H	1:A:600:HIS:HD2	1.29	0.80
1:B:137:HIS:HD2	1:B:307:SER:OG	1.65	0.80
1:B:87:THR:HB	1:B:121:ASN:HD21	1.47	0.79
1:B:572:TRP:H	1:B:600:HIS:CD2	2.02	0.77
1:A:56:ASN:H	1:A:56:ASN:HD22	1.30	0.76
1:B:135:GLY:HA3	1:B:307:SER:HB3	1.67	0.76
1:A:654:CYS:SG	1:A:668:CYS:CB	2.74	0.75
1:B:44:ASN:HD21	1:B:109:ARG:HH22	1.35	0.74
1:A:803:SER:O	1:A:806[A]:VAL:HG23	1.88	0.74
1:B:137:HIS:CD2	1:B:307:SER:OG	2.41	0.73
1:B:518:THR:N	7:B:1101:HOH:O	2.22	0.73
1:A:654:CYS:HG	1:A:668:CYS:CB	2.02	0.73
1:B:114:GLN:NE2	1:B:414:ARG:HH12	1.87	0.73
1:A:206:THR:HB	3:A:902:GOL:H32	1.72	0.71
1:A:515:LEU:O	1:A:519:LEU:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ARG:NE	1:B:664:HIS:HD2	1.84	0.71
1:B:346:ASN:HD22	1:B:346:ASN:H	1.40	0.70
1:A:114:GLN:HE22	1:A:414:ARG:HH22	1.40	0.69
1:B:728:SER:N	1:B:729:PRO:HD3	2.07	0.68
1:A:561:ARG:HE	1:A:664:HIS:HD2	1.43	0.67
1:A:784:GLN:HE21	1:A:793:GLN:HE21	1.42	0.67
1:B:103:TRP:H	1:B:357:ASN:ND2	1.93	0.66
1:B:54:ARG:NE	1:B:70:MET:HE2	2.11	0.65
1:B:149:LEU:HD11	1:B:295:GLY:HA2	1.79	0.65
1:A:578:SER:HB2	4:A:907:SO4:O1	1.98	0.64
1:B:385:GLY:HA2	1:B:387:TRP:CZ3	2.32	0.63
1:A:346:ASN:HD22	1:A:346:ASN:N	1.96	0.63
1:B:590:ARG:HB3	1:B:591:PRO:HD2	1.81	0.63
1:A:202:LYS:HE3	1:A:311:GLU:OE1	1.99	0.63
1:B:728:SER:H	1:B:729:PRO:CD	2.12	0.63
1:B:615:ILE:HG13	1:B:630:TYR:HB3	1.81	0.62
1:A:659:ASP:HB2	1:A:663:GLU:H	1.64	0.62
1:B:591:PRO:HG2	1:B:598:GLU:HG2	1.80	0.62
1:A:451:MET:CE	1:A:544:GLN:HB2	2.30	0.62
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.83	0.61
1:B:94:GLN:OE1	1:B:797:HIS:HE1	1.82	0.61
1:A:720:GLY:HA2	1:A:724:ASN:OD1	2.00	0.60
1:B:728:SER:N	1:B:729:PRO:CD	2.63	0.60
1:B:54:ARG:CZ	1:B:70:MET:HE2	2.32	0.59
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.32	0.59
1:A:56:ASN:H	1:A:56:ASN:ND2	1.99	0.58
1:A:234[B]:THR:HG22	7:B:1102:HOH:O	2.02	0.58
1:A:114:GLN:HE21	1:A:414:ARG:HH12	1.50	0.58
1:A:256:ASP:OD2	1:B:262:LYS:HE3	2.04	0.58
1:B:385:GLY:HA2	1:B:387:TRP:CH2	2.38	0.57
1:A:696:LEU:HG	1:A:703:LEU:HD22	1.86	0.57
1:B:727:ARG:O	1:B:728:SER:HB3	2.05	0.57
1:A:398:GLN:HE22	1:B:241:TRP:HZ2	1.51	0.57
1:B:696:LEU:HG	1:B:703:LEU:HD22	1.88	0.56
1:A:114:GLN:NE2	1:A:414:ARG:HH12	2.03	0.56
1:B:654:CYS:SG	1:B:668:CYS:SG	3.04	0.56
1:A:423:TRP:H	1:A:484:ASN:ND2	2.04	0.56
1:A:110:ARG:HH21	1:A:323:GLN:HG3	1.71	0.56
1:B:256:ASP:O	1:B:259:VAL:HG22	2.06	0.56
1:B:784:GLN:HE21	1:B:793:GLN:HE21	1.52	0.55
1:A:569:ALA:HA	1:A:604:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:MET:HE2	1:A:544:GLN:HB2	1.88	0.55
1:B:568:GLU:HB3	1:B:604:MET:HE1	1.87	0.55
1:A:103:TRP:H	1:A:357:ASN:ND2	2.05	0.55
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.41	0.54
1:A:784:GLN:NE2	1:A:793:GLN:HE21	2.04	0.54
1:B:135:GLY:CA	1:B:307:SER:HB3	2.37	0.54
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.06	0.54
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.89	0.54
1:B:801:TRP:O	1:B:804:LEU:HB2	2.08	0.54
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.56	0.54
1:A:234[B]:THR:CG2	7:B:1102:HOH:O	2.56	0.53
1:B:103:TRP:H	1:B:357:ASN:HD21	1.56	0.53
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.91	0.53
1:A:232:SER:OG	1:A:287:HIS:HD2	1.91	0.52
1:A:103:TRP:H	1:A:357:ASN:HD21	1.57	0.52
1:B:346:ASN:HD22	1:B:346:ASN:N	2.05	0.52
1:A:128:SER:O	1:A:143:ALA:HA	2.09	0.52
1:A:423:TRP:H	1:A:484:ASN:HD22	1.57	0.52
1:B:179:SER:HB3	1:B:185:TYR:CD2	2.44	0.51
1:B:669:HIS:ND1	1:B:716:ASP:OD2	2.26	0.51
1:A:313:THR:O	1:A:316:ASP:HB2	2.10	0.51
1:B:451:MET:CE	1:B:544:GLN:HB2	2.40	0.51
1:A:727:ARG:O	1:A:728:SER:HB3	2.11	0.51
1:A:346:ASN:H	1:A:346:ASN:ND2	2.02	0.50
1:A:672:TYR:CZ	1:A:711:SER:HA	2.47	0.50
1:B:128:SER:O	1:B:143:ALA:HA	2.11	0.50
1:A:232:SER:OG	1:A:287:HIS:CD2	2.65	0.50
1:B:149:LEU:CD1	1:B:295:GLY:HA2	2.40	0.50
1:A:89:ARG:NH2	1:A:98:MET:HE2	2.27	0.50
1:A:572:TRP:H	1:A:600:HIS:CD2	2.19	0.50
1:A:93:GLU:HB3	7:A:1060:HOH:O	2.12	0.49
1:B:784:GLN:NE2	1:B:793:GLN:HE21	2.10	0.49
1:A:588:TYR:CD1	1:A:589:PRO:HD2	2.48	0.49
1:B:742:LEU:HB3	1:B:760:TYR:HB2	1.95	0.49
1:A:94:GLN:OE1	1:A:797:HIS:HE1	1.96	0.48
1:A:654:CYS:SG	1:A:668:CYS:SG	3.10	0.48
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.48	0.48
1:A:578:SER:N	4:A:907:SO4:O1	2.42	0.48
1:A:728:SER:N	1:A:729:PRO:CD	2.76	0.48
1:B:672:TYR:CE1	1:B:711:SER:HA	2.48	0.48
1:B:62:ARG:HD2	1:B:70:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.29	0.48
1:B:542:ARG:NH2	1:B:546:ASP:OD1	2.47	0.48
1:B:106:TYR:HD2	1:B:359:ILE:HG23	1.77	0.48
1:B:678:PHE:HZ	1:B:742:LEU:HD13	1.79	0.48
1:A:594:PRO:HA	1:A:598:GLU:OE1	2.13	0.48
1:B:134:GLY:O	1:B:139:GLY:HA2	2.14	0.48
1:B:203:LEU:HD11	1:B:301:ILE:CG2	2.44	0.47
1:A:451:MET:HE1	1:A:544:GLN:HB2	1.95	0.47
1:A:110:ARG:HH22	1:A:323:GLN:HE21	1.61	0.47
1:B:451:MET:HE2	1:B:544:GLN:HB2	1.96	0.47
1:B:77:LYS:H	1:B:121:ASN:ND2	2.13	0.47
1:A:89:ARG:CZ	1:A:98:MET:CE	2.93	0.46
1:A:145:ILE:O	1:A:298:GLU:HA	2.16	0.46
1:A:575:ARG:HH22	1:A:592:GLN:HE22	1.63	0.46
1:B:672:TYR:CG	1:B:734:ILE:HG21	2.50	0.46
2:A:901:UPH:C16	2:A:901:UPH:C17	2.91	0.46
1:A:561:ARG:HE	1:A:664:HIS:CD2	2.28	0.46
1:A:550:LYS:HE2	7:A:1134:HOH:O	2.16	0.46
1:A:349:LYS:HE2	1:A:349:LYS:HB2	1.70	0.46
1:B:733:ASN:HB3	1:B:734:ILE:H	1.46	0.46
1:A:383:ASN:HD22	1:A:383:ASN:N	2.14	0.46
1:A:537:LEU:HG	1:A:541:LEU:HD13	1.98	0.45
1:A:600:HIS:HA	1:A:655:ASP:OD1	2.16	0.45
1:A:609:VAL:HG23	1:A:680:THR:HB	1.98	0.45
1:B:650:GLU:HG3	1:B:668:CYS:SG	2.56	0.45
1:A:794:ARG:HA	1:A:794:ARG:HD2	1.84	0.45
1:A:575:ARG:HH22	1:A:592:GLN:NE2	2.14	0.45
1:B:569:ALA:HB1	1:B:599:LEU:HD22	1.97	0.45
1:A:598:GLU:OE2	1:A:600:HIS:CE1	2.67	0.45
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.52	0.45
1:B:101:TYR:HA	1:B:115:SER:O	2.17	0.45
1:A:555:ASP:OD2	1:A:558:SER:HB3	2.17	0.45
1:B:140:SER:HB3	1:B:303:PHE:O	2.16	0.45
1:A:234[A]:THR:HG23	1:A:284:GLY:HA2	1.99	0.45
1:A:672:TYR:CE1	1:A:711:SER:HA	2.52	0.45
1:A:641:LEU:HD12	1:A:641:LEU:HA	1.88	0.45
1:A:545:PHE:CZ	1:A:549:ARG:HD2	2.52	0.44
2:B:1003:UPH:C16	2:B:1003:UPH:C17	2.92	0.44
1:B:542:ARG:HD3	1:B:630:TYR:OH	2.18	0.44
1:B:782:TRP:CG	1:B:792:GLY:HA3	2.53	0.44
1:B:270:PRO:HG2	1:B:273:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HB3	4:B:1004:SO4:O4	2.16	0.44
1:B:62:ARG:HD2	1:B:70:MET:HE3	1.99	0.44
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.53	0.44
1:A:444:ILE:HD13	1:A:492:LEU:HD13	2.00	0.44
1:A:604:MET:SD	1:A:641:LEU:HD13	2.59	0.43
1:A:493:ASP:OD1	1:A:613:SER:OG	2.29	0.43
1:B:499:LEU:HD12	1:B:499:LEU:HA	1.78	0.43
1:B:114:GLN:HE21	1:B:414:ARG:HH12	1.60	0.43
1:A:106:TYR:CD2	1:A:360:GLY:HA2	2.53	0.43
1:B:414:ARG:N	1:B:415:PRO:HD2	2.34	0.43
1:A:355:PHE:HB2	1:A:806[B]:VAL:HG11	2.01	0.43
1:B:672:TYR:CE2	1:B:711:SER:HB3	2.54	0.43
1:B:411:ILE:HD12	1:B:418:PRO:HA	2.01	0.43
1:A:110:ARG:HD2	1:A:110:ARG:HA	1.83	0.42
2:A:901:UPH:C10	2:A:901:UPH:O4	2.68	0.42
1:B:407:LEU:HD13	1:B:450:LEU:HD11	2.02	0.42
1:A:678:PHE:HE1	1:A:745:ILE:CD1	2.33	0.42
1:B:194:ARG:HA	1:B:199:GLY:O	2.19	0.42
1:A:499:LEU:HD12	1:A:499:LEU:HA	1.87	0.42
1:B:105:GLU:OE2	1:B:325:THR:HG23	2.19	0.42
1:A:448:TYR:OH	1:A:544:GLN:NE2	2.53	0.41
2:B:1003:UPH:O4	2:B:1003:UPH:C10	2.68	0.41
1:A:137:HIS:HD2	1:A:307:SER:OG	2.03	0.41
1:A:244:LYS:HB3	1:A:245:PRO:HD3	2.01	0.41
1:A:256:ASP:OD2	1:B:262:LYS:CE	2.68	0.41
1:A:52:PRO:HD3	1:A:129:PHE:CE2	2.55	0.41
1:B:179:SER:HB3	1:B:185:TYR:CE2	2.55	0.41
1:B:230:VAL:HA	1:B:288:ILE:O	2.20	0.41
1:B:354:MET:HE1	1:B:802:THR:HG22	2.03	0.41
1:A:234[A]:THR:HG22	1:A:285:ASN:H	1.86	0.41
1:B:239:VAL:HG22	1:B:242:GLN:OE1	2.20	0.41
1:B:727:ARG:O	1:B:728:SER:CB	2.67	0.41
1:A:149:LEU:HD11	1:A:295:GLY:HA2	2.03	0.41
1:A:167:GLN:O	1:A:285:ASN:HB2	2.21	0.41
1:A:637:ILE:HG22	1:A:641:LEU:HD22	2.03	0.41
2:A:901:UPH:O6	2:A:901:UPH:C18	2.58	0.41
1:A:690:LEU:HD11	1:A:745:ILE:HD11	2.03	0.40
1:A:176:ALA:HA	1:A:191:LEU:HD23	2.03	0.40
1:B:244:LYS:HB3	1:B:245:PRO:HD3	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	760/819 (93%)	729 (96%)	27 (4%)	4 (0%)	29	31
1	B	759/819 (93%)	736 (97%)	21 (3%)	2 (0%)	41	47
All	All	1519/1638 (93%)	1465 (96%)	48 (3%)	6 (0%)	34	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	A	728	SER
1	B	728	SER
1	B	733	ASN
1	A	375	TYR
1	A	659	ASP

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	626/707 (88%)	587 (94%)	39 (6%)	18	20
1	B	632/707 (89%)	606 (96%)	26 (4%)	30	38
All	All	1258/1414 (89%)	1193 (95%)	65 (5%)	24	28

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	45	ASN
1	A	56	ASN
1	A	63	PRO
1	A	155	LYS
1	A	202	LYS
1	A	218	ASP
1	A	222	LEU
1	A	237	ASP
1	A	244	LYS
1	A	311	GLU
1	A	320	GLU
1	A	343	GLN
1	A	346	ASN
1	A	349	LYS
1	A	369	SER
1	A	383	ASN
1	A	417	PHE
1	A	423	TRP
1	A	424	ASP
1	A	430	LEU
1	A	438	ASP
1	A	492	LEU
1	A	519	LEU
1	A	541	LEU
1	A	550	LYS
1	A	614	LEU
1	A	624	THR
1	A	641	LEU
1	A	682	LEU
1	A	693	LEU
1	A	703	LEU
1	A	725	TYR
1	A	794	ARG
1	A	801	TRP
1	A	806[A]	VAL
1	A	806[B]	VAL
1	A	807	LYS
1	A	810	SER
1	B	44	ASN
1	B	91	THR
1	B	173	GLU
1	B	186	GLU

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Mol	Chain	Res	Type
1	B	194	ARG
1	B	331	ARG
1	B	346	ASN
1	B	383	ASN
1	B	410	SER
1	B	423	TRP
1	B	424	ASP
1	B	438	ASP
1	B	441	LEU
1	B	449	ASN
1	B	468	ARG
1	B	499	LEU
1	B	518	THR
1	B	575	ARG
1	B	616	SER
1	B	620	LEU
1	B	641	LEU
1	B	676	PHE
1	B	679	LEU
1	B	703	LEU
1	B	742	LEU
1	B	804	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	56	ASN
1	A	85	GLN
1	A	114	GLN
1	A	137	HIS
1	A	157	GLN
1	A	167	GLN
1	A	214	GLN
1	A	287	HIS
1	A	323	GLN
1	A	346	ASN
1	A	357	ASN
1	A	383	ASN
1	A	398	GLN
1	A	484	ASN
1	A	494	ASN

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Mol	Chain	Res	Type
1	A	526	ASN
1	A	544	GLN
1	A	592	GLN
1	A	600	HIS
1	A	664	HIS
1	A	748	GLN
1	A	784	GLN
1	A	797	HIS
1	B	44	ASN
1	B	85	GLN
1	B	114	GLN
1	B	121	ASN
1	B	137	HIS
1	B	157	GLN
1	B	167	GLN
1	B	200	ASN
1	B	214	GLN
1	B	287	HIS
1	B	323	GLN
1	B	346	ASN
1	B	357	ASN
1	B	476	GLN
1	B	484	ASN
1	B	600	HIS
1	B	664	HIS
1	B	748	GLN
1	B	784	GLN
1	B	797	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

16 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	904	-	4,4,4	0.26	0	6,6,6	0.10	0
2	UPH	A	901	-	37,38,38	6.02	14 (37%)	43,53,53	1.66	7 (16%)
4	SO4	B	1007	-	4,4,4	0.38	0	6,6,6	0.14	0
2	UPH	B	1003	-	37,38,38	6.12	20 (54%)	43,53,53	2.09	12 (27%)
4	SO4	A	906	-	4,4,4	0.32	0	6,6,6	0.12	0
4	SO4	A	907	-	4,4,4	0.36	0	6,6,6	0.11	0
4	SO4	B	1004	-	4,4,4	0.36	0	6,6,6	0.14	0
6	NAG	B	1002	1	14,14,15	0.84	0	17,19,21	2.32	5 (29%)
4	SO4	A	908	-	4,4,4	0.31	0	6,6,6	0.10	0
5	BTB	B	1001	-	13,13,13	1.06	1 (7%)	7,16,16	0.88	0
3	GOL	A	902	-	5,5,5	0.11	0	5,5,5	0.49	0
4	SO4	B	1005	-	4,4,4	0.54	0	6,6,6	0.15	0
4	SO4	A	905	-	4,4,4	0.40	0	6,6,6	0.25	0
4	SO4	B	1006	-	4,4,4	0.31	0	6,6,6	0.07	0
4	SO4	B	1008	-	4,4,4	0.27	0	6,6,6	0.11	0
4	SO4	A	903	-	4,4,4	0.35	0	6,6,6	0.08	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	UPH	A	901	-	-	11/18/59/59	0/5/4/4
2	UPH	B	1003	-	-	11/18/59/59	0/5/4/4
6	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
5	BTB	B	1001	-	-	7/21/21/21	-
3	GOL	A	902	-	-	2/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	UPH	C18-N4	-18.36	1.29	1.47
2	A	901	UPH	C18-N4	-17.78	1.30	1.47
2	A	901	UPH	C15-N4	-17.16	1.31	1.47
2	B	1003	UPH	C15-N4	-16.82	1.31	1.47
2	B	1003	UPH	O6-C17	15.51	1.72	1.42
2	A	901	UPH	O6-C17	14.99	1.72	1.42
2	A	901	UPH	O6-C16	14.12	1.70	1.42
2	B	1003	UPH	O6-C16	13.69	1.69	1.42
2	A	901	UPH	C22-C11	9.27	1.55	1.39
2	A	901	UPH	C21-C14	7.82	1.54	1.39
2	B	1003	UPH	C11-C12	-7.66	1.29	1.40
2	A	901	UPH	C13-C12	6.97	1.52	1.39
2	B	1003	UPH	C13-C12	6.67	1.52	1.39
2	B	1003	UPH	C22-C11	6.51	1.50	1.39
2	B	1003	UPH	C21-C14	5.46	1.50	1.39
2	B	1003	UPH	C13-C14	-5.34	1.30	1.39
2	A	901	UPH	C11-C12	-5.26	1.33	1.40
2	B	1003	UPH	C22-C21	-4.47	1.30	1.38
2	A	901	UPH	C13-C14	-4.40	1.31	1.39
2	B	1003	UPH	O1-C1	-3.74	1.34	1.43
2	B	1003	UPH	C19-C20	-3.71	1.43	1.54
2	B	1003	UPH	O2-C2	-3.55	1.34	1.43
2	B	1003	UPH	C23-N1	-3.55	1.41	1.47
2	B	1003	UPH	O7-C24	-3.45	1.36	1.43
2	A	901	UPH	C11-N2	3.31	1.46	1.37
2	A	901	UPH	C19-C20	-3.21	1.45	1.54
2	A	901	UPH	O4-N3	-2.89	1.17	1.22
2	A	901	UPH	C22-C21	-2.87	1.33	1.38
2	B	1003	UPH	C5-N1	-2.82	1.42	1.47
2	B	1003	UPH	C11-N2	2.81	1.45	1.37
2	A	901	UPH	C14-N4	2.59	1.46	1.40
2	B	1003	UPH	C23-C24	-2.44	1.49	1.52
2	B	1003	UPH	O4-N3	-2.42	1.18	1.22
2	B	1003	UPH	C3-N1	-2.33	1.43	1.48
5	B	1001	BTB	C2-N	2.23	1.53	1.48

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1002	NAG	C1-O5-C5	6.71	121.29	112.19
2	B	1003	UPH	O1-C1-C2	-5.51	97.62	110.35
2	B	1003	UPH	C19-C18-C17	-4.69	107.31	111.64
2	A	901	UPH	O6-C17-C18	-4.04	105.56	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	UPH	C16-O6-C17	3.80	117.37	111.52
2	A	901	UPH	C24-C1-C2	-3.79	104.33	110.89
2	A	901	UPH	C16-O6-C17	3.66	117.16	111.52
2	B	1003	UPH	O2-C2-C1	-3.65	101.91	110.35
2	B	1003	UPH	O6-C17-C18	-3.64	106.10	110.99
2	A	901	UPH	C4-C3-C2	-3.62	107.36	112.90
2	B	1003	UPH	C4-C3-C2	-3.31	107.82	112.90
2	B	1003	UPH	C10-N2-C11	3.31	131.34	123.39
2	B	1003	UPH	C23-C24-C1	-3.18	106.61	110.24
2	A	901	UPH	C23-C24-C1	-3.13	106.68	110.24
2	B	1003	UPH	C22-C11-N2	-3.01	116.66	121.80
6	B	1002	NAG	O5-C1-C2	2.97	115.98	111.29
6	B	1002	NAG	C4-C3-C2	2.93	115.32	111.02
2	A	901	UPH	C21-C14-N4	2.92	125.28	121.21
6	B	1002	NAG	O4-C4-C5	2.79	116.24	109.30
2	B	1003	UPH	O2-C2-C3	-2.64	105.07	109.77
2	A	901	UPH	O7-C24-C1	-2.59	104.95	110.14
2	B	1003	UPH	C20-C15-N4	2.49	103.77	102.11
6	B	1002	NAG	C3-C4-C5	-2.47	105.83	110.24
2	B	1003	UPH	C6-C5-N1	-2.09	108.17	113.88

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	UPH	C22-C11-N2-C10
2	A	901	UPH	C12-C11-N2-C10
2	B	1003	UPH	N1-C3-C4-O3
2	B	1003	UPH	C2-C3-C4-O3
2	B	1003	UPH	C22-C11-N2-C10
2	B	1003	UPH	C12-C11-N2-C10
3	A	902	GOL	O1-C1-C2-C3
5	B	1001	BTB	C4-C2-C3-O3
2	A	901	UPH	C13-C14-N4-C15
2	A	901	UPH	N2-C10-C9-C8
2	B	1003	UPH	N1-C5-C6-C7
2	B	1003	UPH	C13-C14-N4-C15
5	B	1001	BTB	N-C5-C6-O6
2	B	1003	UPH	N2-C10-C9-C8
5	B	1001	BTB	N-C7-C8-O8
2	A	901	UPH	C21-C14-N4-C15
2	A	901	UPH	C9-C10-N2-C11

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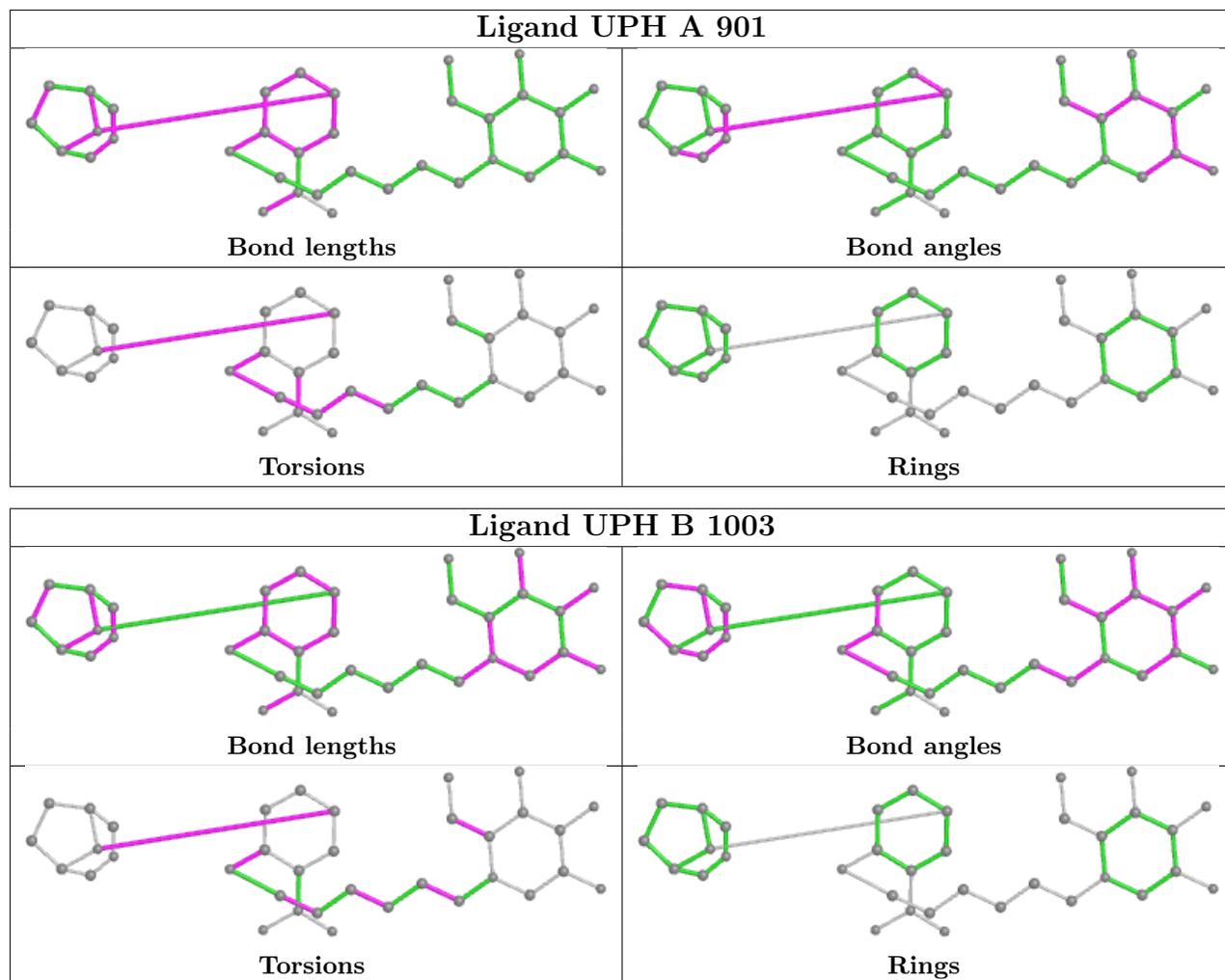
Mol	Chain	Res	Type	Atoms
2	A	901	UPH	C13-C14-N4-C18
2	A	901	UPH	C21-C14-N4-C18
2	B	1003	UPH	C13-C14-N4-C18
2	B	1003	UPH	C21-C14-N4-C15
2	B	1003	UPH	C21-C14-N4-C18
2	A	901	UPH	C13-C12-N3-O4
2	A	901	UPH	C6-C7-C8-C9
2	A	901	UPH	C7-C8-C9-C10
2	B	1003	UPH	C6-C7-C8-C9
5	B	1001	BTB	C1-C2-C3-O3
5	B	1001	BTB	N-C2-C3-O3
5	B	1001	BTB	N-C2-C4-O4
5	B	1001	BTB	C3-C2-C4-O4
3	A	902	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	UPH	5	0
2	B	1003	UPH	4	0
4	A	907	SO4	2	0
4	B	1004	SO4	1	0
5	B	1001	BTB	1	0
3	A	902	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	762/819 (93%)	0.00	32 (4%) 36 47	25, 42, 72, 116	0
1	B	763/819 (93%)	-0.19	6 (0%) 86 90	24, 40, 63, 82	0
All	All	1525/1638 (93%)	-0.09	38 (2%) 57 66	24, 41, 68, 116	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	THR	6.3
1	A	515	LEU	5.5
1	A	40	ILE	3.9
1	A	621	LEU	3.9
1	A	624	THR	3.9
1	B	720	GLY	3.6
1	A	531	LEU	3.3
1	A	43	LEU	3.2
1	A	622	GLY	3.2
1	A	618	GLY	3.1
1	A	41	GLY	3.1
1	A	623	ALA	3.1
1	A	529	VAL	3.0
1	A	516	ASP	2.9
1	A	39	GLU	2.9
1	A	619	SER	2.9
1	A	617	ILE	2.8
1	A	661	PHE	2.7
1	A	306	GLU	2.6
1	A	535	ARG	2.5
1	A	527	PRO	2.4
1	A	499	LEU	2.4
1	A	151	ASP	2.4
1	B	151	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	528	GLU	2.3
1	B	171	ASN	2.3
1	A	520	SER	2.3
1	A	629	PHE	2.3
1	A	668	CYS	2.2
1	A	153	ALA	2.2
1	A	519	LEU	2.2
1	B	216	ASP	2.1
1	A	383	ASN	2.1
1	A	566	THR	2.1
1	B	181	ASN	2.1
1	B	592	GLN	2.1
1	A	155	LYS	2.0
1	A	467	ALA	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.

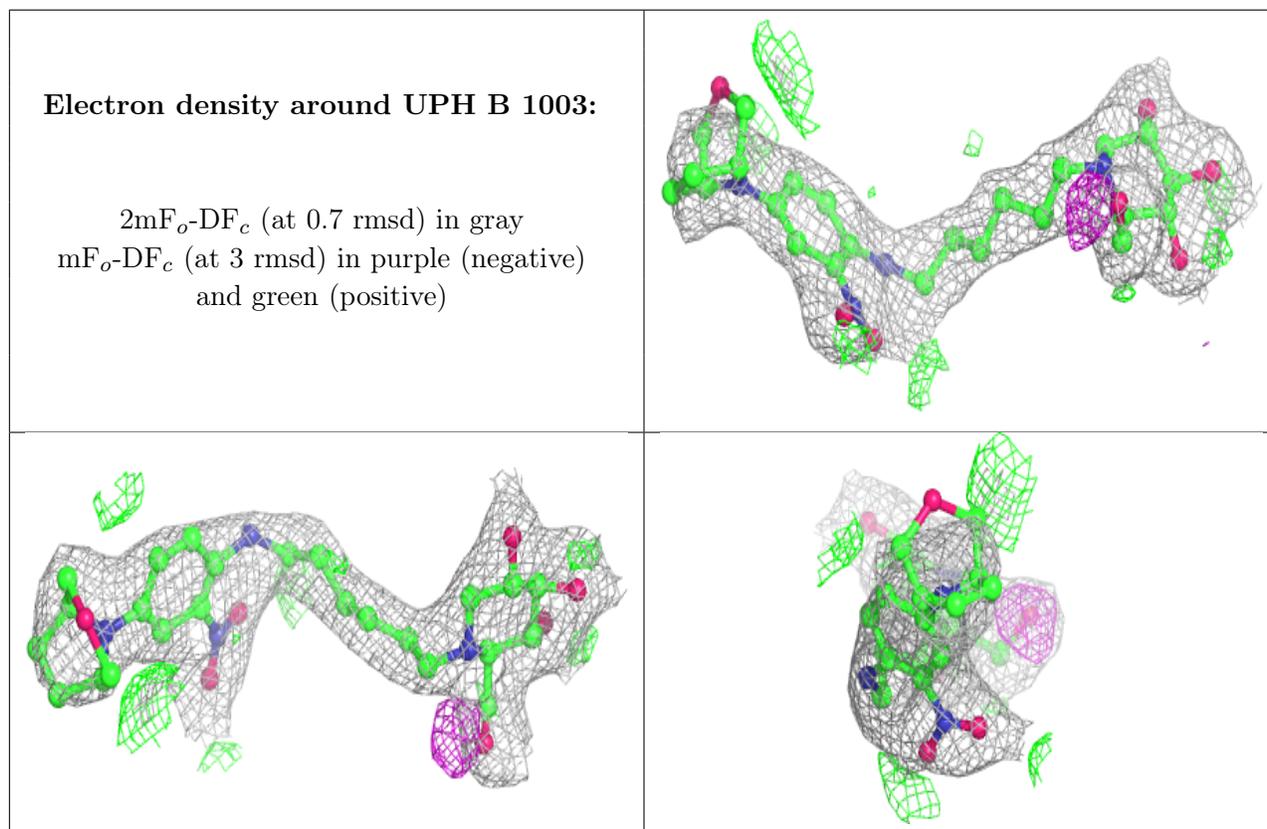
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BTB	B	1001	14/14	0.83	0.22	56,71,78,80	0
6	NAG	B	1002	14/15	0.88	0.22	57,70,77,78	0
4	SO4	A	907	5/5	0.89	0.19	95,101,110,113	0
4	SO4	A	903	5/5	0.92	0.35	92,97,106,110	0
4	SO4	A	908	5/5	0.92	0.24	98,98,100,106	0
3	GOL	A	902	6/6	0.94	0.21	68,75,79,79	0
4	SO4	B	1004	5/5	0.94	0.17	60,66,80,91	0
2	UPH	B	1003	35/35	0.95	0.16	26,64,134,148	0
4	SO4	A	904	5/5	0.96	0.17	75,77,85,92	0

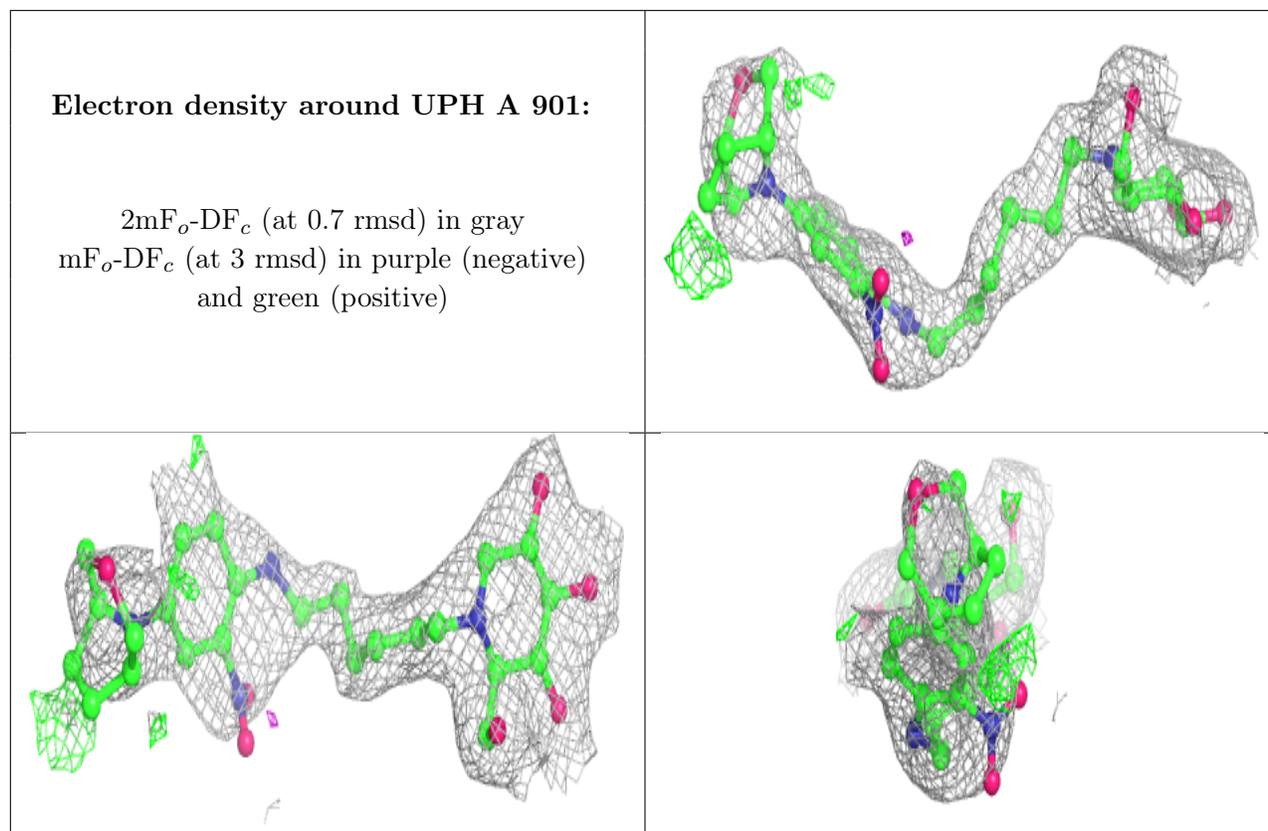
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	1008	5/5	0.96	0.20	51,68,71,73	0
4	SO4	A	906	5/5	0.97	0.12	52,53,70,74	0
2	UPH	A	901	35/35	0.97	0.23	25,73,147,149	0
4	SO4	B	1006	5/5	0.97	0.08	74,77,86,89	0
4	SO4	B	1007	5/5	0.98	0.14	58,60,72,75	0
4	SO4	A	905	5/5	0.98	0.17	41,45,46,51	0
4	SO4	B	1005	5/5	0.99	0.14	38,39,45,52	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.