



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:34 PM EDT

PDB ID : 8E3P  
Title : Co-crystal structure of Chaetomium glucosidase with compound 5  
Authors : Karade, S.S.; Mariuzza, R.A.  
Deposited on : 2022-08-17  
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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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

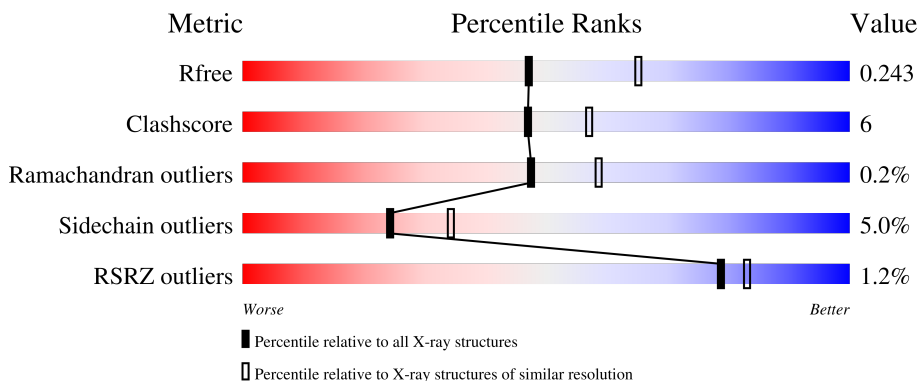
# 1 Overall quality at a glance

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  $\geq 3$ , 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	819	 2% 80% 13% • 6%
1	B	819	 79% 12% • 7%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12647 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	767	6121	3931	1034	1143	13	0	1	0
1	B	764	6076	3898	1017	1148	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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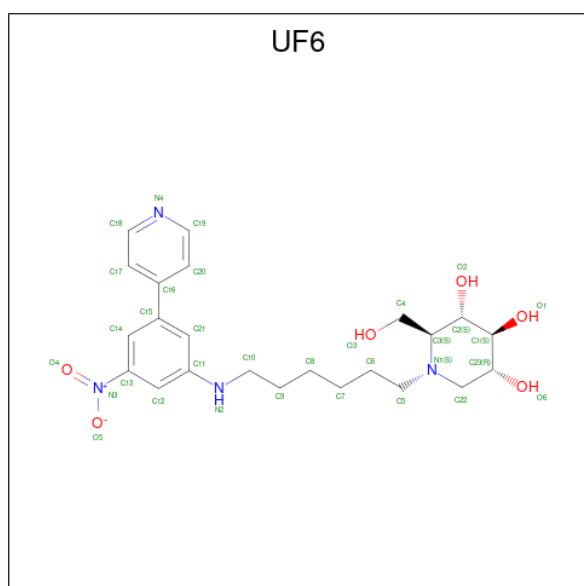
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP 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 (2S,3S,4S,5R)-2-(hydroxymethyl)-1-{6-[3-nitro-5-(pyridin-4-yl)anilino]hexyl}piperidine-3,4,5-triol (three-letter code: UF6) (formula: C<sub>23</sub>H<sub>32</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



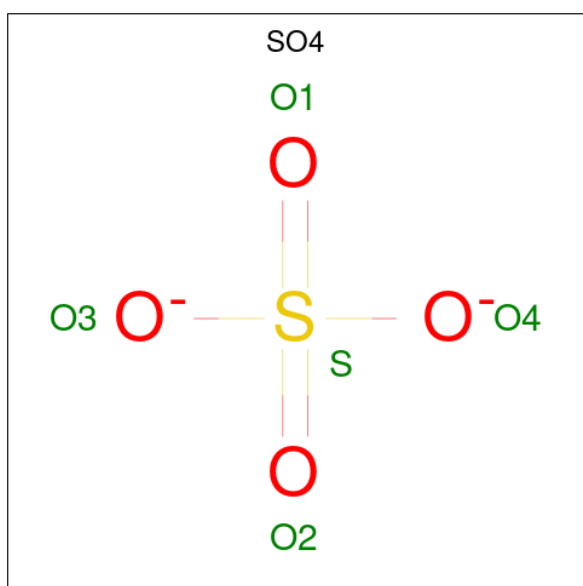
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	23	4	6	0	0
2	B	1	33	23	4	6	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



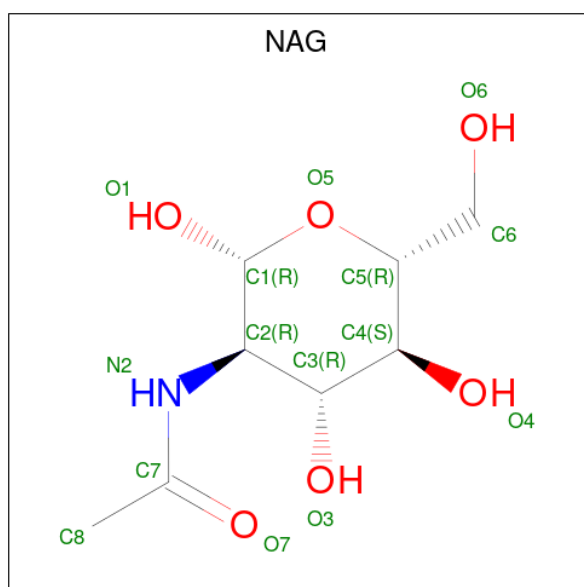
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

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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
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 water.

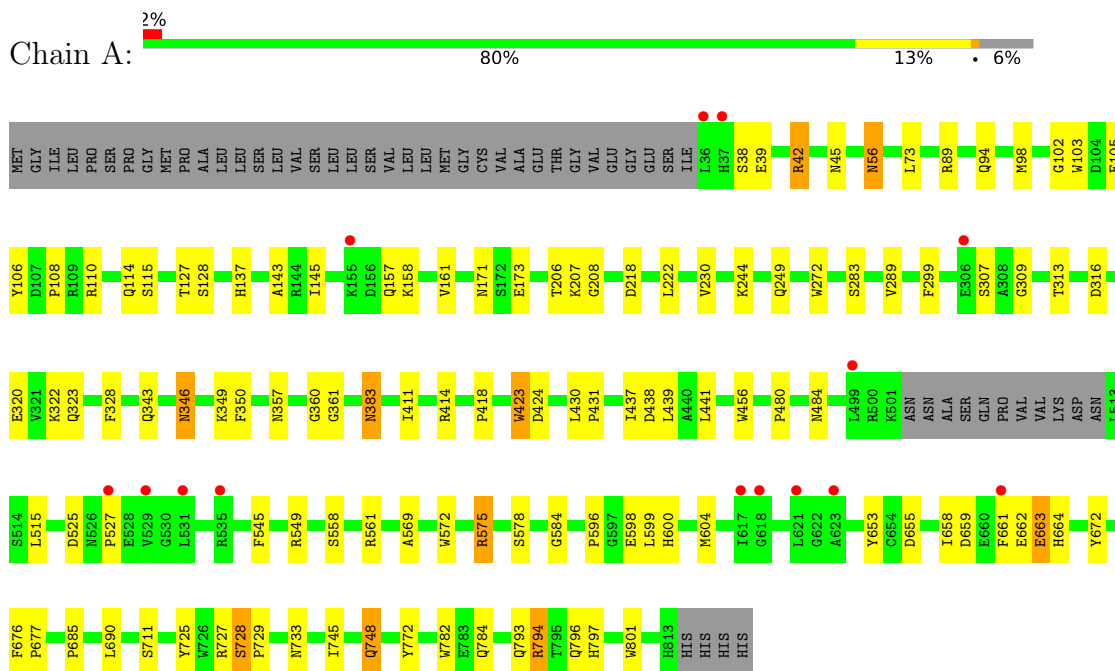
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	141	Total 141	O 141	0	0
6	B	162	Total 162	O 162	0	0



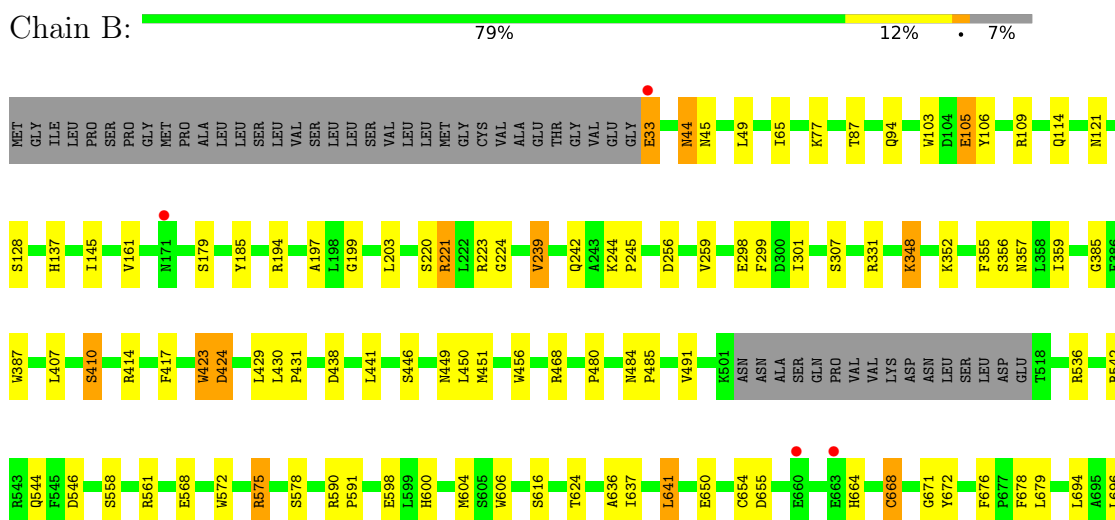
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	137.35Å 178.94Å 180.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 2.30 46.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.96-2.30) 99.7 (46.92-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.195 , 0.243 0.195 , 0.243	Depositor DCC
$R_{free}$ test set	4878 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtrriage
Anisotropy	0.348	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: UF6, SO4, NAG, GOL

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	0.38	0/6300	0.75	1/8570 (0.0%)
1	B	0.39	0/6252	0.77	3/8511 (0.0%)
All	All	0.38	0/12552	0.76	4/17081 (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	A	575	ARG	CB-CA-C	6.18	122.76	110.40
1	B	410	SER	N-CA-CB	-5.36	102.46	110.50
1	B	221	ARG	CB-CA-C	5.21	120.83	110.40
1	B	45	ASN	CB-CA-C	5.05	120.50	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	6121	0	5815	73	0
1	B	6076	0	5725	74	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
3	A	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	25	0	0	2	0
4	B	30	0	0	0	0
5	B	14	0	13	0	0
6	A	141	0	0	2	0
6	B	162	0	0	0	0
All	All	12647	0	11569	147	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 6.

All (147) 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:B:654:CYS:SG	1:B:668:CYS:HB2	1.56	1.44
1:B:654:CYS:SG	1:B:668:CYS:CB	2.25	1.22
1:A:208:GLY:H	3:A:902:GOL:H11	1.18	1.04
1:A:578:SER:HB2	4:A:904:SO4:O1	1.60	1.00
1:A:383:ASN:HD22	1:A:383:ASN:H	1.01	0.96
1:B:572:TRP:H	1:B:600:HIS:HD2	1.19	0.89
1:B:654:CYS:HG	1:B:668:CYS:CB	1.80	0.88
1:A:208:GLY:N	3:A:902:GOL:H11	1.96	0.80
1:B:650:GLU:HG3	1:B:668:CYS:SG	2.21	0.79
1:B:654:CYS:SG	1:B:668:CYS:HB3	2.20	0.78
1:A:383:ASN:HD22	1:A:383:ASN:N	1.80	0.78
1:A:383:ASN:H	1:A:383:ASN:ND2	1.82	0.77
1:A:784:GLN:HE21	1:A:793:GLN:HE21	1.33	0.77
1:B:784:GLN:HE21	1:B:793:GLN:HE21	1.33	0.77
1:B:114:GLN:NE2	1:B:414:ARG:HH12	1.83	0.77
1:B:654:CYS:HG	1:B:668:CYS:HB2	0.94	0.75
1:A:659:ASP:HB3	1:A:661:PHE:H	1.51	0.74
1:B:572:TRP:H	1:B:600:HIS:CD2	2.03	0.74
1:A:572:TRP:H	1:A:600:HIS:HD2	1.35	0.73
1:A:690:LEU:HD11	1:A:745:ILE:HD11	1.71	0.73
1:A:685:PRO:HG3	1:A:748:GLN:HE22	1.55	0.72
1:A:561:ARG:HE	1:A:664:HIS:HD2	1.38	0.71
1:B:94:GLN:OE1	1:B:797:HIS:HE1	1.74	0.71
1:A:784:GLN:NE2	1:A:793:GLN:HE21	1.88	0.70
1:A:423:TRP:H	1:A:484:ASN:ND2	1.89	0.70
1:A:346:ASN:H	1:A:346:ASN:HD22	1.39	0.70
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:H	1:B:121:ASN:ND2	1.93	0.67
1:B:106:TYR:HD2	1:B:359:ILE:HG23	1.60	0.67
1:B:696:LEU:HG	1:B:703:LEU:HD22	1.76	0.66
1:A:423:TRP:H	1:A:484:ASN:HD22	1.44	0.66
1:A:114:GLN:HE22	1:A:414:ARG:HH22	1.44	0.66
1:B:784:GLN:NE2	1:B:793:GLN:HE21	1.94	0.65
1:A:171:ASN:N	4:A:906:SO4:O4	2.26	0.63
1:B:542:ARG:NH2	1:B:546:ASP:OD1	2.34	0.60
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.37	0.60
1:B:678:PHE:HZ	1:B:742:LEU:HD13	1.67	0.60
1:B:87:THR:HB	1:B:121:ASN:HD21	1.67	0.59
1:B:103:TRP:H	1:B:357:ASN:ND2	2.01	0.58
1:A:56:ASN:H	1:A:56:ASN:HD22	1.49	0.58
1:A:659:ASP:HB2	1:A:663:GLU:H	1.69	0.57
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.39	0.57
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.88	0.57
1:B:239:VAL:HG22	1:B:242:GLN:OE1	2.05	0.57
1:B:103:TRP:H	1:B:357:ASN:HD21	1.54	0.55
1:B:137:HIS:HD2	1:B:307:SER:OG	1.89	0.55
1:B:575:ARG:NH1	1:B:598:GLU:OE2	2.39	0.55
1:A:114:GLN:NE2	1:A:414:ARG:HH12	2.04	0.55
1:A:110:ARG:HH22	1:A:323:GLN:HG3	1.72	0.55
1:A:437:ILE:O	1:A:441:LEU:HG	2.08	0.53
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.44	0.53
1:A:108:PRO:HG2	1:A:439:LEU:HD22	1.89	0.53
1:A:561:ARG:HE	1:A:664:HIS:CD2	2.22	0.53
1:B:801:TRP:O	1:B:804:LEU:HB2	2.09	0.53
1:A:114:GLN:HE21	1:A:414:ARG:HH12	1.56	0.53
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.24	0.52
1:A:346:ASN:HD22	1:A:346:ASN:N	2.07	0.52
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.91	0.52
1:A:94:GLN:OE1	1:A:797:HIS:HE1	1.92	0.52
1:B:44:ASN:HD21	1:B:109:ARG:HH22	1.58	0.52
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.57	0.52
1:B:671:GLY:HA2	1:B:703:LEU:HD11	1.92	0.52
1:A:128:SER:O	1:A:143:ALA:HA	2.10	0.51
1:B:114:GLN:HE21	1:B:414:ARG:HH12	1.54	0.51
1:A:230:VAL:HG22	1:A:289:VAL:HG22	1.93	0.51
1:B:727:ARG:O	1:B:728:SER:HB3	2.10	0.51
1:B:728:SER:N	1:B:729:PRO:HD3	2.26	0.50
1:B:733:ASN:HB3	1:B:801:TRP:CG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:SER:N	1:B:729:PRO:CD	2.75	0.50
1:B:348:LYS:HD2	1:B:352:LYS:HE3	1.93	0.49
1:A:456:TRP:CD2	1:A:480:PRO:HA	2.47	0.49
1:A:103:TRP:H	1:A:357:ASN:ND2	2.11	0.49
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.47	0.49
1:B:105:GLU:HA	1:B:356:SER:OG	2.12	0.49
1:A:569:ALA:HA	1:A:604:MET:CE	2.43	0.49
1:A:672:TYR:CZ	1:A:711:SER:HA	2.48	0.49
1:A:584:GLY:O	2:A:901:UF6:O1	2.31	0.48
1:A:598:GLU:OE2	1:A:600:HIS:CE1	2.66	0.48
1:A:206:THR:HB	3:A:902:GOL:H12	1.94	0.48
1:A:361:GLY:HA3	6:A:1067:HOH:O	2.12	0.48
1:A:569:ALA:HB1	1:A:599:LEU:HD22	1.95	0.48
1:B:429:LEU:HB2	1:B:491:VAL:HG21	1.96	0.48
1:A:672:TYR:CE1	1:A:711:SER:HA	2.49	0.48
1:B:424:ASP:OD2	2:B:901:UF6:O3	2.31	0.48
1:B:572:TRP:N	1:B:600:HIS:HD2	2.00	0.48
1:A:161:VAL:HG11	1:A:299:PHE:CE1	2.49	0.47
1:B:244:LYS:HB3	1:B:245:PRO:HD3	1.96	0.47
1:A:137:HIS:HD2	1:A:307:SER:OG	1.97	0.47
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.96	0.47
1:A:411:ILE:HD12	1:A:418:PRO:HA	1.97	0.47
1:A:158:LYS:HD3	1:A:272:TRP:CD1	2.50	0.47
1:B:590:ARG:HB3	1:B:591:PRO:HD2	1.96	0.47
1:B:604:MET:HG2	1:B:641:LEU:HD13	1.97	0.47
1:B:568:GLU:HG3	1:B:636:ALA:HB3	1.97	0.46
1:A:350:PHE:CE1	1:A:772:TYR:HA	2.51	0.46
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.51	0.46
1:A:430:LEU:HB2	1:A:431:PRO:HD3	1.97	0.46
1:A:108:PRO:HG2	1:A:439:LEU:CD2	2.45	0.46
1:B:561:ARG:HE	1:B:664:HIS:CD2	2.28	0.46
1:B:733:ASN:HD22	1:B:733:ASN:H	1.64	0.46
1:B:194:ARG:HA	1:B:199:GLY:O	2.16	0.45
1:A:114:GLN:HB3	1:A:127:THR:OG1	2.16	0.45
1:A:161:VAL:HG11	1:A:299:PHE:HE1	1.81	0.45
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.47	0.45
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.16	0.45
1:A:728:SER:N	1:A:729:PRO:CD	2.79	0.45
1:B:203:LEU:HD11	1:B:301:ILE:CG2	2.46	0.45
1:B:451:MET:CE	1:B:544:GLN:HB2	2.46	0.45
1:B:733:ASN:HD22	1:B:733:ASN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:MET:HE2	1:B:544:GLN:HB2	1.98	0.44
1:B:385:GLY:HA2	1:B:387:TRP:CZ3	2.52	0.44
1:A:313:THR:O	1:A:316:ASP:HB2	2.17	0.44
1:B:728:SER:H	1:B:729:PRO:CD	2.31	0.44
1:A:545:PHE:CZ	1:A:549:ARG:HD2	2.52	0.44
1:A:102:GLY:HA3	1:A:357:ASN:HD21	1.83	0.44
1:B:672:TYR:CG	1:B:734:ILE:HG21	2.53	0.44
1:B:678:PHE:CZ	1:B:742:LEU:HD13	2.51	0.43
1:A:658:ILE:HG23	1:A:662:GLU:HA	1.99	0.43
1:B:220:SER:O	1:B:224:GLY:N	2.52	0.43
1:B:256:ASP:O	1:B:259:VAL:HG22	2.19	0.43
1:B:179:SER:HB3	1:B:185:TYR:CD2	2.53	0.43
1:A:73:LEU:HD22	1:A:145:ILE:HD12	2.00	0.43
1:A:157:GLN:NE2	6:A:1002:HOH:O	2.49	0.43
1:B:407:LEU:HD13	1:B:450:LEU:HD11	2.00	0.43
1:B:33:GLU:N	1:B:536:ARG:HH21	2.17	0.43
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.84	0.43
1:B:355:PHE:HB2	1:B:806:VAL:HG21	2.01	0.42
1:B:385:GLY:HA2	1:B:387:TRP:CH2	2.53	0.42
1:B:423:TRP:H	1:B:484:ASN:ND2	2.17	0.42
1:A:569:ALA:HA	1:A:604:MET:HE1	2.00	0.42
1:B:145:ILE:O	1:B:298:GLU:HA	2.20	0.42
1:A:525:ASP:O	1:A:527:PRO:HD3	2.20	0.42
1:B:714:LYS:HA	1:B:719:TYR:CD1	2.55	0.42
1:A:105:GLU:HG2	1:A:328:PHE:CD1	2.56	0.41
1:A:56:ASN:H	1:A:56:ASN:ND2	2.18	0.41
1:A:106:TYR:CD2	1:A:360:GLY:HA2	2.55	0.41
1:A:349:LYS:HE3	1:A:349:LYS:HB2	1.95	0.41
1:A:794:ARG:HA	1:A:794:ARG:HD2	1.95	0.41
1:B:137:HIS:CD2	1:B:307:SER:OG	2.72	0.41
1:A:727:ARG:O	1:A:728:SER:HB3	2.21	0.41
1:A:89:ARG:CZ	1:A:98:MET:HE2	2.51	0.41
1:A:600:HIS:HA	1:A:655:ASP:OD1	2.22	0.40
1:A:653:TYR:CD2	1:A:677:PRO:HG2	2.57	0.40
1:A:39:GLU:OE2	1:A:42:ARG:NH1	2.54	0.40
1:B:637:ILE:HG22	1:B:641:LEU:HD22	2.03	0.40
1:A:782:TRP:CZ3	1:A:796:GLN:HG3	2.57	0.40
1:B:161:VAL:HG11	1:B:299:PHE:HE1	1.86	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	764/819 (93%)	735 (96%)	27 (4%)	2 (0%)	41	50
1	B	760/819 (93%)	736 (97%)	23 (3%)	1 (0%)	51	64
All	All	1524/1638 (93%)	1471 (96%)	50 (3%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	728	SER
1	B	728	SER
1	A	309	GLY

### 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	637/707 (90%)	608 (95%)	29 (5%)	27	38
1	B	632/707 (89%)	598 (95%)	34 (5%)	22	30
All	All	1269/1414 (90%)	1206 (95%)	63 (5%)	24	34

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	42	ARG
1	A	45	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	56	ASN
1	A	115	SER
1	A	173	GLU
1	A	207	LYS
1	A	218	ASP
1	A	222	LEU
1	A	244	LYS
1	A	249	GLN
1	A	283	SER
1	A	320	GLU
1	A	322	LYS
1	A	343	GLN
1	A	346	ASN
1	A	383	ASN
1	A	423	TRP
1	A	424	ASP
1	A	438	ASP
1	A	515	LEU
1	A	558	SER
1	A	575	ARG
1	A	596	PRO
1	A	663	GLU
1	A	676	PHE
1	A	725	TYR
1	A	748	GLN
1	A	794	ARG
1	B	33	GLU
1	B	44	ASN
1	B	49	LEU
1	B	105	GLU
1	B	128	SER
1	B	221	ARG
1	B	239	VAL
1	B	331	ARG
1	B	348	LYS
1	B	410	SER
1	B	417	PHE
1	B	423	TRP
1	B	424	ASP
1	B	438	ASP
1	B	441	LEU
1	B	446	SER

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Mol	Chain	Res	Type
1	B	449	ASN
1	B	468	ARG
1	B	558	SER
1	B	575	ARG
1	B	578	SER
1	B	616	SER
1	B	624	THR
1	B	641	LEU
1	B	668	CYS
1	B	676	PHE
1	B	679	LEU
1	B	694	LEU
1	B	703	LEU
1	B	733	ASN
1	B	742	LEU
1	B	801	TRP
1	B	804	LEU
1	B	810	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	114	GLN
1	A	137	HIS
1	A	167	GLN
1	A	214	GLN
1	A	242	GLN
1	A	287	HIS
1	A	346	ASN
1	A	357	ASN
1	A	368	HIS
1	A	383	ASN
1	A	398	GLN
1	A	484	ASN
1	A	494	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

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Mol	Chain	Res	Type
1	A	797	HIS
1	B	44	ASN
1	B	114	GLN
1	B	121	ASN
1	B	137	HIS
1	B	157	GLN
1	B	167	GLN
1	B	214	GLN
1	B	287	HIS
1	B	323	GLN
1	B	357	ASN
1	B	476	GLN
1	B	484	ASN
1	B	600	HIS
1	B	664	HIS
1	B	733	ASN
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 [i](#)

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	B	904	-	4,4,4	0.23	0	6,6,6	0.15	0
4	SO4	A	907	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	B	909	-	4,4,4	0.35	0	6,6,6	0.17	0
2	UF6	B	901	-	34,35,35	4.19	8 (23%)	43,47,47	2.19	13 (30%)
4	SO4	A	904	-	4,4,4	0.34	0	6,6,6	0.13	0
2	UF6	A	901	-	34,35,35	4.18	9 (26%)	43,47,47	2.25	10 (23%)
4	SO4	B	905	-	4,4,4	0.48	0	6,6,6	0.21	0
3	GOL	A	902	-	5,5,5	0.14	0	5,5,5	0.25	0
4	SO4	A	903	-	4,4,4	0.39	0	6,6,6	0.33	0
3	GOL	B	903	-	5,5,5	0.27	0	5,5,5	0.38	0
4	SO4	A	906	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	B	908	-	4,4,4	0.32	0	6,6,6	0.09	0
4	SO4	B	907	-	4,4,4	0.33	0	6,6,6	0.11	0
5	NAG	B	902	1	14,14,15	0.52	0	17,19,21	2.06	7 (41%)
4	SO4	B	906	-	4,4,4	0.27	0	6,6,6	0.15	0
4	SO4	A	905	-	4,4,4	0.30	0	6,6,6	0.10	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	UF6	B	901	-	-	7/18/40/40	0/3/3/3
2	UF6	A	901	-	-	9/18/40/40	0/3/3/3
3	GOL	A	902	-	-	1/4/4/4	-
5	NAG	B	902	1	-	2/6/23/26	0/1/1/1
3	GOL	B	903	-	-	4/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	UF6	C5-N1	-18.53	1.14	1.47
2	A	901	UF6	C5-N1	-18.03	1.15	1.47
2	B	901	UF6	O4-N3	9.65	1.39	1.22
2	A	901	UF6	O4-N3	9.34	1.38	1.22
2	A	901	UF6	C23-C1	-7.41	1.41	1.52
2	A	901	UF6	C4-C3	-7.16	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	UF6	C23-C1	-7.15	1.42	1.52
2	B	901	UF6	C4-C3	-6.49	1.42	1.52
2	A	901	UF6	C2-C1	-4.68	1.40	1.52
2	B	901	UF6	C2-C1	-4.55	1.40	1.52
2	A	901	UF6	C22-N1	-2.97	1.42	1.47
2	A	901	UF6	O2-C2	-2.97	1.36	1.43
2	B	901	UF6	C22-N1	-2.93	1.42	1.47
2	A	901	UF6	C11-N2	2.75	1.46	1.38
2	B	901	UF6	C11-N2	2.57	1.46	1.38
2	B	901	UF6	C22-C23	-2.46	1.49	1.52
2	A	901	UF6	O1-C1	2.23	1.48	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	UF6	C12-C13-N3	7.27	125.16	118.75
2	A	901	UF6	C23-C1-C2	-6.33	99.94	110.89
2	A	901	UF6	C12-C13-N3	6.12	124.14	118.75
2	A	901	UF6	O3-C4-C3	-5.35	99.93	111.42
2	B	901	UF6	C1-C2-C3	-5.33	102.37	111.37
2	A	901	UF6	C14-C15-C16	-4.85	112.84	120.86
2	B	901	UF6	O3-C4-C3	-4.38	102.03	111.42
5	B	902	NAG	C1-O5-C5	3.83	117.38	112.19
2	B	901	UF6	C23-C1-C2	-3.77	104.37	110.89
5	B	902	NAG	C2-N2-C7	3.42	127.78	122.90
2	A	901	UF6	C6-C5-N1	-3.29	104.90	113.88
2	A	901	UF6	C21-C15-C16	3.25	126.23	120.86
2	B	901	UF6	C4-C3-C2	3.22	117.83	112.90
2	B	901	UF6	C5-N1-C3	-3.11	104.96	113.29
5	B	902	NAG	C1-C2-N2	-3.06	105.26	110.49
2	B	901	UF6	C23-C22-N1	2.91	115.72	110.54
5	B	902	NAG	C3-C4-C5	-2.85	105.15	110.24
2	A	901	UF6	O2-C2-C3	2.67	114.53	109.77
2	A	901	UF6	C20-C19-N4	-2.61	119.08	123.62
2	A	901	UF6	C14-C13-N3	-2.59	116.46	118.75
2	B	901	UF6	C14-C13-N3	-2.58	116.47	118.75
2	B	901	UF6	C14-C15-C21	2.56	122.09	118.31
2	B	901	UF6	C19-N4-C18	2.45	122.60	116.85
2	B	901	UF6	C17-C18-N4	-2.42	119.41	123.62
2	B	901	UF6	O1-C1-C23	2.38	114.55	109.99
2	A	901	UF6	C20-C16-C15	-2.38	117.24	121.36
5	B	902	NAG	O7-C7-N2	-2.28	117.75	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	NAG	O4-C4-C5	2.24	114.85	109.30
2	B	901	UF6	C14-C15-C16	-2.08	117.42	120.86
5	B	902	NAG	C4-C3-C2	2.01	113.96	111.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

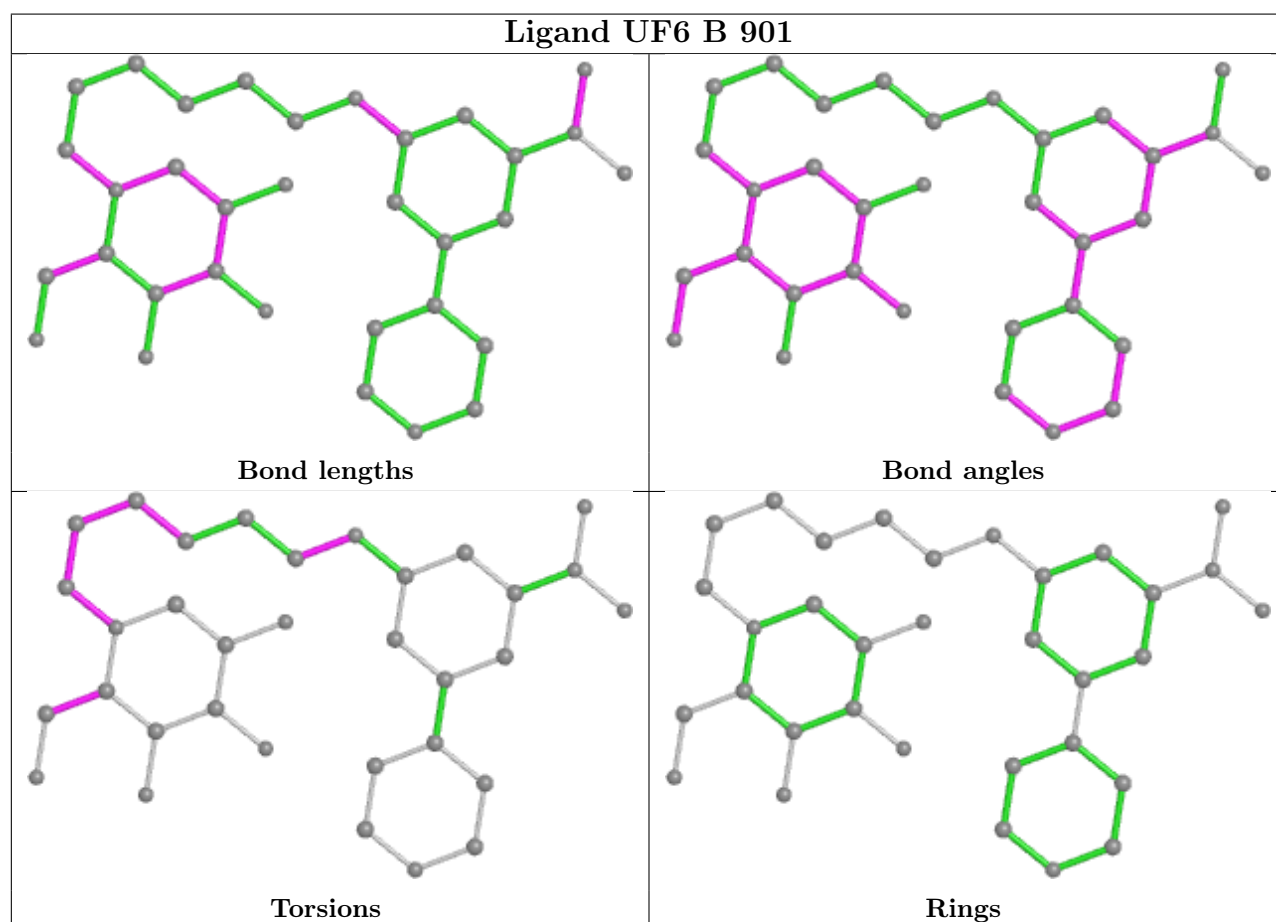
Mol	Chain	Res	Type	Atoms
2	B	901	UF6	N1-C3-C4-O3
2	B	901	UF6	C2-C3-C4-O3
3	B	903	GOL	C1-C2-C3-O3
2	A	901	UF6	C21-C11-N2-C10
2	A	901	UF6	C12-C11-N2-C10
5	B	902	NAG	C8-C7-N2-C2
5	B	902	NAG	O7-C7-N2-C2
2	A	901	UF6	C12-C13-N3-O4
3	B	903	GOL	O1-C1-C2-C3
2	B	901	UF6	C6-C7-C8-C9
3	B	903	GOL	O1-C1-C2-O2
2	A	901	UF6	C14-C13-N3-O4
3	B	903	GOL	O2-C2-C3-O3
2	B	901	UF6	C5-C6-C7-C8
2	B	901	UF6	C9-C10-N2-C11
2	A	901	UF6	C6-C5-N1-C22
2	A	901	UF6	C6-C5-N1-C3
2	A	901	UF6	C6-C7-C8-C9
2	A	901	UF6	N1-C3-C4-O3
2	B	901	UF6	N1-C5-C6-C7
3	A	902	GOL	O2-C2-C3-O3
2	B	901	UF6	C6-C5-N1-C22
2	A	901	UF6	N2-C10-C9-C8

There are no ring outliers.

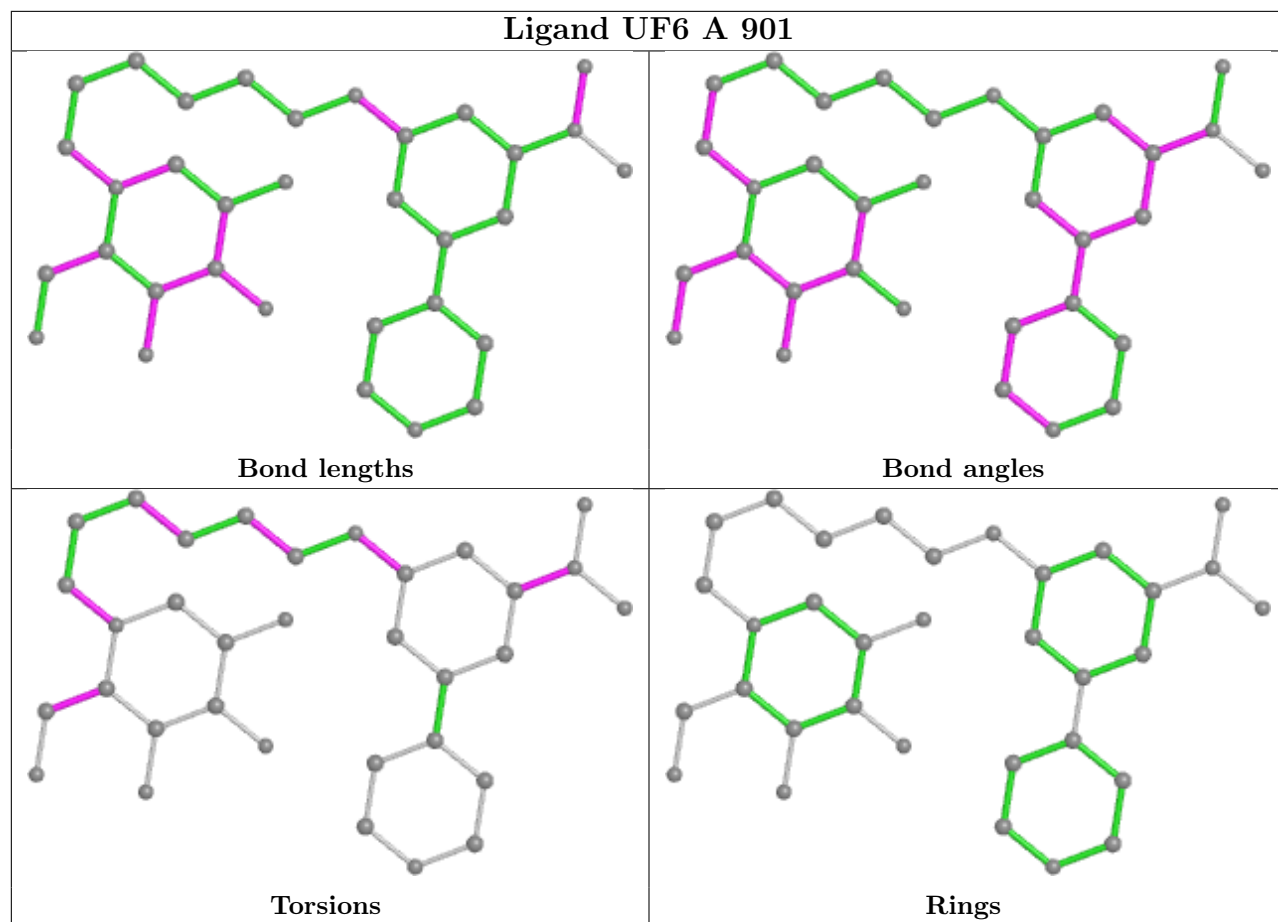
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	UF6	1	0
4	A	904	SO4	1	0
2	A	901	UF6	1	0
3	A	902	GOL	3	0
4	A	906	SO4	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 [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, 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	767/819 (93%)	-0.19	14 (1%) 68 74	31, 48, 73, 106	0
1	B	764/819 (93%)	-0.32	4 (0%) 91 94	33, 48, 71, 115	0
All	All	1531/1638 (93%)	-0.25	18 (1%) 79 83	31, 48, 72, 115	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	LEU	4.0
1	A	531	LEU	3.3
1	A	617	ILE	3.0
1	A	618	GLY	2.8
1	A	37	HIS	2.8
1	A	36	LEU	2.8
1	A	499	LEU	2.7
1	A	306	GLU	2.7
1	A	529	VAL	2.4
1	A	623	ALA	2.4
1	A	661	PHE	2.4
1	B	33	GLU	2.4
1	B	660	GLU	2.3
1	B	171	ASN	2.3
1	A	527	PRO	2.1
1	B	663	GLU	2.1
1	A	535[A]	ARG	2.1
1	A	155	LYS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

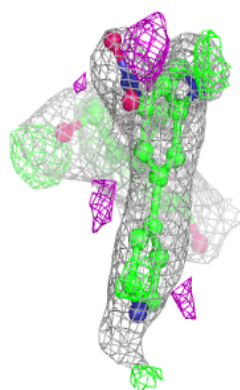
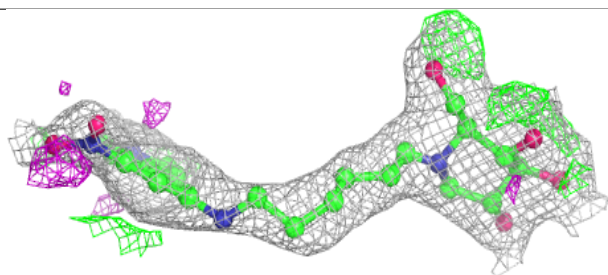
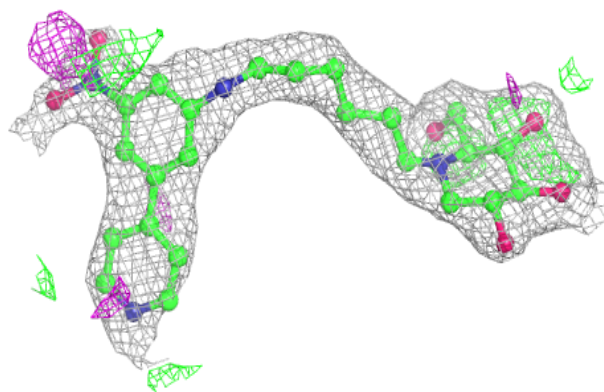
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	SO4	A	904	5/5	0.70	0.20	110,111,121,126	0
4	SO4	B	907	5/5	0.81	0.25	119,120,126,133	0
5	NAG	B	902	14/15	0.89	0.17	77,85,93,96	0
4	SO4	B	908	5/5	0.90	0.12	95,95,101,103	0
4	SO4	B	906	5/5	0.91	0.13	73,81,92,104	0
3	GOL	A	902	6/6	0.92	0.19	56,72,77,97	0
3	GOL	B	903	6/6	0.93	0.19	36,52,56,60	0
2	UF6	A	901	33/33	0.93	0.20	33,54,87,94	0
2	UF6	B	901	33/33	0.94	0.17	37,80,122,128	0
4	SO4	A	906	5/5	0.95	0.17	94,95,100,101	0
4	SO4	A	907	5/5	0.95	0.16	92,102,106,106	0
4	SO4	B	904	5/5	0.97	0.19	57,69,82,82	0
4	SO4	B	909	5/5	0.98	0.17	71,73,77,78	0
4	SO4	A	905	5/5	0.98	0.11	54,58,70,81	0
4	SO4	B	905	5/5	0.99	0.12	44,46,53,56	0
4	SO4	A	903	5/5	0.99	0.14	44,45,48,50	0

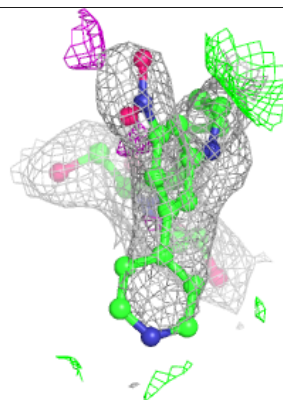
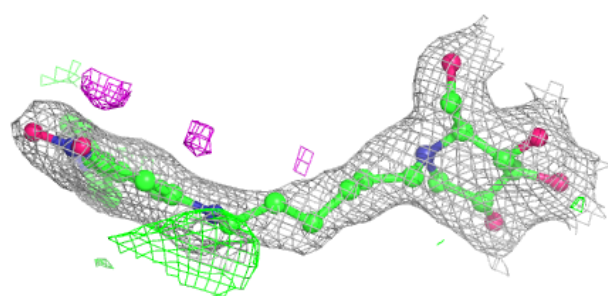
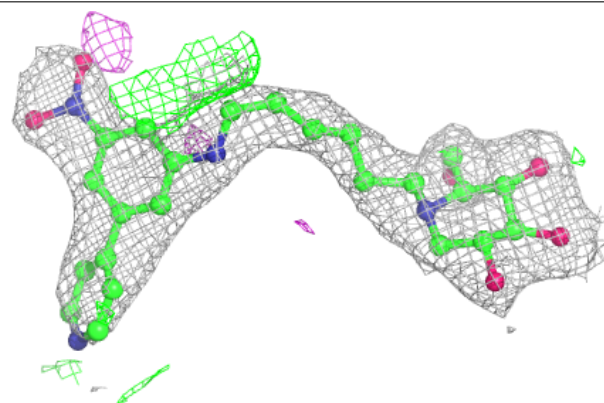
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UF6 A 901:**

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

**Electron density around UF6 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.