Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 09:10 pm BST

PDB ID	:	5OHY
Title	:	A GH31 family sulfoquinovosidase in complex with aza-sugar inhibitor IFGSQ
Authors	:	Jin, Y.; Williams, S.J.; Goddard-Borger, E.; Davies, G.J.
Deposited on	:	2017-07-18
Resolution	:	1.77 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

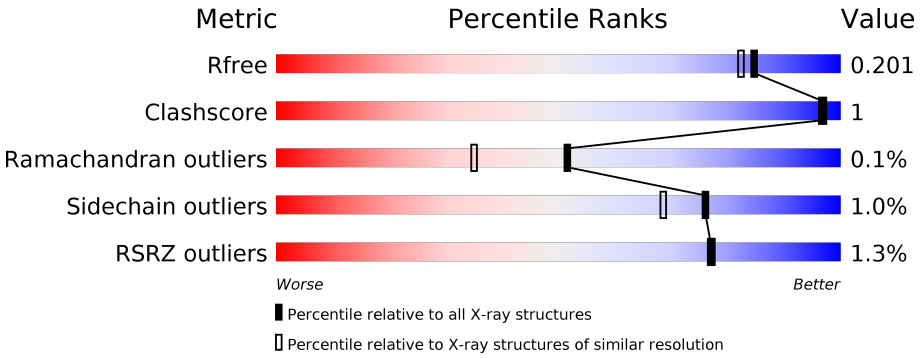
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	672	95%
1	B	672	94%
1	C	672	95%
1	D	672	94%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22718 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 Alpha-glucosidase yihQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	4	0
			5214	3334	899	960	21			
1	B	663	Total	C	N	O	S	0	2	0
			5226	3338	902	965	21			
1	C	660	Total	C	N	O	S	0	4	0
			5192	3320	890	960	22			
1	D	654	Total	C	N	O	S	0	3	0
			5139	3285	884	950	20			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
A	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
A	665	LEU	-	expression tag	UNP A0A083ZKV2
A	666	GLU	-	expression tag	UNP A0A083ZKV2
A	667	HIS	-	expression tag	UNP A0A083ZKV2
A	668	HIS	-	expression tag	UNP A0A083ZKV2
A	669	HIS	-	expression tag	UNP A0A083ZKV2
A	670	HIS	-	expression tag	UNP A0A083ZKV2
A	671	HIS	-	expression tag	UNP A0A083ZKV2
A	672	HIS	-	expression tag	UNP A0A083ZKV2
B	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
B	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
B	665	LEU	-	expression tag	UNP A0A083ZKV2
B	666	GLU	-	expression tag	UNP A0A083ZKV2
B	667	HIS	-	expression tag	UNP A0A083ZKV2
B	668	HIS	-	expression tag	UNP A0A083ZKV2
B	669	HIS	-	expression tag	UNP A0A083ZKV2
B	670	HIS	-	expression tag	UNP A0A083ZKV2
B	671	HIS	-	expression tag	UNP A0A083ZKV2
B	672	HIS	-	expression tag	UNP A0A083ZKV2
C	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2

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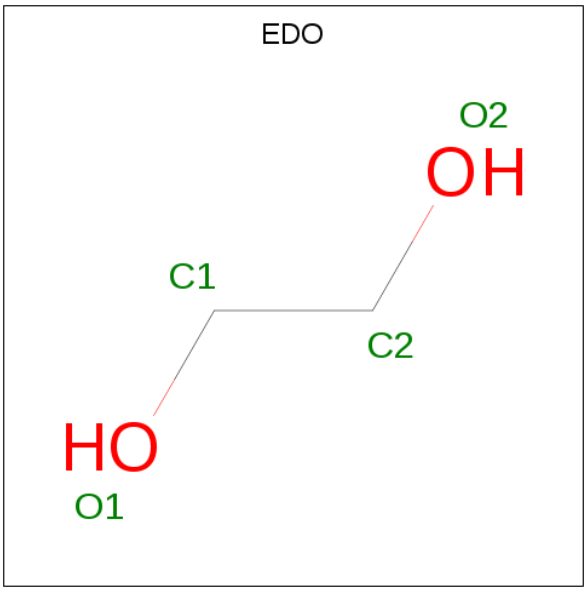
Chain	Residue	Modelled	Actual	Comment	Reference
C	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
C	665	LEU	-	expression tag	UNP A0A083ZKV2
C	666	GLU	-	expression tag	UNP A0A083ZKV2
C	667	HIS	-	expression tag	UNP A0A083ZKV2
C	668	HIS	-	expression tag	UNP A0A083ZKV2
C	669	HIS	-	expression tag	UNP A0A083ZKV2
C	670	HIS	-	expression tag	UNP A0A083ZKV2
C	671	HIS	-	expression tag	UNP A0A083ZKV2
C	672	HIS	-	expression tag	UNP A0A083ZKV2
D	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
D	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
D	665	LEU	-	expression tag	UNP A0A083ZKV2
D	666	GLU	-	expression tag	UNP A0A083ZKV2
D	667	HIS	-	expression tag	UNP A0A083ZKV2
D	668	HIS	-	expression tag	UNP A0A083ZKV2
D	669	HIS	-	expression tag	UNP A0A083ZKV2
D	670	HIS	-	expression tag	UNP A0A083ZKV2
D	671	HIS	-	expression tag	UNP A0A083ZKV2
D	672	HIS	-	expression tag	UNP A0A083ZKV2

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

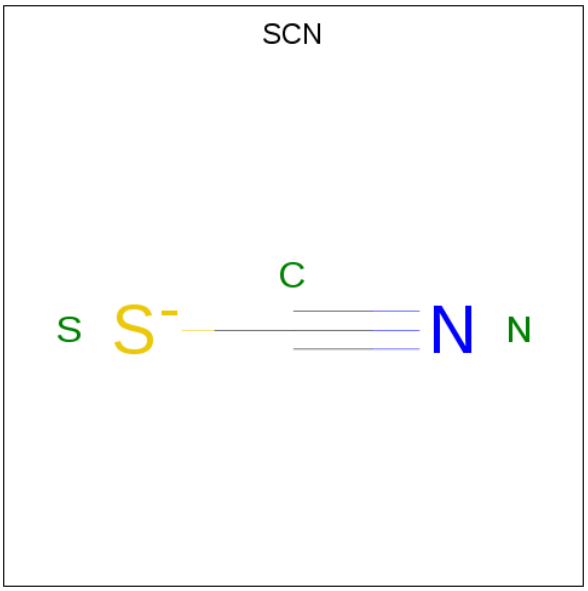
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



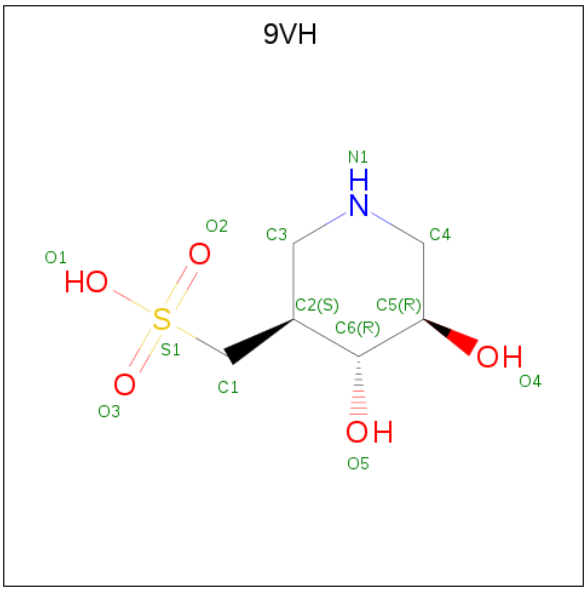
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



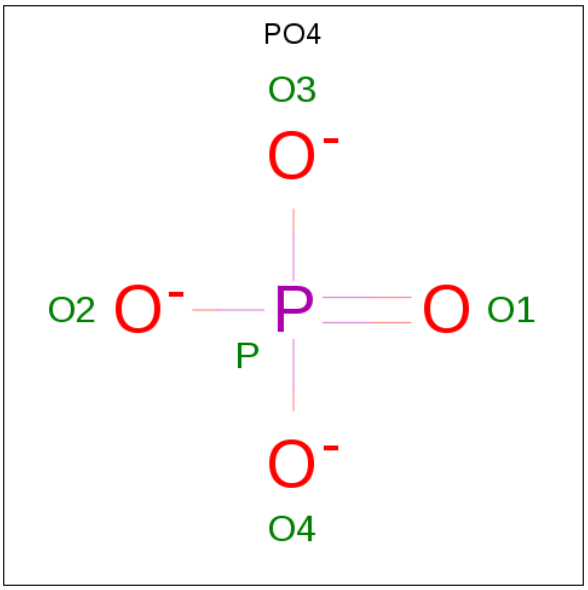
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	C	1	Total C N S 3 1 1 1	0	0
4	C	1	Total C N S 3 1 1 1	0	0

- Molecule 5 is [(3 {S},4 {R},5 {R})-4,5-bis(oxidanyl)piperidin-3-yl]methanesulfonic acid (three-letter code: 9VH) (formula: $C_6H_{13}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	6	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			13	6	1	5	1		
5	C	1	Total	C	N	O	S	0	0
			13	6	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			13	6	1	5	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

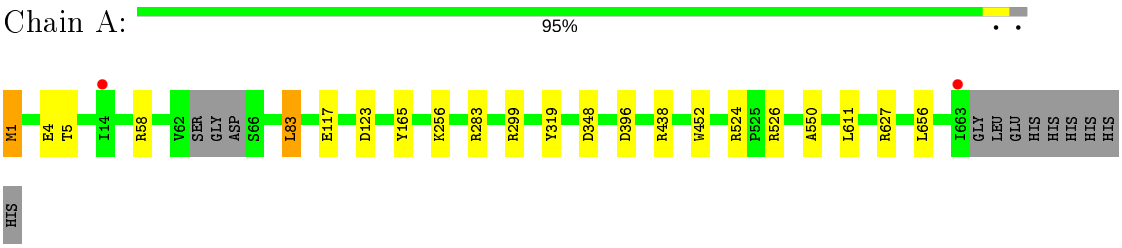
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	526	Total O 528 528	0	2
7	B	500	Total O 501 501	0	1
7	C	409	Total O 409 409	0	0
7	D	383	Total O 383 383	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

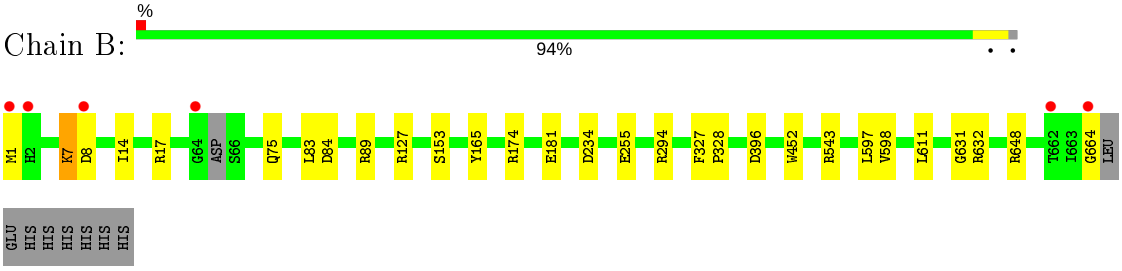
- Molecule 1: Alpha-glucosidase yihQ

Chain A:



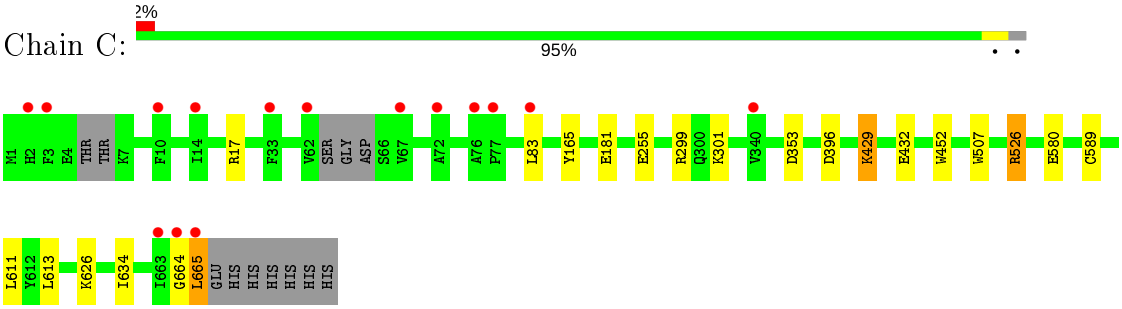
- Molecule 1: Alpha-glucosidase yihQ

Chain B:



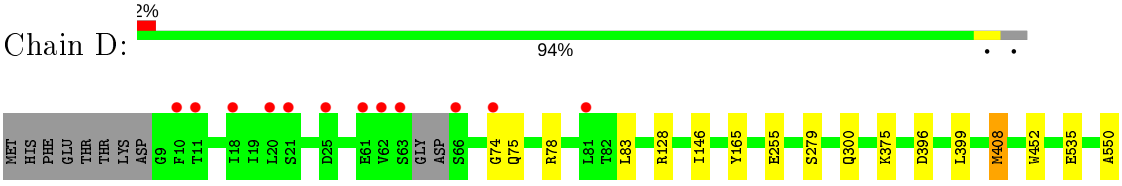
- Molecule 1: Alpha-glucosidase yihQ

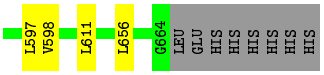
Chain C:



- Molecule 1: Alpha-glucosidase yihQ

Chain D:




L597
V598
L611
L656
G664
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.29Å 168.82Å 101.39Å 90.00° 117.07° 90.00°	Depositor
Resolution (Å)	77.70 – 1.77 77.70 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.70-1.77) 99.9 (77.70-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.177 , 0.195 0.183 , 0.201	Depositor DCC
R_{free} test set	14049 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22718	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, SCN, 9VH, EDO

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	0.88	2/5374 (0.0%)	0.90	10/7305 (0.1%)
1	B	0.85	1/5377 (0.0%)	0.90	10/7307 (0.1%)
1	C	0.88	8/5351 (0.1%)	0.89	5/7276 (0.1%)
1	D	0.81	2/5291 (0.0%)	0.87	4/7198 (0.1%)
All	All	0.86	13/21393 (0.1%)	0.89	29/29086 (0.1%)

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	D	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLU	CD-OE1	10.86	1.37	1.25
1	D	255	GLU	CD-OE2	7.70	1.34	1.25
1	D	279	SER	CB-OG	-7.09	1.33	1.42
1	C	432	GLU	CD-OE1	6.37	1.32	1.25
1	C	589[A]	CYS	CB-SG	-5.97	1.72	1.81
1	C	589[B]	CYS	CB-SG	-5.97	1.72	1.81
1	A	319	TYR	CZ-OH	5.93	1.48	1.37
1	C	255	GLU	CD-OE2	5.87	1.32	1.25
1	C	580	GLU	CD-OE1	-5.71	1.19	1.25
1	B	153	SER	CB-OG	-5.43	1.35	1.42
1	A	117	GLU	CD-OE1	5.38	1.31	1.25
1	C	526	ARG	CZ-NH2	5.32	1.40	1.33
1	C	580	GLU	CD-OE2	-5.04	1.20	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	408	MET	CG-SD-CE	13.12	121.19	100.20
1	D	78	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	348	ASP	CB-CG-OD1	7.81	125.33	118.30
1	C	665	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	627	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	174	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	17	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	396	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	396	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	648	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	299	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	17	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	294	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	127	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	181	GLU	CG-CD-OE1	5.59	129.48	118.30
1	A	524	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	353	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	234	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	283	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	C	396	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	17	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	299	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	535	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	B	127	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	396	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	58	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	123	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	438	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	1	MET	CA-CB-CG	5.00	121.80	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	74	GLY	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	5214	0	4980	4	0
1	B	5226	0	4991	19	0
1	C	5192	0	4927	4	0
1	D	5139	0	4888	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	6	0	0
3	B	12	0	18	0	0
3	C	12	0	18	0	0
3	D	12	0	18	2	0
4	A	3	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
5	A	13	0	0	0	0
5	B	13	0	0	0	0
5	C	13	0	0	0	0
5	D	13	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	A	528	0	0	0	0
7	B	501	0	0	4	0
7	C	409	0	0	1	0
7	D	383	0	0	7	0
All	All	22718	0	19846	38	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 1.

All (38) 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:1:MET:HE1	1:B:14:ILE:CD1	2.23	0.69
1:B:84:ASP:OD2	1:B:89:ARG:NH2	2.27	0.68
1:B:631:GLY:C	1:B:632[B]:ARG:HG3	2.16	0.65
1:B:1:MET:CE	1:B:14:ILE:CD1	2.78	0.62
1:B:89:ARG:NE	7:B:803:HOH:O	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:OE2	7:B:801:HOH:O	2.17	0.57
1:B:89:ARG:NH1	7:B:804:HOH:O	2.36	0.56
1:D:597:LEU:HD23	1:D:598:VAL:N	2.21	0.56
1:B:597:LEU:HD23	1:B:598:VAL:N	2.22	0.53
1:B:1:MET:CE	1:B:14:ILE:HD12	2.41	0.51
1:B:632[B]:ARG:NH2	1:B:632[B]:ARG:HG2	2.26	0.50
1:B:1:MET:HB3	1:B:83:LEU:HD21	1.94	0.50
1:A:1:MET:HB2	1:A:83:LEU:HD21	1.94	0.49
1:D:146[A]:ILE:HD11	7:D:1113:HOH:O	2.13	0.49
1:B:327:PHE:HB3	1:B:328:PRO:HD3	1.96	0.48
1:D:128:ARG:NH1	7:D:804:HOH:O	2.38	0.47
1:B:75:GLN:NE2	7:B:811:HOH:O	2.49	0.46
1:B:543:ARG:HH21	1:B:664:GLY:HA2	1.79	0.46
1:B:1:MET:HE1	1:B:14:ILE:HD11	1.98	0.46
1:B:632[B]:ARG:HH21	1:B:632[B]:ARG:HG2	1.81	0.46
1:B:597:LEU:C	1:B:597:LEU:HD23	2.37	0.45
3:D:703:EDO:H12	7:D:955:HOH:O	2.16	0.45
1:A:256:LYS:HE3	1:A:256:LYS:HB3	1.61	0.45
1:C:526:ARG:NE	1:C:526:ARG:HA	2.32	0.45
1:B:8:ASP:N	1:B:8:ASP:OD1	2.38	0.44
1:A:526:ARG:NE	1:A:526:ARG:HA	2.32	0.44
1:A:550:ALA:O	1:A:656:LEU:HD11	2.18	0.44
1:D:300:GLN:NE2	7:D:801:HOH:O	2.19	0.44
1:C:301:LYS:HA	1:C:301:LYS:HD2	1.89	0.43
1:B:7:LYS:HG3	1:B:8:ASP:N	2.34	0.43
1:C:429:LYS:HD2	7:C:1170:HOH:O	2.20	0.42
1:D:550:ALA:O	1:D:656:LEU:HD11	2.19	0.42
1:C:613:LEU:HD11	1:C:634:ILE:HD13	2.01	0.42
1:D:375:LYS:HE3	7:D:1150:HOH:O	2.19	0.41
1:D:399:LEU:HD13	1:D:408:MET:HG3	2.03	0.41
3:D:703:EDO:C1	7:D:955:HOH:O	2.68	0.41
1:D:128:ARG:NE	7:D:804:HOH:O	2.37	0.41
1:D:597:LEU:HD23	1:D:597:LEU:C	2.41	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	660/672 (98%)	638 (97%)	22 (3%)	0	100	100
1	B	661/672 (98%)	638 (96%)	22 (3%)	1 (0%)	47	32
1	C	658/672 (98%)	638 (97%)	19 (3%)	1 (0%)	47	32
1	D	653/672 (97%)	633 (97%)	20 (3%)	0	100	100
All	All	2632/2688 (98%)	2547 (97%)	83 (3%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	LYS
1	C	664	GLY

5.3.2 Protein sidechains

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	532/545 (98%)	526 (99%)	6 (1%)	73	65
1	B	534/545 (98%)	531 (99%)	3 (1%)	86	82
1	C	527/545 (97%)	519 (98%)	8 (2%)	65	53
1	D	523/545 (96%)	518 (99%)	5 (1%)	76	68
All	All	2116/2180 (97%)	2094 (99%)	22 (1%)	76	68

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	5	THR
1	A	83	LEU
1	A	165	TYR
1	A	452	TRP
1	A	611	LEU
1	B	165	TYR
1	B	452	TRP
1	B	611	LEU
1	C	83	LEU
1	C	165	TYR
1	C	429	LYS
1	C	452	TRP
1	C	507	TRP
1	C	611	LEU
1	C	626	LYS
1	C	665	LEU
1	D	75	GLN
1	D	83	LEU
1	D	165	TYR
1	D	452	TRP
1	D	611	LEU

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

Mol	Chain	Res	Type
1	A	300	GLN
1	D	164	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	B	702	-	3,3,3	0.74	0	2,2,2	0.20	0
6	PO4	C	708	-	4,4,4	1.11	0	6,6,6	0.46	0
3	EDO	C	704	-	3,3,3	0.38	0	2,2,2	0.52	0
3	EDO	B	703	-	3,3,3	0.62	0	2,2,2	0.38	0
4	SCN	A	703	-	1,2,2	0.42	0	0,1,1	0.00	-
3	EDO	D	703	-	3,3,3	1.06	0	2,2,2	0.57	0
3	EDO	C	702	-	3,3,3	0.66	0	2,2,2	0.59	0
3	EDO	D	702	-	3,3,3	0.77	0	2,2,2	0.22	0
4	SCN	C	706	-	1,2,2	0.56	0	0,1,1	0.00	-
5	9VH	A	704	-	11,13,13	1.31	2 (18%)	14,19,19	1.03	0
3	EDO	D	704	-	3,3,3	0.31	0	2,2,2	0.58	0
5	9VH	B	707	-	11,13,13	1.22	2 (18%)	14,19,19	1.59	2 (14%)
6	PO4	B	708	-	4,4,4	1.24	0	6,6,6	1.09	0
4	SCN	B	705	-	1,2,2	0.47	0	0,1,1	0.00	-
4	SCN	C	705	-	1,2,2	0.81	0	0,1,1	0.00	-
3	EDO	C	703	-	3,3,3	0.53	0	2,2,2	0.37	0
4	SCN	B	706	-	1,2,2	0.71	0	0,1,1	0.00	-
6	PO4	A	705	-	4,4,4	1.30	0	6,6,6	0.94	0
3	EDO	A	702	-	3,3,3	0.72	0	2,2,2	0.98	0
5	9VH	D	705	-	11,13,13	1.21	1 (9%)	14,19,19	2.04	6 (42%)
3	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.18	0
5	9VH	C	707	-	11,13,13	1.51	1 (9%)	14,19,19	1.66	2 (14%)

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	EDO	C	704	-	-	0/1/1/1	-
3	EDO	D	703	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	702	-	-	0/1/1/1	-
5	9VH	D	705	-	-	0/5/19/19	0/1/1/1
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	D	702	-	-	0/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
5	9VH	A	704	-	-	0/5/19/19	0/1/1/1
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	D	704	-	-	0/1/1/1	-
5	9VH	B	707	-	-	1/5/19/19	0/1/1/1
5	9VH	C	707	-	-	0/5/19/19	0/1/1/1
3	EDO	B	703	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	707	9VH	O3-S1	4.35	1.57	1.45
5	D	705	9VH	O3-S1	2.71	1.53	1.45
5	B	707	9VH	O3-S1	2.68	1.52	1.45
5	A	704	9VH	C4-N1	2.66	1.50	1.46
5	B	707	9VH	C4-N1	2.10	1.49	1.46
5	A	704	9VH	O1-S1	2.07	1.55	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	707	9VH	O1-S1-O2	4.26	121.68	111.27
5	D	705	9VH	O3-S1-C1	-4.05	102.12	106.94
5	C	707	9VH	O1-S1-O2	3.82	120.61	111.27
5	C	707	9VH	O3-S1-O2	-3.51	101.81	113.95
5	D	705	9VH	O4-C5-C4	-3.48	102.82	109.61
5	B	707	9VH	O3-S1-O2	-3.13	103.12	113.95
5	D	705	9VH	O4-C5-C6	2.59	115.33	110.14
5	D	705	9VH	O5-C6-C2	-2.52	105.82	110.08
5	D	705	9VH	O5-C6-C5	2.18	114.16	109.99
5	D	705	9VH	O1-S1-C1	2.04	108.99	105.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	707	9VH	C2-C1-S1-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	703	EDO	2	0

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	660/672 (98%)	-0.42	2 (0%)	94	93	18, 27, 48, 83	0
1	B	663/672 (98%)	-0.40	6 (0%)	84	84	18, 28, 48, 81	1 (0%)
1	C	660/672 (98%)	-0.26	15 (2%)	60	60	18, 30, 67, 97	0
1	D	654/672 (97%)	-0.16	12 (1%)	68	68	20, 36, 75, 99	0
All	All	2637/2688 (98%)	-0.31	35 (1%)	77	77	18, 29, 64, 99	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	5.1
1	D	10	PHE	4.7
1	B	664	GLY	4.2
1	C	3	PHE	3.9
1	C	14	ILE	3.5
1	D	18	ILE	3.4
1	B	64	GLY	3.3
1	D	21	SER	3.2
1	C	663	ILE	3.1
1	C	83	LEU	3.0
1	D	81	LEU	2.9
1	C	62	VAL	2.8
1	C	76	ALA	2.8
1	D	63	SER	2.8
1	C	665	LEU	2.7
1	D	66	SER	2.6
1	C	67	VAL	2.5
1	C	72	ALA	2.5
1	D	74	GLY	2.4
1	A	663	ILE	2.4
1	C	664	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	25	ASP	2.4
1	A	14	ILE	2.3
1	C	77	PRO	2.2
1	D	20	LEU	2.2
1	C	340	VAL	2.2
1	D	11	THR	2.2
1	C	33	PHE	2.1
1	B	8	ASP	2.1
1	C	2	HIS	2.1
1	D	61	GLU	2.0
1	B	1	MET	2.0
1	C	10	PHE	2.0
1	B	2	HIS	2.0
1	B	662	THR	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	B	708	5/5	0.82	0.37	45,53,60,63	5
3	EDO	D	704	4/4	0.85	0.14	33,34,39,48	0
3	EDO	D	703	4/4	0.90	0.15	33,39,41,56	0
4	SCN	C	706	3/3	0.91	0.14	44,44,46,56	3
3	EDO	B	703	4/4	0.93	0.08	31,37,40,43	0
3	EDO	C	702	4/4	0.93	0.10	31,34,41,44	0
2	K	D	701	1/1	0.93	0.09	35,35,35,35	0
3	EDO	B	704	4/4	0.93	0.10	32,33,33,37	0
2	K	C	701	1/1	0.94	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	A	705	5/5	0.94	0.12	41,43,49,52	5
3	EDO	C	704	4/4	0.94	0.11	38,38,40,48	0
3	EDO	D	702	4/4	0.94	0.11	21,22,27,31	0
6	PO4	C	708	5/5	0.95	0.20	43,43,52,52	5
2	K	A	701	1/1	0.95	0.10	33,33,33,33	0
3	EDO	A	702	4/4	0.97	0.08	24,24,31,32	0
4	SCN	B	706	3/3	0.97	0.11	41,41,54,58	0
5	9VH	D	705	13/13	0.97	0.11	19,24,30,30	0
5	9VH	B	707	13/13	0.97	0.10	17,19,23,23	0
5	9VH	A	704	13/13	0.98	0.09	18,20,22,22	0
2	K	B	701	1/1	0.98	0.07	32,32,32,32	0
4	SCN	C	705	3/3	0.98	0.09	26,26,28,40	0
3	EDO	C	703	4/4	0.98	0.07	24,24,28,29	0
3	EDO	B	702	4/4	0.98	0.08	18,22,23,25	0
5	9VH	C	707	13/13	0.98	0.08	18,21,24,24	0
4	SCN	B	705	3/3	0.99	0.12	33,33,37,54	0
4	SCN	A	703	3/3	0.99	0.10	30,30,36,46	0

6.5 Other polymers

There are no such residues in this entry.