



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2017 – 03:48 PM EST

PDB ID : 5H47  
Title : Crystal structure of AOL complexed with 2-MeSe-Fuc  
Authors : Kato, R.; Nishikawa, Y.; Makyio, H.  
Deposited on : 2016-10-31  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

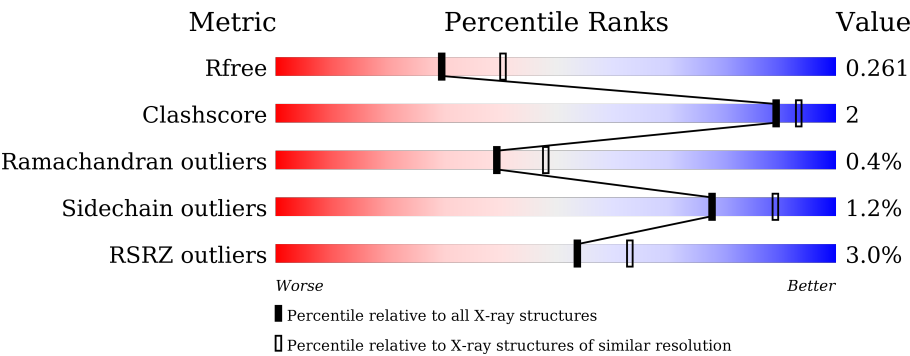
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



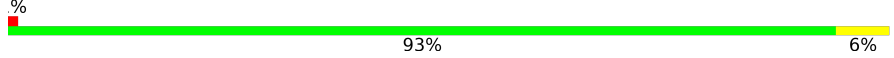
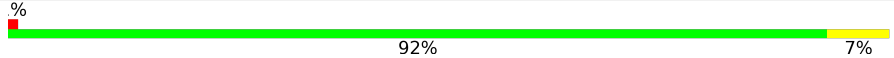
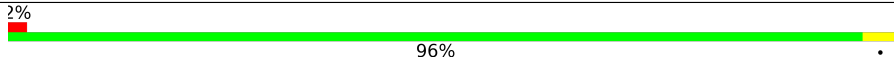
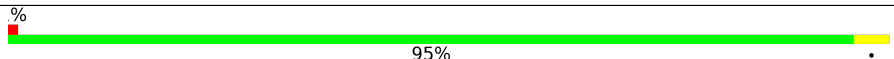
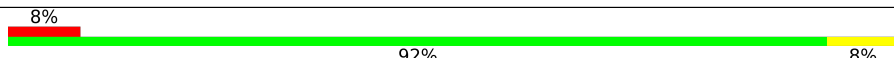
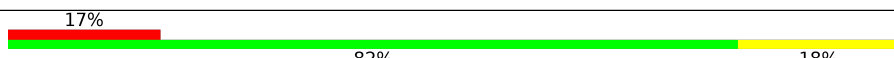
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	311	<div><div>%</div><div><div></div><div>94%</div><div>6%</div></div></div>
1	B	311	<div><div></div><div><div>95%</div><div>5%</div></div></div>
1	C	311	<div><div></div><div><div>93%</div><div>7%</div></div></div>
1	D	311	<div><div>%</div><div><div></div><div>94%</div><div>6%</div></div></div>
1	E	311	<div><div>%</div><div><div></div><div>93%</div><div>7%</div></div></div>
1	F	311	<div><div>3%</div><div><div></div><div>94%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	311	
1	H	311	
1	I	311	
1	J	311	
1	K	311	
1	L	311	

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
2	FSW	A	1006	-	-	-	X
2	FSW	B	1001	-	-	-	X
2	FSW	B	1005	-	-	-	X
2	FSW	B	1006	-	-	-	X
2	FSW	C	1001	-	-	-	X
2	FSW	C	1005	-	-	-	X
2	FSW	C	1006	-	-	-	X
2	FSW	D	1006	-	-	-	X
2	FSW	E	1001	-	-	-	X
2	FSW	E	1003	-	-	-	X
2	FSW	E	1005	-	-	-	X
2	FSW	E	1006	-	-	-	X
2	FSW	F	1001	-	-	-	X
2	FSW	F	1005	-	-	-	X
2	FSW	F	1006	-	-	-	X
2	FSW	G	1001	-	-	-	X
2	FSW	G	1005	-	-	-	X
2	FSW	G	1006	-	-	-	X
2	FSW	H	1001	-	-	-	X
2	FSW	H	1002	-	-	-	X
2	FSW	H	1003	-	-	-	X
2	FSW	H	1005	-	-	-	X
2	FSW	H	1006	-	-	-	X
2	FSW	I	1001	-	-	-	X
2	FSW	I	1002	-	-	-	X
2	FSW	I	1005	-	-	-	X
2	FSW	I	1006	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FSW	J	1001	-	-	-	X
2	FSW	J	1005	-	-	-	X
2	FSW	J	1006	-	-	-	X

## 2 Entry composition

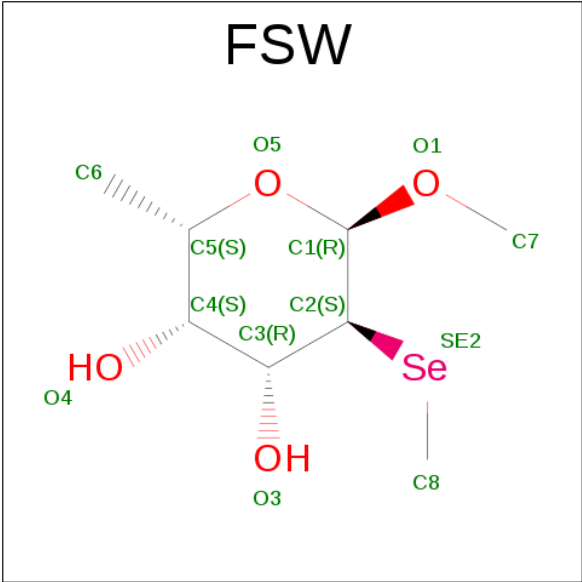
There are 3 unique types of molecules in this entry. The entry contains 31809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	B	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	C	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	D	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	E	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	F	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	G	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	H	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	I	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	J	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	K	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	L	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			

- Molecule 2 is (2S,3S,4R,5S,6R)-6-methoxy-2-methyl-5-methylselanyl-oxane-3,4-diol (three-letter code: FSW) (formula: C<sub>8</sub>H<sub>16</sub>O<sub>4</sub>Se).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	C	1	Total	C	O	Se	0	0
			13	8	4	1		
2	C	1	Total	C	O	Se	0	0
			13	8	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	J	1	Total 13	C 8	O 4	Se 1	0	0
2	J	1	Total 13	C 8	O 4	Se 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total	O	0	0
			209	209		
3	B	188	Total	O	0	0
			188	188		
3	C	156	Total	O	0	0
			156	156		

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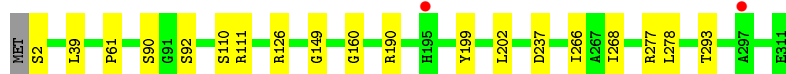
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	179	Total 179	O 179	0	0
3	E	150	Total 150	O 150	0	0
3	F	160	Total 160	O 160	0	0
3	G	121	Total 121	O 121	0	0
3	H	139	Total 139	O 139	0	0
3	I	124	Total 124	O 124	0	0
3	J	107	Total 107	O 107	0	0
3	K	61	Total 61	O 61	0	0
3	L	47	Total 47	O 47	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 errors 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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein

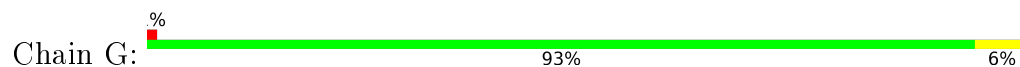


- Molecule 1: Uncharacterized protein





- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



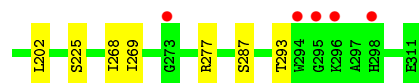
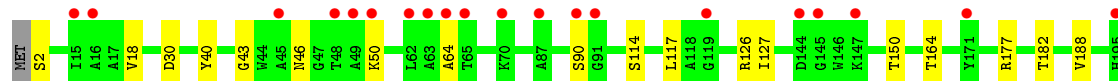
- Molecule 1: Uncharacterized protein



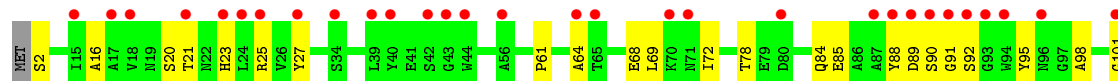
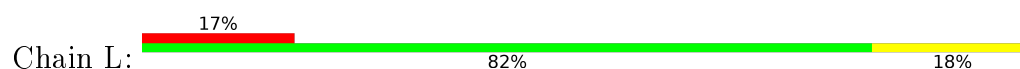
- Molecule 1: Uncharacterized protein

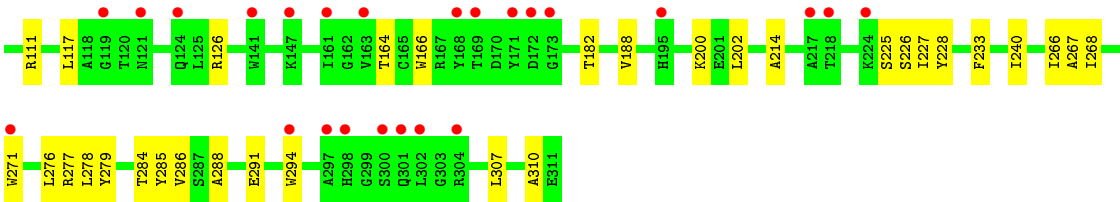


- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.97Å 214.32Å 126.53Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	39.99 – 2.30 39.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.99-2.30) 100.0 (39.38-2.30)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.216 , 0.258 0.219 , 0.261	Depositor DCC
$R_{free}$ test set	11931 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.78% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FSW

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	0.70	0/2504	0.85	2/3413 (0.1%)
1	B	0.69	0/2504	0.83	0/3413
1	C	0.68	0/2504	0.81	0/3413
1	D	0.71	0/2504	0.86	5/3413 (0.1%)
1	E	0.67	0/2504	0.82	3/3413 (0.1%)
1	F	0.66	0/2504	0.82	0/3413
1	G	0.63	0/2504	0.81	3/3413 (0.1%)
1	H	0.66	0/2504	0.81	1/3413 (0.0%)
1	I	0.65	0/2504	0.80	2/3413 (0.1%)
1	J	0.71	0/2504	0.84	1/3413 (0.0%)
1	K	0.67	0/2504	0.85	2/3413 (0.1%)
1	L	0.69	0/2504	0.85	1/3413 (0.0%)
All	All	0.68	0/30048	0.83	20/40956 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	30	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	183	ASP	CB-CG-OD1	6.44	124.09	118.30
1	E	177	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	73	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	E	177	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	12	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	G	39	LEU	CA-CB-CG	5.62	128.22	115.30
1	G	278	LEU	CA-CB-CG	5.61	128.19	115.30
1	D	25	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	I	30	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	25	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	39	LEU	CA-CB-CG	5.37	127.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	H	126	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	126	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	K	177	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	J	126	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	304	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	L	25	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	I	126	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2436	0	2348	8	0
1	B	2436	0	2348	9	0
1	C	2436	0	2348	16	0
1	D	2436	0	2348	8	0
1	E	2436	0	2348	10	0
1	F	2436	0	2348	10	0
1	G	2436	0	2348	14	0
1	H	2436	0	2348	16	0
1	I	2436	0	2348	7	0
1	J	2436	0	2348	5	0
1	K	2436	0	2348	10	0
1	L	2436	0	2348	32	0
2	A	78	0	0	2	0
2	B	78	0	0	0	0
2	C	78	0	0	4	0
2	D	78	0	0	1	0
2	E	78	0	0	2	0
2	F	78	0	0	2	0
2	G	78	0	0	2	0
2	H	78	0	0	4	0
2	I	78	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	78	0	0	0	0
2	K	78	0	0	0	0
2	L	78	0	0	6	0
3	A	209	0	0	2	0
3	B	188	0	0	3	0
3	C	156	0	0	1	0
3	D	179	0	0	0	0
3	E	150	0	0	0	0
3	F	160	0	0	1	0
3	G	121	0	0	5	0
3	H	139	0	0	4	0
3	I	124	0	0	2	0
3	J	107	0	0	0	0
3	K	61	0	0	1	0
3	L	47	0	0	3	0
All	All	31809	0	28176	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (142) 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:L:88:TYR:CZ	2:L:1001:FSW:O4	1.99	1.15
1:C:2:SER:N	3:C:1101:HOH:O	1.99	0.96
1:L:88:TYR:CE1	2:L:1001:FSW:O4	2.20	0.93
1:B:2:SER:N	3:B:1101:HOH:O	2.06	0.87
1:L:88:TYR:CE2	2:L:1001:FSW:O4	2.31	0.83
1:C:140:MET:CE	1:C:149:GLY:HA3	2.10	0.81
1:H:2:SER:N	3:H:1102:HOH:O	2.16	0.77
1:H:272:GLU:O	3:H:1101:HOH:O	2.08	0.72
1:A:2:SER:N	3:A:1102:HOH:O	2.23	0.71
1:L:268:ILE:HD13	1:L:278:LEU:HD13	1.73	0.70
1:I:190:ARG:HD3	1:I:202:LEU:HD23	1.72	0.70
1:F:291:GLU:OE1	2:F:1006:FSW:O3	2.09	0.70
1:L:23:HIS:HB3	1:L:69:LEU:HD11	1.76	0.66
1:E:167:ARG:NH1	1:E:171:TYR:O	2.30	0.65
1:L:276:LEU:HD12	1:L:294:TRP:HB3	1.80	0.63
1:C:140:MET:HE1	1:C:149:GLY:HA3	1.81	0.63
1:G:111:ARG:HG3	1:G:159:THR:O	2.02	0.60
1:I:300:SER:HB2	3:I:1203:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:268:ILE:HD12	1:L:277:ARG:O	2.02	0.59
1:B:190:ARG:HD2	1:B:202:LEU:HD23	1.86	0.58
1:L:166:TRP:CD1	1:L:227:ILE:HD13	2.39	0.58
1:F:168:TYR:HB2	1:F:171:TYR:HB2	1.86	0.57
1:L:188:VAL:HG21	1:L:202:LEU:HD22	1.85	0.57
1:A:190:ARG:HD2	1:A:202:LEU:HD23	1.84	0.57
1:G:268:ILE:HD13	1:G:278:LEU:HD13	1.84	0.57
1:B:268:ILE:HD13	1:B:278:LEU:HD13	1.86	0.57
1:A:237:ASP:OD2	3:A:1101:HOH:O	2.17	0.56
1:L:95:TYR:HE2	2:L:1002:FSW:C8	2.18	0.56
1:C:140:MET:HE3	1:C:149:GLY:HA3	1.86	0.55
1:H:98:ALA:HB2	2:H:1002:FSW:C8	2.38	0.54
1:L:111:ARG:HD2	3:L:1108:HOH:O	2.07	0.53
1:I:190:ARG:CD	1:I:202:LEU:HD23	2.36	0.53
1:C:291:GLU:OE1	2:C:1006:FSW:O3	2.27	0.52
1:B:130:GLN:OE1	3:B:1102:HOH:O	2.18	0.52
1:C:140:MET:CE	1:C:149:GLY:CA	2.86	0.52
1:C:95:TYR:HE1	2:C:1002:FSW:C8	2.21	0.52
1:K:268:ILE:HD12	1:K:277:ARG:O	2.10	0.52
1:B:111:ARG:HG3	1:B:160:GLY:HA2	1.90	0.52
1:L:284:THR:O	1:L:288:ALA:HB3	2.10	0.52
1:C:268:ILE:HD12	1:C:277:ARG:O	2.10	0.51
1:E:35:ILE:HD12	1:E:62:LEU:HD11	1.91	0.51
1:L:78:THR:HG22	1:L:84:GLN:OE1	2.10	0.51
1:C:140:MET:HE1	1:C:149:GLY:CA	2.40	0.51
1:L:88:TYR:CD1	2:L:1001:FSW:O4	2.64	0.51
1:G:2:SER:N	3:G:1104:HOH:O	2.43	0.51
1:L:214:ALA:O	1:L:233:PHE:HA	2.10	0.50
2:A:1004:FSW:O1	2:A:1004:FSW:C8	2.60	0.50
1:G:277:ARG:CD	1:G:293:THR:HG22	2.42	0.50
1:L:285:TYR:HA	3:L:1105:HOH:O	2.11	0.50
1:H:305:ARG:NH2	3:H:1104:HOH:O	2.36	0.50
1:A:268:ILE:HD13	1:A:278:LEU:HD13	1.93	0.49
1:C:36:ARG:HD3	1:C:48:THR:O	2.13	0.49
1:K:188:VAL:HG21	1:K:202:LEU:HD22	1.93	0.49
1:I:111:ARG:HG3	1:I:160:GLY:HA2	1.94	0.49
1:H:98:ALA:CB	2:H:1002:FSW:C8	2.90	0.49
1:H:170:ASP:HB3	1:H:224:LYS:HG3	1.94	0.49
1:I:111:ARG:NH1	3:I:1105:HOH:O	2.44	0.49
1:C:138:GLU:OE1	2:C:1003:FSW:O3	2.31	0.48
1:G:189:GLN:NE2	1:G:251:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:MET:HE3	2:G:1003:FSW:SE2	2.64	0.48
1:C:111:ARG:HG3	1:C:159:THR:O	2.14	0.47
1:J:2:SER:OG	1:J:3:THR:N	2.46	0.47
1:L:117:LEU:HD21	1:L:126:ARG:CG	2.45	0.47
1:H:111:ARG:HD2	3:H:1146:HOH:O	2.13	0.47
1:K:277:ARG:CD	1:K:293:THR:HG22	2.44	0.47
2:G:1005:FSW:O1	3:G:1102:HOH:O	2.20	0.47
1:B:111:ARG:NH1	3:B:1106:HOH:O	2.44	0.47
1:A:111:ARG:HG3	1:A:160:GLY:HA2	1.97	0.47
1:E:277:ARG:CD	1:E:293:THR:HG22	2.45	0.46
1:L:117:LEU:HD21	1:L:126:ARG:HG3	1.97	0.46
1:L:21:THR:O	1:L:271:TRP:CE2	2.68	0.46
1:F:111:ARG:HG3	1:F:159:THR:O	2.15	0.46
1:H:111:ARG:HG3	1:H:160:GLY:HA2	1.97	0.46
1:L:16:ALA:HB1	1:L:64:ALA:HB3	1.98	0.46
1:L:27:TYR:OH	1:L:72:ILE:HG21	2.15	0.46
1:L:61:PRO:HB3	1:L:111:ARG:HA	1.98	0.46
1:C:3:THR:HG21	1:C:310:ALA:O	2.16	0.46
1:K:117:LEU:HD21	1:K:126:ARG:CG	2.46	0.46
1:L:240:ILE:HG12	1:L:266:ILE:HD11	1.97	0.46
1:K:50:LYS:NZ	3:K:1102:HOH:O	2.38	0.46
1:H:193:ASP:OD2	1:H:199:TYR:OH	2.13	0.46
1:K:40:TYR:HA	1:K:43:GLY:O	2.17	0.45
1:F:111:ARG:HD2	3:F:1190:HOH:O	2.16	0.45
1:F:126:ARG:CD	1:F:140:MET:HB3	2.46	0.45
1:L:98:ALA:O	1:L:101:GLY:N	2.50	0.45
1:D:111:ARG:HG3	1:D:159:THR:O	2.17	0.45
1:E:111:ARG:HG3	1:E:159:THR:O	2.17	0.45
1:B:266:ILE:HG22	1:B:267:ALA:N	2.30	0.45
1:D:268:ILE:HD12	1:D:277:ARG:O	2.17	0.45
1:F:268:ILE:HD12	1:F:277:ARG:O	2.16	0.45
1:E:138:GLU:OE1	2:E:1003:FSW:O3	2.35	0.45
1:E:179:TRP:CZ2	1:E:231:ILE:HD11	2.51	0.44
1:I:111:ARG:HG3	1:I:159:THR:O	2.17	0.44
1:D:190:ARG:HD2	1:D:202:LEU:HD23	1.99	0.44
1:G:7:GLN:NE2	1:J:134:ASN:HD21	2.16	0.44
1:G:7:GLN:HE22	1:J:134:ASN:HD21	1.64	0.44
1:G:11:PHE:HB2	1:J:212:ARG:NH1	2.33	0.44
1:F:189:GLN:OE1	2:F:1004:FSW:O4	2.36	0.44
1:D:61:PRO:HB3	1:D:111:ARG:HA	1.99	0.44
1:H:111:ARG:HG3	1:H:159:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:TYR:OH	3:G:1103:HOH:O	2.20	0.43
1:F:163:VAL:HA	1:F:177:ARG:O	2.17	0.43
1:G:305:ARG:HD3	3:G:1217:HOH:O	2.17	0.43
1:H:278:LEU:HB2	1:H:292:TRP:HB3	2.01	0.43
1:G:277:ARG:HD3	1:G:293:THR:HG22	2.01	0.43
1:H:189:GLN:NE2	2:H:1004:FSW:O4	2.49	0.43
1:K:117:LEU:HD21	1:K:126:ARG:HG2	1.99	0.43
1:L:2:SER:N	3:L:1105:HOH:O	2.50	0.43
1:L:89:ASP:O	1:L:91:GLY:N	2.51	0.43
1:I:277:ARG:CD	1:I:293:THR:HG22	2.49	0.43
1:D:40:TYR:HA	1:D:43:GLY:O	2.20	0.42
1:J:27:TYR:CD2	1:J:27:TYR:N	2.87	0.42
1:L:266:ILE:HG22	1:L:267:ALA:N	2.35	0.42
1:B:30:ASP:OD1	1:B:30:ASP:C	2.58	0.42
1:C:191:ALA:HB3	1:C:199:TYR:CD2	2.55	0.42
1:L:307:LEU:O	1:L:310:ALA:HB3	2.18	0.42
1:L:20:SER:OG	1:L:68:GLU:OE1	2.27	0.42
1:L:85:GLU:OE2	2:L:1002:FSW:O4	2.37	0.42
1:B:205:ILE:HG22	1:B:251:TYR:CE2	2.55	0.42
1:E:175:SER:OG	1:E:193:ASP:OD1	2.35	0.42
1:K:269:ILE:HG13	1:K:277:ARG:HB2	2.00	0.42
1:G:111:ARG:HD2	3:G:1127:HOH:O	2.19	0.42
1:H:291:GLU:OE1	2:H:1006:FSW:O3	2.38	0.42
1:A:149:GLY:HA2	2:A:1003:FSW:C8	2.50	0.41
1:E:212:ARG:NH1	1:H:11:PHE:HB2	2.35	0.41
1:D:126:ARG:HD3	1:D:140:MET:HB3	2.02	0.41
1:G:193:ASP:HB2	1:G:196:THR:CG2	2.51	0.41
1:C:83:LEU:HB3	1:C:99:LEU:HD21	2.01	0.41
1:E:291:GLU:OE1	2:E:1006:FSW:O3	2.39	0.41
1:E:2:SER:CB	1:H:157:PRO:HG2	2.50	0.41
1:K:18:VAL:HG13	1:K:64:ALA:HB1	2.03	0.41
1:H:39:LEU:HD13	1:H:41:GLU:HG2	2.03	0.41
1:L:228:TYR:N	1:L:228:TYR:CD1	2.88	0.41
1:A:277:ARG:CD	1:A:293:THR:HG22	2.51	0.40
1:L:279:TYR:CE1	1:L:291:GLU:HG3	2.56	0.40
1:D:189:GLN:OE1	2:D:1004:FSW:O4	2.40	0.40
1:F:192:TYR:CE2	1:F:197:GLY:HA2	2.55	0.40
1:D:190:ARG:CD	1:D:202:LEU:HD23	2.52	0.40
1:K:114:SER:HA	1:K:127:ILE:HD13	2.02	0.40
1:A:61:PRO:HG3	1:A:110:SER:O	2.22	0.40
1:C:37:GLU:OE1	2:C:1001:FSW:O4	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:TRP:CZ2	1:F:231:ILE:HD11	2.56	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	308/311 (99%)	302 (98%)	6 (2%)	0	100	100
1	B	308/311 (99%)	299 (97%)	8 (3%)	1 (0%)	46	57
1	C	308/311 (99%)	298 (97%)	9 (3%)	1 (0%)	46	57
1	D	308/311 (99%)	293 (95%)	14 (4%)	1 (0%)	46	57
1	E	308/311 (99%)	297 (96%)	9 (3%)	2 (1%)	30	36
1	F	308/311 (99%)	296 (96%)	11 (4%)	1 (0%)	46	57
1	G	308/311 (99%)	301 (98%)	7 (2%)	0	100	100
1	H	308/311 (99%)	296 (96%)	11 (4%)	1 (0%)	46	57
1	I	308/311 (99%)	296 (96%)	12 (4%)	0	100	100
1	J	308/311 (99%)	290 (94%)	14 (4%)	4 (1%)	15	15
1	K	308/311 (99%)	283 (92%)	23 (8%)	2 (1%)	30	36
1	L	308/311 (99%)	281 (91%)	25 (8%)	2 (1%)	30	36
All	All	3696/3732 (99%)	3532 (96%)	149 (4%)	15 (0%)	39	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	90	SER
1	B	46	ASN
1	J	42	SER

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Mol	Chain	Res	Type
1	J	46	ASN
1	D	46	ASN
1	E	46	ASN
1	H	46	ASN
1	K	46	ASN
1	C	46	ASN
1	J	308	PRO
1	K	225	SER
1	L	286	VAL
1	F	46	ASN
1	J	92	SER
1	E	286	VAL

### 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	251/252 (100%)	247 (98%)	4 (2%)	70	84
1	B	251/252 (100%)	250 (100%)	1 (0%)	93	97
1	C	251/252 (100%)	250 (100%)	1 (0%)	93	97
1	D	251/252 (100%)	249 (99%)	2 (1%)	86	94
1	E	251/252 (100%)	248 (99%)	3 (1%)	78	89
1	F	251/252 (100%)	249 (99%)	2 (1%)	86	94
1	G	251/252 (100%)	248 (99%)	3 (1%)	78	89
1	H	251/252 (100%)	249 (99%)	2 (1%)	86	94
1	I	251/252 (100%)	250 (100%)	1 (0%)	93	97
1	J	251/252 (100%)	247 (98%)	4 (2%)	70	84
1	K	251/252 (100%)	245 (98%)	6 (2%)	57	74
1	L	251/252 (100%)	245 (98%)	6 (2%)	57	74
All	All	3012/3024 (100%)	2977 (99%)	35 (1%)	78	89

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	92	SER
1	A	199	TYR
1	A	266	ILE
1	B	258	THR
1	C	62	LEU
1	D	39	LEU
1	D	90	SER
1	E	62	LEU
1	E	182	THR
1	E	201	GLU
1	F	196	THR
1	F	258	THR
1	G	90	SER
1	G	120	THR
1	G	199	TYR
1	H	24	LEU
1	H	266	ILE
1	I	42	SER
1	J	42	SER
1	J	50	LYS
1	J	182	THR
1	J	201	GLU
1	K	2	SER
1	K	90	SER
1	K	150	THR
1	K	164	THR
1	K	182	THR
1	K	287	SER
1	L	92	SER
1	L	164	THR
1	L	182	THR
1	L	200	LYS
1	L	225	SER
1	L	226	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	242	GLN
1	B	301	GLN
1	D	121	ASN
1	F	124	GLN

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Mol	Chain	Res	Type
1	G	7	GLN
1	G	189	GLN
1	H	189	GLN
1	J	249	GLN
1	K	124	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

72 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	$\# Z  > 2$
2	FSW	A	1001	-	10,13,13	0.90	1 (10%)	13,18,18	2.75	5 (38%)
2	FSW	A	1002	-	10,13,13	0.85	0	13,18,18	2.44	6 (46%)
2	FSW	A	1003	-	10,13,13	0.92	1 (10%)	13,18,18	2.39	4 (30%)
2	FSW	A	1004	-	10,13,13	1.08	2 (20%)	13,18,18	1.98	1 (7%)
2	FSW	A	1005	-	10,13,13	1.15	1 (10%)	13,18,18	2.54	6 (46%)
2	FSW	A	1006	-	10,13,13	1.08	2 (20%)	13,18,18	2.34	2 (15%)
2	FSW	B	1001	-	10,13,13	1.31	1 (10%)	13,18,18	3.03	5 (38%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FSW	B	1002	-	10,13,13	0.52	0	13,18,18	2.12	2 (15%)
2	FSW	B	1003	-	10,13,13	1.10	2 (20%)	13,18,18	2.30	4 (30%)
2	FSW	B	1004	-	10,13,13	1.09	1 (10%)	13,18,18	0.89	1 (7%)
2	FSW	B	1005	-	10,13,13	1.19	2 (20%)	13,18,18	2.51	5 (38%)
2	FSW	B	1006	-	10,13,13	1.28	1 (10%)	13,18,18	2.77	4 (30%)
2	FSW	C	1001	-	10,13,13	1.19	1 (10%)	13,18,18	2.99	6 (46%)
2	FSW	C	1002	-	10,13,13	0.86	1 (10%)	13,18,18	0.74	0
2	FSW	C	1003	-	10,13,13	0.91	0	13,18,18	2.19	2 (15%)
2	FSW	C	1004	-	10,13,13	0.87	1 (10%)	13,18,18	0.49	0
2	FSW	C	1005	-	10,13,13	1.59	1 (10%)	13,18,18	3.79	7 (53%)
2	FSW	C	1006	-	10,13,13	0.65	0	13,18,18	0.74	0
2	FSW	D	1001	-	10,13,13	1.73	2 (20%)	13,18,18	3.18	7 (53%)
2	FSW	D	1002	-	10,13,13	1.67	1 (10%)	13,18,18	2.12	3 (23%)
2	FSW	D	1003	-	10,13,13	0.95	1 (10%)	13,18,18	2.19	5 (38%)
2	FSW	D	1004	-	10,13,13	1.03	1 (10%)	13,18,18	2.39	2 (15%)
2	FSW	D	1005	-	10,13,13	1.21	1 (10%)	13,18,18	2.28	6 (46%)
2	FSW	D	1006	-	10,13,13	0.94	1 (10%)	13,18,18	2.67	5 (38%)
2	FSW	E	1001	-	10,13,13	0.65	0	13,18,18	0.75	0
2	FSW	E	1002	-	10,13,13	1.33	2 (20%)	13,18,18	2.27	3 (23%)
2	FSW	E	1003	-	10,13,13	0.81	0	13,18,18	2.17	3 (23%)
2	FSW	E	1004	-	10,13,13	0.77	0	13,18,18	2.62	4 (30%)
2	FSW	E	1005	-	10,13,13	1.03	1 (10%)	13,18,18	1.94	5 (38%)
2	FSW	E	1006	-	10,13,13	0.64	0	13,18,18	0.75	0
2	FSW	F	1001	-	10,13,13	0.64	0	13,18,18	0.74	0
2	FSW	F	1002	-	10,13,13	0.90	1 (10%)	13,18,18	2.31	3 (23%)
2	FSW	F	1003	-	10,13,13	0.62	0	13,18,18	2.24	2 (15%)
2	FSW	F	1004	-	10,13,13	0.92	1 (10%)	13,18,18	2.44	4 (30%)
2	FSW	F	1005	-	10,13,13	1.30	1 (10%)	13,18,18	1.29	1 (7%)
2	FSW	F	1006	-	10,13,13	0.65	0	13,18,18	0.75	0
2	FSW	G	1001	-	10,13,13	0.64	0	13,18,18	0.74	0
2	FSW	G	1002	-	10,13,13	0.73	0	13,18,18	1.04	1 (7%)
2	FSW	G	1003	-	10,13,13	1.00	1 (10%)	13,18,18	0.95	1 (7%)
2	FSW	G	1004	-	10,13,13	1.04	1 (10%)	13,18,18	2.48	4 (30%)
2	FSW	G	1005	-	10,13,13	1.29	2 (20%)	13,18,18	3.16	6 (46%)
2	FSW	G	1006	-	10,13,13	0.64	0	13,18,18	0.75	0
2	FSW	H	1001	-	10,13,13	1.11	1 (10%)	13,18,18	3.07	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FSW	H	1002	-	10,13,13	0.65	0	13,18,18	0.75	0
2	FSW	H	1003	-	10,13,13	1.22	2 (20%)	13,18,18	2.48	5 (38%)
2	FSW	H	1004	-	10,13,13	1.12	1 (10%)	13,18,18	1.23	1 (7%)
2	FSW	H	1005	-	10,13,13	1.39	1 (10%)	13,18,18	3.00	4 (30%)
2	FSW	H	1006	-	10,13,13	0.63	0	13,18,18	0.74	0
2	FSW	I	1001	-	10,13,13	1.10	1 (10%)	13,18,18	2.67	4 (30%)
2	FSW	I	1002	-	10,13,13	1.20	1 (10%)	13,18,18	3.09	5 (38%)
2	FSW	I	1003	-	10,13,13	0.83	0	13,18,18	2.32	3 (23%)
2	FSW	I	1004	-	10,13,13	0.99	1 (10%)	13,18,18	2.48	3 (23%)
2	FSW	I	1005	-	10,13,13	0.64	0	13,18,18	0.74	0
2	FSW	I	1006	-	10,13,13	0.94	1 (10%)	13,18,18	2.39	3 (23%)
2	FSW	J	1001	-	10,13,13	1.50	1 (10%)	13,18,18	2.96	5 (38%)
2	FSW	J	1002	-	10,13,13	0.93	1 (10%)	13,18,18	1.28	1 (7%)
2	FSW	J	1003	-	10,13,13	0.97	1 (10%)	13,18,18	2.56	4 (30%)
2	FSW	J	1004	-	10,13,13	1.05	1 (10%)	13,18,18	2.44	4 (30%)
2	FSW	J	1005	-	10,13,13	0.63	0	13,18,18	0.74	0
2	FSW	J	1006	-	10,13,13	0.64	0	13,18,18	0.75	0
2	FSW	K	1001	-	10,13,13	0.65	0	13,18,18	0.74	0
2	FSW	K	1002	-	10,13,13	0.69	0	13,18,18	1.60	4 (30%)
2	FSW	K	1003	-	10,13,13	1.27	1 (10%)	13,18,18	2.67	7 (53%)
2	FSW	K	1004	-	10,13,13	1.02	1 (10%)	13,18,18	2.33	3 (23%)
2	FSW	K	1005	-	10,13,13	0.98	1 (10%)	13,18,18	1.51	3 (23%)
2	FSW	K	1006	-	10,13,13	1.09	1 (10%)	13,18,18	1.29	1 (7%)
2	FSW	L	1001	-	10,13,13	0.63	0	13,18,18	0.70	0
2	FSW	L	1002	-	10,13,13	0.69	0	13,18,18	1.58	3 (23%)
2	FSW	L	1003	-	10,13,13	1.32	1 (10%)	13,18,18	1.62	3 (23%)
2	FSW	L	1004	-	10,13,13	0.65	0	13,18,18	0.74	0
2	FSW	L	1005	-	10,13,13	0.65	0	13,18,18	0.75	0
2	FSW	L	1006	-	10,13,13	1.17	1 (10%)	13,18,18	1.93	5 (38%)

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	FSW	A	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1002	-	-	0/2/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FSW	A	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1002	-	-	0/2/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FSW	H	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	J	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	J	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	J	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	J	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	J	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	J	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1006	-	-	0/2/24/24	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FSW	O1-C1	2.04	1.43	1.40
2	D	1001	FSW	O5-C1	2.05	1.47	1.41
2	F	1004	FSW	O1-C1	2.06	1.43	1.40
2	B	1003	FSW	O5-C1	2.07	1.47	1.41
2	H	1003	FSW	O5-C1	2.08	1.47	1.41
2	C	1004	FSW	O1-C1	2.09	1.43	1.40
2	J	1003	FSW	O1-C1	2.10	1.43	1.40
2	D	1003	FSW	O1-C1	2.12	1.43	1.40
2	A	1006	FSW	O5-C1	2.15	1.47	1.41
2	A	1004	FSW	O1-C1	2.18	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1004	FSW	O1-C1	2.20	1.43	1.40
2	E	1002	FSW	O5-C1	2.21	1.47	1.41
2	F	1002	FSW	O1-C1	2.23	1.44	1.40
2	K	1005	FSW	O1-C1	2.24	1.44	1.40
2	H	1004	FSW	O1-C1	2.25	1.44	1.40
2	A	1004	FSW	O5-C1	2.26	1.47	1.41
2	B	1005	FSW	O5-C1	2.26	1.47	1.41
2	J	1004	FSW	O1-C1	2.26	1.44	1.40
2	D	1004	FSW	O1-C1	2.26	1.44	1.40
2	G	1005	FSW	O5-C1	2.29	1.47	1.41
2	A	1003	FSW	O1-C1	2.32	1.44	1.40
2	C	1002	FSW	O1-C1	2.32	1.44	1.40
2	A	1006	FSW	O1-C1	2.35	1.44	1.40
2	B	1003	FSW	O1-C1	2.37	1.44	1.40
2	K	1004	FSW	O1-C1	2.40	1.44	1.40
2	J	1002	FSW	O1-C1	2.41	1.44	1.40
2	D	1006	FSW	O1-C1	2.50	1.44	1.40
2	I	1006	FSW	O1-C1	2.51	1.44	1.40
2	B	1005	FSW	O1-C1	2.52	1.44	1.40
2	H	1001	FSW	O1-C1	2.58	1.44	1.40
2	H	1003	FSW	O1-C1	2.61	1.44	1.40
2	E	1005	FSW	O1-C1	2.63	1.44	1.40
2	G	1004	FSW	O1-C1	2.69	1.44	1.40
2	G	1003	FSW	O1-C1	2.71	1.44	1.40
2	C	1001	FSW	O1-C1	2.74	1.44	1.40
2	D	1005	FSW	O1-C1	2.89	1.45	1.40
2	I	1001	FSW	O1-C1	2.95	1.45	1.40
2	B	1004	FSW	O1-C1	2.99	1.45	1.40
2	K	1006	FSW	O1-C1	3.06	1.45	1.40
2	A	1005	FSW	O1-C1	3.10	1.45	1.40
2	G	1005	FSW	O1-C1	3.11	1.45	1.40
2	L	1006	FSW	O1-C1	3.12	1.45	1.40
2	E	1002	FSW	O1-C1	3.17	1.45	1.40
2	K	1003	FSW	O1-C1	3.18	1.45	1.40
2	B	1006	FSW	O1-C1	3.19	1.45	1.40
2	L	1003	FSW	O1-C1	3.22	1.45	1.40
2	I	1002	FSW	O1-C1	3.42	1.46	1.40
2	B	1001	FSW	O1-C1	3.44	1.46	1.40
2	F	1005	FSW	O1-C1	3.50	1.46	1.40
2	H	1005	FSW	O1-C1	3.59	1.46	1.40
2	J	1001	FSW	O1-C1	3.59	1.46	1.40
2	C	1005	FSW	O1-C1	4.04	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1002	FSW	O1-C1	4.88	1.48	1.40
2	D	1001	FSW	O1-C1	4.90	1.48	1.40

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1005	FSW	O4-C4-C3	-9.29	89.41	110.36
2	C	1005	FSW	O4-C4-C3	-7.26	93.99	110.36
2	C	1005	FSW	O4-C4-C5	-5.34	97.49	109.67
2	E	1005	FSW	O4-C4-C3	-4.03	101.26	110.36
2	D	1005	FSW	O5-C5-C4	-2.87	104.62	109.58
2	L	1002	FSW	O5-C5-C4	-2.71	104.89	109.58
2	B	1003	FSW	O5-C5-C4	-2.60	105.07	109.58
2	K	1002	FSW	C3-C4-C5	-2.60	105.78	109.66
2	K	1003	FSW	O5-C5-C4	-2.50	105.25	109.58
2	F	1004	FSW	O5-C5-C4	-2.46	105.33	109.58
2	D	1003	FSW	O5-C5-C4	-2.34	105.53	109.58
2	K	1002	FSW	O5-C5-C4	-2.30	105.60	109.58
2	L	1003	FSW	O5-C5-C4	-2.16	105.83	109.58
2	J	1004	FSW	O5-C5-C4	-2.14	105.88	109.58
2	D	1001	FSW	O5-C5-C4	-2.12	105.90	109.58
2	K	1002	FSW	O5-C1-O1	-2.11	105.83	110.92
2	A	1002	FSW	O5-C5-C4	-2.07	105.99	109.58
2	A	1002	FSW	O3-C3-C4	2.00	114.87	110.36
2	A	1003	FSW	O3-C3-C4	2.01	114.88	110.36
2	H	1003	FSW	O3-C3-C2	2.01	113.70	108.44
2	A	1002	FSW	O5-C1-C2	2.03	114.40	109.87
2	G	1003	FSW	O1-C1-C2	2.03	111.81	108.11
2	E	1005	FSW	C7-O1-C1	2.03	116.63	113.32
2	A	1005	FSW	O5-C5-C6	2.04	110.90	106.57
2	G	1004	FSW	O5-C5-C6	2.05	110.92	106.57
2	B	1001	FSW	C6-C5-C4	2.05	117.00	113.02
2	D	1005	FSW	O3-C3-C2	2.05	113.81	108.44
2	G	1005	FSW	C3-C4-C5	2.06	112.73	109.66
2	J	1003	FSW	O3-C3-C4	2.08	115.06	110.36
2	H	1003	FSW	C1-O5-C5	2.08	117.57	113.76
2	A	1001	FSW	O5-C5-C6	2.08	110.99	106.57
2	A	1003	FSW	O3-C3-C2	2.09	113.89	108.44
2	E	1005	FSW	C3-C4-C5	2.11	112.81	109.66
2	C	1005	FSW	O3-C3-C2	2.11	113.96	108.44
2	D	1005	FSW	C3-C4-C5	2.12	112.82	109.66
2	G	1004	FSW	O4-C4-C3	2.15	115.21	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1005	FSW	O3-C3-C4	2.15	115.22	110.36
2	E	1004	FSW	O5-C5-C6	2.18	111.20	106.57
2	E	1003	FSW	O5-C5-C6	2.19	111.21	106.57
2	D	1005	FSW	O3-C3-C4	2.20	115.33	110.36
2	J	1001	FSW	C7-O1-C1	2.22	116.94	113.32
2	H	1001	FSW	O3-C3-C2	2.23	114.28	108.44
2	B	1005	FSW	C1-O5-C5	2.24	117.86	113.76
2	B	1004	FSW	O5-C1-O1	2.25	116.35	110.92
2	B	1005	FSW	O5-C5-C6	2.25	111.35	106.57
2	A	1005	FSW	C3-C4-C5	2.27	113.04	109.66
2	B	1006	FSW	O3-C3-C2	2.27	114.39	108.44
2	D	1002	FSW	C7-O1-C1	2.29	117.05	113.32
2	A	1003	FSW	O4-C4-C5	2.29	114.89	109.67
2	H	1005	FSW	O4-C4-C5	2.30	114.92	109.67
2	B	1001	FSW	C7-O1-C1	2.30	117.07	113.32
2	I	1002	FSW	C7-O1-C1	2.32	117.09	113.32
2	L	1003	FSW	C1-O5-C5	2.33	118.02	113.76
2	I	1003	FSW	O3-C3-C2	2.34	114.55	108.44
2	H	1004	FSW	O4-C4-C5	2.34	115.00	109.67
2	K	1005	FSW	O4-C4-C3	2.35	115.65	110.36
2	B	1003	FSW	O5-C5-C6	2.35	111.56	106.57
2	I	1004	FSW	O4-C4-C3	2.36	115.68	110.36
2	A	1006	FSW	O4-C4-C3	2.37	115.70	110.36
2	G	1002	FSW	O3-C3-C2	2.38	114.65	108.44
2	H	1005	FSW	C3-C4-C5	2.44	113.30	109.66
2	L	1002	FSW	O1-C1-C2	2.44	112.57	108.11
2	D	1006	FSW	C3-C4-C5	2.48	113.37	109.66
2	L	1002	FSW	O5-C5-C6	2.50	111.87	106.57
2	J	1003	FSW	C1-O5-C5	2.52	118.37	113.76
2	J	1002	FSW	O3-C3-C2	2.52	115.04	108.44
2	F	1004	FSW	O5-C5-C6	2.53	111.93	106.57
2	K	1003	FSW	C7-O1-C1	2.55	117.47	113.32
2	C	1001	FSW	O3-C3-C2	2.55	115.10	108.44
2	E	1004	FSW	O3-C3-C2	2.56	115.14	108.44
2	E	1005	FSW	O3-C3-C2	2.57	115.15	108.44
2	C	1005	FSW	C7-O1-C1	2.57	117.50	113.32
2	K	1004	FSW	C3-C4-C5	2.57	113.50	109.66
2	B	1005	FSW	O3-C3-C2	2.58	115.19	108.44
2	L	1006	FSW	O5-C5-C4	2.58	114.05	109.58
2	I	1003	FSW	O4-C4-C3	2.60	116.23	110.36
2	J	1004	FSW	O5-C5-C6	2.64	112.16	106.57
2	K	1003	FSW	O3-C3-C2	2.64	115.34	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	FSW	O3-C3-C2	2.64	115.34	108.44
2	I	1001	FSW	O3-C3-C2	2.65	115.38	108.44
2	L	1003	FSW	C7-O1-C1	2.68	117.69	113.32
2	K	1003	FSW	O5-C5-C6	2.71	112.31	106.57
2	C	1001	FSW	O5-C5-C6	2.72	112.35	106.57
2	I	1006	FSW	O4-C4-C3	2.74	116.55	110.36
2	G	1005	FSW	O5-C5-C6	2.76	112.42	106.57
2	E	1005	FSW	O4-C4-C5	2.76	115.96	109.67
2	D	1003	FSW	O5-C5-C6	2.76	112.43	106.57
2	A	1005	FSW	O4-C4-C5	2.77	115.99	109.67
2	C	1001	FSW	C1-O5-C5	2.80	118.88	113.76
2	I	1002	FSW	O3-C3-C2	2.81	115.80	108.44
2	G	1004	FSW	O3-C3-C2	2.82	115.81	108.44
2	L	1006	FSW	O4-C4-C5	2.83	116.13	109.67
2	F	1002	FSW	O3-C3-C2	2.89	116.00	108.44
2	I	1004	FSW	O3-C3-C2	2.89	116.00	108.44
2	C	1005	FSW	C1-O5-C5	2.90	119.07	113.76
2	G	1005	FSW	O5-C1-C2	2.93	116.41	109.87
2	L	1006	FSW	C7-O1-C1	2.96	118.14	113.32
2	A	1005	FSW	O3-C3-C4	3.00	117.14	110.36
2	F	1003	FSW	O4-C4-C3	3.04	117.21	110.36
2	D	1006	FSW	O3-C3-C2	3.09	116.52	108.44
2	K	1002	FSW	O5-C1-C2	3.09	116.78	109.87
2	B	1001	FSW	O1-C1-C2	3.11	113.78	108.11
2	H	1005	FSW	C7-O1-C1	3.11	118.38	113.32
2	K	1006	FSW	O1-C1-C2	3.16	113.87	108.11
2	A	1001	FSW	O1-C1-C2	3.16	113.88	108.11
2	D	1003	FSW	C3-C4-C5	3.20	114.44	109.66
2	D	1006	FSW	O1-C1-C2	3.20	113.95	108.11
2	L	1006	FSW	C1-O5-C5	3.22	119.65	113.76
2	D	1001	FSW	C7-O1-C1	3.26	118.63	113.32
2	A	1001	FSW	C7-O1-C1	3.26	118.63	113.32
2	L	1006	FSW	O1-C1-C2	3.27	114.07	108.11
2	C	1001	FSW	O1-C1-C2	3.27	114.08	108.11
2	D	1001	FSW	O1-C1-C2	3.29	114.12	108.11
2	D	1002	FSW	O3-C3-C2	3.31	117.11	108.44
2	B	1006	FSW	O4-C4-C3	3.34	117.89	110.36
2	D	1004	FSW	O4-C4-C3	3.35	117.91	110.36
2	E	1002	FSW	O3-C3-C2	3.36	117.24	108.44
2	K	1005	FSW	O1-C1-C2	3.38	114.27	108.11
2	C	1003	FSW	O4-C4-C3	3.39	118.01	110.36
2	C	1005	FSW	O1-C1-C2	3.39	114.30	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1003	FSW	O4-C4-C3	3.40	118.02	110.36
2	F	1005	FSW	O1-C1-C2	3.40	114.32	108.11
2	D	1005	FSW	O4-C4-C5	3.40	117.42	109.67
2	A	1005	FSW	O1-C1-C2	3.41	114.34	108.11
2	I	1006	FSW	O1-C1-C2	3.42	114.36	108.11
2	H	1003	FSW	O5-C5-C6	3.49	113.98	106.57
2	G	1005	FSW	C7-O1-C1	3.50	119.02	113.32
2	A	1002	FSW	O4-C4-C3	3.55	118.37	110.36
2	I	1001	FSW	O1-C1-C2	3.56	114.61	108.11
2	H	1003	FSW	O4-C4-C3	3.57	118.41	110.36
2	B	1006	FSW	O1-C1-C2	3.65	114.77	108.11
2	K	1003	FSW	C3-C4-C5	3.65	115.11	109.66
2	E	1002	FSW	O4-C4-C3	3.72	118.75	110.36
2	A	1001	FSW	O4-C4-C3	3.75	118.82	110.36
2	D	1001	FSW	O3-C3-C2	3.82	118.44	108.44
2	B	1003	FSW	O4-C4-C3	3.87	119.08	110.36
2	D	1003	FSW	O4-C4-C5	3.87	118.50	109.67
2	B	1005	FSW	O4-C4-C3	3.97	119.31	110.36
2	D	1003	FSW	O4-C4-C3	4.04	119.46	110.36
2	J	1001	FSW	O3-C3-C2	4.13	119.26	108.44
2	D	1001	FSW	O5-C5-C6	4.14	115.36	106.57
2	B	1002	FSW	O4-C4-C3	4.17	119.77	110.36
2	J	1001	FSW	O1-C1-C2	4.19	115.76	108.11
2	K	1003	FSW	O4-C4-C3	4.22	119.87	110.36
2	G	1005	FSW	C1-O5-C5	4.25	121.54	113.76
2	E	1004	FSW	O4-C4-C3	4.41	120.30	110.36
2	B	1001	FSW	O4-C4-C3	4.48	120.45	110.36
2	F	1002	FSW	O4-C4-C5	4.48	119.88	109.67
2	D	1006	FSW	O4-C4-C3	4.48	120.46	110.36
2	I	1002	FSW	O4-C4-C3	4.67	120.89	110.36
2	J	1001	FSW	O4-C4-C5	4.84	120.71	109.67
2	D	1005	FSW	O4-C4-C3	4.85	121.30	110.36
2	J	1004	FSW	O4-C4-C3	4.87	121.34	110.36
2	F	1004	FSW	O4-C4-C3	4.87	121.35	110.36
2	C	1001	FSW	O4-C4-C3	5.10	121.86	110.36
2	K	1004	FSW	O4-C4-C5	5.14	121.40	109.67
2	B	1002	FSW	O4-C4-C5	5.15	121.41	109.67
2	D	1001	FSW	O4-C4-C3	5.18	122.04	110.36
2	J	1003	FSW	O4-C4-C5	5.23	121.60	109.67
2	H	1001	FSW	O4-C4-C5	5.29	121.73	109.67
2	K	1004	FSW	O4-C4-C3	5.35	122.42	110.36
2	F	1002	FSW	O4-C4-C3	5.40	122.53	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1003	FSW	O4-C4-C5	5.47	122.14	109.67
2	E	1002	FSW	O4-C4-C5	5.53	122.29	109.67
2	I	1001	FSW	O4-C4-C5	5.54	122.30	109.67
2	H	1001	FSW	O1-C1-C2	5.59	118.31	108.11
2	A	1002	FSW	O4-C4-C5	5.60	122.45	109.67
2	B	1003	FSW	O4-C4-C5	5.67	122.59	109.67
2	E	1003	FSW	O4-C4-C5	5.67	122.59	109.67
2	F	1004	FSW	O4-C4-C5	5.75	122.77	109.67
2	D	1006	FSW	O4-C4-C5	5.89	123.11	109.67
2	I	1001	FSW	O4-C4-C3	5.93	123.72	110.36
2	D	1002	FSW	O1-C1-C2	5.97	119.01	108.11
2	J	1003	FSW	O4-C4-C3	6.03	123.96	110.36
2	A	1004	FSW	O4-C4-C5	6.05	123.46	109.67
2	I	1002	FSW	O1-C1-C2	6.08	119.21	108.11
2	H	1003	FSW	O4-C4-C5	6.08	123.54	109.67
2	J	1004	FSW	O4-C4-C5	6.13	123.64	109.67
2	A	1005	FSW	O4-C4-C3	6.26	124.47	110.36
2	B	1005	FSW	O4-C4-C5	6.35	124.14	109.67
2	F	1003	FSW	O4-C4-C5	6.35	124.16	109.67
2	C	1003	FSW	O4-C4-C5	6.38	124.21	109.67
2	I	1002	FSW	O4-C4-C5	6.54	124.59	109.67
2	J	1001	FSW	O4-C4-C3	6.60	125.24	110.36
2	D	1001	FSW	O4-C4-C5	6.60	124.72	109.67
2	I	1006	FSW	O4-C4-C5	6.63	124.78	109.67
2	D	1004	FSW	O4-C4-C5	6.84	125.27	109.67
2	E	1004	FSW	O4-C4-C5	6.89	125.38	109.67
2	H	1001	FSW	O4-C4-C3	6.90	125.92	110.36
2	A	1001	FSW	O4-C4-C5	6.93	125.48	109.67
2	C	1001	FSW	O4-C4-C5	6.99	125.61	109.67
2	I	1003	FSW	O4-C4-C5	7.01	125.67	109.67
2	I	1004	FSW	O4-C4-C5	7.33	126.39	109.67
2	A	1003	FSW	O4-C4-C3	7.36	126.97	110.36
2	A	1006	FSW	O4-C4-C5	7.52	126.82	109.67
2	G	1004	FSW	O4-C4-C5	7.55	126.88	109.67
2	B	1006	FSW	O4-C4-C5	7.91	127.70	109.67
2	G	1005	FSW	O4-C4-C5	8.28	128.54	109.67
2	B	1001	FSW	O4-C4-C5	8.33	128.66	109.67
2	C	1005	FSW	C3-C4-C5	8.38	122.18	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	FSW	1	0
2	A	1004	FSW	1	0
2	C	1001	FSW	1	0
2	C	1002	FSW	1	0
2	C	1003	FSW	1	0
2	C	1006	FSW	1	0
2	D	1004	FSW	1	0
2	E	1003	FSW	1	0
2	E	1006	FSW	1	0
2	F	1004	FSW	1	0
2	F	1006	FSW	1	0
2	G	1003	FSW	1	0
2	G	1005	FSW	1	0
2	H	1002	FSW	2	0
2	H	1004	FSW	1	0
2	H	1006	FSW	1	0
2	L	1001	FSW	4	0
2	L	1002	FSW	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	310/311 (99%)	-0.28	2 (0%) 90 93	20, 29, 46, 79	0
1	B	310/311 (99%)	-0.32	0 100 100	21, 31, 49, 82	0
1	C	310/311 (99%)	-0.22	1 (0%) 94 96	24, 37, 55, 80	0
1	D	310/311 (99%)	-0.03	3 (0%) 84 88	23, 36, 60, 82	0
1	E	310/311 (99%)	-0.11	4 (1%) 79 84	24, 37, 59, 79	0
1	F	310/311 (99%)	0.04	9 (2%) 55 64	24, 41, 64, 84	0
1	G	310/311 (99%)	-0.15	2 (0%) 90 93	27, 40, 58, 83	0
1	H	310/311 (99%)	-0.04	4 (1%) 79 84	26, 41, 63, 84	0
1	I	310/311 (99%)	0.00	6 (1%) 70 76	25, 41, 63, 112	0
1	J	310/311 (99%)	0.13	3 (0%) 84 88	29, 46, 66, 90	0
1	K	310/311 (99%)	0.52	25 (8%) 15 21	31, 55, 81, 94	0
1	L	310/311 (99%)	0.95	54 (17%) 2 3	30, 65, 101, 123	0
All	All	3720/3732 (99%)	0.04	113 (3%) 54 63	20, 40, 74, 123	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	298	HIS	5.2
1	L	39	LEU	4.9
1	L	173	GLY	4.8
1	L	88	TYR	4.5
1	L	27	TYR	4.4
1	L	119	GLY	4.4
1	H	200	LYS	4.3
1	I	195	HIS	4.2
1	L	195	HIS	4.0
1	K	295	GLY	3.7
1	K	145	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	87	ALA	3.6
1	E	298	HIS	3.5
1	L	93	GLY	3.5
1	K	45	ALA	3.5
1	L	297	ALA	3.4
1	E	297	ALA	3.4
1	L	44	TRP	3.4
1	L	271	TRP	3.3
1	L	23	HIS	3.3
1	L	147	LYS	3.3
1	L	101	GLY	3.2
1	K	90	SER	3.2
1	K	49	ALA	3.2
1	K	91	GLY	3.2
1	L	43	GLY	3.1
1	K	195	HIS	3.1
1	K	64	ALA	3.1
1	K	294	TRP	3.0
1	K	298	HIS	3.0
1	L	70	LYS	3.0
1	K	50	LYS	2.9
1	F	172	ASP	2.9
1	L	96	ASN	2.9
1	L	17	ALA	2.9
1	L	141	TRP	2.9
1	L	168	TYR	2.9
1	L	121	ASN	2.8
1	L	218	THR	2.8
1	F	119	GLY	2.8
1	L	40	TYR	2.7
1	L	304	ARG	2.7
1	L	90	SER	2.7
1	J	195	HIS	2.7
1	L	94	TRP	2.7
1	L	71	ASN	2.7
1	L	25	ARG	2.6
1	F	297	ALA	2.6
1	L	91	GLY	2.6
1	K	70	LYS	2.6
1	L	42	SER	2.6
1	L	15	ILE	2.6
1	E	91	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	273	GLY	2.6
1	L	171	TYR	2.5
1	L	124	GLN	2.5
1	L	21	THR	2.5
1	C	200	LYS	2.5
1	H	298	HIS	2.4
1	K	119	GLY	2.4
1	L	169	THR	2.4
1	K	296	LYS	2.4
1	F	200	LYS	2.4
1	F	266	ILE	2.4
1	K	15	ILE	2.3
1	L	24	LEU	2.3
1	L	300	SER	2.3
1	F	298	HIS	2.3
1	I	101	GLY	2.3
1	E	195	HIS	2.3
1	L	217	ALA	2.3
1	L	89	ASP	2.3
1	L	301	GLN	2.3
1	J	298	HIS	2.3
1	K	65	THR	2.2
1	L	18	VAL	2.2
1	D	161	ILE	2.2
1	L	64	ALA	2.2
1	F	295	GLY	2.2
1	I	200	LYS	2.2
1	K	16	ALA	2.2
1	K	63	ALA	2.2
1	L	56	ALA	2.2
1	L	163	VAL	2.2
1	G	200	LYS	2.2
1	K	144	ASP	2.2
1	A	195	HIS	2.2
1	L	80	ASP	2.2
1	L	172	ASP	2.2
1	A	297	ALA	2.1
1	L	161	ILE	2.1
1	H	297	ALA	2.1
1	J	50	LYS	2.1
1	L	224	LYS	2.1
1	I	15	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	62	LEU	2.1
1	D	195	HIS	2.1
1	L	65	THR	2.1
1	L	294	TRP	2.1
1	F	215	ILE	2.1
1	G	298	HIS	2.1
1	K	48	THR	2.1
1	D	63	ALA	2.1
1	F	173	GLY	2.1
1	K	171	TYR	2.1
1	L	302	LEU	2.0
1	I	103	LYS	2.0
1	I	59	GLY	2.0
1	K	87	ALA	2.0
1	L	34	SER	2.0
1	L	92	SER	2.0
1	H	214	ALA	2.0
1	K	147	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FSW	B	1001	13/13	0.94	0.19	14.65	35,39,49,53	0
2	FSW	E	1006	13/13	0.89	0.24	8.48	52,62,69,76	0
2	FSW	E	1001	13/13	0.87	0.23	8.30	51,60,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FSW	C	1006	13/13	0.88	0.19	7.08	34,39,50,57	0
2	FSW	J	1001	13/13	0.83	0.29	6.94	55,67,80,83	0
2	FSW	G	1006	13/13	0.84	0.20	5.83	40,51,66,69	0
2	FSW	H	1006	13/13	0.86	0.24	5.80	44,54,70,77	0
2	FSW	I	1005	13/13	0.92	0.19	5.07	40,47,60,68	0
2	FSW	F	1006	13/13	0.86	0.26	5.03	55,65,76,77	0
2	FSW	F	1001	13/13	0.89	0.23	5.02	56,60,75,75	0
2	FSW	A	1006	13/13	0.91	0.16	4.81	28,35,50,54	0
2	FSW	J	1006	13/13	0.83	0.26	4.45	48,56,82,84	0
2	FSW	H	1001	13/13	0.93	0.22	4.28	50,57,67,69	0
2	FSW	D	1006	13/13	0.91	0.24	4.18	47,54,65,70	0
2	FSW	H	1002	13/13	0.94	0.18	3.78	43,48,52,57	0
2	FSW	I	1001	13/13	0.88	0.19	3.77	40,47,61,61	0
2	FSW	B	1006	13/13	0.91	0.18	3.71	30,41,56,60	0
2	FSW	I	1006	13/13	0.92	0.15	3.18	35,39,56,58	0
2	FSW	G	1001	13/13	0.88	0.19	3.10	50,54,73,74	0
2	FSW	C	1001	13/13	0.92	0.16	3.04	36,40,53,57	0
2	FSW	B	1005	13/13	0.94	0.14	3.02	41,46,56,59	0
2	FSW	H	1003	13/13	0.89	0.17	2.96	36,44,57,70	0
2	FSW	H	1005	13/13	0.93	0.19	2.94	51,61,70,71	0
2	FSW	C	1005	13/13	0.94	0.16	2.93	33,40,49,51	0
2	FSW	G	1005	13/13	0.91	0.20	2.65	51,57,73,80	0
2	FSW	J	1005	13/13	0.89	0.19	2.57	57,63,72,72	0
2	FSW	E	1005	13/13	0.93	0.16	2.43	47,52,60,61	0
2	FSW	F	1005	13/13	0.95	0.18	2.31	56,64,72,73	0
2	FSW	E	1003	13/13	0.96	0.13	2.05	34,39,46,61	0
2	FSW	I	1002	13/13	0.88	0.19	2.01	41,60,73,75	0
2	FSW	A	1005	13/13	0.96	0.13	1.91	33,43,52,55	0
2	FSW	D	1005	13/13	0.96	0.13	1.77	42,49,54,55	0
2	FSW	K	1002	13/13	0.76	0.23	1.65	78,91,109,185	0
2	FSW	K	1006	13/13	0.89	0.26	1.63	64,76,88,92	0
2	FSW	A	1001	13/13	0.95	0.13	1.62	30,38,52,55	0
2	FSW	K	1001	13/13	0.88	0.25	1.58	78,89,94,94	0
2	FSW	F	1003	13/13	0.94	0.15	1.56	36,39,49,50	0
2	FSW	K	1005	13/13	0.94	0.23	1.52	58,67,78,84	0
2	FSW	D	1001	13/13	0.88	0.19	1.43	50,57,69,79	0
2	FSW	L	1005	13/13	0.83	0.20	1.37	66,74,85,88	0
2	FSW	L	1001	13/13	0.59	0.39	1.35	88,110,127,130	0
2	FSW	L	1002	13/13	0.83	0.28	1.34	105,123,133,136	0
2	FSW	C	1003	13/13	0.94	0.14	1.30	34,38,51,57	0
2	FSW	D	1003	13/13	0.94	0.14	1.29	34,38,44,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FSW	D	1002	13/13	0.89	0.17	1.24	52,67,88,93	0
2	FSW	K	1003	13/13	0.89	0.18	1.06	52,57,70,80	0
2	FSW	B	1003	13/13	0.95	0.12	1.00	29,33,42,53	0
2	FSW	J	1002	13/13	0.93	0.16	0.97	47,54,60,62	0
2	FSW	A	1004	13/13	0.95	0.12	0.95	25,28,37,49	0
2	FSW	E	1002	13/13	0.96	0.12	0.54	30,37,40,44	0
2	FSW	I	1003	13/13	0.95	0.15	0.49	40,52,59,60	0
2	FSW	F	1004	13/13	0.95	0.14	0.41	37,40,44,45	0
2	FSW	A	1003	13/13	0.97	0.12	0.34	32,34,39,42	0
2	FSW	H	1004	13/13	0.94	0.15	0.18	34,36,40,42	0
2	FSW	L	1006	13/13	0.92	0.26	0.16	77,89,100,100	0
2	FSW	F	1002	13/13	0.97	0.11	-0.06	34,39,44,47	0
2	FSW	G	1003	13/13	0.96	0.12	-0.09	37,40,52,53	0
2	FSW	J	1003	13/13	0.94	0.14	-0.10	40,43,53,53	0
2	FSW	G	1004	13/13	0.96	0.11	-0.24	35,40,42,43	0
2	FSW	D	1004	13/13	0.97	0.11	-0.28	30,32,36,37	0
2	FSW	L	1004	13/13	0.95	0.13	-0.43	47,54,56,57	0
2	FSW	A	1002	13/13	0.98	0.10	-0.43	25,27,32,37	0
2	FSW	L	1003	13/13	0.88	0.17	-0.60	43,46,55,68	0
2	FSW	E	1004	13/13	0.97	0.09	-0.65	30,32,35,36	0
2	FSW	G	1002	13/13	0.97	0.10	-0.68	37,38,40,40	0
2	FSW	K	1004	13/13	0.97	0.11	-0.70	42,48,53,54	0
2	FSW	B	1004	13/13	0.97	0.10	-0.82	24,27,28,31	0
2	FSW	C	1002	13/13	0.96	0.09	-1.03	32,38,48,50	0
2	FSW	I	1004	13/13	0.96	0.11	-1.09	34,41,45,48	0
2	FSW	B	1002	13/13	0.98	0.09	-1.16	25,27,30,30	0
2	FSW	C	1004	13/13	0.98	0.10	-1.30	28,33,36,37	0
2	FSW	J	1004	13/13	0.98	0.09	-1.55	35,41,43,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.