



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2025 – 11:29 pm BST

PDB ID : 4AGI / pdb\_00004agi  
Title : Crystal Structure of Fucose binding lectin from Aspergillus Fumigatus (AFL) in complex with seleno fucoside.  
Authors : Houser, J.; Komarek, J.; Kostlanova, N.; Lahmann, M.; Cioci, G.; Varrot, A.; Imberty, A.; Wimmerova, M.  
Deposited on : 2012-01-30  
Resolution : 1.60 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

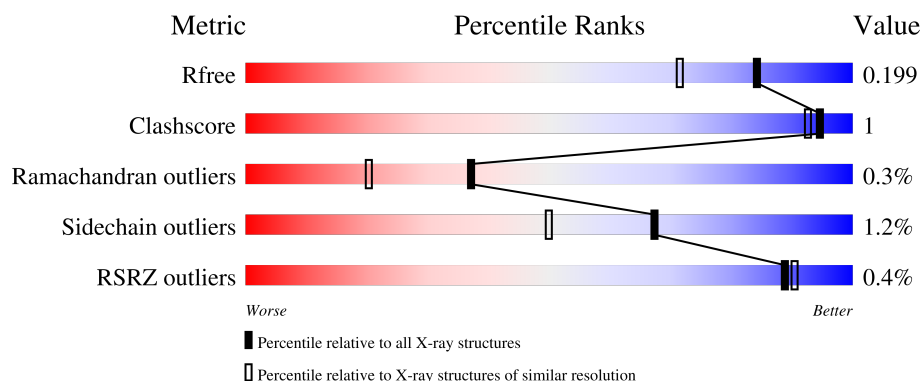
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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	315	<div> <div style="width: 96%;"></div> <div>96%</div> </div>
1	B	315	<div> <div style="width: 92%;"></div> <div>92%</div> <div style="width: 7%;"></div> <div>7%</div> </div>
1	C	315	<div> <div style="width: 94%;"></div> <div>94%</div> <div style="width: 5%;"></div> <div>5%</div> </div>
1	D	315	<div> <div style="width: 95%;"></div> <div>95%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11266 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.

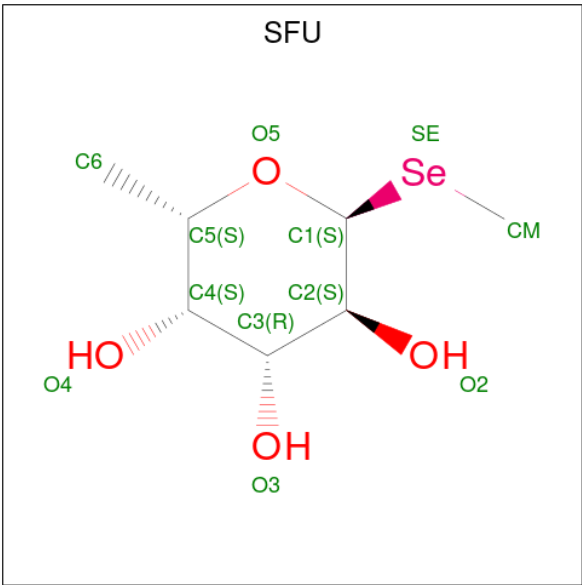
- Molecule 1 is a protein called FUCOSE-SPECIFIC LECTIN FLEA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	Se	0	2	0
			2446	1559	419	463	4	1			
1	B	314	Total	C	N	O	S	Se	0	1	0
			2436	1554	418	459	4	1			
1	C	314	Total	C	N	O	S	Se	0	1	0
			2446	1558	422	461	4	1			
1	D	314	Total	C	N	O	S	Se	0	3	0
			2465	1568	423	469	4	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	LEU	conflict	UNP Q4WW81
A	111	CSK	ARG	engineered mutation	UNP Q4WW81
B	20	SER	LEU	conflict	UNP Q4WW81
B	111	CSK	ARG	engineered mutation	UNP Q4WW81
C	20	SER	LEU	conflict	UNP Q4WW81
C	111	CSK	ARG	engineered mutation	UNP Q4WW81
D	20	SER	LEU	conflict	UNP Q4WW81
D	111	CSK	ARG	engineered mutation	UNP Q4WW81

- Molecule 2 is methyl 1-seleno-alpha-L-fucopyranoside (CCD ID: SFU) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>4</sub>Se).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	Se	0	0
			12	7	4	1		
2	A	1	Total	C	O	Se	0	0
			12	7	4	1		
2	A	1	Total	C	O	Se	0	0
			12	7	4	1		
2	A	1	Total	C	O	Se	0	0
			12	7	4	1		
2	A	1	Total	C	O	Se	0	0
			12	7	4	1		
2	A	1	Total	C	O	Se	0	0
			12	7	4	1		
2	B	1	Total	C	O	Se	0	0
			12	7	4	1		
2	B	1	Total	C	O	Se	0	0
			12	7	4	1		
2	B	1	Total	C	O	Se	0	0
			12	7	4	1		
2	B	1	Total	C	O	Se	0	0
			12	7	4	1		
2	B	1	Total	C	O	Se	0	0
			12	7	4	1		
2	C	1	Total	C	O	Se	0	0
			12	7	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 12	C 7	O 4	Se 1	0	0
2	C	1	Total 12	C 7	O 4	Se 1	0	0
2	C	1	Total 12	C 7	O 4	Se 1	0	0
2	C	1	Total 12	C 7	O 4	Se 1	0	0
2	C	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0
2	D	1	Total 12	C 7	O 4	Se 1	0	0

- Molecule 3 is water.

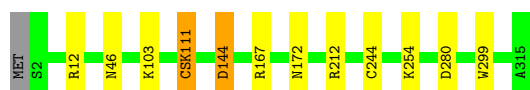
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	345	Total 345	O 345	0	0
3	B	234	Total 234	O 234	0	0
3	C	308	Total 308	O 308	0	0
3	D	274	Total 274	O 274	0	0

### 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.

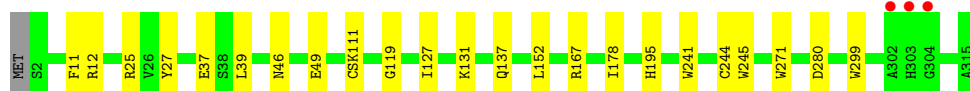
#### • Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

Chain A:  96%



#### • Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

Chain B:  92% 7%



#### • Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

Chain C:  94% 5%



#### • Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

Chain D:  95%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.69Å 79.85Å 84.39Å 91.09° 88.89° 103.00°	Depositor
Resolution (Å)	84.22 – 1.60 84.22 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (84.22-1.60) 95.8 (84.22-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.152 , 0.185 0.170 , 0.199	Depositor DCC
$R_{free}$ test set	7525 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.128 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: SFU, CSD, CSK

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	0.86	1/2506 (0.0%)	0.87	3/3416 (0.1%)
1	B	0.83	4/2490 (0.2%)	0.87	3/3395 (0.1%)
1	C	0.85	0/2503	0.88	4/3411 (0.1%)
1	D	0.82	1/2519 (0.0%)	0.87	5/3433 (0.1%)
All	All	0.84	6/10018 (0.1%)	0.87	15/13655 (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	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	TRP	CD2-CE2	5.66	1.48	1.41
1	B	245	TRP	CD2-CE2	5.37	1.47	1.41
1	B	241	TRP	CD2-CE2	5.24	1.47	1.41
1	D	241	TRP	CD2-CE2	5.12	1.47	1.41
1	B	299	TRP	CD2-CE2	5.07	1.47	1.41
1	B	271	TRP	CD2-CE2	5.04	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	C	12	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	39	LEU	CA-CB-CG	7.99	133.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	D	12	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	B	39	LEU	CA-CB-CG	6.12	129.36	115.30
1	C	186	LYS	CD-CE-NZ	6.11	125.75	111.70
1	D	126	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	25	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	39	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	201	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	25	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	12	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	144[A]	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	144[B]	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	CSK	Mainchain

## 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	2446	0	2318	4	1
1	B	2436	0	2303	7	0
1	C	2446	0	2327	8	0
1	D	2465	0	2330	4	0
2	A	84	0	70	0	0
2	B	72	0	60	1	0
2	C	72	0	60	0	0
2	D	84	0	70	0	0
3	A	345	0	0	2	1
3	B	234	0	0	2	0
3	C	308	0	0	2	0
3	D	274	0	0	1	1
All	All	11266	0	9538	23	2

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 (23) 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:C:184:ASP:OD1	1:C:186:LYS:HG3	1.95	0.66
1:C:246:ASP:OD2	1:C:252:HIS:HE1	1.77	0.66
2:B:940:SFU:O2	2:B:940:SFU:CM	2.44	0.66
1:C:67:LYS:NZ	3:C:2100:HOH:O	2.28	0.65
1:D:184:ASP:OD2	1:D:186:LYS:HE2	2.01	0.60
1:B:119:GLY:HA3	1:B:167:ARG:HD3	1.88	0.55
1:B:152:LEU:HD13	1:B:178:ILE:HD11	1.90	0.54
1:A:167:ARG:NH2	1:A:172:ASN:HA	2.23	0.53
1:D:2:SER:N	3:D:2001:HOH:O	2.41	0.53
1:C:184:ASP:CG	1:C:186:LYS:HG3	2.30	0.51
1:C:152:LEU:HD13	1:C:178:ILE:HD11	1.96	0.47
1:B:131:LYS:HE3	1:B:137:GLN:HG2	1.97	0.46
1:D:131:LYS:HE3	1:D:137:GLN:HG2	1.98	0.45
1:A:111:CSK:SE	3:A:2168:HOH:O	2.84	0.45
1:A:212:ARG:O	3:A:2240:HOH:O	2.21	0.45
1:B:49:GLU:CG	3:B:2044:HOH:O	2.65	0.44
1:C:172:ASN:HD22	1:C:172:ASN:HA	1.64	0.44
1:A:212:ARG:NH1	1:B:11:PHE:HB2	2.35	0.42
1:D:276[A]:ASN:O	1:D:276[A]:ASN:OD1	2.38	0.42
1:B:111:CSK:SE	3:B:2112:HOH:O	2.88	0.41
1:B:27:TYR:CE1	1:B:37:GLU:HG3	2.56	0.41
1:C:119:GLY:HA3	1:C:167:ARG:HD3	2.02	0.41
1:C:23:HIS:NE2	3:C:2045:HOH:O	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2072:HOH:O	3:A:2198:HOH:O[1_655]	1.76	0.44
1:A:144[B]:ASP:OD1	3:D:2252:HOH:O[1_545]	1.88	0.32

## 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	312/315 (99%)	304 (97%)	7 (2%)	1 (0%)	37	20
1	B	311/315 (99%)	304 (98%)	6 (2%)	1 (0%)	37	20
1	C	311/315 (99%)	303 (97%)	7 (2%)	1 (0%)	37	20
1	D	313/315 (99%)	308 (98%)	4 (1%)	1 (0%)	37	20
All	All	1247/1260 (99%)	1219 (98%)	24 (2%)	4 (0%)	37	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	46	ASN
1	A	46	ASN
1	D	46	ASN
1	B	46	ASN

### 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	246/248 (99%)	243 (99%)	3 (1%)	67	50
1	B	243/248 (98%)	240 (99%)	3 (1%)	67	50
1	C	247/248 (100%)	243 (98%)	4 (2%)	58	37
1	D	249/248 (100%)	247 (99%)	2 (1%)	79	66
All	All	985/992 (99%)	973 (99%)	12 (1%)	67	50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	254	LYS
1	A	280	ASP
1	B	127	ILE
1	B	195	HIS
1	B	280	ASP
1	C	39	LEU
1	C	103	LYS
1	C	157	PRO
1	C	280	ASP
1	D	195	HIS
1	D	280	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	172	ASN
1	B	105	GLN
1	C	55	ASN
1	C	105	GLN
1	C	172	ASN
1	C	189	GLN
1	C	252	HIS
1	D	46	ASN
1	D	55	ASN
1	D	303	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSK	B	111	1	3,7,8	1.01	0	1,7,9	0.37	0
1	CSK	A	111	1	3,7,8	1.27	0	1,7,9	0.94	0
1	CSD	A	244	1	3,7,8	1.19	0	1,8,10	2.76	1 (100%)
1	CSD	D	244	1	3,7,8	0.85	0	1,8,10	0.87	0
1	CSD	C	244	1	3,7,8	1.43	0	1,8,10	1.80	0
1	CSK	C	111	1	3,7,8	1.48	1 (33%)	1,7,9	0.60	0
1	CSK	D	111	1	3,7,8	1.27	0	1,7,9	0.62	0
1	CSD	B	244	1	3,7,8	1.65	1 (33%)	1,8,10	2.42	1 (100%)

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
1	CSK	B	111	1	-	0/0/6/8	-
1	CSK	A	111	1	-	0/0/6/8	-
1	CSD	A	244	1	-	0/2/6/8	-
1	CSD	D	244	1	-	0/2/6/8	-
1	CSD	C	244	1	-	0/2/6/8	-
1	CSK	C	111	1	-	0/0/6/8	-
1	CSK	D	111	1	-	0/0/6/8	-
1	CSD	B	244	1	-	0/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	CSK	CA-N	-2.32	1.41	1.48
1	B	244	CSD	CB-SG	-2.11	1.67	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	CSD	OD1-SG-CB	2.76	110.79	105.54
1	B	244	CSD	OD1-SG-CB	2.42	110.13	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	111	CSK	1	0
1	A	111	CSK	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

26 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	SFU	A	950	-	9,12,12	0.88	0	15,17,17	1.04	0
2	SFU	C	920	-	9,12,12	0.92	0	15,17,17	1.03	1 (6%)
2	SFU	D	990	-	9,12,12	0.56	0	15,17,17	1.22	1 (6%)
2	SFU	B	960	-	9,12,12	0.97	1 (11%)	15,17,17	0.92	1 (6%)
2	SFU	C	960	-	9,12,12	0.74	0	15,17,17	1.21	2 (13%)
2	SFU	B	930	-	9,12,12	0.51	0	15,17,17	0.87	1 (6%)
2	SFU	B	950	-	9,12,12	0.42	0	15,17,17	1.22	2 (13%)
2	SFU	B	910	-	9,12,12	0.77	0	15,17,17	0.92	1 (6%)
2	SFU	D	920	-	9,12,12	0.86	0	15,17,17	1.10	1 (6%)
2	SFU	D	930	-	9,12,12	0.60	0	15,17,17	0.86	1 (6%)
2	SFU	C	910	-	9,12,12	0.47	0	15,17,17	0.80	0
2	SFU	A	960	-	9,12,12	0.36	0	15,17,17	0.85	0
2	SFU	B	940	-	9,12,12	0.55	0	15,17,17	0.97	0
2	SFU	A	990	-	9,12,12	0.63	0	15,17,17	1.40	1 (6%)
2	SFU	A	930	-	9,12,12	0.46	0	15,17,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SFU	D	910	-	9,12,12	0.80	0	15,17,17	0.95	0
2	SFU	D	950	-	9,12,12	0.99	1 (11%)	15,17,17	1.24	2 (13%)
2	SFU	B	920	-	9,12,12	0.77	0	15,17,17	0.89	0
2	SFU	C	930	-	9,12,12	0.78	0	15,17,17	0.92	1 (6%)
2	SFU	D	940	-	9,12,12	0.66	0	15,17,17	1.01	2 (13%)
2	SFU	C	950	-	9,12,12	0.53	0	15,17,17	1.09	2 (13%)
2	SFU	A	940	-	9,12,12	0.60	0	15,17,17	1.09	0
2	SFU	A	920	-	9,12,12	0.63	0	15,17,17	0.86	0
2	SFU	C	940	-	9,12,12	0.68	0	15,17,17	0.90	0
2	SFU	D	960	-	9,12,12	0.54	0	15,17,17	1.08	0
2	SFU	A	910	-	9,12,12	0.71	0	15,17,17	0.97	1 (6%)

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	SFU	A	950	-	-	0/0/22/22	0/1/1/1
2	SFU	C	920	-	-	0/0/22/22	0/1/1/1
2	SFU	D	990	-	-	0/0/22/22	0/1/1/1
2	SFU	B	960	-	-	0/0/22/22	0/1/1/1
2	SFU	C	960	-	-	0/0/22/22	0/1/1/1
2	SFU	B	930	-	-	0/0/22/22	0/1/1/1
2	SFU	B	950	-	-	0/0/22/22	0/1/1/1
2	SFU	B	910	-	-	0/0/22/22	0/1/1/1
2	SFU	D	920	-	-	0/0/22/22	0/1/1/1
2	SFU	D	930	-	-	0/0/22/22	0/1/1/1
2	SFU	C	910	-	-	0/0/22/22	0/1/1/1
2	SFU	A	960	-	-	0/0/22/22	0/1/1/1
2	SFU	B	940	-	-	0/0/22/22	0/1/1/1
2	SFU	A	990	-	-	0/0/22/22	0/1/1/1
2	SFU	A	930	-	-	0/0/22/22	0/1/1/1
2	SFU	D	910	-	-	0/0/22/22	0/1/1/1
2	SFU	D	950	-	-	0/0/22/22	0/1/1/1
2	SFU	B	920	-	-	0/0/22/22	0/1/1/1
2	SFU	C	930	-	-	0/0/22/22	0/1/1/1
2	SFU	D	940	-	-	0/0/22/22	0/1/1/1
2	SFU	C	950	-	-	0/0/22/22	0/1/1/1
2	SFU	A	940	-	-	0/0/22/22	0/1/1/1
2	SFU	A	920	-	-	0/0/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SFU	C	940	-	-	0/0/22/22	0/1/1/1
2	SFU	D	960	-	-	0/0/22/22	0/1/1/1
2	SFU	A	910	-	-	0/0/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	950	SFU	O2-C2	2.49	1.48	1.43
2	B	960	SFU	O5-C5	-2.05	1.39	1.44

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	990	SFU	O4-C4-C3	-3.54	102.17	110.35
2	D	990	SFU	O5-C5-C6	3.12	113.44	106.70
2	C	930	SFU	C3-C2-C1	2.93	114.87	109.33
2	B	950	SFU	C5-O5-C1	2.81	119.94	113.31
2	D	950	SFU	O5-C5-C4	2.80	114.55	109.52
2	D	920	SFU	C5-O5-C1	2.63	119.49	113.31
2	C	950	SFU	C5-O5-C1	2.58	119.38	113.31
2	A	910	SFU	C5-O5-C1	2.51	119.22	113.31
2	B	910	SFU	C3-C2-C1	2.50	114.05	109.33
2	D	950	SFU	O5-C1-C2	2.22	115.79	109.85
2	D	940	SFU	C4-C3-C2	-2.22	106.95	110.82
2	D	930	SFU	C3-C2-C1	2.18	113.47	109.33
2	B	950	SFU	O5-C5-C6	2.13	111.31	106.70
2	C	960	SFU	C5-O5-C1	2.13	118.32	113.31
2	C	950	SFU	O2-C2-C3	2.12	115.25	110.35
2	B	960	SFU	C5-O5-C1	2.09	118.24	113.31
2	C	920	SFU	C3-C2-C1	2.09	113.29	109.33
2	D	940	SFU	O2-C2-C3	2.08	115.15	110.35
2	B	930	SFU	C3-C2-C1	2.03	113.17	109.33
2	C	960	SFU	O3-C3-C4	2.02	115.03	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	940	SFU	1	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 [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	312/315 (99%)	-0.62	0 100 100	6, 9, 18, 24	2 (0%)
1	B	312/315 (99%)	-0.29	3 (0%) 79 82	7, 12, 24, 39	1 (0%)
1	C	312/315 (99%)	-0.47	2 (0%) 85 88	7, 11, 21, 33	1 (0%)
1	D	312/315 (99%)	-0.56	0 100 100	6, 10, 18, 32	3 (0%)
All	All	1248/1260 (99%)	-0.48	5 (0%) 89 90	6, 11, 21, 39	7 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	ALA	2.7
1	B	302	ALA	2.6
1	B	303	HIS	2.6
1	C	303	HIS	2.2
1	B	304	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	B	244	8/9	0.92	0.10	15,16,19,27	0
1	CSD	C	244	8/9	0.94	0.09	11,12,15,22	0
1	CSD	A	244	8/9	0.95	0.07	8,9,10,18	0
1	CSD	D	244	8/9	0.95	0.08	8,9,10,19	0
1	CSK	B	111	8/9	0.97	0.07	7,9,10,12	2
1	CSK	C	111	8/9	0.97	0.07	6,7,11,11	2
1	CSK	A	111	8/9	0.98	0.06	6,7,12,13	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSK	D	111	8/9	0.98	0.06	7,8,9,11	2

## 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( $\text{\AA}^2$ )	Q<0.9
2	SFU	A	990	12/12	0.95	0.10	22,24,26,27	0
2	SFU	B	950	12/12	0.95	0.09	17,20,24,26	0
2	SFU	B	910	12/12	0.98	0.07	12,15,19,19	0
2	SFU	B	940	12/12	0.98	0.07	15,18,21,25	0
2	SFU	A	960	12/12	0.98	0.05	9,10,16,18	0
2	SFU	B	960	12/12	0.98	0.06	13,14,16,18	0
2	SFU	C	930	12/12	0.98	0.06	11,12,15,16	0
2	SFU	C	940	12/12	0.98	0.06	12,14,18,22	0
2	SFU	C	950	12/12	0.98	0.07	13,14,18,19	0
2	SFU	D	910	12/12	0.98	0.06	12,13,16,16	0
2	SFU	D	960	12/12	0.98	0.06	10,12,16,17	0
2	SFU	D	990	12/12	0.98	0.08	14,17,18,18	0
2	SFU	A	910	12/12	0.99	0.04	10,10,11,13	0
2	SFU	C	910	12/12	0.99	0.05	11,13,16,16	0
2	SFU	C	920	12/12	0.99	0.05	11,11,12,17	0
2	SFU	A	920	12/12	0.99	0.04	8,8,9,13	0
2	SFU	A	930	12/12	0.99	0.04	9,9,12,13	0
2	SFU	B	920	12/12	0.99	0.04	10,12,14,17	0
2	SFU	C	960	12/12	0.99	0.05	10,11,15,19	0
2	SFU	B	930	12/12	0.99	0.05	10,11,13,13	0
2	SFU	D	920	12/12	0.99	0.05	10,11,14,16	0
2	SFU	D	930	12/12	0.99	0.05	10,10,13,14	0
2	SFU	D	940	12/12	0.99	0.05	9,11,13,15	0
2	SFU	D	950	12/12	0.99	0.04	9,10,11,15	0
2	SFU	A	940	12/12	0.99	0.05	10,11,14,18	0
2	SFU	A	950	12/12	0.99	0.05	9,10,12,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.