Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:34 am BST

PDB ID	:	6M9S
Title	:	Crystal structure of SeMet SznF from Streptomyces achromogenes var. streptozoticus NRRL 2697
Authors	:	Rohac, R.; Mitchell, A.J.; Boal, A.K.
Deposited on	:	2018-08-24
Resolution	:	2.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

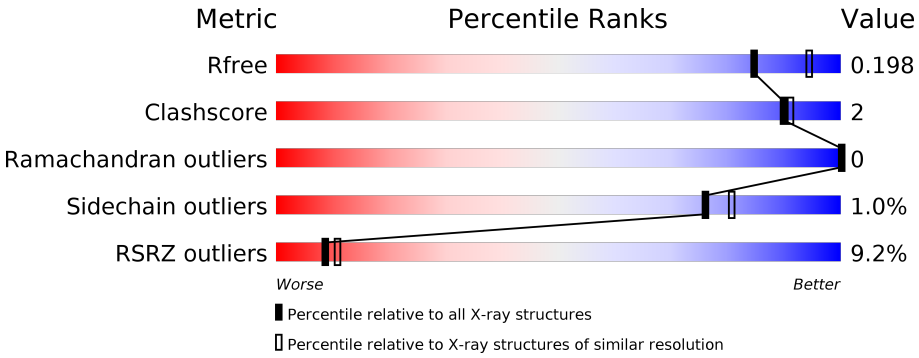
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	488	5% 90% • 6%
1	B	488	11% 88% 5% 8%
1	C	488	12% 91% • 6%
1	D	488	6% 90% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16254 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.

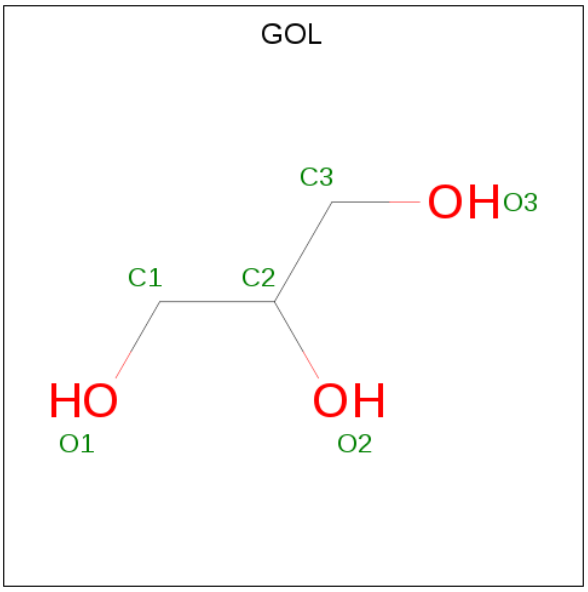
- Molecule 1 is a protein called SznF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	Se	0	8	1
			3727	2369	644	702	5	7			
1	B	450	Total	C	N	O	S	Se	0	5	1
			3648	2324	628	682	5	9			
1	C	459	Total	C	N	O	S	Se	0	13	0
			3820	2422	671	714	5	8			
1	D	457	Total	C	N	O	S	Se	0	10	0
			3749	2379	649	707	5	9			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

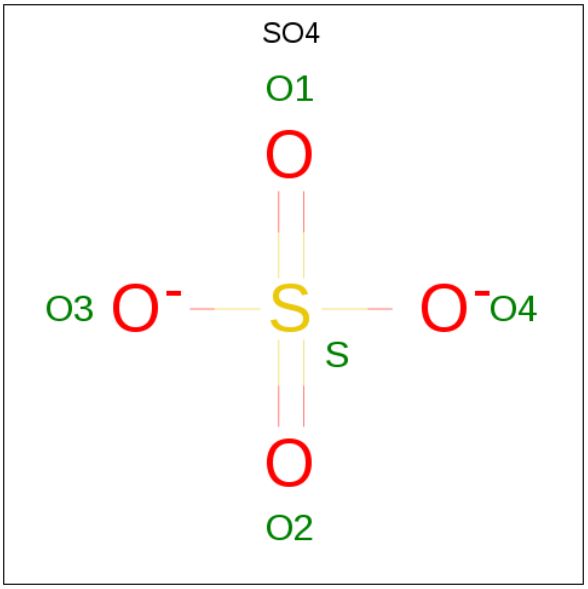
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



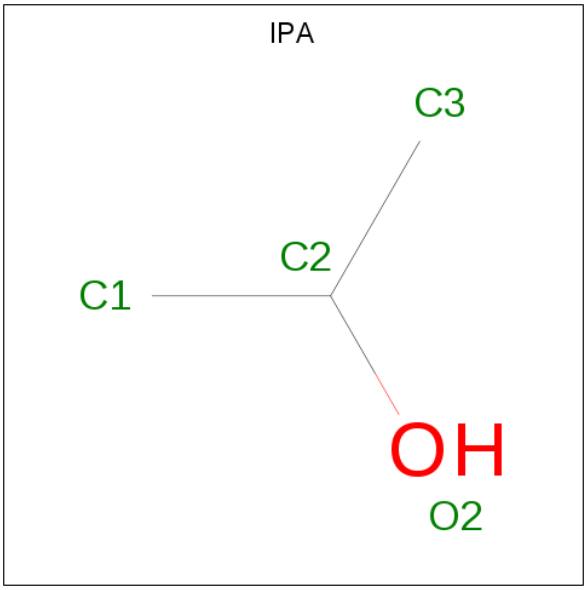
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	300	Total O 300 300	0	0
6	B	226	Total O 226 226	0	0
6	C	350	Total O 351 351	0	3

Continued on next page...

Continued from previous page...

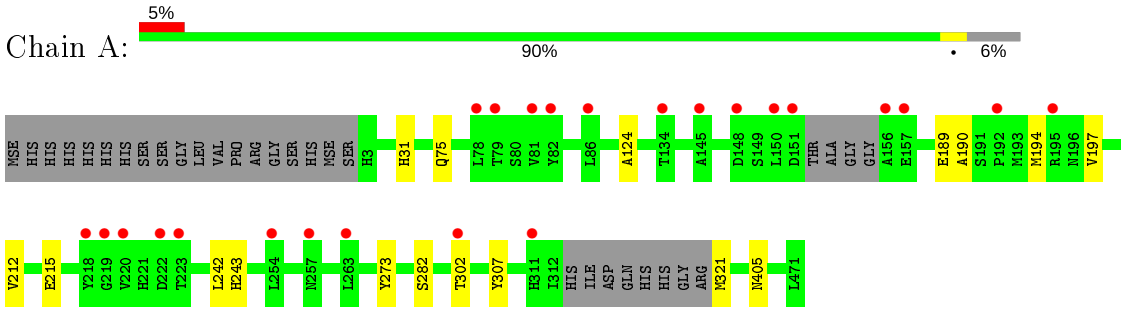
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	361	Total	O	0	1
			362	362		

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.

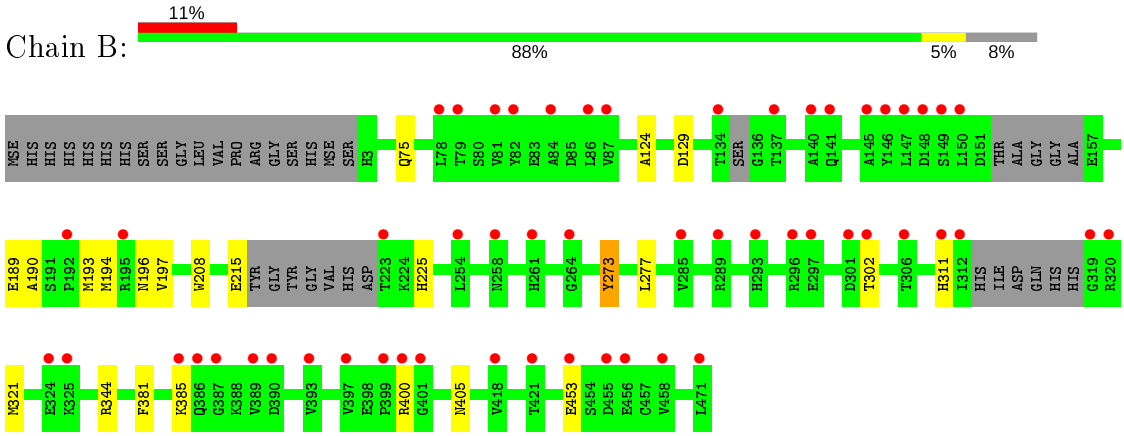
- Molecule 1: SznF

Chain A:



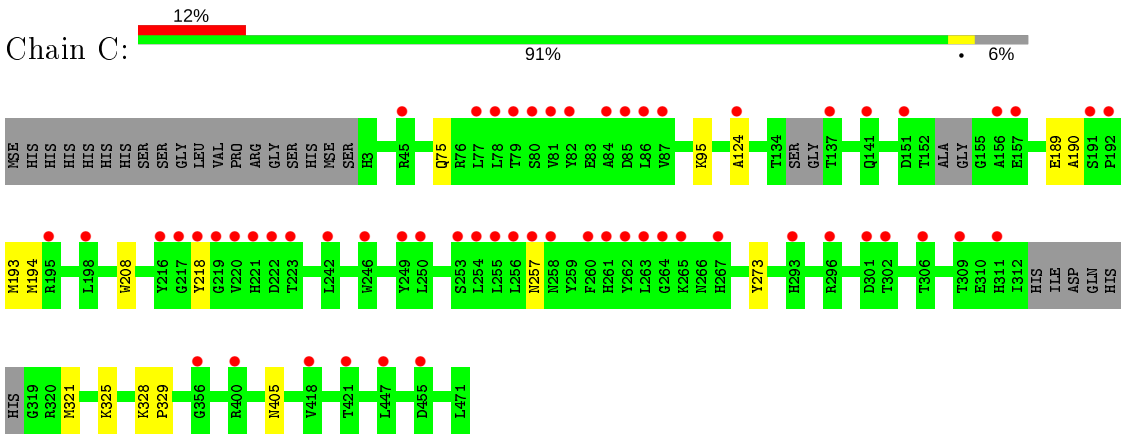
- Molecule 1: SznF

Chain B:



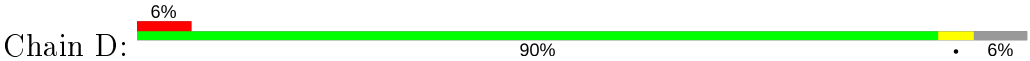
- Molecule 1: SznF

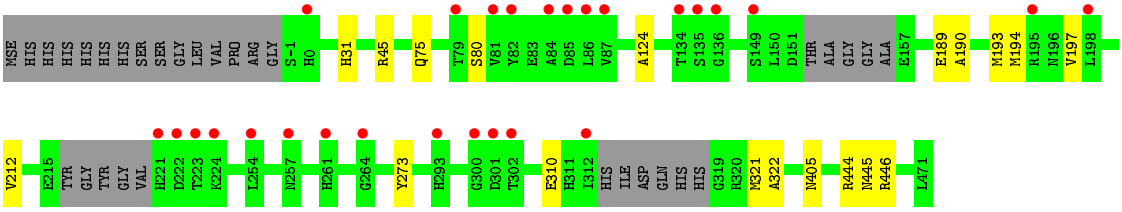
Chain C:



• Molecule 1: SznF

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.51Å 109.46Å 365.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.08 49.09 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.09-2.08) 99.9 (49.09-2.08)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.189 0.186 , 0.198	Depositor DCC
R_{free} test set	7469 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16254	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: GOL, IPA, FE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/3829	0.61	0/5185
1	B	0.37	0/3734	0.62	0/5049
1	C	0.39	0/3911	0.59	0/5289
1	D	0.39	0/3845	0.60	0/5200
All	All	0.39	0/15319	0.60	0/20723

There are no bond length outliers.

There are no bond angle outliers.

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	3727	0	3550	15	0
1	B	3648	0	3489	17	0
1	C	3820	0	3634	13	0
1	D	3749	0	3561	14	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	12	0	16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	4	0	8	0	0
5	C	4	0	8	0	0
6	A	300	0	0	2	0
6	B	226	0	0	0	0
6	C	351	0	0	4	0
6	D	362	0	0	4	0
All	All	16254	0	14290	53	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 (53) 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:193:MSE:HG2	1:C:208[B]:TRP:CZ3	2.03	0.92
1:C:321[B]:MSE:HE3	6:C:605:HOH:O	1.73	0.87
1:C:193:MSE:HG2	1:C:208[B]:TRP:HZ3	1.39	0.86
1:B:193[B]:MSE:SE	1:B:277:LEU:HD13	2.38	0.73
1:A:189:GLU:OE2	1:A:307:TYR:OH	2.04	0.73
1:B:196:ASN:ND2	1:B:273:TYR:CD2	2.60	0.69
1:C:321[B]:MSE:CE	6:C:605:HOH:O	2.37	0.66
1:A:194[B]:MSE:HE1	1:B:197:VAL:CG1	2.28	0.64
1:A:189:GLU:OE1	2:A:502:FE:FE	1.49	0.63
1:D:31:HIS:CD2	6:D:660:HOH:O	2.52	0.61
1:D:31:HIS:HD2	6:D:660:HOH:O	1.83	0.61
1:A:194[A]:MSE:HE3	1:A:212:VAL:HG11	1.84	0.60
1:C:328:LYS:HB2	1:C:329:PRO:HD3	1.83	0.59
1:A:194[B]:MSE:HE1	1:B:197:VAL:HG12	1.85	0.59
1:D:446[B]:ARG:NE	1:D:446[B]:ARG:HA	2.17	0.58
1:B:321[B]:MSE:SE	1:B:321[B]:MSE:C	2.95	0.55
1:D:31:HIS:NE2	6:D:602:HOH:O	2.33	0.55
1:C:194[A]:MSE:SE	1:D:197:VAL:HG12	2.60	0.52
1:D:45[A]:ARG:HD3	1:D:80[A]:SER:OG	2.10	0.51
1:A:194[B]:MSE:HE1	1:B:197:VAL:HG11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE1	1:A:215:GLU:OE1	2.31	0.49
1:A:31:HIS:HD2	6:A:618:HOH:O	1.95	0.49
1:B:400:ARG:NH1	1:B:453:GLU:O	2.45	0.49
1:D:194[B]:MSE:SE	1:D:212:VAL:HG11	2.63	0.49
1:A:31:HIS:CD2	6:A:618:HOH:O	2.65	0.49
1:A:194[A]:MSE:HE2	1:A:194[A]:MSE:HA	1.94	0.49
1:B:193[B]:MSE:HG2	1:B:273:TYR:OH	2.12	0.49
1:C:189:GLU:HB3	6:C:822:HOH:O	2.14	0.48
1:D:321[B]:MSE:SE	1:D:321[B]:MSE:C	3.02	0.48
1:B:215:GLU:HB3	1:B:225:HIS:CE1	2.50	0.47
1:A:194[B]:MSE:HG2	1:B:194[B]:MSE:HE1	1.95	0.47
1:A:194[A]:MSE:HE2	1:A:197:VAL:HB	1.96	0.47
1:C:194[A]:MSE:SE	1:D:197:VAL:CG1	3.13	0.47
1:A:189:GLU:O	1:A:190:ALA:HB3	2.16	0.46
1:D:321[B]:MSE:SE	1:D:322:ALA:N	2.98	0.46
1:C:321[B]:MSE:HE2	1:C:325:LYS:HB2	1.98	0.46
1:D:446[B]:ARG:HD3	6:D:666:HOH:O	2.16	0.45
1:C:257[B]:ASN:ND2	6:C:610[B]:HOH:O	2.44	0.45
1:B:381:PHE:O	1:B:385:LYS:HG3	2.17	0.44
1:C:75:GLN:HE22	1:C:124:ALA:HB1	1.83	0.43
1:A:75:GLN:HE22	1:A:124:ALA:HB1	1.83	0.43
1:B:197:VAL:CG2	1:B:208:TRP:CD1	3.02	0.43
1:C:189:GLU:O	1:C:190:ALA:HB3	2.19	0.43
1:D:75:GLN:HE22	1:D:124:ALA:HB1	1.83	0.43
1:B:75:GLN:HE22	1:B:124:ALA:HB1	1.84	0.43
1:B:197:VAL:CG2	1:B:208:TRP:HD1	2.32	0.43
1:B:189:GLU:O	1:B:190:ALA:HB3	2.18	0.42
1:D:189:GLU:O	1:D:190:ALA:HB3	2.19	0.42
1:A:242:LEU:HA	1:A:243:HIS:HA	1.87	0.42
1:D:444:ARG:CZ	1:D:445:ASN:HD21	2.33	0.41
1:B:129:ASP:OD1	1:B:344[A]:ARG:NH2	2.53	0.41
1:C:321[B]:MSE:SE	1:C:321[B]:MSE:C	3.09	0.41
1:B:225:HIS:ND1	1:B:311:HIS:CE1	2.89	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	459/488 (94%)	451 (98%)	8 (2%)	0	100	100
1	B	445/488 (91%)	440 (99%)	5 (1%)	0	100	100
1	C	464/488 (95%)	458 (99%)	6 (1%)	0	100	100
1	D	459/488 (94%)	453 (99%)	6 (1%)	0	100	100
All	All	1827/1952 (94%)	1802 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	396/412 (96%)	391 (99%)	5 (1%)	69	74
1	B	386/412 (94%)	383 (99%)	3 (1%)	81	85
1	C	404/412 (98%)	400 (99%)	4 (1%)	76	81
1	D	399/412 (97%)	395 (99%)	4 (1%)	76	81
All	All	1585/1648 (96%)	1569 (99%)	16 (1%)	76	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	TYR
1	A	282	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	302	THR
1	A	321	MSE
1	A	405	ASN
1	B	273	TYR
1	B	302	THR
1	B	405	ASN
1	C	95	LYS
1	C	218	TYR
1	C	273	TYR
1	C	405	ASN
1	D	193	MSE
1	D	273	TYR
1	D	310	GLU
1	D	405	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	B	445	ASN
1	D	445	ASN

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)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	SO4	B	504	-	4,4,4	0.42	0	6,6,6	0.14	0
4	SO4	A	505	-	4,4,4	0.36	0	6,6,6	0.19	0
4	SO4	C	504	-	4,4,4	0.44	0	6,6,6	0.26	0
3	GOL	B	503	-	5,5,5	0.33	0	5,5,5	0.55	0
4	SO4	D	504	-	4,4,4	0.49	0	6,6,6	0.17	0
3	GOL	C	503	-	5,5,5	0.28	0	5,5,5	0.49	0
4	SO4	D	505	-	4,4,4	0.34	0	6,6,6	0.16	0
3	GOL	A	503	-	5,5,5	0.46	0	5,5,5	0.49	0
3	GOL	D	503	-	5,5,5	0.32	0	5,5,5	0.45	0
5	IPA	C	505	-	3,3,3	0.61	0	3,3,3	0.37	0
3	GOL	A	504	-	5,5,5	0.27	0	5,5,5	0.47	0
5	IPA	A	506	-	3,3,3	0.55	0	3,3,3	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	A	504	-	-	3/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
3	GOL	D	503	-	-	0/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-C3
3	A	504	GOL	C1-C2-C3-O3
3	A	503	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O2-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	504	GOL	O2-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	451/488 (92%)	0.12	24 (5%) 26 31	31, 43, 74, 110	2 (0%)
1	B	444/488 (90%)	0.51	55 (12%) 4 5	33, 51, 80, 98	0
1	C	453/488 (92%)	0.51	59 (13%) 3 4	25, 42, 72, 104	0
1	D	450/488 (92%)	0.13	27 (6%) 21 26	26, 41, 71, 96	0
All	All	1798/1952 (92%)	0.32	165 (9%) 9 11	25, 44, 77, 110	2 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	VAL	6.5
1	C	218	TYR	6.5
1	A	218	TYR	5.8
1	C	222	ASP	5.5
1	C	216	TYR	5.1
1	C	257[A]	ASN	5.0
1	A	222	ASP	5.0
1	B	137	THR	4.8
1	D	136	GLY	4.7
1	A	219	GLY	4.6
1	C	254	LEU	4.5
1	D	0	HIS	4.2
1	C	79	THR	4.2
1	B	418	VAL	4.1
1	D	301	ASP	4.1
1	B	141	GLN	4.1
1	B	81	VAL	4.1
1	B	293	HIS	4.0
1	D	222	ASP	4.0
1	A	223	THR	4.0
1	C	151	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	223	THR	3.9
1	C	86	LEU	3.9
1	A	220	VAL	3.9
1	C	302	THR	3.9
1	C	78	LEU	3.9
1	C	82	TYR	3.9
1	C	223	THR	3.7
1	B	145	ALA	3.6
1	B	397	VAL	3.6
1	B	312	ILE	3.6
1	C	246	TRP	3.5
1	B	78	LEU	3.5
1	C	301[A]	ASP	3.5
1	C	219	GLY	3.5
1	B	86	LEU	3.4
1	C	81	VAL	3.4
1	B	82	TYR	3.4
1	D	221	HIS	3.4
1	C	137	THR	3.4
1	B	140	ALA	3.3
1	D	86	LEU	3.3
1	C	255	LEU	3.3
1	C	306	THR	3.3
1	C	250	LEU	3.3
1	B	150	LEU	3.2
1	B	390	ASP	3.2
1	B	389	VAL	3.2
1	C	249	TYR	3.2
1	A	82	TYR	3.2
1	B	84	ALA	3.1
1	B	400	ARG	3.1
1	A	302	THR	3.1
1	C	263	LEU	3.1
1	D	134	THR	3.1
1	C	256	LEU	3.1
1	B	301	ASP	3.1
1	C	84	ALA	3.0
1	B	421	THR	3.0
1	B	386	GLN	3.0
1	A	157	GLU	3.0
1	D	81	VAL	3.0
1	B	455	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	258	ASN	2.9
1	B	296	ARG	2.9
1	B	311	HIS	2.9
1	B	453	GLU	2.9
1	D	302	THR	2.8
1	D	82	TYR	2.8
1	A	78	LEU	2.8
1	A	311	HIS	2.7
1	D	312	ILE	2.7
1	B	254	LEU	2.7
1	C	221	HIS	2.7
1	C	141	GLN	2.7
1	A	257[A]	ASN	2.7
1	A	151	ASP	2.7
1	A	86	LEU	2.6
1	B	458	VAL	2.6
1	C	198	LEU	2.6
1	C	455	ASP	2.6
1	B	195	ARG	2.6
1	D	264	GLY	2.6
1	B	134	THR	2.6
1	B	456	GLU	2.6
1	A	156	ALA	2.5
1	C	253	SER	2.5
1	B	146	TYR	2.5
1	A	79	THR	2.5
1	D	198	LEU	2.5
1	B	261	HIS	2.5
1	D	84	ALA	2.5
1	B	306	THR	2.5
1	C	262	TYR	2.5
1	D	195	ARG	2.5
1	B	387	GLY	2.5
1	C	260	PHE	2.5
1	C	264	GLY	2.5
1	C	265	LYS	2.5
1	B	285	VAL	2.5
1	C	261	HIS	2.5
1	C	242	LEU	2.4
1	C	192	PRO	2.4
1	B	297	GLU	2.4
1	C	418	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	195	ARG	2.4
1	A	192	PRO	2.4
1	C	400	ARG	2.4
1	A	134	THR	2.4
1	A	254	LEU	2.4
1	B	324	GLU	2.4
1	B	401	GLY	2.4
1	C	195	ARG	2.4
1	A	81	VAL	2.4
1	B	325	LYS	2.4
1	B	79	THR	2.4
1	D	79	THR	2.4
1	C	217	GLY	2.4
1	B	319	GLY	2.4
1	B	258	ASN	2.3
1	B	149	SER	2.3
1	C	447	LEU	2.3
1	D	257[A]	ASN	2.3
1	D	293	HIS	2.3
1	B	393	VAL	2.3
1	B	223	THR	2.3
1	D	261	HIS	2.3
1	A	145	ALA	2.2
1	C	87	VAL	2.2
1	C	156	ALA	2.2
1	C	356	GLY	2.2
1	A	148	ASP	2.2
1	D	300	GLY	2.2
1	C	293	HIS	2.2
1	C	124	ALA	2.2
1	B	385	LYS	2.2
1	C	421	THR	2.2
1	D	85	ASP	2.2
1	C	80[A]	SER	2.2
1	B	147	LEU	2.1
1	B	264	GLY	2.1
1	B	302	THR	2.1
1	C	85	ASP	2.1
1	C	311	HIS	2.1
1	D	224	LYS	2.1
1	C	296[A]	ARG	2.1
1	B	471	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	77	LEU	2.1
1	D	135	SER	2.1
1	B	87	VAL	2.1
1	B	399	PRO	2.1
1	D	149	SER	2.1
1	B	289	ARG	2.0
1	B	192	PRO	2.0
1	B	320	ARG	2.0
1	C	267	HIS	2.0
1	C	157	GLU	2.0
1	C	191	SER	2.0
1	A	150	LEU	2.0
1	A	263	LEU	2.0
1	C	309	THR	2.0
1	D	254	LEU	2.0
1	C	45[A]	ARG	2.0
1	B	148	ASP	2.0
1	D	87	VAL	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
5	IPA	A	506	4/4	0.79	0.19	73,77,78,80	0
5	IPA	C	505	4/4	0.85	0.12	52,52,54,55	0
4	SO4	C	504	5/5	0.86	0.18	64,65,69,75	0
3	GOL	C	503	6/6	0.88	0.13	37,42,46,53	0
3	GOL	A	504	6/6	0.88	0.16	59,65,68,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	503	6/6	0.91	0.11	43,52,59,66	0
3	GOL	D	503	6/6	0.91	0.18	37,42,46,53	0
4	SO4	B	504	5/5	0.91	0.16	72,76,78,85	0
2	FE	A	502	1/1	0.93	0.08	51,51,51,51	1
3	GOL	B	503	6/6	0.93	0.12	44,47,53,60	0
2	FE	B	502	1/1	0.94	0.05	65,65,65,65	1
2	FE	D	502	1/1	0.94	0.06	53,53,53,53	1
4	SO4	A	505	5/5	0.95	0.07	64,67,69,72	0
2	FE	B	501	1/1	0.95	0.12	52,52,52,52	0
4	SO4	D	504	5/5	0.96	0.12	54,59,64,67	0
4	SO4	D	505	5/5	0.97	0.18	66,67,71,74	0
2	FE	A	501	1/1	0.98	0.12	42,42,42,42	0
2	FE	C	502	1/1	0.98	0.05	53,53,53,53	1
2	FE	D	501	1/1	0.98	0.14	41,41,41,41	0
2	FE	C	501	1/1	0.98	0.15	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.