



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 10:25 AM JST

PDB ID : 6A6G
Title : Crystal structure of thermostable FiSufS-SufU complex from thermophilic *Ferrobacterium Islandicum* AW-1
Authors : Dhanasingh, I.; Jin, H.S.; Lee, D.W.; Lee, S.H.
Deposited on : 2018-06-27
Resolution : 2.49 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 ⓘ](#)) 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 : 2.14.6
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) : 2.14.6

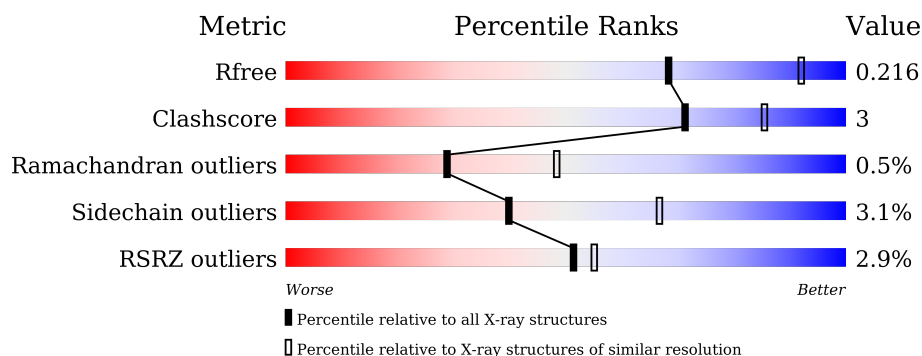
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	425	<div> <div></div> <div>92% 6% ..</div> </div>
1	B	425	<div> <div>%</div> <div>92% 6% ..</div> </div>
2	C	138	<div> <div>8%</div> <div>81% 15% ...</div> </div>
2	D	138	<div> <div>11%</div> <div>80% 15% . .</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9343 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3330	2140	550	629	11			
1	B	422	Total	C	N	O	S	0	0	0
			3340	2146	553	630	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP A0A1B0VPZ3
A	-2	SER	-	expression tag	UNP A0A1B0VPZ3
A	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
A	0	HIS	-	expression tag	UNP A0A1B0VPZ3
B	-3	SER	-	expression tag	UNP A0A1B0VPZ3
B	-2	SER	-	expression tag	UNP A0A1B0VPZ3
B	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
B	0	HIS	-	expression tag	UNP A0A1B0VPZ3

- Molecule 2 is a protein called Iron-sulfur cluster assembly scaffold protein NifU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	136	Total	C	N	O	S	0	0	0
			1091	702	175	202	12			
2	D	133	Total	C	N	O	S	0	0	0
			1071	691	170	198	12			

There are 6 discrepancies between the modelled and reference sequences:

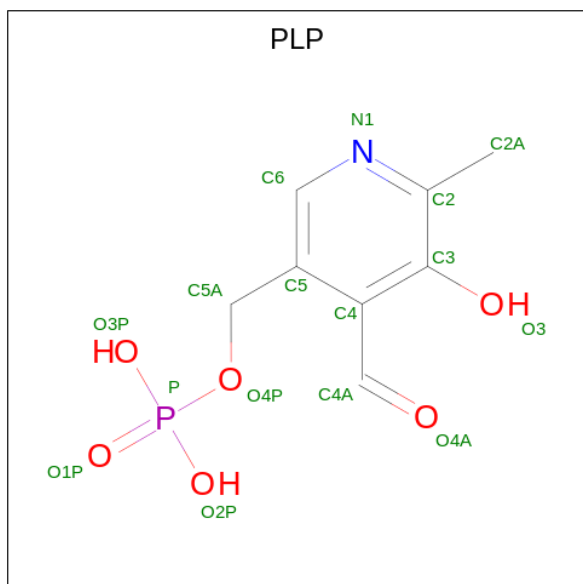
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A1B0VLW5
C	-1	SER	-	expression tag	UNP A0A1B0VLW5
C	0	HIS	-	expression tag	UNP A0A1B0VLW5
D	-2	GLY	-	expression tag	UNP A0A1B0VLW5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP A0A1B0VLW5
D	0	HIS	-	expression tag	UNP A0A1B0VLW5

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



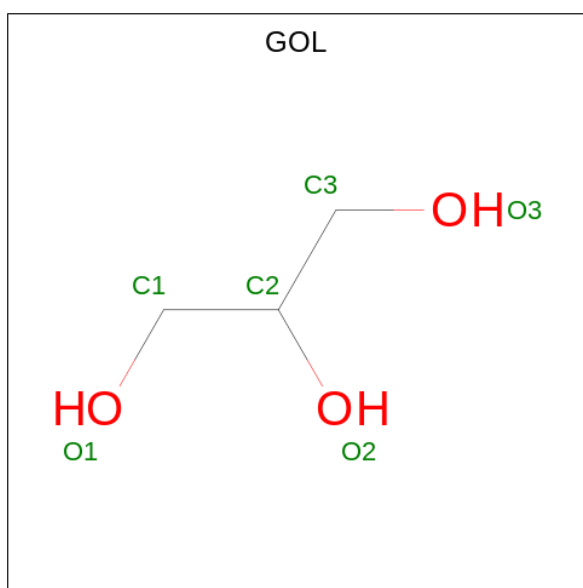
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Zn 1	0	0
6	C	2	Total 2	Zn 2	0	0

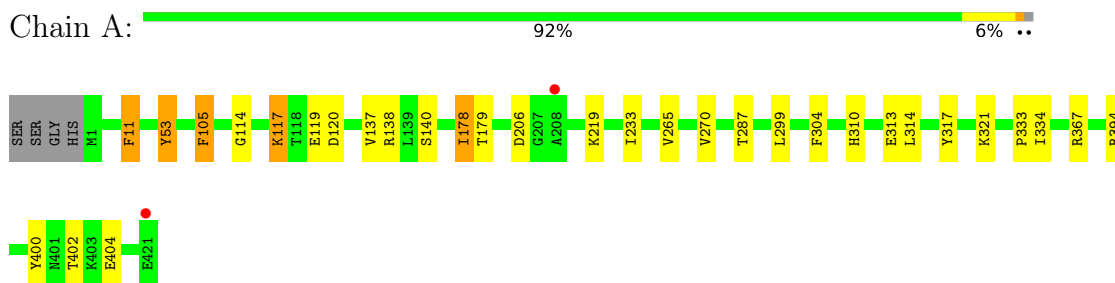
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total 209	O 209	0	0
7	B	193	Total 193	O 193	0	0
7	C	37	Total 37	O 37	0	0
7	D	19	Total 19	O 19	0	0

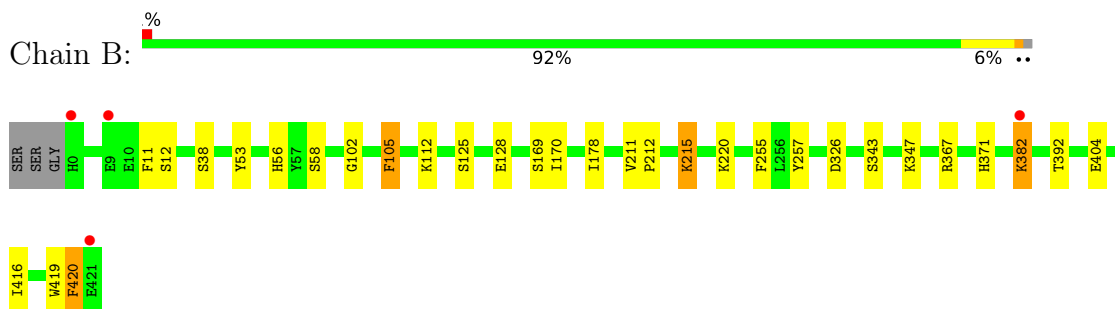
3 Residue-property plots [i](#)

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.

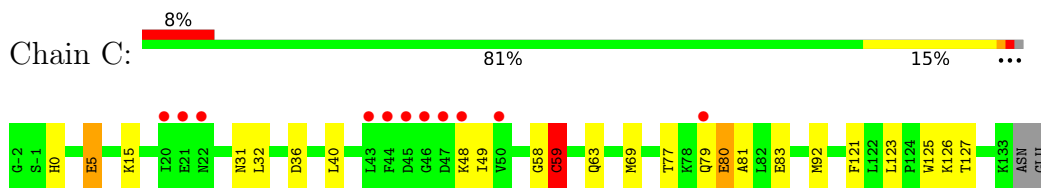
- Molecule 1: Cysteine desulfurase



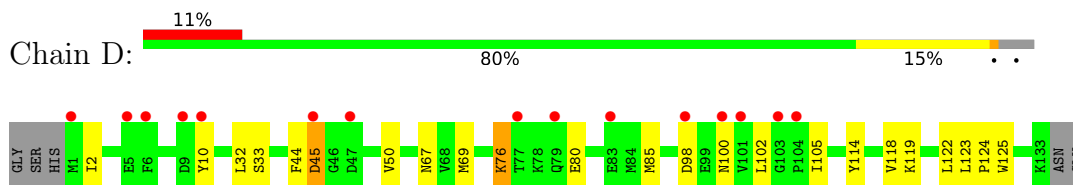
- Molecule 1: Cysteine desulfurase



- Molecule 2: Iron-sulfur cluster assembly scaffold protein NifU



- Molecule 2: Iron-sulfur cluster assembly scaffold protein NifU



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.27Å 76.97Å 192.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.49 29.62 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.62-2.49) 98.9 (29.62-2.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.146 , 0.214 0.154 , 0.216	Depositor DCC
R_{free} test set	1912 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9343	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, ZN, PEG, CSS, PLP

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	0.68	0/3392	0.76	0/4590
1	B	0.67	0/3403	0.75	1/4605 (0.0%)
2	C	0.61	1/1104 (0.1%)	0.74	2/1476 (0.1%)
2	D	0.51	0/1083	0.63	0/1448
All	All	0.65	1/8982 (0.0%)	0.74	3/12119 (0.0%)

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
2	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	59	CYS	CB-SG	-7.35	1.69	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	59	CYS	N-CA-CB	-6.15	99.53	110.60
2	C	59	CYS	CB-CA-C	-5.83	98.74	110.40
1	B	326	ASP	CB-CG-OD1	5.61	123.35	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	58	GLY	Peptide

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	3330	0	3337	20	0
1	B	3340	0	3344	18	0
2	C	1091	0	1093	12	0
2	D	1071	0	1078	13	0
3	A	15	0	6	1	0
3	B	15	0	7	0	0
4	A	14	0	20	0	0
5	B	6	0	8	0	0
6	C	2	0	0	1	0
6	D	1	0	0	0	0
7	A	209	0	0	5	0
7	B	193	0	0	1	0
7	C	37	0	0	1	0
7	D	19	0	0	0	0
All	All	9343	0	8893	62	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 3.

All (62) 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)
2:C:5:GLU:OE2	6:C:201:ZN:ZN	1.43	0.67
2:D:76:LYS:HE3	2:D:80:GLU:HB3	1.78	0.66
1:B:343:SER:HB3	1:B:392:THR:HG21	1.79	0.64
1:A:334:ILE:HD12	1:A:334:ILE:O	2.00	0.61
1:A:394:ARG:HD2	7:A:718:HOH:O	2.02	0.58
1:B:56:HIS:NE2	7:B:602:HOH:O	2.32	0.58
1:A:53:TYR:CE2	1:A:287:THR:HG21	2.40	0.56
1:B:419:TRP:O	1:B:420:PHE:CB	2.54	0.56
2:D:69:MET:HG3	2:D:125:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:LYS:HE3	2:D:80:GLU:CB	2.37	0.55
1:B:419:TRP:O	1:B:420:PHE:HB3	2.07	0.54
2:C:0:HIS:HE1	2:C:5:GLU:OE2	1.91	0.54
1:A:313:GLU:OE2	7:A:601:HOH:O	2.18	0.53
1:A:265:VAL:HG22	1:A:270:VAL:HG23	1.91	0.52
1:A:333:PRO:O	1:A:334:ILE:HG13	2.10	0.52
1:A:310:HIS:NE2	1:A:314:LEU:HD11	2.24	0.52
2:D:10:TYR:O	2:D:67:ASN:ND2	2.41	0.50
2:C:77:THR:HG23	2:C:80:GLU:OE2	2.12	0.50
2:C:48:LYS:HG3	2:C:49:ILE:N	2.26	0.50
1:B:128:GLU:OE2	1:B:178:ILE:HD12	2.11	0.50
2:D:123:LEU:N	2:D:124:PRO:HD2	2.27	0.49
1:A:404:GLU:HG2	7:A:663:HOH:O	2.11	0.49
2:C:36:ASP:OD1	2:C:59:CYS:HB2	2.13	0.49
2:D:102:LEU:HB3	2:D:105:ILE:HB	1.94	0.49
2:D:44:PHE:O	2:D:50:VAL:HG23	2.13	0.49
1:B:416:ILE:O	1:B:419:TRP:O	2.31	0.48
1:A:137:VAL:O	1:A:140:SER:OG	2.26	0.48
2:D:44:PHE:O	2:D:45:ASP:HB2	2.13	0.48
1:B:382:LYS:HE3	1:B:382:LYS:HA	1.95	0.48
2:C:77:THR:OG1	2:C:80:GLU:HB2	2.12	0.48
2:C:79:GLN:C	2:C:81:ALA:H	2.16	0.48
2:D:33:SER:HA	2:D:119:LYS:HD2	1.95	0.47
1:A:114:GLY:O	1:A:117:LYS:HE2	2.13	0.47
1:A:138:ARG:HG2	1:B:257:TYR:CE1	2.49	0.47
2:D:32:LEU:HD12	2:D:32:LEU:O	2.13	0.47
1:B:105:PHE:C	1:B:105:PHE:CD1	2.87	0.46
2:C:92:MET:HG3	2:C:121:PHE:CD2	2.50	0.46
2:D:118:VAL:HG12	2:D:122:LEU:HD12	1.96	0.46
2:C:123:LEU:HD13	7:C:311:HOH:O	2.15	0.46
2:D:69:MET:HG3	2:D:125:TRP:CH2	2.50	0.46
7:A:758:HOH:O	1:B:112:LYS:HD3	2.16	0.46
1:B:170:ILE:HG22	1:B:170:ILE:O	2.15	0.45
1:B:211:VAL:N	1:B:212:PRO:CD	2.79	0.45
1:A:11:PHE:CZ	1:A:402:THR:HG22	2.53	0.44
1:A:394:ARG:CD	7:A:718:HOH:O	2.64	0.43
2:C:31:ASN:ND2	2:C:31:ASN:O	2.52	0.43
1:B:125:SER:HB3	1:B:178:ILE:CD1	2.49	0.42
2:C:69:MET:HG3	2:C:125:TRP:CH2	2.54	0.42
2:C:40:LEU:HD12	2:C:127:THR:HG22	2.02	0.42
1:B:215:LYS:HD3	1:B:215:LYS:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:HIS:NE2	1:B:392:THR:HG22	2.35	0.42
2:D:2:ILE:HD12	2:D:114:TYR:CD2	2.55	0.42
1:A:317:TYR:CZ	1:A:321:LYS:HE3	2.55	0.41
1:A:105:PHE:CD1	1:A:105:PHE:C	2.94	0.41
1:B:102:GLY:O	1:B:105:PHE:HB3	2.21	0.41
1:B:105:PHE:HA	1:B:255:PHE:CD2	2.56	0.41
1:B:367:ARG:HG2	1:B:371:HIS:HD1	1.85	0.41
1:A:178:ILE:HG13	1:A:179:THR:N	2.35	0.41
1:A:233:ILE:HG23	1:A:233:ILE:O	2.21	0.41
1:A:117:LYS:HG2	1:A:120:ASP:OD2	2.20	0.40
1:A:206:ASP:OD2	3:A:501:PLP:N1	2.55	0.40
1:A:299:LEU:HD13	1:A:304:PHE:HE1	1.86	0.40

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	418/425 (98%)	400 (96%)	18 (4%)	0	100	100
1	B	419/425 (99%)	401 (96%)	17 (4%)	1 (0%)	47	68
2	C	133/138 (96%)	120 (90%)	10 (8%)	3 (2%)	6	10
2	D	130/138 (94%)	120 (92%)	8 (6%)	2 (2%)	10	18
All	All	1100/1126 (98%)	1041 (95%)	53 (5%)	6 (0%)	29	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	59	CYS
2	D	100	ASN
1	B	420	PHE

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Mol	Chain	Res	Type
2	C	15	LYS
2	D	98	ASP
2	C	80	GLU

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	369/372 (99%)	360 (98%)	9 (2%)	49	74
1	B	370/372 (100%)	358 (97%)	12 (3%)	39	65
2	C	119/121 (98%)	113 (95%)	6 (5%)	24	46
2	D	117/121 (97%)	114 (97%)	3 (3%)	46	72
All	All	975/986 (99%)	945 (97%)	30 (3%)	40	67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	53	TYR
1	A	105	PHE
1	A	117	LYS
1	A	119	GLU
1	A	178	ILE
1	A	219	LYS
1	A	367	ARG
1	A	400	TYR
1	B	11	PHE
1	B	12	SER
1	B	38	SER
1	B	53	TYR
1	B	58	SER
1	B	105	PHE
1	B	169	SER
1	B	215	LYS
1	B	220	LYS

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Mol	Chain	Res	Type
1	B	347	LYS
1	B	382	LYS
1	B	404	GLU
2	C	5	GLU
2	C	32	LEU
2	C	59	CYS
2	C	63	GLN
2	C	83	GLU
2	C	126	LYS
2	D	45	ASP
2	D	76	LYS
2	D	85	MET

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

Mol	Chain	Res	Type
1	B	352	HIS
2	C	0	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CSS	A	372	1	4,6,7	1.01	0	1,6,8	0.19	0
2	CSS	C	34	2	4,6,7	0.90	0	1,6,8	1.07	0
1	CSS	B	372	1	4,6,7	0.63	0	1,6,8	0.08	0
2	CSS	D	34	2	4,6,7	0.71	0	1,6,8	1.20	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
1	CSS	A	372	1	-	0/1/5/7	-
2	CSS	C	34	2	-	0/1/5/7	-
1	CSS	B	372	1	-	0/1/5/7	-
2	CSS	D	34	2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	34	CSS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PLP	B	501	1	15,15,16	2.56	3 (20%)	20,22,23	1.47	4 (20%)
4	PEG	A	503	-	6,6,6	0.62	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	A	501	1	15,15,16	2.59	4 (26%)	20,22,23	1.50	4 (20%)
4	PEG	A	502	-	6,6,6	0.54	0	5,5,5	0.26	0
5	GOL	B	502	-	5,5,5	0.33	0	5,5,5	0.47	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	PLP	B	501	1	-	2/6/6/8	0/1/1/1
4	PEG	A	503	-	-	2/4/4/4	-
3	PLP	A	501	1	-	2/6/6/8	0/1/1/1
4	PEG	A	502	-	-	2/4/4/4	-
5	GOL	B	502	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PLP	C3-C2	6.75	1.47	1.40
3	B	501	PLP	C5-C4	6.41	1.47	1.40
3	B	501	PLP	C3-C2	6.26	1.47	1.40
3	A	501	PLP	C5-C4	5.59	1.46	1.40
3	A	501	PLP	C3-C4	3.77	1.48	1.40
3	B	501	PLP	C3-C4	3.49	1.47	1.40
3	A	501	PLP	C4A-C4	-2.25	1.47	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PLP	O4P-C5A-C5	3.20	115.44	109.35
3	A	501	PLP	C6-N1-C2	3.18	125.05	119.17
3	B	501	PLP	C6-N1-C2	2.60	123.99	119.17
3	B	501	PLP	O4P-C5A-C5	2.55	114.21	109.35
3	A	501	PLP	O3P-P-O2P	2.47	117.08	107.64
3	A	501	PLP	O3-C3-C2	2.42	122.76	117.49
3	B	501	PLP	C4-C3-C2	-2.17	116.86	120.07
3	B	501	PLP	C6-C5-C4	2.05	119.77	118.16

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	PLP	C4-C5-C5A-O4P
5	B	502	GOL	C1-C2-C3-O3
5	B	502	GOL	O2-C2-C3-O3
4	A	503	PEG	O2-C3-C4-O4
4	A	502	PEG	O2-C3-C4-O4
3	B	501	PLP	C5A-O4P-P-O1P
3	A	501	PLP	C6-C5-C5A-O4P
4	A	503	PEG	O1-C1-C2-O2
4	A	502	PEG	O1-C1-C2-O2
3	B	501	PLP	C5A-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PLP	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 ⓘ

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, 95th 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	420/425 (98%)	-0.40	2 (0%) 91 91	19, 28, 49, 76	0
1	B	421/425 (99%)	-0.38	4 (0%) 82 84	18, 30, 49, 93	0
2	C	135/138 (97%)	0.27	11 (8%) 12 12	26, 53, 86, 100	0
2	D	132/138 (95%)	0.68	15 (11%) 5 4	33, 64, 91, 104	0
All	All	1108/1126 (98%)	-0.18	32 (2%) 51 55	18, 32, 75, 104	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	22	ASN	4.2
2	D	79	GLN	3.9
2	C	46	GLY	3.7
2	C	44	PHE	3.7
2	D	98	ASP	3.6
1	B	421	GLU	3.5
1	A	421	GLU	3.3
2	D	100	ASN	3.2
1	B	9	GLU	3.2
2	C	50	VAL	3.2
2	C	47	ASP	3.1
2	C	45	ASP	3.0
2	D	45	ASP	2.9
1	B	0	HIS	2.8
1	A	208	ALA	2.8
2	D	6	PHE	2.7
2	C	21	GLU	2.5
2	D	77	THR	2.5
2	D	1	MET	2.4
2	D	10	TYR	2.4
2	D	47	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	101	VAL	2.3
2	D	9	ASP	2.3
2	D	5	GLU	2.3
2	C	48	LYS	2.2
2	D	103	GLY	2.2
1	B	382	LYS	2.2
2	D	83	GLU	2.1
2	C	20	ILE	2.1
2	C	79	GLN	2.1
2	C	43	LEU	2.1
2	D	104	PRO	2.0

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, 95th 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
2	CSS	D	34	7/8	0.88	0.18	61,67,77,100	0
2	CSS	C	34	7/8	0.89	0.17	56,64,94,105	0
1	CSS	B	372	7/8	0.94	0.12	32,34,41,48	0
1	CSS	A	372	7/8	0.96	0.15	30,31,44,46	0

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, 95th 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
4	PEG	A	503	7/7	0.67	0.35	61,72,78,81	0
4	PEG	A	502	7/7	0.83	0.25	65,68,72,73	0
5	GOL	B	502	6/6	0.87	0.15	63,66,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PLP	A	501	15/16	0.98	0.20	23,25,27,29	0
3	PLP	B	501	15/16	0.98	0.17	22,30,36,37	0
6	ZN	C	202	1/1	1.00	0.06	31,31,31,31	0
6	ZN	C	201	1/1	1.00	0.06	25,25,25,25	0
6	ZN	D	201	1/1	1.00	0.07	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.