W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2016 – 06:22 AM EDT

PDB ID	:	5FEW
Title	:	HydE from T. maritima in complex with S-adenosyl-L-cysteine (final product)
Authors	:	Rohac, R.; Amara, P.; Benjdia, A.; Martin, L.; Ruffie, P.; Favier, A.; Berteau, O.; Mouesca, J.M.; Fontecilla-Camps, J.C.; Nicolet, Y.
Deposited on	:	2015-12-17
Resolution	:	1.17 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

http://wwpdb.org/validation/2016/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:

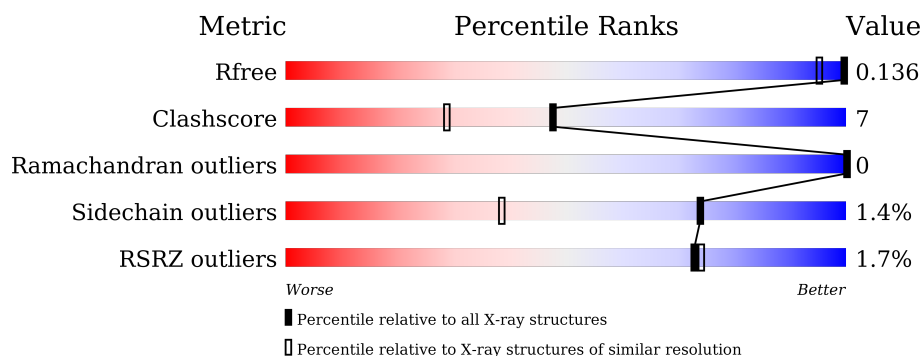|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027257
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027257

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.17 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	Percentile Ranks	Value
Rfree		0.136
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		1.4%
RSRZ outliers		1.7%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1018 (1.22-1.14)
Clashscore	102246	1094 (1.22-1.14)
Ramachandran outliers	100387	1047 (1.22-1.14)
Sidechain outliers	100360	1046 (1.22-1.14)
RSRZ outliers	91569	1020 (1.22-1.14)

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. 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	358	2%　81%　14%　·　·

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
3	CPS	A	406[A]	-	-	-	X
3	CPS	A	406[B]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MET	A	409[A]	-	-	-	X
7	SAH	A	411[B]	-	-	-	X
8	41K	A	412[B]	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3631 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 [FeFe] hydrogenase maturase subunit HydE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	346	2930	1872	502	537	19	0	33	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q9X0Z6
A	-8	TRP	-	expression tag	UNP Q9X0Z6
A	-7	SER	-	expression tag	UNP Q9X0Z6
A	-6	HIS	-	expression tag	UNP Q9X0Z6
A	-5	PRO	-	expression tag	UNP Q9X0Z6
A	-4	GLN	-	expression tag	UNP Q9X0Z6
A	-3	PHE	-	expression tag	UNP Q9X0Z6
A	-2	GLU	-	expression tag	UNP Q9X0Z6
A	-1	LYS	-	expression tag	UNP Q9X0Z6
A	0	ALA	-	expression tag	UNP Q9X0Z6
A	1	SER	-	expression tag	UNP Q9X0Z6
A	311	SER	CYS	engineered mutation	UNP Q9X0Z6
A	319	SER	CYS	engineered mutation	UNP Q9X0Z6
A	322	SER	CYS	engineered mutation	UNP Q9X0Z6

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
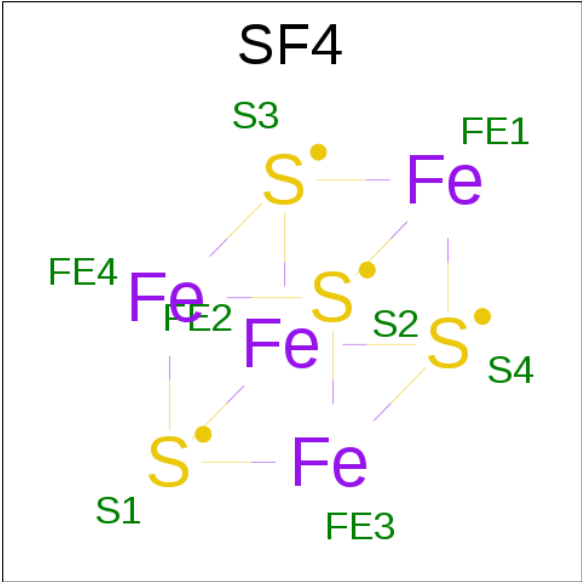
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4			0	0

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).
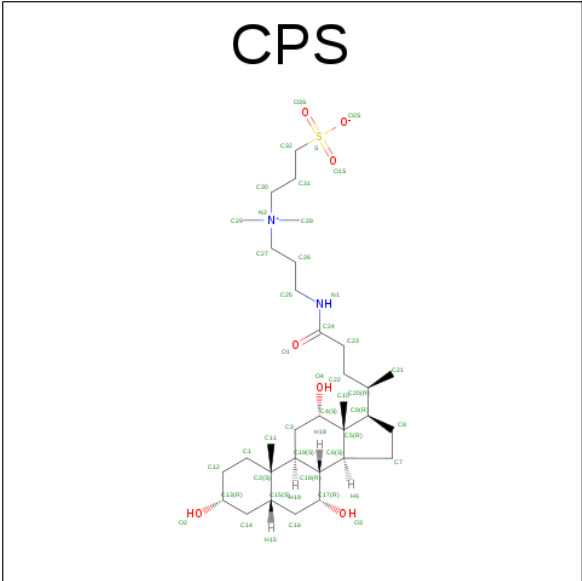
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total C N O S 42 32 2 7 1					0	0
3	A	1	Total C N O S 42 32 2 7 1					0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 29	C 24	N 1	O 4	0	0
3	A	1	Total 29	C 24	N 1	O 4	0	0
3	A	1	Total 50	C 44	O 6		0	1

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0

- Molecule 5 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).
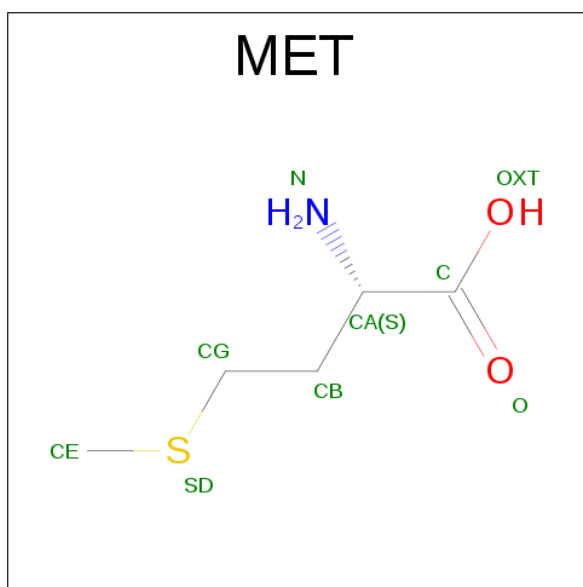
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 9	C 5	N 1	O 2	S 1	0	1

- Molecule 6 is S-adenosyl-L-cysteine (three-letter code: 5X8) (formula: $C_{13}H_{18}N_6O_5S$).
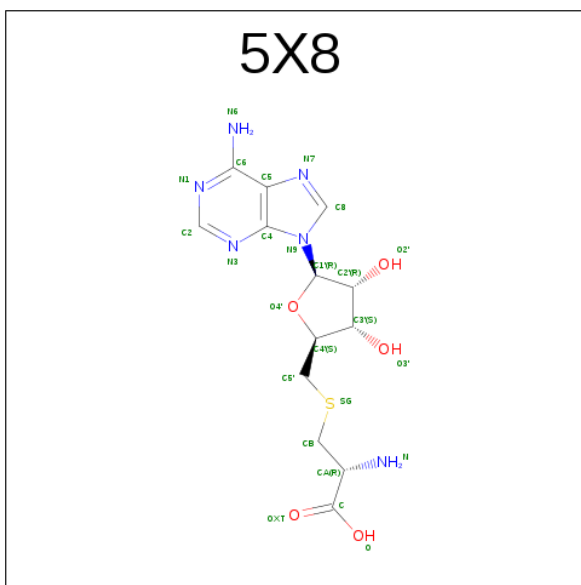
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	25	13	6	5	1	0	1

- Molecule 7 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).
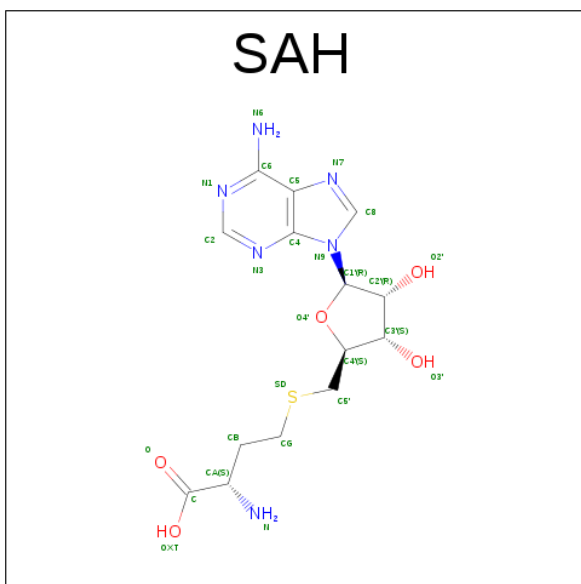
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	A	1	26	14	6	5	1	0	1

- Molecule 8 is (2R,4R)-2-methyl-1,3-thiazolidine-2,4-dicarboxylic acid (three-letter code: 41K) (formula: $C_6H_9NO_4S$).
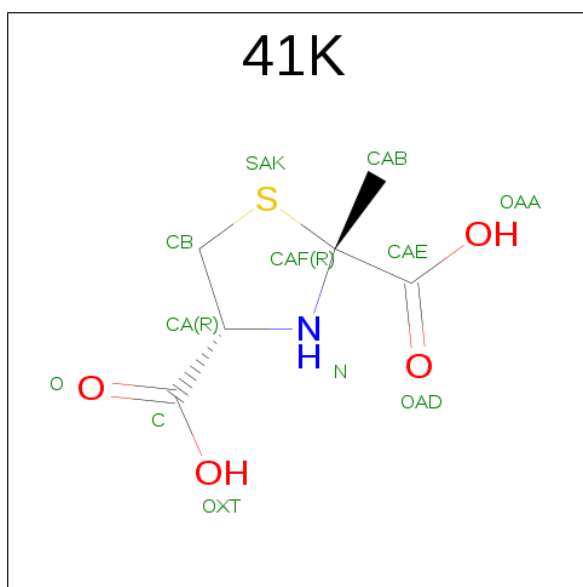
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 12	C 6	N 1	O 4	S 1	0	1

• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	424	Total 427	O 427	0	13

3 Residue-property plots ⓘ

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: [FeFe] hydrogenase maturase subunit HydE
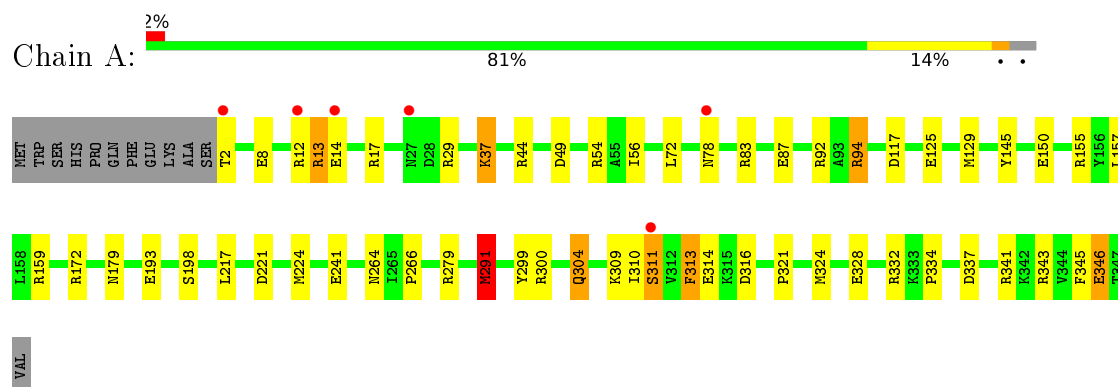
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.99Å 78.97Å 86.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 1.17	Depositor
	43.90 – 1.17	EDS
% Data completeness	99.7 (43.90-1.17)	Depositor
(in resolution range)	99.7 (43.90-1.17)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.13 (at 1.17Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.110 , 0.132	Depositor
	0.111 , 0.136	DCC
R_{free} test set	5529 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	11.7	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.6	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3631	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, CL, SF4, 5X8, 41K, CPS

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	1.82	14/3048 (0.5%)	1.33	36/4117 (0.9%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304[A]	GLN	CB-CG	50.52	2.88	1.52
1	A	304[B]	GLN	CB-CG	50.52	2.88	1.52
1	A	92	ARG	CZ-NH2	-8.01	1.22	1.33
1	A	346	GLU	CD-OE1	-7.18	1.17	1.25
1	A	13	ARG	CZ-NH2	6.79	1.41	1.33
1	A	328	GLU	CD-OE1	-6.63	1.18	1.25
1	A	341	ARG	CG-CD	-6.05	1.36	1.51
1	A	346	GLU	CD-OE2	-6.05	1.19	1.25
1	A	125	GLU	CD-OE1	-5.95	1.19	1.25
1	A	78[A]	ASN	C-O	5.93	1.34	1.23
1	A	78[B]	ASN	C-O	5.93	1.34	1.23
1	A	300	ARG	CZ-NH2	-5.85	1.25	1.33
1	A	241	GLU	CD-OE2	-5.50	1.19	1.25
1	A	17	ARG	CZ-NH1	5.16	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304[A]	GLN	CA-CB-CG	-19.09	71.39	113.40
1	A	304[B]	GLN	CA-CB-CG	-19.09	71.39	113.40
1	A	13	ARG	NE-CZ-NH1	-10.29	115.15	120.30
1	A	300	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	A	29	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	337	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	29	ARG	NE-CZ-NH2	-8.48	116.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	155	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	241	GLU	OE1-CD-OE2	-7.65	114.12	123.30
1	A	117	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	279	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	54	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	117	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	49	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	44	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	332	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	345	PHE	CB-CG-CD2	-6.41	116.32	120.80
1	A	83	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	299	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	A	72	LEU	CB-CG-CD2	6.17	121.50	111.00
1	A	291[A]	MET	CG-SD-CE	5.82	109.51	100.20
1	A	291[B]	MET	CG-SD-CE	5.82	109.51	100.20
1	A	94	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	A	343	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	313	PHE	CB-CG-CD1	5.65	124.75	120.80
1	A	221	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	44	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	92	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	279	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	299	TYR	CG-CD2-CE2	-5.43	116.95	121.30
1	A	145	TYR	CB-CG-CD1	5.27	124.16	121.00
1	A	172	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	155	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	193[A]	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	193[B]	GLU	OE1-CD-OE2	-5.02	117.28	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2930	0	2950	41	1
2	A	8	0	0	0	0
3	A	192	0	225	16	0
4	A	2	0	0	0	0
5	A	9	0	8	0	0
6	A	25	0	0	0	0
7	A	26	0	19	0	0
8	A	12	0	7	1	0
9	A	427	0	0	19	2
All	All	3631	0	3209	47	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 7.

All (47) 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:A:324[B]:MET:CE	3:A:406[B]:CPS:C11	2.34	1.04
1:A:324[B]:MET:HE2	3:A:406[B]:CPS:H11B	1.42	1.02
1:A:324[B]:MET:CE	3:A:406[B]:CPS:H11B	1.98	0.92
1:A:324[B]:MET:HE2	3:A:406[B]:CPS:C11	1.97	0.91
1:A:324[B]:MET:HE3	3:A:406[B]:CPS:C11	2.01	0.91
1:A:150:GLU:OE1	9:A:501:HOH:O	1.96	0.82
1:A:321:PRO:HB3	3:A:406[A]:CPS:H11A	1.66	0.77
1:A:334:PRO:HA	9:A:607[B]:HOH:O	1.88	0.73
1:A:309:LYS:CD	9:A:634:HOH:O	2.35	0.73
1:A:314:GLU:O	9:A:502[B]:HOH:O	2.07	0.71
1:A:157:LEU:HD23	1:A:224[A]:MET:HE2	1.72	0.71
1:A:314:GLU:OE2	9:A:503:HOH:O	2.08	0.71
1:A:87[B]:GLU:HG3	9:A:741:HOH:O	1.91	0.70
1:A:334:PRO:CA	9:A:607[B]:HOH:O	2.39	0.70
1:A:334:PRO:CB	9:A:607[B]:HOH:O	2.40	0.70
1:A:324[B]:MET:CE	3:A:406[B]:CPS:H11	2.24	0.64
1:A:217:LEU:HD11	9:A:504:HOH:O	1.97	0.62
1:A:157:LEU:CD2	1:A:224[A]:MET:HE2	2.29	0.62
1:A:159:ARG:NH2	8:A:412[B]:41K:OAA	2.28	0.62
1:A:12:ARG:NH2	9:A:506:HOH:O	2.32	0.61
1:A:291[B]:MET:CE	9:A:898:HOH:O	2.49	0.59
1:A:324[B]:MET:HE3	3:A:406[B]:CPS:H11A	1.84	0.56
1:A:291[B]:MET:HE1	9:A:898:HOH:O	2.03	0.56
1:A:266[B]:PRO:HG3	9:A:898:HOH:O	2.06	0.55
1:A:94:ARG:HG3	1:A:129[B]:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:406[B]:CPS:H16A	9:A:703:HOH:O	2.08	0.53
1:A:14:GLU:HG2	1:A:14:GLU:O	2.08	0.52
1:A:56[A]:ILE:HD12	1:A:291[A]:MET:HE1	1.90	0.52
3:A:406[A]:CPS:H21A	3:A:406[A]:CPS:H4	1.91	0.52
1:A:13:ARG:NH1	1:A:346:GLU:OE1	2.44	0.51
1:A:8:GLU:O	1:A:12:ARG:HG3	2.11	0.50
1:A:324[B]:MET:HE3	3:A:406[B]:CPS:H11	1.84	0.48
1:A:157:LEU:HD23	1:A:224[A]:MET:CE	2.41	0.48
1:A:37[A]:LYS:HE3	9:A:591:HOH:O	2.13	0.47
3:A:405:CPS:H21A	3:A:405:CPS:H4	1.97	0.47
1:A:324[B]:MET:HE2	3:A:406[B]:CPS:H11	1.88	0.47
1:A:157:LEU:CD2	1:A:224[A]:MET:CE	2.93	0.45
3:A:406[B]:CPS:H21A	3:A:406[B]:CPS:H4	1.99	0.44
1:A:56[A]:ILE:HD12	1:A:291[A]:MET:CE	2.47	0.44
1:A:198:SER:OG	9:A:504:HOH:O	2.21	0.43
1:A:179[A]:ASN:CG	9:A:505:HOH:O	2.57	0.43
1:A:304[A]:GLN:HB3	9:A:728:HOH:O	2.19	0.43
1:A:291[B]:MET:HE3	9:A:898:HOH:O	2.15	0.42
1:A:224[B]:MET:HA	1:A:264:ASN:O	2.19	0.41
3:A:403[A]:CPS:H31A	3:A:403[A]:CPS:H272	1.85	0.41
3:A:404:CPS:H21A	3:A:404:CPS:H4	2.02	0.40
1:A:310:ILE:O	1:A:311:SER:CB	2.70	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)
9:A:738:HOH:O	9:A:865:HOH:O[2_655]	1.94	0.26
1:A:313:PHE:O	9:A:737:HOH:O[3_755]	1.97	0.23

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	374/358 (104%)	363 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	320/313 (102%)	314 (98%)	6 (2%)	65	25

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	37[A]	LYS
1	A	37[B]	LYS
1	A	291[A]	MET
1	A	291[B]	MET
1	A	311	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	#$|Z| > 2$
2	SF4	A	401	1,5,7	0,12,12	0.00	-	0,24,24	0.00	-
3	CPS	A	402	-	45,45,45	1.95	7 (15%)	69,70,70	1.28	8 (11%)
3	CPS	A	403[A]	-	45,45,45	1.65	7 (15%)	69,70,70	1.63	16 (23%)
3	CPS	A	404	-	32,32,45	1.10	1 (3%)	51,51,70	0.99	2 (3%)
3	CPS	A	405	-	32,32,45	1.32	2 (6%)	51,51,70	1.51	6 (11%)
3	CPS	A	406[A]	-	28,28,45	1.80	7 (25%)	46,46,70	2.28	20 (43%)
3	CPS	A	406[B]	-	28,28,45	1.25	3 (10%)	46,46,70	1.46	10 (21%)
5	MET	A	409[A]	2	5,8,8	0.89	0	3,9,9	1.17	0
6	5X8	A	410[A]	-	21,27,27	1.45	4 (19%)	18,39,39	1.95	5 (27%)
7	SAH	A	411[B]	2	22,28,28	1.33	3 (13%)	18,40,40	2.14	7 (38%)
8	41K	A	412[B]	4	4,12,12	1.81	2 (50%)	2,18,18	1.88	1 (50%)

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	SF4	A	401	1,5,7	-	0/0/48/48	0/6/5/5
3	CPS	A	402	-	-	0/25/90/90	0/4/4/4
3	CPS	A	403[A]	-	-	0/25/90/90	0/4/4/4
3	CPS	A	404	-	-	0/9/74/90	0/4/4/4
3	CPS	A	405	-	-	0/9/74/90	0/4/4/4
3	CPS	A	406[A]	-	-	0/4/69/90	0/4/4/4
3	CPS	A	406[B]	-	-	0/4/69/90	0/4/4/4
5	MET	A	409[A]	2	-	0/4/8/8	0/0/0/0
6	5X8	A	410[A]	-	-	0/6/30/30	0/3/3/3
7	SAH	A	411[B]	2	-	0/7/31/31	0/3/3/3
8	41K	A	412[B]	4	-	0/0/21/21	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	CPS	C32-S	-9.97	1.62	1.77
3	A	403[A]	CPS	C32-S	-6.30	1.68	1.77
3	A	406[A]	CPS	C18-C17	-4.56	1.45	1.53
3	A	403[A]	CPS	O3S-S	-3.81	1.34	1.45
3	A	406[A]	CPS	C3-C4	-3.56	1.47	1.53
3	A	406[B]	CPS	C5-C6	-3.40	1.49	1.55
7	A	411[B]	SAH	CG-SD	-3.19	1.69	1.81
6	A	410[A]	5X8	C4-N3	-2.94	1.31	1.35
3	A	402	CPS	C14-C15	-2.88	1.48	1.53
8	A	412[B]	41K	CB-SAK	-2.73	1.77	1.80
3	A	406[B]	CPS	C16-C17	-2.57	1.48	1.52
3	A	403[A]	CPS	C24-N1	-2.47	1.27	1.33
7	A	411[B]	SAH	O4'-C4'	-2.37	1.39	1.45
3	A	402	CPS	C20-C9	-2.30	1.50	1.54
3	A	406[A]	CPS	C2-C19	-2.23	1.51	1.56
3	A	403[A]	CPS	C18-C6	-2.22	1.49	1.53
3	A	406[B]	CPS	C7-C6	-2.06	1.50	1.54
3	A	402	CPS	C12-C13	-2.03	1.46	1.51
3	A	403[A]	CPS	C14-C15	-2.00	1.50	1.53
3	A	406[A]	CPS	C18-C19	2.21	1.58	1.53
6	A	410[A]	5X8	O3'-C3'	2.26	1.48	1.43
3	A	402	CPS	C31-C32	2.28	1.59	1.52
3	A	403[A]	CPS	C25-N1	2.30	1.51	1.46
8	A	412[B]	41K	CAF-N	2.31	1.48	1.46
3	A	406[A]	CPS	C14-C13	2.33	1.56	1.51
3	A	406[A]	CPS	C11-C2	2.35	1.58	1.54
3	A	406[A]	CPS	O3-C17	2.44	1.48	1.43
3	A	403[A]	CPS	C20-C9	2.47	1.58	1.54
3	A	405	CPS	C23-C24	2.57	1.61	1.51
6	A	410[A]	5X8	O4'-C4'	2.59	1.51	1.45
3	A	402	CPS	C29-N2	2.97	1.57	1.50
3	A	402	CPS	C1-C2	3.00	1.59	1.54
3	A	404	CPS	O4-C4	3.06	1.48	1.43
3	A	405	CPS	C3-C4	3.06	1.58	1.53
6	A	410[A]	5X8	C2'-C1'	3.29	1.58	1.53
7	A	411[B]	SAH	C5-C4	3.36	1.48	1.40

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	CPS	C3-C19-C2	-5.42	108.13	113.77
3	A	406[A]	CPS	C22-C20-C9	-5.40	97.89	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	410[A]	5X8	C1'-N9-C4	-5.38	120.80	126.81
3	A	402	CPS	O1S-S-C32	-4.27	103.85	106.87
3	A	406[A]	CPS	C8-C9-C5	-4.24	99.50	103.59
3	A	406[A]	CPS	C9-C5-C4	-4.04	114.13	117.68
3	A	402	CPS	O3S-S-C32	-4.04	104.01	106.87
3	A	406[A]	CPS	C3-C19-C2	-3.93	109.68	113.77
3	A	406[A]	CPS	C11-C2-C1	-3.71	101.95	108.23
3	A	403[A]	CPS	O2S-S-O1S	-3.68	103.11	111.26
3	A	403[A]	CPS	O1-C24-C23	-3.60	115.71	121.97
3	A	406[A]	CPS	C14-C13-C12	-3.24	106.38	110.53
3	A	403[A]	CPS	C23-C22-C20	-3.05	108.79	114.46
3	A	403[A]	CPS	C25-N1-C24	-2.98	116.88	122.79
6	A	410[A]	5X8	O4'-C4'-C3'	-2.93	99.23	105.16
3	A	406[B]	CPS	C10-C5-C9	-2.87	106.68	111.20
6	A	410[A]	5X8	N3-C2-N1	-2.86	126.62	128.87
6	A	410[A]	5X8	C4'-O4'-C1'	-2.86	106.61	109.64
6	A	410[A]	5X8	O2'-C2'-C1'	-2.69	103.21	111.61
3	A	402	CPS	C29-N2-C27	-2.63	102.51	109.42
3	A	405	CPS	C19-C3-C4	-2.63	111.08	114.38
3	A	406[B]	CPS	C1-C2-C15	-2.63	104.87	107.76
3	A	406[A]	CPS	C1-C12-C13	-2.61	106.94	110.41
3	A	406[A]	CPS	C5-C6-C18	-2.59	111.33	114.73
3	A	403[A]	CPS	C5-C9-C20	-2.57	116.30	119.44
7	A	411[B]	SAH	O3'-C3'-C4'	-2.39	103.88	111.01
3	A	402	CPS	C23-C24-N1	-2.30	112.46	116.46
3	A	406[A]	CPS	C8-C7-C6	-2.29	100.51	105.11
3	A	405	CPS	C5-C6-C18	-2.26	111.76	114.73
3	A	406[A]	CPS	C10-C5-C4	-2.22	106.87	109.09
7	A	411[B]	SAH	O4'-C4'-C3'	-2.21	100.67	105.16
3	A	402	CPS	C26-C25-N1	-2.20	106.06	112.29
3	A	406[A]	CPS	C14-C15-C2	-2.18	110.32	112.66
3	A	403[A]	CPS	C22-C23-C24	-2.17	108.30	113.26
3	A	405	CPS	C23-C24-N1	-2.10	109.46	116.54
3	A	406[A]	CPS	C19-C3-C4	-2.08	111.77	114.38
3	A	406[B]	CPS	C14-C13-C12	-2.07	107.88	110.53
3	A	404	CPS	C23-C22-C20	-2.04	110.67	114.46
3	A	403[A]	CPS	C21-C20-C9	-2.00	109.90	112.99
3	A	402	CPS	C3-C19-C2	-2.00	111.69	113.77
3	A	406[B]	CPS	C6-C5-C4	2.02	109.20	107.37
3	A	402	CPS	C31-C32-S	2.04	116.47	113.15
3	A	406[A]	CPS	C16-C15-C2	2.05	114.86	112.66
3	A	406[B]	CPS	C7-C6-C5	2.09	105.61	103.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	406[A]	CPS	C1-C2-C19	2.10	114.77	111.43
3	A	406[B]	CPS	C10-C5-C6	2.12	114.54	111.20
3	A	404	CPS	C1-C2-C15	2.18	110.16	107.76
3	A	406[B]	CPS	C3-C19-C18	2.23	113.98	110.77
3	A	406[A]	CPS	C21-C20-C9	2.23	118.33	112.35
3	A	403[A]	CPS	C21-C20-C22	2.28	114.03	110.33
7	A	411[B]	SAH	C2'-C3'-C4'	2.31	107.36	102.64
3	A	403[A]	CPS	C3-C19-C18	2.39	114.21	110.77
3	A	403[A]	CPS	C19-C18-C6	2.51	113.16	109.63
3	A	406[B]	CPS	C11-C2-C19	2.64	114.68	111.20
8	A	412[B]	41K	CB-SAK-CAF	2.64	96.48	91.36
3	A	406[A]	CPS	C19-C18-C17	2.73	115.19	111.89
3	A	405	CPS	C23-C22-C20	2.74	119.55	114.46
3	A	406[A]	CPS	C7-C8-C9	2.76	110.67	105.11
3	A	403[A]	CPS	O2S-S-C32	2.79	110.78	104.99
3	A	402	CPS	C29-N2-C30	2.84	116.89	109.42
3	A	403[A]	CPS	C23-C24-N1	2.90	121.50	116.46
3	A	406[A]	CPS	C11-C2-C19	3.02	115.19	111.20
3	A	403[A]	CPS	C31-C32-S	3.07	118.15	113.15
3	A	406[B]	CPS	C14-C15-C2	3.30	116.19	112.66
3	A	406[B]	CPS	C12-C1-C2	3.33	118.78	112.81
7	A	411[B]	SAH	C4'-O4'-C1'	3.35	113.20	109.64
3	A	405	CPS	C6-C5-C4	3.39	110.44	107.37
7	A	411[B]	SAH	C5'-C4'-C3'	3.46	123.95	114.98
3	A	403[A]	CPS	C9-C5-C4	3.48	120.73	117.68
3	A	406[A]	CPS	C3-C19-C18	3.52	115.83	110.77
3	A	403[A]	CPS	O3S-S-C32	3.57	109.39	106.87
7	A	411[B]	SAH	C1'-N9-C4	3.62	130.85	126.81
3	A	403[A]	CPS	C8-C9-C5	3.67	107.13	103.59
3	A	406[A]	CPS	C6-C5-C4	4.03	111.02	107.37
7	A	411[B]	SAH	C4'-C5'-SD	4.58	127.64	113.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403[A]	CPS	1	0
3	A	404	CPS	1	0
3	A	405	CPS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406[A]	CPS	2	0
3	A	406[B]	CPS	11	0
8	A	412[B]	41K	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, 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	346/358 (96%)	-0.15	6 (1%)	73	74	9, 14, 28, 46	12 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	SER	3.7
1	A	78[A]	ASN	3.4
1	A	2	THR	2.5
1	A	27[A]	ASN	2.3
1	A	14	GLU	2.2
1	A	12	ARG	2.1

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, 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	LLDF	B-factors(Å²)	Q<0.9
3	CPS	A	406[B]	25/42	0.88	0.15	4.95	18,21,30,37	25
5	MET	A	409[A]	9/9	0.97	0.11	4.88	12,14,19,20	9
3	CPS	A	406[A]	25/42	0.88	0.15	4.49	9,11,14,16	25
7	SAH	A	411[B]	26/26	0.97	0.08	2.40	5,11,14,15	26
8	41K	A	412[B]	12/12	0.98	0.09	2.37	11,16,19,22	12
4	CL	A	408	1/1	0.97	0.08	1.01	27,27,27,27	1
6	5X8	A	410[A]	25/25	0.97	0.07	0.98	13,15,20,22	25
3	CPS	A	403[A]	42/42	0.95	0.08	0.54	12,16,25,37	13
3	CPS	A	405	29/42	0.93	0.10	0.44	14,17,24,46	0
3	CPS	A	404	29/42	0.96	0.07	0.35	12,14,39,43	0
3	CPS	A	402	42/42	0.97	0.07	-0.19	9,13,24,31	5
2	SF4	A	401	8/8	1.00	0.04	-1.69	11,11,12,12	0
4	CL	A	407	1/1	0.99	0.03	-3.73	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.