



Full wwPDB X-ray Structure Validation Report

Jun 19, 2014 – 09:06 AM EDT

PDB ID : 4M6X
Title : Mutant structure of methyltransferase from *Streptomyces hygroscopicus* complexed with S-adenosyl-L-homocysteine and methylphenylpyruvic acid
Authors : Liu, Y.C.; Zou, X.W.; Chan, H.C.; Huang, C.J.; Li, T.L.
Deposited on : 2013-08-12
Resolution : 2.30 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

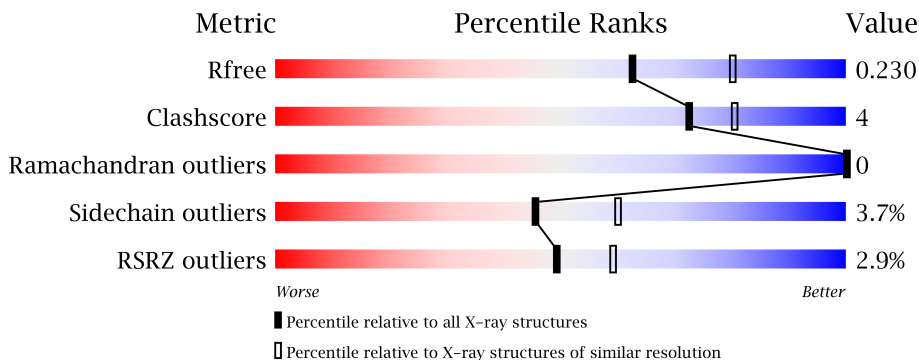
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	56D	B	402	-	X
6	CA	B	406	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5768 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

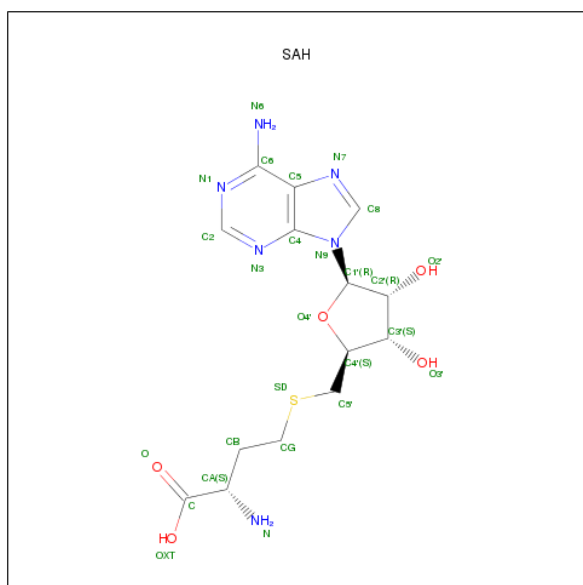
- Molecule 1 is a protein called Methyltransferase MppJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2639	1665	470	492	12			
1	B	333	Total	C	N	O	S	0	0	0
			2593	1639	462	481	11			

There are 4 discrepancies between the modelled and reference sequences:

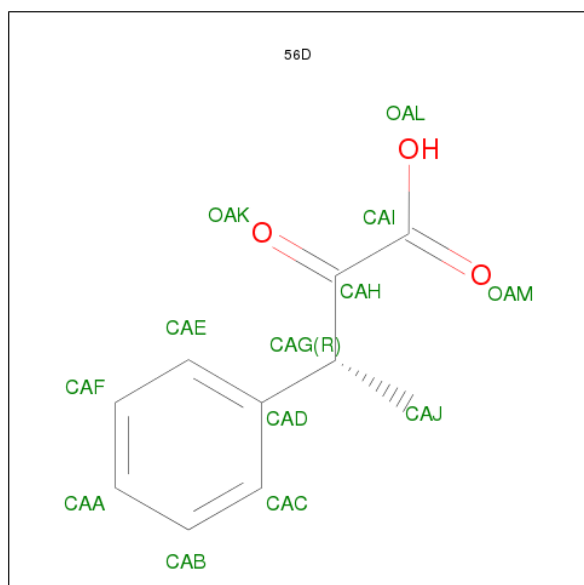
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q643C8
A	0	HIS	-	EXPRESSION TAG	UNP Q643C8
A	244	GLU	ASP	ENGINEERED MUTATION	UNP Q643C8
B	244	GLU	ASP	ENGINEERED MUTATION	UNP Q643C8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is (3R)-2-OXO-3-PHENYLBUTANOICACID (three-letter code: 56D) (formula: $C_{10}H_{10}O_3$).

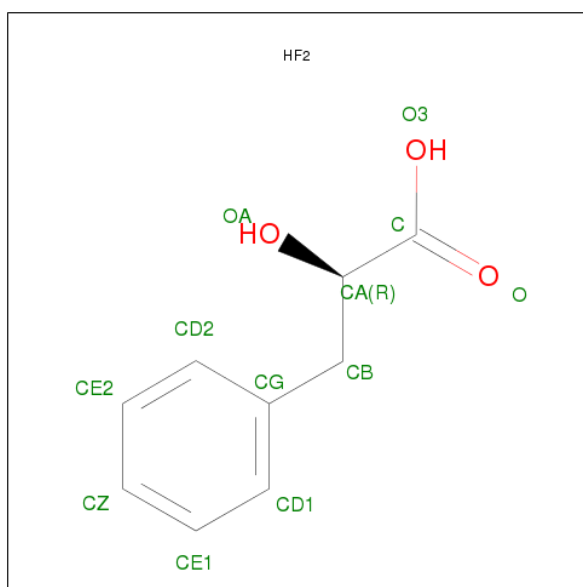


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	10	3		
3	B	1	Total	C	O	0	0
			13	10	3		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is (2R)-2-HYDROXY-3-PHENYLPROPANOICACID (three-letter code: HF2) (formula: $C_9H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	9	3		
5	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Ca	0	0
			3	3		
6	A	2	Total	Ca	0	0
			2	2		

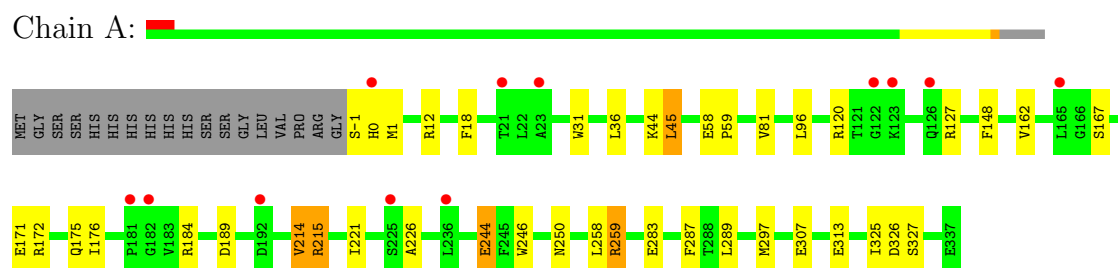
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	196	Total	O	0	0
			196	196		
7	B	231	Total	O	0	0
			231	231		

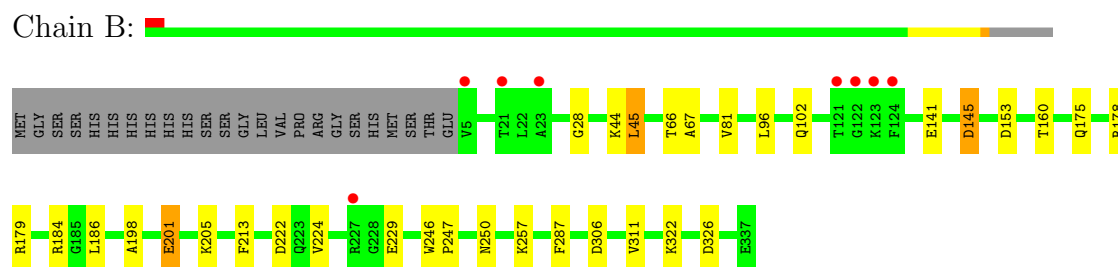
3 Residue-property plots

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: Methyltransferase MppJ



- Molecule 1: Methyltransferase MppJ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.01Å 90.22Å 136.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.94 – 2.30 27.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.94-2.30) 99.6 (27.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.162 , 0.227 0.168 , 0.230	Depositor DCC
R_{free} test set	1616 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31880 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5768	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SAH, 56D, HF2, FE

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	0.52	0/2699	0.69	0/3652
1	B	0.53	0/2652	0.72	1/3589 (0.0%)
All	All	0.52	0/5351	0.71	1/7241 (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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	45	LEU	CA-CB-CG	6.48	130.21	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2552	28	0
1	B	2593	0	2510	18	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
3	A	13	0	0	0	0
3	B	13	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	7	0	0
5	B	12	0	7	2	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
7	A	196	0	0	6	0
7	B	231	0	0	2	0
All	All	5768	0	5114	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:153:ASP:OD1	1:B:179:ARG:NH2	2.08	0.86
1:A:1:MET:HA	7:A:686:HOH:O	1.90	0.70
1:A:244:GLU:HG2	7:A:624:HOH:O	1.92	0.70
1:A:325:ILE:O	7:A:644:HOH:O	2.08	0.70
1:A:148:PHE:HZ	1:A:176:ILE:HD11	1.61	0.65
1:A:120:ARG:NH2	1:A:297:MET:O	2.34	0.61
1:B:160:THR:HG22	7:B:602:HOH:O	2.00	0.60
1:B:186:LEU:HD22	1:B:229:GLU:HG2	1.83	0.59
1:A:214:VAL:HG11	1:A:226:ALA:HB2	1.87	0.56
1:B:322:LYS:HE3	5:B:404:HF2:HA	1.87	0.56
1:A:0:HIS:ND1	1:A:0:HIS:N	2.48	0.56
1:A:148:PHE:CZ	1:A:176:ILE:HD11	2.41	0.55
1:A:96:LEU:HD13	1:A:287:PHE:HB2	1.90	0.54
1:B:96:LEU:HD13	1:B:287:PHE:HB2	1.91	0.53
1:A:120:ARG:NH1	7:A:646:HOH:O	2.26	0.51
1:B:322:LYS:CE	5:B:404:HF2:HA	2.41	0.51
1:A:0:HIS:NE2	1:A:283:GLU:OE2	2.44	0.50
1:B:246:TRP:HA	1:B:247:PRO:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:GLU:OE2	1:A:175:GLN:NE2	2.46	0.49
1:A:172:ARG:O	1:A:176:ILE:HG12	2.13	0.48
1:A:45:LEU:CD2	1:A:81:VAL:HB	2.45	0.47
1:A:259:ARG:O	1:A:259:ARG:HD3	2.15	0.46
1:A:45:LEU:HD23	1:A:45:LEU:C	2.35	0.46
1:B:198:ALA:HB1	1:B:213:PHE:CZ	2.50	0.46
1:A:0:HIS:O	7:A:686:HOH:O	2.20	0.45
1:B:184:ARG:HD2	7:B:666:HOH:O	2.15	0.45
1:A:221:ILE:HG21	1:A:258:LEU:HD23	1.98	0.45
1:B:250:ASN:H	1:B:250:ASN:HD22	1.64	0.45
1:A:127:ARG:HD3	7:A:538:HOH:O	2.16	0.45
1:A:162:VAL:HG11	1:A:176:ILE:HG21	1.99	0.44
1:A:31:TRP:HB2	1:A:36:LEU:HD12	1.99	0.44
1:B:201:GLU:HG3	1:B:205:LYS:HE2	2.00	0.43
1:A:45:LEU:HD22	1:A:81:VAL:HB	2.01	0.42
1:A:189:ASP:O	1:A:215:ARG:HA	2.20	0.42
1:B:141:GLU:O	1:B:145:ASP:HB2	2.20	0.42
1:B:222:ASP:OD2	1:B:257:LYS:HE3	2.20	0.42
1:A:289:LEU:HD21	1:B:67:ALA:HA	2.02	0.41
1:B:175:GLN:HE22	1:B:178:ARG:HH11	1.68	0.41
2:A:401:SAH:HG1	2:A:401:SAH:H4'	1.58	0.41
1:A:58:GLU:N	1:A:59:PRO:CD	2.83	0.41
1:A:250:ASN:H	1:A:250:ASN:HD22	1.67	0.41
1:A:246:TRP:CH2	1:A:307:GLU:HB3	2.56	0.41
1:B:44:LYS:HA	1:B:81:VAL:O	2.21	0.40
1:A:18:PHE:CZ	1:B:287:PHE:HA	2.56	0.40
1:B:28:GLY:HA3	1:B:102:GLN:NE2	2.36	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	337/357 (94%)	325 (96%)	12 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	331/357 (93%)	321 (97%)	10 (3%)	0	100	100
All	All	668/714 (94%)	646 (97%)	22 (3%)	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	270/285 (95%)	258 (96%)	12 (4%)	39	51
1	B	264/285 (93%)	256 (97%)	8 (3%)	53	70
All	All	534/570 (94%)	514 (96%)	20 (4%)	45	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	12	ARG
1	A	44	LYS
1	A	45	LEU
1	A	167	SER
1	A	184	ARG
1	A	214	VAL
1	A	215	ARG
1	A	244	GLU
1	A	259	ARG
1	A	313	GLU
1	A	327	SER
1	B	45	LEU
1	B	66	THR
1	B	145	ASP
1	B	201	GLU
1	B	224	VAL
1	B	306	ASP
1	B	311	VAL
1	B	326	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	250	ASN
1	A	264	ASN
1	B	92	HIS
1	B	102	GLN
1	B	119	ASN
1	B	175	GLN
1	B	250	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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, 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	339/357 (94%)	-0.05	12 (3%)	42 52	22, 35, 61, 89	0
1	B	333/357 (93%)	-0.27	8 (2%)	56 66	20, 29, 48, 73	0
All	All	672/714 (94%)	-0.16	20 (2%)	49 58	20, 31, 56, 89	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	GLN	4.4
1	B	227	ARG	3.7
1	B	5	VAL	3.3
1	A	122	GLY	3.1
1	B	123	LYS	2.8
1	A	181	PRO	2.8
1	A	182	GLY	2.8
1	A	23	ALA	2.7
1	A	165	LEU	2.6
1	B	21	THR	2.6
1	A	236	LEU	2.6
1	A	192	ASP	2.5
1	B	124	PHE	2.4
1	A	225	SER	2.3
1	A	123	LYS	2.3
1	A	21	THR	2.3
1	B	122	GLY	2.2
1	B	121	THR	2.1
1	B	23	ALA	2.1
1	A	0	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	CA	B	406	1/1	0.12	3.17	73,73,73,73	0
3	56D	B	402	13/13	0.18	2.91	33,45,47,47	0
3	56D	A	402	13/13	0.17	1.70	51,56,60,66	0
5	HF2	A	404	12/12	0.11	0.33	31,34,36,40	0
4	FE	A	403	1/1	0.08	-0.33	32,32,32,32	0
2	SAH	B	401	26/26	0.10	-0.45	28,33,48,52	0
6	CA	B	407	1/1	0.09	-0.78	77,77,77,77	0
2	SAH	A	401	26/26	0.10	-0.92	36,45,68,71	0
6	CA	B	405	1/1	0.06	-1.19	71,71,71,71	0
5	HF2	B	404	12/12	0.08	-1.20	31,35,38,39	0
6	CA	A	406	1/1	0.10	-1.64	69,69,69,69	0
4	FE	B	403	1/1	0.08	-1.73	28,28,28,28	0
6	CA	A	405	1/1	0.04	-1.96	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.