



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:56 AM UTC

PDB ID : 5CJM / pdb_00005cjm
Title : Crystal structure of Mycobacterium tuberculosis malate synthase in complex with 4H-thieno[3,2-b]pyrrole-5-carboxylic acid
Authors : Huang, H.-L.; Sacchettini, J.C.
Deposited on : 2015-07-14
Resolution : 2.13 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

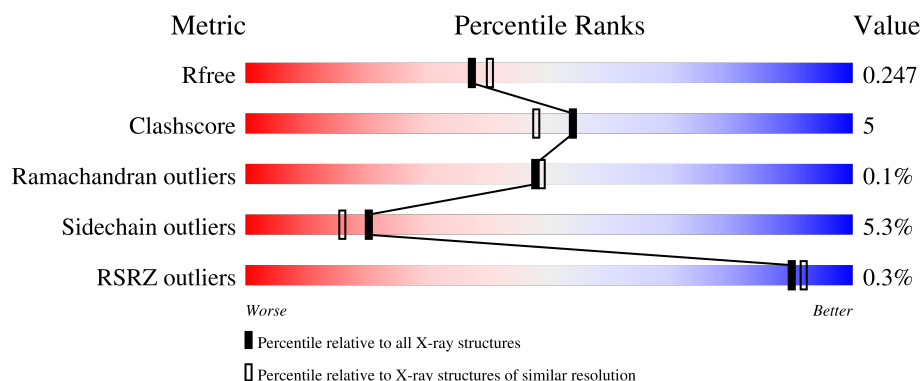
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	741	 81% 13% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5835 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 Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	711	5446	3417	959	1048	22	0	1	0

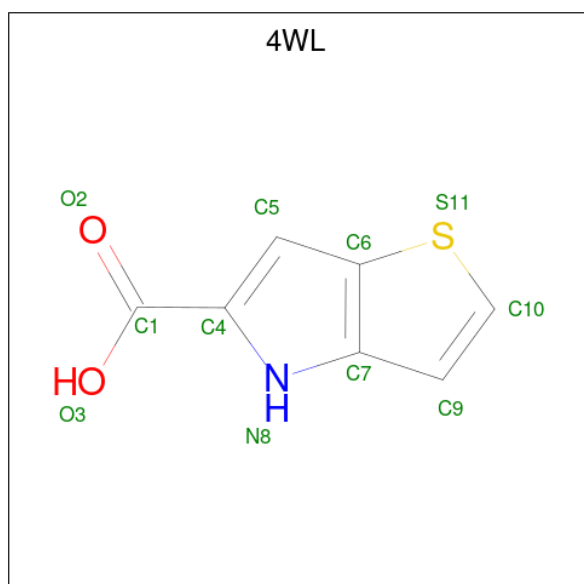
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	ALA	CYS	engineered mutation	UNP P9WK17

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 4H-THIENO[3,2-B]PYROLE-5-CARBOXYLIC ACID (CCD ID: 4WL) (formula: C₇H₅NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			11	7	1	2	1		

- Molecule 4 is water.

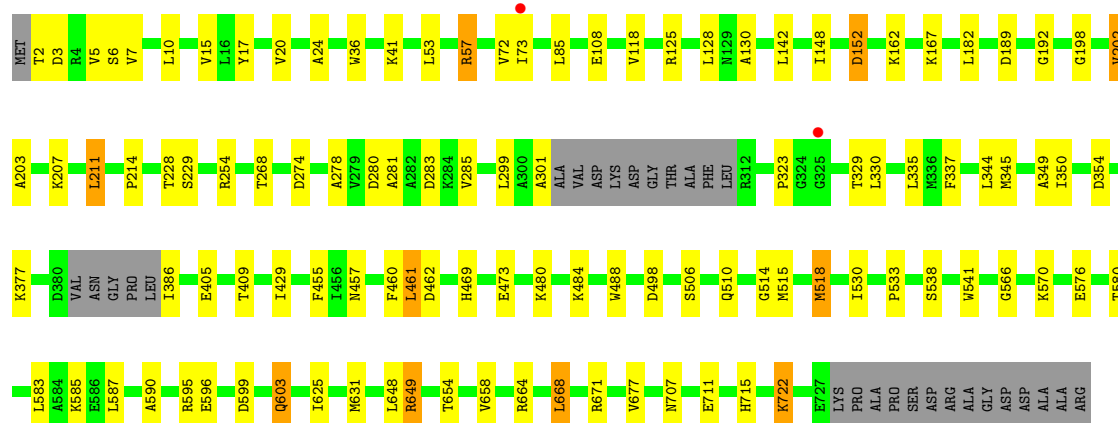
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	376	Total	O	0	0
			376	376		

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: Malate synthase G

Chain A:  81% 13% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.78Å 80.78Å 226.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.22 – 2.13 40.22 – 2.13	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.22-2.13) 98.2 (40.22-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.219 , 0.301 (Not available) , 0.247	Depositor DCC
R_{free} test set	2126 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5835	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CSO, MG, 4WL

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	0.50	0/5543	0.87	7/7534 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	LEU	N-CA-C	5.79	117.28	110.97
1	A	337	PHE	N-CA-C	-5.56	101.97	110.14
1	A	514	GLY	N-CA-C	5.52	121.58	112.30
1	A	274	ASP	N-CA-C	5.21	118.74	112.38
1	A	344	LEU	N-CA-C	5.11	116.70	111.03
1	A	590	ALA	CA-C-N	5.01	126.11	119.84
1	A	590	ALA	C-N-CA	5.01	126.11	119.84

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	5446	0	5386	53	0
2	A	2	0	0	0	0
3	A	11	0	4	2	0
4	A	376	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5835	0	5390	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 5.

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:A:386:ILE:N	4:A:903:HOH:O	2.18	0.75
1:A:480:LYS:O	4:A:902:HOH:O	2.10	0.69
1:A:299:LEU:O	4:A:901:HOH:O	2.10	0.67
1:A:53:LEU:HD22	1:A:405:GLU:HG2	1.78	0.65
1:A:211:LEU:HD13	1:A:214:PRO:HA	1.79	0.64
1:A:518:MET:SD	4:A:1213:HOH:O	2.55	0.64
1:A:211:LEU:HD12	1:A:211:LEU:H	1.63	0.62
1:A:386:ILE:N	4:A:914:HOH:O	2.30	0.62
1:A:57:ARG:HD2	1:A:405:GLU:OE1	2.00	0.62
1:A:455:PHE:CZ	1:A:457:ASN:HB2	2.37	0.60
1:A:7:VAL:HG11	1:A:36:TRP:HB3	1.82	0.60
1:A:345:MET:HE2	1:A:711:GLU:HB3	1.87	0.56
1:A:530:ILE:O	1:A:533:PRO:HD2	2.06	0.56
1:A:603:GLN:HG2	1:A:625:ILE:HB	1.88	0.55
1:A:108:GLU:HB2	1:A:335:LEU:HD13	1.89	0.54
1:A:280:ASP:OD2	1:A:722:LYS:NZ	2.41	0.54
1:A:281:ALA:HB2	1:A:349:ALA:HA	1.91	0.53
1:A:15:VAL:HG22	1:A:285:VAL:HG11	1.93	0.51
1:A:498:ASP:OD2	4:A:904:HOH:O	2.19	0.50
1:A:473:GLU:OE2	1:A:649:ARG:NH2	2.42	0.49
1:A:377:LYS:NZ	4:A:936:HOH:O	2.44	0.49
1:A:72:VAL:HG23	1:A:73:ILE:HG13	1.95	0.48
1:A:20:VAL:HA	1:A:24:ALA:HB3	1.95	0.48
1:A:5:VAL:HG21	1:A:17:TYR:CD2	2.50	0.47
1:A:130:ALA:HB1	1:A:268:THR:HG21	1.96	0.47
1:A:192:GLY:N	1:A:203:ALA:HB3	2.30	0.47
1:A:469:HIS:CD2	1:A:707:ASN:HA	2.49	0.47
1:A:142:LEU:HB3	1:A:148:ILE:HD13	1.97	0.47
1:A:668:LEU:HD22	1:A:671:ARG:HH22	1.80	0.46
1:A:198:GLY:HA2	1:A:323:PRO:O	2.15	0.46
1:A:707:ASN:ND2	4:A:910:HOH:O	2.27	0.46
1:A:278:ALA:HA	1:A:283:ASP:HB3	1.98	0.45
1:A:631:MET:O	3:A:803:4WL:H5	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ASP:OD1	1:A:664:ARG:NH2	2.47	0.45
1:A:125:ARG:CZ	1:A:301:ALA:HB1	2.47	0.45
1:A:668:LEU:HD22	1:A:671:ARG:NH2	2.32	0.45
1:A:182:LEU:HD22	1:A:202:VAL:HG11	1.99	0.44
1:A:715:HIS:NE2	4:A:924:HOH:O	2.36	0.44
1:A:108:GLU:OE2	1:A:108:GLU:N	2.44	0.43
1:A:167:LYS:HG3	4:A:907:HOH:O	2.18	0.43
1:A:10:LEU:HD13	1:A:350:ILE:HG21	2.00	0.43
1:A:189:ASP:HA	1:A:254:ARG:HH21	1.84	0.42
1:A:462:ASP:N	4:A:946:HOH:O	2.52	0.42
1:A:460:PHE:CD2	1:A:461:LEU:HD23	2.55	0.42
1:A:484:LYS:HG3	4:A:902:HOH:O	2.18	0.42
1:A:409:THR:HG21	1:A:429:ILE:HD12	2.01	0.42
1:A:455:PHE:HD1	1:A:510:GLN:HB2	1.84	0.41
1:A:566:GLY:O	1:A:570:LYS:NZ	2.53	0.41
1:A:118:VAL:HG11	3:A:803:4WL:H9	2.02	0.41
1:A:329:THR:O	1:A:330:LEU:HD23	2.20	0.41
1:A:488:TRP:HB3	1:A:580:THR:O	2.20	0.41
1:A:515:MET:HE2	1:A:541:TRP:HB3	2.03	0.41
1:A:654:THR:O	1:A:658:VAL:HG23	2.20	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	705/741 (95%)	679 (96%)	25 (4%)	1 (0%)	48 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASP

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	572/592 (97%)	542 (95%)	30 (5%)	21	16

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	ASP
1	A	6	SER
1	A	41	LYS
1	A	57	ARG
1	A	85	LEU
1	A	128	LEU
1	A	152	ASP
1	A	162	LYS
1	A	202	VAL
1	A	207	LYS
1	A	211	LEU
1	A	228	THR
1	A	229	SER
1	A	354	ASP
1	A	506	SER
1	A	518	MET
1	A	538	SER
1	A	576	GLU
1	A	583	LEU
1	A	585	LYS
1	A	587	LEU
1	A	595	ARG
1	A	596	GLU
1	A	603	GLN
1	A	648	LEU
1	A	649	ARG
1	A	668	LEU
1	A	677	VAL
1	A	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	83	GLN
1	A	129	ASN
1	A	340	ASN
1	A	685	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSO	A	410	1	3,6,7	0.53	0	1,6,8	1.23	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	CSO	A	410	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	4WL	A	803	-	12,12,12	2.05	2 (16%)	15,17,17	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4WL	A	803	-	-	0/4/4/4	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	4WL	C4-C1	5.48	1.61	1.48
3	A	803	4WL	C7-C6	2.71	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	4WL	C5-C6-S11	2.17	144.32	135.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	4WL	2	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	710/741 (95%)	-0.32	2 (0%) 90 92	10, 24, 47, 69	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	GLY	3.1
1	A	73	ILE	2.3

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
1	CSO	A	410	7/8	0.91	0.06	14,15,20,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	4WL	A	803	11/11	0.91	0.06	17,28,32,46	0
2	MG	A	802	1/1	0.95	0.04	12,12,12,12	0
2	MG	A	801	1/1	0.95	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.