



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:23 AM UTC

PDB ID : 4I6W / pdb_00004i6w
Title : 3-hydroxy-3-methylglutaryl (HMG) Coenzyme-A reductase complexed with
thioimevalonate
Authors : Steussy, C.N.; Stauffacher, C.V.; Schmidt, T.; Burgner II, J.W.; Rodwell,
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Deposited on : 2012-11-30
Resolution : 1.66 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

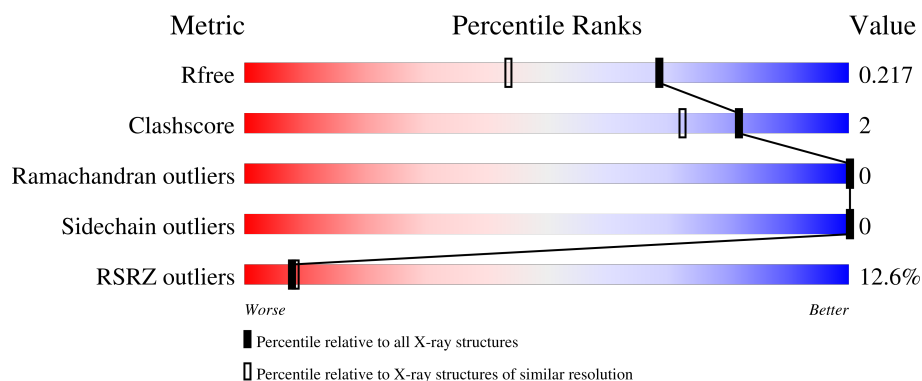
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	428	
1	B	428	

2 Entry composition [i](#)

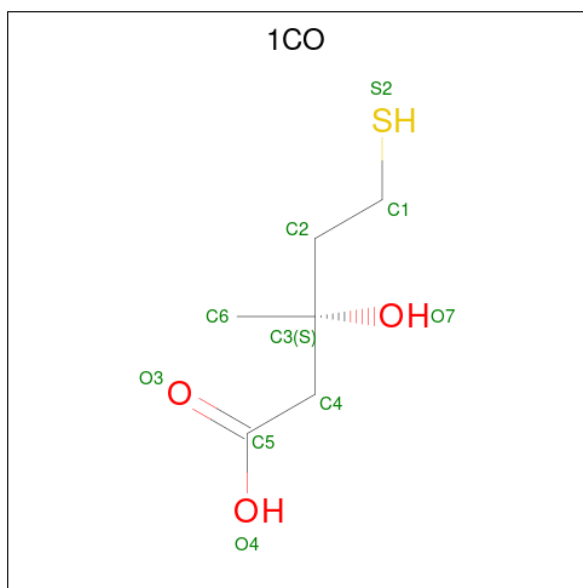
There are 5 unique types of molecules in this entry. The entry contains 6340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	2	0
			2784	1743	504	522	15			
1	B	376	Total	C	N	O	S	0	1	0
			2797	1751	505	526	15			

- Molecule 2 is (3S)-3-hydroxy-3-methyl-5-sulfanylpentanoic acid (CCD ID: 1CO) (formula: C₆H₁₂O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			10	6	3	1		
2	B	1	Total	C	O	S	0	0
			10	6	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

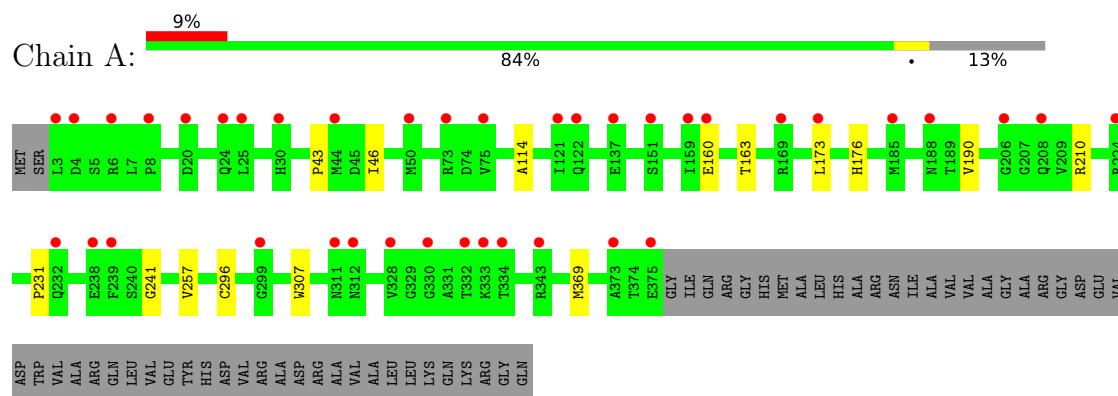
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	376	Total 380	O 380	0	4
5	B	325	Total 327	O 327	0	2

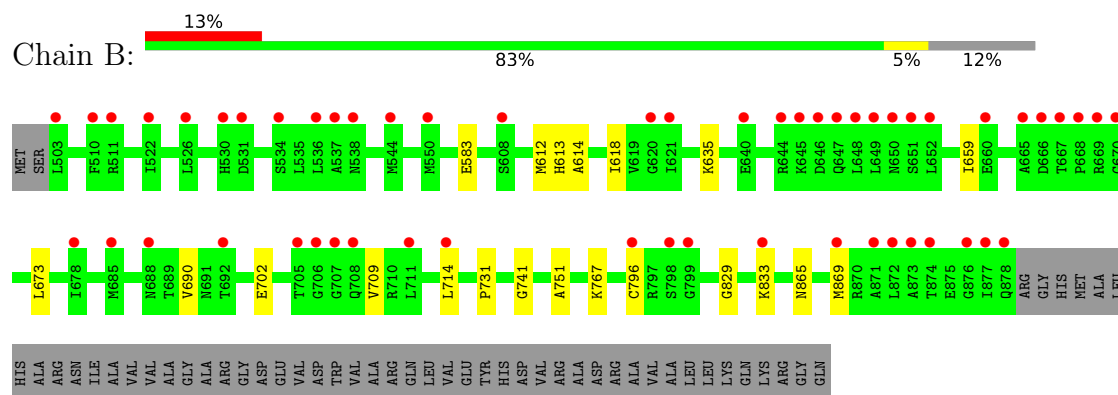
3 Residue-property plots [i](#)

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: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	226.10Å 226.10Å 226.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 – 1.66 38.78 – 1.66	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.78-1.66) 99.4 (38.78-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.193 , 0.218 0.193 , 0.217	Depositor DCC
R_{free} test set	2527 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6340	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: SO4, GOL, 1CO

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	0.45	0/2830	0.74	0/3849
1	B	0.44	0/2840	0.77	0/3863
All	All	0.44	0/5670	0.75	0/7712

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	2784	0	2827	12	0
1	B	2797	0	2836	16	0
2	A	10	0	11	0	0
2	B	10	0	11	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	380	0	0	1	0
5	B	327	0	0	1	0
All	All	6340	0	5701	28	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 (28) 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:B:612:MET:HE3	1:B:714:LEU:HD11	1.54	0.89
1:B:829:GLY:H	1:B:833:LYS:HE3	1.45	0.80
1:B:635:LYS:HG3	1:B:659:ILE:HG12	1.69	0.74
1:A:307:TRP:NE1	1:A:369:MET:HE1	2.08	0.68
1:B:583:GLU:OE2	2:B:1001:1CO:S2	2.49	0.65
1:B:618:ILE:HD12	1:B:673:LEU:HD22	1.83	0.61
1:A:296[B]:CYS:SG	1:A:296[B]:CYS:O	2.61	0.59
1:B:614:ALA:HB2	1:B:690:VAL:HB	1.85	0.57
1:A:114:ALA:HB2	1:A:190:VAL:HB	1.86	0.57
1:A:163:THR:HG22	1:A:173:LEU:HD13	1.88	0.56
1:B:731:PRO:O	1:B:741:GLY:HA3	2.07	0.54
1:A:163:THR:HG22	1:A:173:LEU:CD1	2.39	0.53
1:B:796[A]:CYS:SG	1:B:796[A]:CYS:O	2.66	0.53
1:B:612:MET:HE3	1:B:714:LEU:CD1	2.34	0.52
1:A:210:ARG:HD2	5:B:1414:HOH:O	2.12	0.50
1:B:829:GLY:N	1:B:833:LYS:HE3	2.19	0.49
1:A:231:PRO:O	1:A:241:GLY:HA3	2.12	0.49
1:A:160:GLU:HG3	1:A:176:HIS:HB2	1.96	0.47
1:A:307:TRP:CD1	1:A:369:MET:HE1	2.50	0.47
1:A:257:VAL:HG13	5:A:716:HOH:O	2.15	0.46
1:B:751:ALA:HB3	1:B:869:MET:HE2	1.98	0.45
1:B:767:LYS:NZ	2:B:1001:1CO:S2	2.81	0.45
1:B:613:HIS:O	1:B:714:LEU:HD12	2.19	0.42
1:A:43:PRO:HG2	1:A:46:ILE:HG12	2.02	0.42
1:B:865:ASN:O	1:B:869:MET:HG3	2.20	0.42
1:B:702:GLU:HG3	1:B:709:VAL:HG23	2.01	0.41
1:B:829:GLY:H	1:B:833:LYS:CE	2.23	0.41
1:A:369:MET:HB2	1:A:369:MET:HE3	1.82	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	373/428 (87%)	363 (97%)	10 (3%)	0	100	100
1	B	375/428 (88%)	366 (98%)	9 (2%)	0	100	100
All	All	748/856 (87%)	729 (98%)	19 (2%)	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	288/327 (88%)	288 (100%)	0	100	100
1	B	289/327 (88%)	289 (100%)	0	100	100
All	All	577/654 (88%)	577 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	115	GLN
1	A	126	ASN
1	A	150	ASN
1	B	567	ASN
1	B	662	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands 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	$\# Z > 2$
3	SO4	B	1003	-	4,4,4	0.44	0	6,6,6	0.10	0
3	SO4	B	1002	-	4,4,4	0.39	0	6,6,6	0.20	0
2	1CO	A	501	-	8,9,9	0.92	0	7,12,12	0.99	0
3	SO4	A	502	-	4,4,4	0.42	0	6,6,6	0.27	0
3	SO4	A	503	-	4,4,4	0.42	0	6,6,6	0.09	0
4	GOL	A	504	-	5,5,5	0.30	0	5,5,5	0.26	0
4	GOL	B	1004	-	5,5,5	0.31	0	5,5,5	0.18	0
2	1CO	B	1001	-	8,9,9	0.95	0	7,12,12	1.79	1 (14%)

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
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	1004	-	-	2/4/4/4	-
2	1CO	B	1001	-	-	3/9/9/9	-
2	1CO	A	501	-	-	1/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	1CO	C2-C1-S2	-4.26	109.30	113.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	1CO	S2-C1-C2-C3
2	B	1001	1CO	S2-C1-C2-C3
4	B	1004	GOL	C1-C2-C3-O3
4	B	1004	GOL	O2-C2-C3-O3
2	B	1001	1CO	C3-C4-C5-O4
2	B	1001	1CO	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	1CO	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

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	373/428 (87%)	0.49	39 (10%)	11 12	10, 23, 37, 51	28 (7%)
1	B	376/428 (87%)	0.67	55 (14%)	6 6	11, 26, 48, 72	28 (7%)
All	All	749/856 (87%)	0.58	94 (12%)	8 8	10, 24, 45, 72	56 (7%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	ILE	12.2
1	A	75	VAL	11.3
1	A	159	ILE	10.2
1	B	648	LEU	8.6
1	B	669	ARG	8.2
1	A	334	THR	8.2
1	A	169	ARG	8.1
1	A	151	SER	7.7
1	B	608	SER	7.6
1	B	685	MET	7.2
1	A	332	THR	7.0
1	B	550	MET	6.9
1	B	833	LYS	6.7
1	A	44	MET	6.5
1	B	647	GLN	6.5
1	A	137	GLU	6.5
1	A	188	ASN	6.4
1	A	122	GLN	6.3
1	A	160	GLU	6.2
1	B	660	GLU	6.2
1	A	50	MET	6.0
1	B	544	MET	6.0
1	A	224	ARG	5.6
1	B	878	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	665	ALA	4.8
1	B	645	LYS	4.7
1	B	646	ASP	4.7
1	B	649	LEU	4.4
1	B	537	ALA	4.1
1	B	536	LEU	4.0
1	B	871	ALA	3.9
1	B	640	GLU	3.8
1	A	311	ASN	3.6
1	A	6	ARG	3.6
1	B	799	GLY	3.5
1	B	538	ASN	3.4
1	B	666	ASP	3.4
1	B	650	ASN	3.4
1	A	343[A]	ARG	3.3
1	B	711	LEU	3.3
1	B	872	LEU	3.2
1	B	869	MET	3.0
1	A	185	MET	3.0
1	B	877	ILE	3.0
1	A	330	GLY	3.0
1	A	173	LEU	2.9
1	B	503	LEU	2.9
1	B	707	GLY	2.9
1	B	798	SER	2.8
1	A	299	GLY	2.8
1	B	644	ARG	2.8
1	A	232	GLN	2.7
1	A	312	ASN	2.7
1	B	688	ASN	2.7
1	A	239	PHE	2.6
1	B	651	SER	2.6
1	B	714	LEU	2.6
1	B	873	ALA	2.6
1	B	652	LEU	2.5
1	A	208	GLN	2.5
1	B	534	SER	2.5
1	B	670	GLY	2.5
1	B	705	THR	2.5
1	B	874	THR	2.5
1	B	706	GLY	2.4
1	B	667	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	121	ILE	2.4
1	A	333	LYS	2.4
1	A	30	HIS	2.4
1	A	8	PRO	2.4
1	A	24	GLN	2.3
1	B	708	GLN	2.3
1	B	620	GLY	2.3
1	A	3	LEU	2.3
1	A	25	LEU	2.3
1	B	876	GLY	2.3
1	A	375	GLU	2.2
1	B	531	ASP	2.2
1	B	796[A]	CYS	2.2
1	A	238	GLU	2.1
1	A	73	ARG	2.1
1	A	4	ASP	2.1
1	A	20	ASP	2.1
1	B	668	PRO	2.1
1	B	511	ARG	2.1
1	B	526	LEU	2.1
1	B	692	THR	2.1
1	A	206	GLY	2.1
1	A	328	VAL	2.1
1	A	373	ALA	2.0
1	B	510	PHE	2.0
1	B	522	ILE	2.0
1	B	621	ILE	2.0
1	B	530	HIS	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 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	SO4	B	1003	5/5	0.74	0.12	68,68,69,69	0
3	SO4	A	503	5/5	0.79	0.14	69,70,71,72	0
4	GOL	A	504	6/6	0.85	0.14	28,36,38,42	0
4	GOL	B	1004	6/6	0.87	0.13	31,37,39,40	0
2	1CO	B	1001	10/10	0.88	0.12	21,25,34,41	0
3	SO4	B	1002	5/5	0.89	0.12	33,33,35,37	0
2	1CO	A	501	10/10	0.89	0.11	24,27,34,40	0
3	SO4	A	502	5/5	0.90	0.16	27,29,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.