



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 2OWN / pdb_00002own
Title : Crystal structure of oleoyl thioesterase (putative) (NP_784467.1) from Lactobacillus plantarum at 2.00 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-02-16
Resolution : 2.00 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

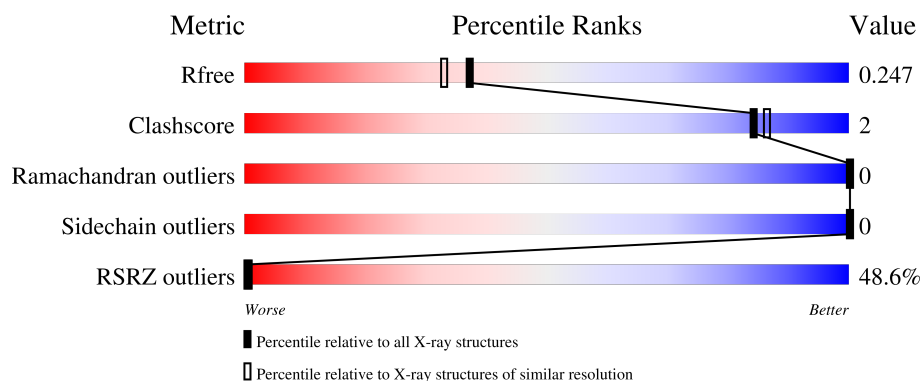
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	262	23% 94% .
1	B	262	71% 89% 10% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4679 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 Putative Oleoyl-[acyl-carrier protein] thioesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	Se	0	4	0
			2062	1321	343	391	3	4			
1	B	258	Total	C	N	O	S	Se	0	3	0
			2070	1322	349	392	3	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q88YP1
A	1	MSE	MET	modified residue	UNP Q88YP1
A	54	MSE	MET	modified residue	UNP Q88YP1
A	74	MSE	MET	modified residue	UNP Q88YP1
A	118	MSE	MET	modified residue	UNP Q88YP1
A	119	MSE	MET	modified residue	UNP Q88YP1
B	0	GLY	-	expression tag	UNP Q88YP1
B	1	MSE	MET	modified residue	UNP Q88YP1
B	54	MSE	MET	modified residue	UNP Q88YP1
B	74	MSE	MET	modified residue	UNP Q88YP1
B	118	MSE	MET	modified residue	UNP Q88YP1
B	119	MSE	MET	modified residue	UNP Q88YP1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			9	9		
4	B	1	Total	O	0	0
			9	9		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	245	Total	O	0	0
			245	245		
6	B	198	Total	O	0	0
			198	198		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	106.52Å 106.52Å 234.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.55 – 2.00 72.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.55-2.00) 99.6 (72.55-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.242 0.209 , 0.247	Depositor DCC
R_{free} test set	2725 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.131	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	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4679	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 3.00% 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: ACT, GOL, UNL, SO4

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	1.03	0/2120	1.18	4/2896 (0.1%)
1	B	1.08	0/2125	1.19	3/2903 (0.1%)
All	All	1.06	0/4245	1.18	7/5799 (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	B	87	GLY	N-CA-C	-6.21	98.46	113.18
1	A	87	GLY	N-CA-C	-5.93	99.14	113.18
1	B	72	THR	N-CA-C	-5.82	104.30	111.40
1	A	72	THR	N-CA-C	-5.81	103.68	112.04
1	A	89	ALA	N-CA-C	5.73	116.97	108.60
1	B	88	SER	N-CA-C	5.32	116.76	111.07
1	A	91	ASN	CB-CA-C	5.16	120.33	110.17

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	2062	0	2004	4	0
1	B	2070	0	1997	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	0	0	0
2	B	5	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	1	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	30	0	40	0	0
5	B	18	0	24	0	0
6	A	245	0	0	0	0
6	B	198	0	0	0	0
All	All	4679	0	4071	19	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 (19) 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:3:THR:HG23	1:B:6:ALA:HB2	1.65	0.77
1:B:3:THR:CG2	1:B:6:ALA:HB2	2.35	0.56
1:B:218:VAL:HG12	1:B:241:VAL:HG22	1.89	0.54
1:B:167:VAL:HG21	1:B:212:VAL:HG12	1.95	0.48
1:A:167:VAL:HG21	1:A:212:VAL:HG12	1.96	0.48
1:B:218:VAL:HG12	1:B:241:VAL:CG2	2.45	0.47
1:B:94:PHE:CE1	3:B:263:ACT:H1	2.51	0.46
1:B:83:ILE:HG23	1:B:101:ILE:HD13	1.99	0.45
1:B:71:ILE:HD13	1:B:74:MSE:SE	2.67	0.44
1:A:172:ILE:HD13	1:A:178[B]:VAL:HG22	1.98	0.44
1:B:63:VAL:HG21	1:B:119:MSE:HG3	2.00	0.44
1:B:118:MSE:HE1	1:B:133:LEU:CD1	2.49	0.42
1:B:68:ALA:HB3	1:B:113:THR:OG1	2.19	0.42
1:B:10:LEU:HD11	1:B:84:ALA:HB1	2.00	0.42
1:B:37:ALA:HB1	1:B:99:PHE:CD2	2.56	0.41
1:B:60:VAL:CG1	1:B:127:VAL:HG21	2.51	0.41
1:A:83:ILE:HG23	1:A:101:ILE:HD13	2.02	0.41
1:A:83:ILE:HG23	1:A:101:ILE:CD1	2.51	0.40
1:B:83:ILE:HG23	1:B:101:ILE:CD1	2.51	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	258/262 (98%)	253 (98%)	5 (2%)	0	100	100
1	B	257/262 (98%)	250 (97%)	7 (3%)	0	100	100
All	All	515/524 (98%)	503 (98%)	12 (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	224/228 (98%)	224 (100%)	0	100	100
1	B	223/228 (98%)	223 (100%)	0	100	100
All	All	447/456 (98%)	447 (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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	B	66	GLN
1	B	108	GLN
1	B	121	GLN
1	B	166	HIS
1	B	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are unknown - leaving 16 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	$\# Z > 2$
5	GOL	B	267	-	5,5,5	0.39	0	5,5,5	0.56	0
5	GOL	A	273	-	5,5,5	0.37	0	5,5,5	0.50	0
5	GOL	A	270	5	5,5,5	0.40	0	5,5,5	0.43	0
2	SO4	A	265	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	B	262	-	4,4,4	0.21	0	6,6,6	0.12	0
3	ACT	B	263	-	3,3,3	0.81	0	3,3,3	1.49	0
5	GOL	B	265	-	5,5,5	0.39	0	5,5,5	0.25	0
2	SO4	A	263	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	262	-	4,4,4	0.30	0	6,6,6	0.27	0
2	SO4	A	266	-	4,4,4	0.24	0	6,6,6	0.08	0
5	GOL	A	269	5	5,5,5	0.40	0	5,5,5	0.43	0
3	ACT	A	267	-	3,3,3	0.81	0	3,3,3	1.37	0
5	GOL	A	272	-	5,5,5	0.41	0	5,5,5	0.66	0
2	SO4	A	264	-	4,4,4	0.23	0	6,6,6	0.12	0
5	GOL	A	271	-	5,5,5	0.52	0	5,5,5	0.67	0
5	GOL	B	266	-	5,5,5	0.37	0	5,5,5	0.54	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
5	GOL	B	267	-	-	0/4/4/4	-
5	GOL	A	273	-	-	4/4/4/4	-
5	GOL	A	270	5	-	2/4/4/4	-
5	GOL	B	265	-	-	0/4/4/4	-
5	GOL	A	269	5	-	0/4/4/4	-
5	GOL	A	272	-	-	2/4/4/4	-
5	GOL	A	271	-	-	0/4/4/4	-
5	GOL	B	266	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	270	GOL	C1-C2-C3-O3
5	A	272	GOL	C1-C2-C3-O3
5	A	273	GOL	O1-C1-C2-C3
5	A	272	GOL	O1-C1-C2-O2
5	A	273	GOL	O1-C1-C2-O2
5	A	270	GOL	O2-C2-C3-O3
5	A	273	GOL	C1-C2-C3-O3
5	A	273	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	263	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

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	252/262 (96%)	1.50	60 (23%)	2 2	21, 36, 54, 66	4 (1%)
1	B	254/262 (96%)	2.99	186 (73%)	0 0	20, 35, 53, 65	3 (1%)
All	All	506/524 (96%)	2.25	246 (48%)	0 1	20, 36, 54, 66	7 (1%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	THR	7.3
1	B	174	PRO	7.2
1	B	126	ILE	7.0
1	B	59	GLY	6.7
1	B	177	HIS	6.6
1	B	178	VAL	6.6
1	B	260	ILE	6.5
1	B	141	VAL	6.5
1	B	4	LEU	6.0
1	B	193	ALA	5.8
1	B	131	PRO	5.8
1	A	174	PRO	5.5
1	B	93	TYR	5.4
1	B	192	PRO	5.4
1	B	90	TYR	5.4
1	A	173	ASP	5.3
1	B	92	PRO	5.3
1	B	256	LEU	5.3
1	B	197	LEU	5.3
1	A	3	THR	5.2
1	B	194	THR	5.2
1	B	122	THR	5.2
1	B	23	ASP	5.1
1	A	122	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	195	PHE	5.0
1	A	123	THR	5.0
1	B	243	ASP	4.8
1	B	255	THR	4.8
1	B	124	ARG	4.8
1	B	62	TRP	4.8
1	B	121	GLN	4.8
1	B	127	VAL	4.8
1	A	126	ILE	4.7
1	B	173	ASP	4.7
1	B	242	ASP	4.7
1	B	63	VAL	4.7
1	B	24	ARG	4.7
1	B	175	ASN	4.7
1	B	53	GLU	4.6
1	A	124	ARG	4.6
1	B	142	VAL	4.6
1	B	191	LEU	4.6
1	B	25	THR	4.6
1	B	76	ARG	4.5
1	B	241	VAL	4.5
1	B	52	THR	4.5
1	B	261	GLN	4.4
1	B	106	GLY	4.4
1	B	170	PHE	4.4
1	B	196	LEU	4.4
1	B	20	TYR	4.4
1	B	160	THR	4.3
1	B	56	GLN	4.3
1	B	26	GLY	4.3
1	B	75	PRO	4.3
1	B	27	ARG	4.2
1	A	228	GLU	4.2
1	B	22	CYS	4.2
1	B	117	VAL	4.2
1	B	94	PHE	4.1
1	A	215	GLY	4.1
1	B	158	ASP	4.1
1	B	8	ALA	4.1
1	B	19	TYR	4.1
1	B	3	THR	4.1
1	B	259	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	176	ARG	4.0
1	B	199	HIS	4.0
1	B	218	VAL	4.0
1	B	140	GLU	4.0
1	B	202	VAL	4.0
1	A	178[A]	VAL	3.9
1	B	81	VAL	3.9
1	A	143	LYS	3.9
1	B	87	GLY	3.9
1	B	6	ALA	3.9
1	B	144	ARG	3.9
1	A	177	HIS	3.8
1	B	28	ALA	3.8
1	B	198	GLN	3.8
1	B	71	ILE	3.8
1	B	172	ILE	3.8
1	B	101	ILE	3.8
1	B	166	HIS	3.8
1	B	5	GLY	3.7
1	A	180	ASN	3.7
1	B	224	ILE	3.7
1	B	215	GLY	3.7
1	B	120	SER	3.7
1	B	61	GLY	3.7
1	B	78	ASP	3.7
1	B	156	ALA	3.7
1	B	48	LEU	3.6
1	A	125	ARG	3.6
1	B	147[A]	ARG	3.6
1	B	18	THR	3.6
1	B	132	GLU	3.6
1	B	188	VAL	3.5
1	B	229	VAL	3.5
1	B	42	GLU	3.5
1	B	109	LEU	3.5
1	B	189	ASP	3.5
1	B	80	VAL	3.5
1	B	258	GLU	3.5
1	B	17	ILE	3.5
1	A	27	ARG	3.5
1	B	16	ARG	3.5
1	B	128	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	139	SER	3.4
1	B	73	ARG	3.4
1	A	257	PRO	3.4
1	B	145	ILE	3.4
1	B	257	PRO	3.4
1	A	176	ARG	3.4
1	B	254	ARG	3.4
1	B	95	ALA	3.4
1	B	77	GLN	3.4
1	B	65	THR	3.4
1	B	214	TYR	3.4
1	B	201	LEU	3.4
1	A	258	GLU	3.3
1	B	60	VAL	3.3
1	B	230	ALA	3.3
1	B	58	HIS	3.3
1	B	233	VAL	3.3
1	B	30	LEU	3.3
1	B	72	THR	3.3
1	B	225	LEU	3.3
1	A	175	ASN	3.3
1	B	107	GLN	3.3
1	A	226	PRO	3.2
1	A	230	ALA	3.2
1	B	253	TRP	3.1
1	B	161	ILE	3.1
1	A	73	ARG	3.1
1	B	10	LEU	3.1
1	B	129	ILE	3.1
1	B	102[A]	ARG	3.1
1	B	200	ASP	3.1
1	B	209	GLU	3.1
1	A	229	VAL	3.0
1	B	88	SER	3.0
1	A	172	ILE	3.0
1	B	7	ASN	2.9
1	B	36	ILE	2.9
1	B	32	THR	2.9
1	A	243	ASP	2.9
1	B	29	THR	2.9
1	B	184	PHE	2.9
1	B	227	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	167	VAL	2.8
1	B	190	THR	2.8
1	A	127	VAL	2.8
1	A	254[A]	ARG	2.8
1	B	222	ALA	2.8
1	A	131	PRO	2.8
1	A	134	VAL	2.8
1	B	100	TRP	2.8
1	B	14	GLN	2.8
1	A	130	LEU	2.8
1	B	136	PRO	2.8
1	A	129	ILE	2.8
1	B	116	TRP	2.8
1	B	231	ASP	2.7
1	B	31	THR	2.7
1	A	242	ASP	2.7
1	A	227	SER	2.7
1	B	134	VAL	2.7
1	A	42	GLU	2.6
1	B	47	ALA	2.6
1	B	133	LEU	2.6
1	A	120	SER	2.6
1	A	121	GLN	2.6
1	B	135	ALA	2.6
1	B	159	THR	2.6
1	A	153	SER	2.6
1	B	234	THR	2.6
1	B	57	SER	2.6
1	B	165	TYR	2.6
1	A	194	THR	2.6
1	B	244	GLU	2.5
1	A	179	ASN	2.5
1	B	153	SER	2.5
1	A	60	VAL	2.5
1	B	157	THR	2.5
1	B	220	ALA	2.5
1	B	83	ILE	2.5
1	B	91	ASN	2.5
1	B	96	TYR	2.5
1	B	187	LEU	2.5
1	B	217	THR	2.4
1	B	146	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	164	PRO	2.4
1	B	169	PHE	2.4
1	B	50	LEU	2.4
1	B	210	ASN	2.4
1	B	163	LYS	2.4
1	B	245	LYS	2.4
1	A	93	TYR	2.4
1	B	89	ALA	2.4
1	B	130	LEU	2.4
1	A	59	GLY	2.4
1	A	170	PHE	2.4
1	A	90	TYR	2.3
1	A	225	LEU	2.3
1	B	103	ASP	2.3
1	B	212	VAL	2.3
1	B	211	GLU	2.3
1	B	183	TYR	2.3
1	A	147	ARG	2.3
1	A	152	ILE	2.3
1	A	218	VAL	2.3
1	B	235	THR	2.3
1	B	246	CYS	2.3
1	A	24	ARG	2.3
1	B	155	GLU	2.3
1	A	52	THR	2.3
1	B	86	ARG	2.3
1	A	4	LEU	2.3
1	B	213	LYS	2.2
1	A	47	ALA	2.2
1	B	105	ASP	2.2
1	B	104	ALA	2.2
1	B	208	TYR	2.2
1	B	162	THR	2.2
1	A	256	LEU	2.2
1	B	9	SER	2.2
1	B	11	TYR	2.2
1	A	184	PHE	2.1
1	A	211	GLU	2.1
1	B	251	ILE	2.1
1	B	240	GLU	2.1
1	B	232	GLN	2.1
1	A	169	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	154	PHE	2.1
1	A	181	ALA	2.1
1	A	61	GLY	2.1
1	A	150	ARG	2.1
1	B	186	TRP	2.1
1	A	155	GLU	2.1
1	B	179	ASN	2.1
1	B	239	ILE	2.1
1	B	21	GLU	2.0
1	B	238	LEU	2.0
1	B	82	THR	2.0
1	B	55	VAL	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(Å ²)	Q<0.9
3	ACT	A	267	4/4	0.53	0.35	89,90,90,90	0
2	SO4	A	264	5/5	0.61	0.21	93,94,94,95	0
3	ACT	B	263	4/4	0.63	0.29	62,63,63,64	0
2	SO4	A	266	5/5	0.67	0.16	106,109,109,109	0
5	GOL	B	266	6/6	0.67	0.24	67,68,71,72	0
5	GOL	A	272	6/6	0.76	0.21	39,49,51,52	0
5	GOL	A	271	6/6	0.76	0.22	49,50,51,51	0
4	UNL	B	264	9/-	0.78	0.18	56,58,64,64	0
2	SO4	A	263	5/5	0.78	0.17	75,76,78,79	0
2	SO4	B	262	5/5	0.79	0.17	70,71,72,73	0
5	GOL	B	267	6/6	0.80	0.18	51,53,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	262	5/5	0.81	0.20	45,45,57,59	0
5	GOL	A	273	6/6	0.81	0.22	67,68,69,72	0
2	SO4	A	265	5/5	0.83	0.15	50,52,56,60	0
5	GOL	B	265	6/6	0.85	0.16	52,54,56,58	0
4	UNL	A	268	9/-	0.90	0.13	24,32,39,41	0
5	GOL	A	269	6/6	0.93	0.10	10,11,16,17	6
5	GOL	A	270	6/6	0.95	0.18	68,69,70,70	6

6.5 Other polymers [i](#)

There are no such residues in this entry.