



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:07 PM UTC

PDB ID : 2X1C / pdb_00002x1c
Title : The crystal structure of precursor acyl coenzyme A:isopenicillin N acyltransferase from *Penicillium chrysogenum*
Authors : Bokhove, M.; Yoshida, H.; Hensgens, C.M.H.; van der Laan, J.M.; Sutherland, J.D.; Dijkstra, B.W.
Deposited on : 2009-12-23
Resolution : 1.85 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

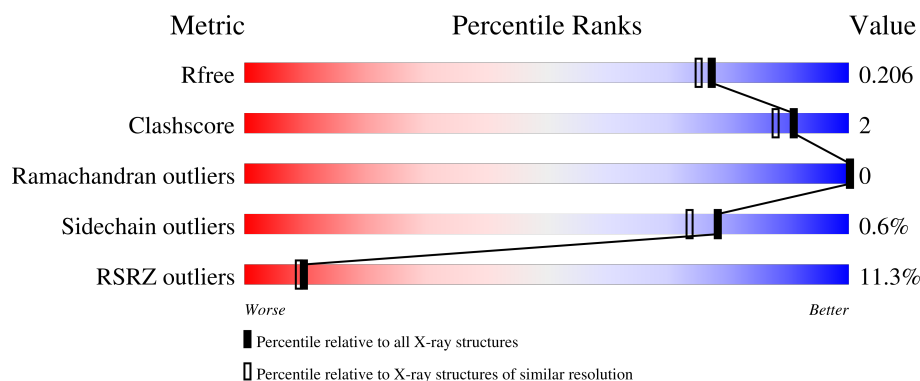
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	357	6% 96% ..
1	B	357	4% 94% 5% ..
1	C	357	6% 95% ..
1	D	357	29% 95% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12046 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 ACYL-COENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	5	0
			2833	1777	512	531	13			
1	B	356	Total	C	N	O	S	0	9	0
			2877	1803	518	542	14			
1	C	355	Total	C	N	O	S	0	7	0
			2842	1782	509	538	13			
1	D	355	Total	C	N	O	S	0	5	0
			2836	1778	513	533	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	CYS	engineered mutation	UNP P15802
B	103	ALA	CYS	engineered mutation	UNP P15802
C	103	ALA	CYS	engineered mutation	UNP P15802
D	103	ALA	CYS	engineered mutation	UNP P15802

- 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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	221	Total	O	0	0
			221	221		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	138	Total 138	O 138	0	0
5	D	65	Total 65	O 65	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.22Å 68.23Å 151.28Å 90.00° 129.57° 90.00°	Depositor
Resolution (Å)	48.80 – 1.85 48.80 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.80-1.85) 98.4 (48.80-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.169 , 0.193 0.189 , 0.206	Depositor DCC
R_{free} test set	7647 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12046	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 4.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, CL

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	0.59	0/2890	0.74	0/3900
1	B	0.64	0/2934	0.75	0/3959
1	C	0.55	0/2899	0.72	0/3915
1	D	0.49	0/2893	0.73	0/3905
All	All	0.57	0/11616	0.73	0/15679

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 [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	2833	0	2782	12	0
1	B	2877	0	2815	13	0
1	C	2842	0	2778	8	0
1	D	2836	0	2780	7	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
2	D	5	0	0	0	0
3	A	6	0	8	1	0
3	B	18	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	16	0	0
4	B	2	0	0	0	0
5	A	161	0	0	0	0
5	B	221	0	0	1	0
5	C	138	0	0	0	0
5	D	65	0	0	0	0
All	All	12046	0	11203	39	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 (39) 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:236:LEU:HD23	1:A:242[B]:MET:HG3	1.54	0.88
1:A:214:MET:HE2	1:A:242[B]:MET:HE2	1.59	0.84
1:B:350:ARG:HD3	1:B:356:ARG:HB3	1.68	0.76
1:D:236:LEU:HD23	1:D:242:MET:HG3	1.75	0.68
1:B:236:LEU:HD23	1:B:242[A]:MET:HG3	1.76	0.66
1:B:283:LYS:HE2	1:B:320:ASP:CG	2.21	0.66
1:B:283:LYS:HE2	1:B:320:ASP:OD1	1.98	0.62
1:A:214:MET:HE2	1:A:242[B]:MET:CE	2.32	0.59
1:C:275:LEU:HB3	1:C:289:LEU:HD22	1.86	0.56
1:A:236:LEU:HD23	1:A:242[B]:MET:CG	2.29	0.56
1:B:100:ARG:HE	3:B:1360:GOL:C1	2.21	0.54
1:B:100:ARG:HE	3:B:1360:GOL:H12	1.71	0.54
1:C:235:VAL:C	1:C:242:MET:HE2	2.33	0.53
1:B:133:LEU:HD12	1:B:145:PHE:CZ	2.44	0.52
1:A:133:LEU:HD12	1:A:145:PHE:CZ	2.45	0.52
3:B:1360:GOL:H11	5:B:2074:HOH:O	2.10	0.52
1:C:89:ARG:NH2	1:C:148:GLU:OE1	2.42	0.51
1:A:353:LEU:HG	1:D:112[B]:ASN:ND2	2.27	0.50
1:B:258:GLU:HG2	1:B:261:PRO:HG3	1.94	0.49
1:A:39:LYS:NZ	1:A:98:ALA:H	2.10	0.49
1:B:115:LEU:HD21	1:B:283:LYS:HE3	1.95	0.48
1:A:39:LYS:HZ1	1:A:98:ALA:H	1.61	0.48
1:A:98:ALA:HB1	1:A:310:ARG:HH12	1.79	0.47
1:B:275:LEU:HB3	1:B:289:LEU:HD22	1.97	0.47
1:C:252:HIS:HB3	1:C:256:GLU:HG3	1.98	0.46
1:A:134:THR:HG21	3:A:1360:GOL:H32	1.98	0.46
1:B:112:ASN:ND2	1:C:353:LEU:HG	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ASP:O	1:D:349:GLU:HG2	2.17	0.44
1:A:236:LEU:CD2	1:A:242[B]:MET:HG3	2.37	0.44
1:C:167:ASN:HB2	1:C:212:PHE:HB3	2.00	0.43
1:C:133:LEU:HD12	1:C:145:PHE:CZ	2.53	0.43
1:C:148:GLU:HB2	1:C:151:ILE:HD12	2.00	0.43
1:A:242[B]:MET:HE3	1:A:242[B]:MET:HB3	1.78	0.42
1:D:211:ALA:HB3	1:D:226:PHE:CZ	2.54	0.42
1:B:108:CYS:SG	1:B:276:LEU:HD22	2.60	0.42
1:B:214:MET:HE2	1:B:242[B]:MET:SD	2.60	0.41
1:D:272:MET:HE2	1:D:300:ILE:HD13	2.02	0.41
1:D:25:ILE:HG13	1:D:149:ALA:HB1	2.02	0.41
1:D:325:GLU:HG2	1:D:343:ARG:HG2	2.03	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	358/357 (100%)	347 (97%)	11 (3%)	0	100	100
1	B	363/357 (102%)	355 (98%)	8 (2%)	0	100	100
1	C	360/357 (101%)	351 (98%)	9 (2%)	0	100	100
1	D	358/357 (100%)	351 (98%)	7 (2%)	0	100	100
All	All	1439/1428 (101%)	1404 (98%)	35 (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	294/291 (101%)	293 (100%)	1 (0%)	86	85
1	B	299/291 (103%)	298 (100%)	1 (0%)	86	85
1	C	296/291 (102%)	294 (99%)	2 (1%)	76	70
1	D	294/291 (101%)	291 (99%)	3 (1%)	68	60
All	All	1183/1164 (102%)	1176 (99%)	7 (1%)	78	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	PHE
1	B	157	PHE
1	C	157	PHE
1	C	279	PHE
1	D	24	VAL
1	D	157	PHE
1	D	277	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	172	GLN
1	A	219	HIS
1	A	234	GLN
1	B	219	HIS
1	B	234	GLN
1	B	251	GLN
1	B	284	GLN
1	B	288	GLN
1	C	219	HIS
1	C	234	GLN
1	D	219	HIS
1	D	234	GLN

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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	SO4	B	1357	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	A	1359	-	4,4,4	0.26	0	6,6,6	0.07	0
3	GOL	B	1361	-	5,5,5	0.45	0	5,5,5	0.43	0
3	GOL	A	1360	-	5,5,5	0.41	0	5,5,5	0.36	0
3	GOL	C	1356	-	5,5,5	0.47	0	5,5,5	0.54	0
2	SO4	A	1357	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	A	1356	-	4,4,4	0.15	0	6,6,6	0.36	0
3	GOL	B	1359	-	5,5,5	0.44	0	5,5,5	0.80	0
2	SO4	A	1358	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	B	1358	-	4,4,4	0.25	0	6,6,6	0.07	0
3	GOL	B	1360	-	5,5,5	0.42	0	5,5,5	0.44	0
2	SO4	D	1356	-	4,4,4	0.28	0	6,6,6	0.29	0
3	GOL	C	1357	-	5,5,5	0.37	0	5,5,5	0.38	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
3	GOL	B	1361	-	-	4/4/4/4	-
3	GOL	C	1356	-	-	4/4/4/4	-
3	GOL	B	1359	-	-	4/4/4/4	-
3	GOL	A	1360	-	-	0/4/4/4	-
3	GOL	B	1360	-	-	0/4/4/4	-
3	GOL	C	1357	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1359	GOL	C1-C2-C3-O3
3	B	1359	GOL	O2-C2-C3-O3
3	B	1361	GOL	O1-C1-C2-C3
3	B	1361	GOL	C1-C2-C3-O3
3	C	1356	GOL	O1-C1-C2-C3
3	C	1357	GOL	C1-C2-C3-O3
3	C	1357	GOL	O1-C1-C2-O2
3	B	1359	GOL	O1-C1-C2-C3
3	C	1356	GOL	C1-C2-C3-O3
3	C	1357	GOL	O1-C1-C2-C3
3	B	1359	GOL	O1-C1-C2-O2
3	B	1361	GOL	O1-C1-C2-O2
3	B	1361	GOL	O2-C2-C3-O3
3	C	1356	GOL	O2-C2-C3-O3
3	C	1357	GOL	O2-C2-C3-O3
3	C	1356	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1360	GOL	1	0
3	B	1360	GOL	3	0

5.7 Other polymers

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	355/357 (99%)	0.17	21 (5%)	28	31	9, 24, 42, 58	5 (1%)
1	B	356/357 (99%)	-0.02	13 (3%)	45	49	8, 21, 36, 50	9 (2%)
1	C	355/357 (99%)	0.46	22 (6%)	26	29	9, 28, 49, 66	7 (1%)
1	D	355/357 (99%)	1.47	104 (29%)	1	1	11, 37, 63, 79	5 (1%)
All	All	1421/1428 (99%)	0.52	160 (11%)	10	9	8, 27, 50, 79	26 (1%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	8.6
1	D	43	THR	6.0
1	D	298	PHE	5.1
1	A	96	LEU	5.0
1	C	355	ALA	4.9
1	D	26	ALA	4.6
1	D	304	TYR	4.5
1	D	312	ALA	4.2
1	D	40	THR	4.1
1	D	24	VAL	4.0
1	D	303	ALA	4.0
1	D	38	GLY	4.0
1	D	47	LEU	4.0
1	A	97	LYS	3.8
1	D	36	ILE	3.8
1	D	262	LEU	3.8
1	C	307	GLY	3.6
1	D	311	GLY	3.6
1	D	2	LEU	3.6
1	A	43	THR	3.6
1	D	98	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	95	GLY	3.5
1	D	92	PHE	3.5
1	D	23	ALA	3.5
1	D	29	ILE	3.4
1	D	15	TYR	3.4
1	B	307	GLY	3.4
1	D	355	ALA	3.4
1	C	310	ARG	3.3
1	D	18	GLY	3.3
1	A	38	GLY	3.3
1	D	79	ASP	3.3
1	D	37	ARG	3.3
1	A	41	LYS	3.2
1	D	296	TYR	3.2
1	D	51	LEU	3.2
1	D	31	PHE	3.2
1	D	310	ARG	3.2
1	C	254	LYS	3.1
1	D	41	LYS	3.1
1	D	76	ALA	3.1
1	D	307	GLY	3.1
1	D	306	GLU	3.1
1	D	19	SER	3.1
1	D	209	ALA	3.1
1	C	306	GLU	3.0
1	B	112	ASN	3.0
1	C	41	LYS	3.0
1	B	306	GLU	3.0
1	D	123	PHE	3.0
1	D	266	TRP	3.0
1	A	355	ALA	3.0
1	C	354	ASN	3.0
1	A	44	ASP	2.9
1	D	75	GLY	2.9
1	D	219	HIS	2.9
1	D	308	LYS	2.9
1	D	25	ILE	2.9
1	D	73	ALA	2.9
1	C	222	PHE	2.8
1	B	262	LEU	2.8
1	D	33	VAL	2.8
1	D	278	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	42	LYS	2.8
1	D	20	ALA	2.7
1	D	174	LEU	2.7
1	D	337	ASP	2.7
1	D	255	ASN	2.7
1	C	40	THR	2.7
1	D	125	ALA	2.6
1	D	264	ASP	2.6
1	A	37	ARG	2.6
1	D	35	LEU	2.6
1	D	94	TYR	2.6
1	B	254	LYS	2.6
1	D	124	SER	2.6
1	B	356	ARG	2.6
1	D	309	SER	2.6
1	D	122	PHE	2.6
1	D	49	GLN	2.6
1	D	77	GLU	2.6
1	A	34	ASP	2.5
1	C	255	ASN	2.5
1	D	129	ASN	2.5
1	D	285	ALA	2.5
1	D	52	SER	2.5
1	D	284	GLN	2.5
1	D	34	ASP	2.5
1	D	274	PHE	2.5
1	D	54	LEU	2.5
1	C	36	ILE	2.5
1	D	354	ASN	2.5
1	B	38	GLY	2.5
1	C	47	LEU	2.5
1	D	80	VAL	2.5
1	D	97	LYS	2.5
1	A	112	ASN	2.4
1	B	346[A]	GLU	2.4
1	D	21	ALA	2.4
1	D	50	VAL	2.4
1	D	267	ASN	2.4
1	D	301	CYS	2.4
1	D	305	GLU	2.4
1	A	353	LEU	2.4
1	C	43	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	37	ARG	2.4
1	D	253	GLY	2.4
1	D	260	ASP	2.4
1	B	219	HIS	2.4
1	C	308	LYS	2.4
1	C	44	ASP	2.3
1	B	37	ARG	2.3
1	D	314	LEU	2.3
1	D	90	THR	2.3
1	D	7	GLN	2.3
1	D	295	ASN	2.3
1	D	261	PRO	2.3
1	D	1	MET	2.3
1	D	95	GLY	2.3
1	D	78	ARG	2.3
1	C	172	GLN	2.3
1	C	259	LEU	2.3
1	D	55	GLY	2.3
1	D	96	LEU	2.3
1	C	257	LYS	2.3
1	D	22	LYS	2.3
1	B	310	ARG	2.3
1	A	277	ASP	2.3
1	D	346	GLU	2.3
1	A	40	THR	2.3
1	A	42	LYS	2.3
1	D	259	LEU	2.3
1	D	315	PHE	2.2
1	D	4	ILE	2.2
1	D	334	THR	2.2
1	D	28	SER	2.2
1	B	304	TYR	2.2
1	D	39	LYS	2.2
1	B	347	GLU	2.2
1	D	210	SER	2.2
1	D	11	PHE	2.2
1	C	266	TRP	2.2
1	A	284	GLN	2.2
1	A	36	ILE	2.1
1	D	290	TRP	2.1
1	D	126	THR	2.1
1	D	130	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	257	LYS	2.1
1	D	347[A]	GLU	2.1
1	A	251	GLN	2.1
1	D	30	ASP	2.1
1	A	347	GLU	2.1
1	A	354	ASN	2.1
1	C	98	ALA	2.1
1	C	49	GLN	2.0
1	D	120	TRP	2.0
1	D	44	ASP	2.0
1	D	67	GLU	2.0
1	D	173	GLY	2.0
1	D	27	ARG	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	GOL	C	1357	6/6	0.76	0.22	49,52,53,54	0
3	GOL	B	1360	6/6	0.77	0.16	43,44,46,47	0
3	GOL	B	1359	6/6	0.79	0.17	36,42,43,45	0
2	SO4	B	1358	5/5	0.81	0.14	73,73,73,73	0
2	SO4	A	1359	5/5	0.83	0.12	72,72,72,72	0
3	GOL	B	1361	6/6	0.87	0.14	31,36,38,40	0
3	GOL	C	1356	6/6	0.89	0.12	38,41,41,42	0
3	GOL	A	1360	6/6	0.91	0.10	34,36,36,36	0
2	SO4	A	1358	5/5	0.91	0.14	38,38,40,40	0
4	CL	B	1363	1/1	0.94	0.26	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1356	5/5	0.95	0.11	35,35,35,37	0
2	SO4	A	1357	5/5	0.95	0.16	32,32,34,35	0
2	SO4	B	1357	5/5	0.96	0.09	25,28,30,30	0
2	SO4	A	1356	5/5	0.98	0.06	25,27,27,28	0
4	CL	B	1362	1/1	1.00	0.02	16,16,16,16	1

6.5 Other polymers [i](#)

There are no such residues in this entry.