



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2023 – 08:01 pm GMT

PDB ID : 2X1E
Title : The crystal structure of mature acyl coenzyme A:isopenicillin N acyltransferase from *Penicillium chrysogenum* in complex 6- aminopenicillanic acid
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 : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

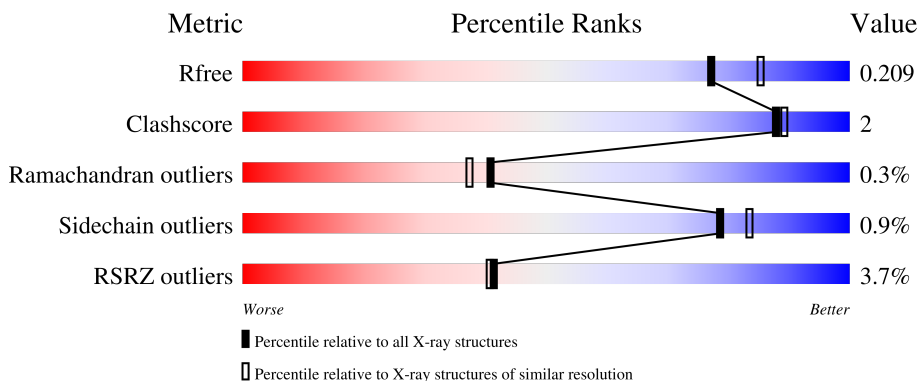
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	357	 92% 8% .
1	B	357	 4% 94% 5% .
1	C	357	 5% 94% . .
1	D	357	 3% 91% 7% .

2 Entry composition [i](#)

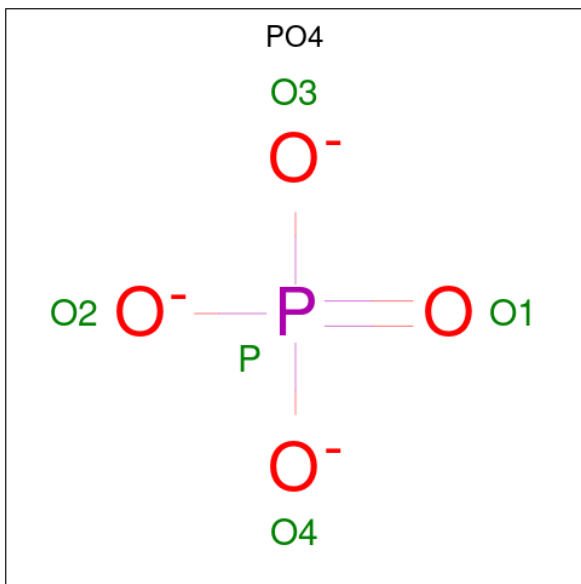
There are 6 unique types of molecules in this entry. The entry contains 11691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	354	Total 2849	C 1789	N 513	O 533	S 14	0	7	0
1	B	352	Total 2791	C 1753	N 500	O 523	S 15	0	2	0
1	C	350	Total 2782	C 1747	N 496	O 525	S 14	0	3	0
1	D	351	Total 2802	C 1760	N 503	O 525	S 14	0	4	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



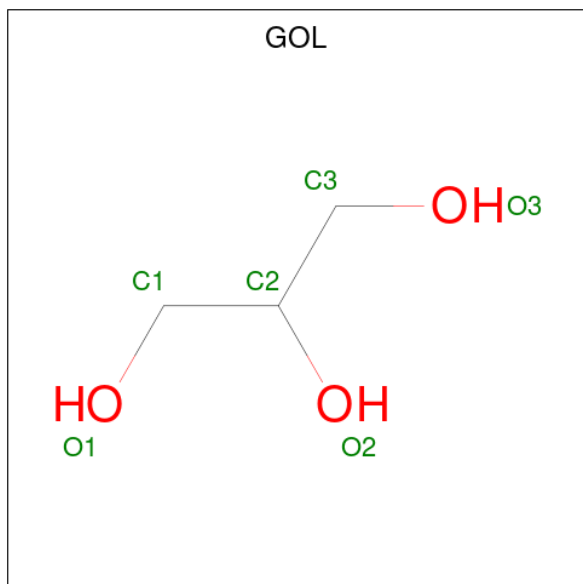
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

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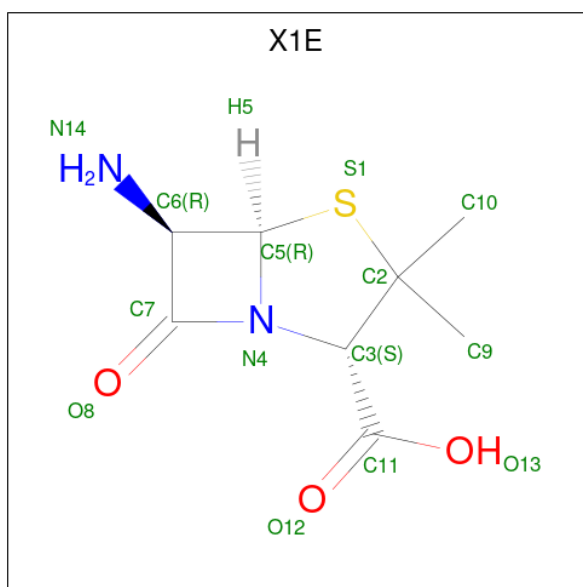
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	D	1	5	4	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is (2S,5R,6R)-6-AMINO-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (three-letter code: X1E) (formula: C₈H₁₂N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	14	8	2	3	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	B	1	1	1	0	0

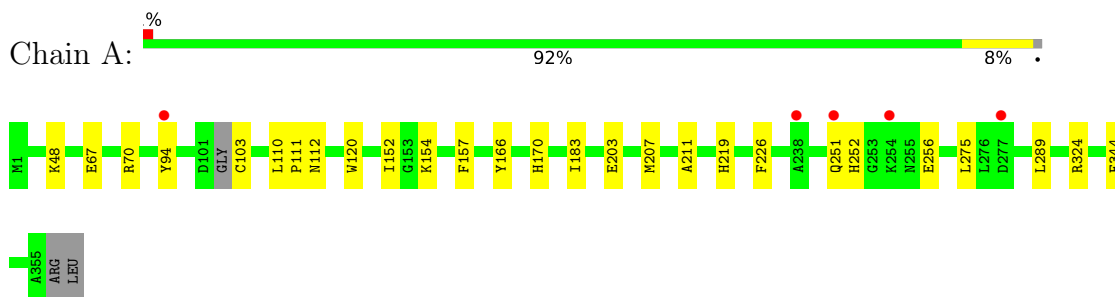
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	97	97	97	0	0
6	B	107	107	107	0	0
6	C	99	99	99	0	0
6	D	92	92	92	0	0

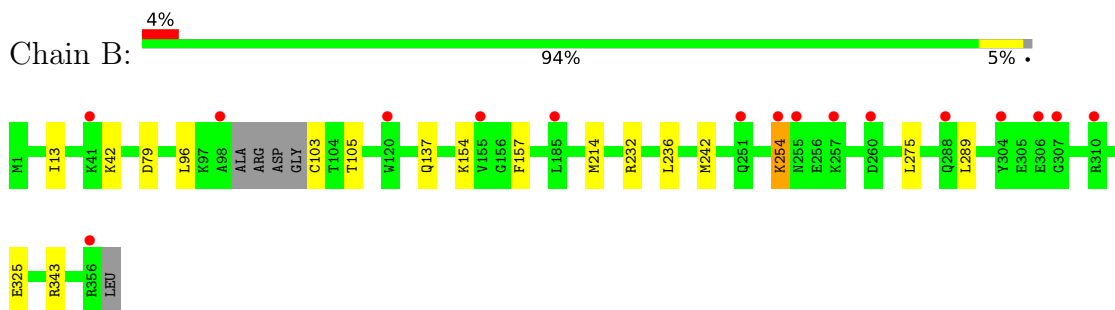
3 Residue-property plots [i](#)

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.

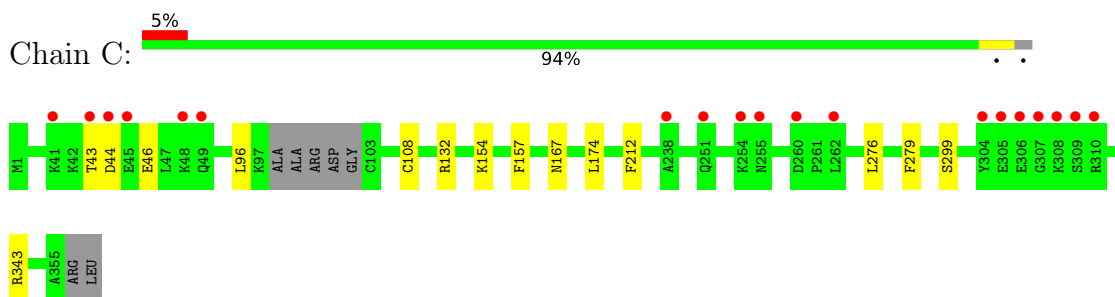
- Molecule 1: ACYL-COENZYME



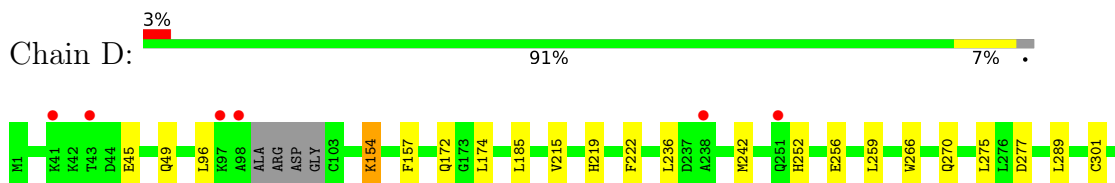
- Molecule 1: ACYL-COENZYME



- Molecule 1: ACYL-COENZYME



- Molecule 1: ACYL-COENZYME





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.18Å 68.38Å 146.57Å 90.00° 128.81° 90.00°	Depositor
Resolution (Å)	33.63 – 2.00 33.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.63-2.00) 98.7 (33.59-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.202 0.188 , 0.209	Depositor DCC
R_{free} test set	5157 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11691	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: PO4, CL, GOL, CSD, X1E

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	0.41	0/2904	0.53	0/3922
1	B	0.43	0/2840	0.54	0/3834
1	C	0.43	0/2831	0.53	0/3823
1	D	0.41	0/2854	0.52	0/3852
All	All	0.42	0/11429	0.53	0/15431

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	2849	0	2788	18	0
1	B	2791	0	2742	10	0
1	C	2782	0	2725	6	0
1	D	2802	0	2755	12	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
3	A	12	0	16	1	0
3	C	24	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	0	0
4	A	14	0	11	1	0
5	B	1	0	0	0	0
6	A	97	0	0	2	0
6	B	107	0	0	1	0
6	C	99	0	0	0	0
6	D	92	0	0	0	0
All	All	11691	0	11077	45	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.

The worst 5 of 45 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:324[B]:ARG:HD3	1:A:344:PHE:HD2	1.46	0.78
1:A:324[B]:ARG:HD3	1:A:344:PHE:CD2	2.22	0.75
1:A:94[A]:TYR:CE2	1:A:170[A]:HIS:CD2	2.76	0.74
1:B:325:GLU:HG2	1:B:343:ARG:HG2	1.71	0.72
1:D:45:GLU:O	1:D:49:GLN:HG2	1.90	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	357/357 (100%)	348 (98%)	8 (2%)	1 (0%)	41 37
1	B	350/357 (98%)	343 (98%)	6 (2%)	1 (0%)	41 37
1	C	349/357 (98%)	342 (98%)	6 (2%)	1 (0%)	41 37
1	D	351/357 (98%)	342 (97%)	8 (2%)	1 (0%)	41 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1407/1428 (98%)	1375 (98%)	28 (2%)	4 (0%)	41 37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	B	154	LYS
1	C	154	LYS
1	D	154	LYS

5.3.2 Protein sidechains [i](#)

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	296/291 (102%)	294 (99%)	2 (1%)	84 88
1	B	290/291 (100%)	288 (99%)	2 (1%)	84 88
1	C	290/291 (100%)	286 (99%)	4 (1%)	67 72
1	D	291/291 (100%)	289 (99%)	2 (1%)	84 88
All	All	1167/1164 (100%)	1157 (99%)	10 (1%)	78 83

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	299	SER
1	D	157	PHE
1	D	277	ASP
1	B	254	LYS
1	C	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN

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Mol	Chain	Res	Type
1	C	170	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues 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$
1	CSD	D	103	1	3,7,8	1.26	0	1,8,10	1.55	0
1	CSD	A	103	1	3,7,8	1.33	1 (33%)	1,8,10	1.60	0
1	CSD	B	103	1	3,7,8	1.30	1 (33%)	1,8,10	0.88	0
1	CSD	C	103	1	3,7,8	1.18	0	1,8,10	0.30	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	CSD	D	103	1	-	0/2/6/8	-
1	CSD	A	103	1	-	0/2/6/8	-
1	CSD	B	103	1	-	0/2/6/8	-
1	CSD	C	103	1	-	0/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	CSD	CB-SG	-2.02	1.67	1.79
1	A	103	CSD	CB-SG	-2.00	1.67	1.79

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	GOL	C	1357	-	5,5,5	0.43	0	5,5,5	0.23	0
2	PO4	D	1356	-	4,4,4	0.85	0	6,6,6	0.58	0
4	X1E	A	1358	-	15,15,15	1.69	3 (20%)	24,25,25	3.04	10 (41%)
3	GOL	C	1358	-	5,5,5	0.33	0	5,5,5	0.61	0
3	GOL	A	1357	-	5,5,5	0.34	0	5,5,5	0.34	0
2	PO4	B	1357	-	4,4,4	0.90	0	6,6,6	0.37	0
3	GOL	D	1357	-	5,5,5	0.35	0	5,5,5	0.35	0
3	GOL	C	1356	-	5,5,5	0.35	0	5,5,5	0.54	0
3	GOL	C	1359	-	5,5,5	0.35	0	5,5,5	0.16	0
2	PO4	A	1356	-	4,4,4	0.93	0	6,6,6	0.60	0
3	GOL	A	1359	-	5,5,5	0.33	0	5,5,5	0.35	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	C	1357	-	-	0/4/4/4	-
4	X1E	A	1358	-	-	0/4/35/35	0/2/2/2
3	GOL	C	1358	-	-	4/4/4/4	-
3	GOL	A	1357	-	-	0/4/4/4	-
3	GOL	D	1357	-	-	0/4/4/4	-
3	GOL	C	1356	-	-	0/4/4/4	-
3	GOL	C	1359	-	-	0/4/4/4	-
3	GOL	A	1359	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1358	X1E	C2-S1	-3.75	1.77	1.85
4	A	1358	X1E	C5-S1	-2.94	1.76	1.81
4	A	1358	X1E	C7-N4	-2.76	1.31	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1358	X1E	S1-C5-N4	-9.34	92.55	105.10
4	A	1358	X1E	C2-C3-N4	-5.52	98.16	106.49
4	A	1358	X1E	C5-N4-C3	4.85	123.30	117.26
4	A	1358	X1E	C2-S1-C5	3.56	101.89	94.08
4	A	1358	X1E	C3-N4-C7	3.54	136.66	126.35

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1359	GOL	O1-C1-C2-O2
3	A	1359	GOL	O1-C1-C2-C3
3	C	1358	GOL	O1-C1-C2-C3
3	C	1358	GOL	C1-C2-C3-O3
3	C	1358	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1358	X1E	1	0
3	C	1358	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1356	GOL	1	0
3	A	1359	GOL	1	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	353/357 (98%)	-0.12	5 (1%) 75 74	19, 28, 40, 50	0
1	B	351/357 (98%)	-0.06	16 (4%) 32 31	18, 26, 41, 54	0
1	C	349/357 (97%)	-0.01	19 (5%) 25 24	16, 27, 49, 61	0
1	D	350/357 (98%)	-0.07	12 (3%) 45 44	20, 29, 43, 57	0
All	All	1403/1428 (98%)	-0.07	52 (3%) 41 41	16, 28, 43, 61	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	TYR	5.1
1	C	308	LYS	4.9
1	B	306	GLU	4.8
1	D	306	GLU	4.7
1	C	254	LYS	4.5

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	CSD	C	103	8/9	0.98	0.13	24,25,27,29	0
1	CSD	D	103	8/9	0.98	0.08	24,25,27,27	0
1	CSD	A	103	8/9	0.99	0.10	23,23,25,27	0
1	CSD	B	103	8/9	0.99	0.11	23,24,26,29	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
3	GOL	A	1359	6/6	0.81	0.12	45,47,48,48	0
4	X1E	A	1358	14/14	0.81	0.17	55,57,57,58	0
2	PO4	B	1357	5/5	0.82	0.26	70,70,71,71	0
3	GOL	D	1357	6/6	0.87	0.14	45,46,48,49	0
2	PO4	A	1356	5/5	0.87	0.20	33,39,40,40	0
3	GOL	C	1359	6/6	0.89	0.10	38,39,41,41	0
3	GOL	A	1357	6/6	0.92	0.14	35,36,37,38	0
3	GOL	C	1358	6/6	0.93	0.10	33,35,35,36	0
3	GOL	C	1357	6/6	0.94	0.10	30,31,31,31	0
2	PO4	D	1356	5/5	0.96	0.16	39,41,41,41	0
3	GOL	C	1356	6/6	0.97	0.11	29,32,33,35	0
5	CL	B	1358	1/1	0.99	0.05	24,24,24,24	1

6.5 Other polymers [i](#)

There are no such residues in this entry.