



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:20 am BST

PDB ID : 4PKC
Title : Benzylsuccinate alpha-gamma complex
Authors : Funk, M.A.; Drennan, C.L.
Deposited on : 2014-05-14
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

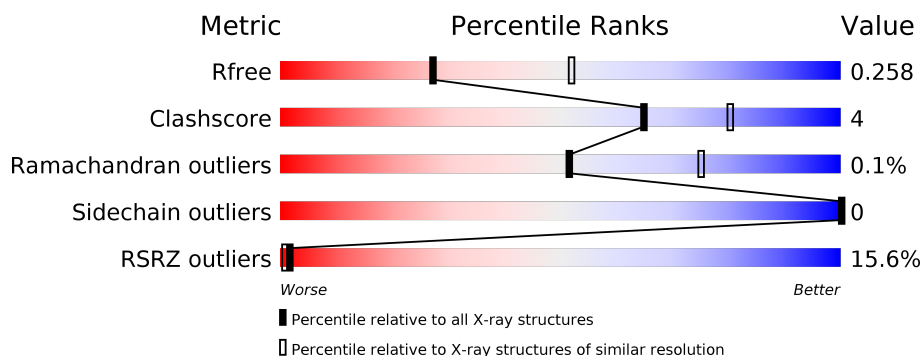
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	878	<div> <div>15%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	C	60	<div> <div>3%</div> <div>55%</div> <div>13%</div> <div>32%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	901	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7193 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 TutD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6672	4212	1156	1266	38			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	ILE	MET	variant	UNP O68395
A	866	SER	-	expression tag	UNP O68395
A	867	GLY	-	expression tag	UNP O68395
A	868	THR	-	expression tag	UNP O68395
A	869	GLY	-	expression tag	UNP O68395
A	870	SER	-	expression tag	UNP O68395
A	871	GLY	-	expression tag	UNP O68395
A	872	SER	-	expression tag	UNP O68395
A	873	SER	-	expression tag	UNP O68395
A	874	HIS	-	expression tag	UNP O68395
A	875	HIS	-	expression tag	UNP O68395
A	876	HIS	-	expression tag	UNP O68395
A	877	HIS	-	expression tag	UNP O68395
A	878	HIS	-	expression tag	UNP O68395
A	879	HIS	-	expression tag	UNP O68395

- Molecule 2 is a protein called TutF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	41	Total	C	N	O	S	0	0	0
			320	204	52	63	1			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	185	Total O 185 185	0	0
5	C	9	Total O 9 9	0	0

- Molecule 1: TutD



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.86 Å 154.86 Å 82.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.60 48.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.97-2.60) 85.1 (48.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.217 , 0.257 0.222 , 0.258	Depositor DCC
R_{free} test set	3083 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	1.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.8	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	0.94	EDS
Total number of atoms	7193	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: GOL, 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	0.21	0/6825	0.36	0/9224
2	C	0.20	0/328	0.33	0/442
All	All	0.21	0/7153	0.36	0/9666

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	6672	0	6508	54	0
2	C	320	0	291	6	0
3	A	1	0	0	2	0
4	A	6	0	8	0	0
5	A	185	0	0	3	0
5	C	9	0	0	1	0
All	All	7193	0	6807	57	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 4.

All (57) 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:375:ALA:O	1:A:382:ARG:NH1	2.12	0.83
2:C:44:LYS:NZ	5:C:109:HOH:O	2.10	0.79
1:A:123:ASP:OD2	5:A:1181:HOH:O	2.11	0.69
1:A:494:MET:HE1	1:A:709:VAL:HB	1.78	0.65
1:A:666:PRO:HB2	1:A:675:ALA:HB2	1.79	0.64
1:A:297:ARG:NH2	5:A:1138:HOH:O	2.28	0.64
1:A:623:ALA:HB1	1:A:679:ILE:HG13	1.79	0.64
1:A:631:LYS:NZ	1:A:636:GLU:OE1	2.27	0.64
1:A:542:THR:HG22	1:A:560:LYS:HD3	1.81	0.62
1:A:313:LYS:NZ	1:A:366:GLU:OE2	2.23	0.61
1:A:655:PHE:HB3	1:A:658:MET:HB3	1.83	0.61
1:A:709:VAL:HG13	1:A:711:LEU:HD23	1.82	0.61
1:A:270:LEU:HD13	2:C:43:SER:HB2	1.84	0.59
1:A:520:LEU:HD12	1:A:561:GLN:HB3	1.84	0.58
1:A:737:ILE:HD13	1:A:755:VAL:HG13	1.85	0.58
1:A:412:ASP:OD2	1:A:439:LYS:NZ	2.31	0.56
1:A:419:LYS:HD2	1:A:446:GLU:HB3	1.88	0.56
1:A:400:ASN:HD21	1:A:404:GLU:HB2	1.71	0.56
1:A:509:SER:OG	1:A:580:GLU:OE2	2.23	0.55
1:A:335:ASP:OD1	1:A:336:THR:N	2.38	0.55
1:A:384:ILE:HG21	1:A:711:LEU:HD22	1.88	0.54
1:A:548:LEU:HD21	1:A:554:VAL:HB	1.88	0.54
1:A:604:CYS:SG	5:A:1116:HOH:O	2.59	0.53
1:A:492:LEU:HB2	3:A:901:CL:CL	2.45	0.53
2:C:23:GLU:OE2	2:C:47:PHE:HZ	1.93	0.52
1:A:130:TYR:CE1	1:A:326:TYR:HB2	2.48	0.49
1:A:186:SER:HB2	1:A:519:LYS:HE2	1.95	0.49
1:A:31:PRO:HB2	1:A:34:GLU:HG2	1.94	0.48
1:A:518:ALA:HA	1:A:622:ALA:HB2	1.96	0.48
1:A:533:TYR:OH	1:A:718:ARG:NH2	2.47	0.47
2:C:10:ALA:HA	2:C:31:ARG:HG2	1.94	0.47
1:A:19:ASN:HD22	1:A:21:THR:HG22	1.79	0.47
1:A:319:ILE:HD13	1:A:323:ILE:HD12	1.97	0.47
1:A:614:HIS:O	1:A:616:PRO:HD3	2.16	0.46
1:A:834:PHE:O	1:A:842:GLN:NE2	2.41	0.45
1:A:21:THR:OG1	1:A:28:GLU:OE1	2.34	0.45
1:A:640:THR:HG23	1:A:643:GLN:H	1.81	0.44
1:A:76:MET:HB3	1:A:157:ILE:HG21	1.99	0.44
1:A:559:ARG:HG3	1:A:686:ILE:HD12	2.00	0.44
1:A:766:LEU:HA	1:A:799:HIS:HB3	1.99	0.44
1:A:265:ARG:NH2	2:C:20:ASP:OD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PHE:HE1	1:A:709:VAL:HG22	1.84	0.43
1:A:459:HIS:HE1	1:A:461:GLU:HB2	1.83	0.43
1:A:502:ARG:HG2	1:A:503:LYS:HG3	2.00	0.42
1:A:273:ILE:HG21	2:C:30:VAL:HG21	2.02	0.42
1:A:516:PHE:CE1	1:A:715:VAL:HG21	2.54	0.42
1:A:447:CYS:HB2	1:A:455:PRO:HD3	2.01	0.41
1:A:434:LYS:NZ	1:A:794:ASP:OD1	2.40	0.41
1:A:421:ILE:HA	1:A:421:ILE:HD12	1.97	0.41
1:A:716:GLY:HA2	1:A:719:THR:HG22	2.02	0.41
1:A:517:PRO:HD2	1:A:617:ILE:O	2.20	0.41
1:A:740:TYR:HB3	1:A:743:THR:HG21	2.03	0.41
1:A:807:THR:HG23	1:A:846:ILE:HG23	2.04	0.40
1:A:494:MET:HG2	3:A:901:CL:CL	2.59	0.40
1:A:438:GLU:OE2	1:A:442:ARG:NH1	2.46	0.40
1:A:78:TYR:O	1:A:101:ASN:ND2	2.44	0.40
1:A:150:PRO:HB2	1:A:152:ASP:OD1	2.21	0.40

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	839/878 (96%)	805 (96%)	33 (4%)	1 (0%)	51	75
2	C	39/60 (65%)	37 (95%)	2 (5%)	0	100	100
All	All	878/938 (94%)	842 (96%)	35 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	723	PRO

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	706/741 (95%)	706 (100%)	0	100	100
2	C	31/51 (61%)	31 (100%)	0	100	100
All	All	737/792 (93%)	737 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	643	GLN
1	A	849	GLN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	GOL	A	902	-	5,5,5	0.36	0	5,5,5	0.28	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
4	GOL	A	902	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	GOL	O1-C1-C2-C3
4	A	902	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	843/878 (96%)	0.90	136 (16%) 1 1	45, 68, 161, 240	0
2	C	41/60 (68%)	0.30	2 (4%) 29 23	52, 69, 94, 119	0
All	All	884/938 (94%)	0.87	138 (15%) 2 1	45, 68, 161, 240	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	GLY	19.6
1	A	741	MET	17.8
1	A	743	THR	15.4
1	A	668	TRP	11.8
1	A	732	ALA	11.6
1	A	860	PHE	9.5
1	A	728	GLY	9.4
1	A	740	TYR	9.2
1	A	850	GLU	8.2
1	A	744	ASP	8.1
1	A	755	VAL	8.0
1	A	737	ILE	7.9
1	A	758	VAL	7.9
1	A	637	LYS	7.7
1	A	666	PRO	7.3
1	A	745	LYS	7.2
1	A	706	GLY	7.2
1	A	752	LEU	7.0
1	A	856	SER	7.0
1	A	708	ALA	6.8
1	A	712	TYR	6.7
1	A	858	LEU	6.4
1	A	714	GLU	6.4
1	A	784	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	710	GLY	6.1
1	A	747	GLY	6.0
1	A	855	ALA	6.0
1	A	678	ILE	5.8
1	A	655	PHE	5.7
1	A	861	LEU	5.7
1	A	18	LEU	5.6
1	A	674	TYR	5.6
1	A	766	LEU	5.6
1	A	739	PRO	5.5
1	A	865	ILE	5.4
1	A	686	ILE	5.4
1	A	665	ALA	5.4
1	A	675	ALA	5.4
1	A	653	GLU	5.3
1	A	754	SER	5.2
1	A	863	VAL	5.2
1	A	854	SER	5.1
1	A	664	ARG	5.0
1	A	662	PHE	4.8
1	A	715	VAL	4.7
1	A	748	PRO	4.5
1	A	746	LYS	4.5
1	A	862	ASN	4.4
1	A	724	ASP	4.4
1	A	494	MET	4.3
1	A	759	GLN	4.3
1	A	657	GLU	4.3
1	A	738	SER	4.2
1	A	493	CYS	4.2
1	A	658	MET	4.1
1	A	857	ASP	4.1
1	A	713	MET	4.1
1	A	628	ALA	4.0
1	A	652	TRP	4.0
1	A	723	PRO	4.0
1	A	749	THR	3.9
1	A	711	LEU	3.8
1	A	629	ILE	3.8
1	A	733	ASP	3.8
1	A	792	TRP	3.7
1	A	327	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	705	THR	3.7
1	A	634	PHE	3.6
1	A	552	GLU	3.6
1	A	19	ASN	3.6
1	A	828	SER	3.5
1	A	734	ASP	3.5
1	A	626	LEU	3.4
1	A	853	PHE	3.3
1	A	682	PHE	3.3
1	A	328	SER	3.3
1	A	651	ASN	3.3
1	A	859	GLU	3.3
1	A	864	GLU	3.2
1	A	725	GLY	3.2
1	A	756	SER	3.2
1	A	549	LYS	3.1
1	A	512	GLY	3.1
1	A	736	GLY	3.0
1	A	648	LEU	3.0
1	A	846	ILE	2.9
1	A	379	ARG	2.9
1	A	283	LYS	2.9
1	A	673	ASP	2.9
1	A	707	GLN	2.8
1	A	554	VAL	2.8
1	A	383	GLU	2.7
1	A	521	LEU	2.7
1	A	727	PHE	2.6
1	A	718	ARG	2.6
1	A	783	GLU	2.5
1	A	492	LEU	2.5
2	C	47	PHE	2.5
1	A	735	GLY	2.5
1	A	777	ARG	2.5
2	C	9	CYS	2.5
1	A	613	TRP	2.5
1	A	731	ALA	2.4
1	A	280	THR	2.4
1	A	393	ILE	2.4
1	A	331	ALA	2.4
1	A	381	TYR	2.4
1	A	852	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	829	GLY	2.4
1	A	680	THR	2.4
1	A	683	TYR	2.4
1	A	388	SER	2.4
1	A	33	ASP	2.3
1	A	201	VAL	2.3
1	A	849	GLN	2.3
1	A	805	VAL	2.3
1	A	650	ALA	2.3
1	A	789	ILE	2.3
1	A	709	VAL	2.3
1	A	538	LEU	2.2
1	A	649	LYS	2.2
1	A	788	TYR	2.2
1	A	802	PHE	2.2
1	A	533	TYR	2.2
1	A	553	ASP	2.2
1	A	819	LYS	2.2
1	A	390	ASP	2.2
1	A	633	VAL	2.1
1	A	639	TYR	2.1
1	A	555	TRP	2.1
1	A	730	GLU	2.1
1	A	20	PHE	2.1
1	A	495	SER	2.1
1	A	619	THR	2.1
1	A	135	HIS	2.1
1	A	751	VAL	2.1
1	A	810	MET	2.1
1	A	636	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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	CL	A	901	1/1	0.73	0.48	85,85,85,85	0
4	GOL	A	902	6/6	0.81	0.25	63,72,73,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.