



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 4KE4 / pdb_00004ke4
Title : Elucidation of the structure and reaction mechanism of Sorghum bicolor hydroxycinnamoyltransferase and its structural relationship to other CoA-dependent transferases and synthases
Authors : Walker, A.M.; Hayes, R.P.; Youn, B.; Vermerris, W.; Sattler, S.E.; Kang, C.
Deposited on : 2013-04-25
Resolution : 2.01 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

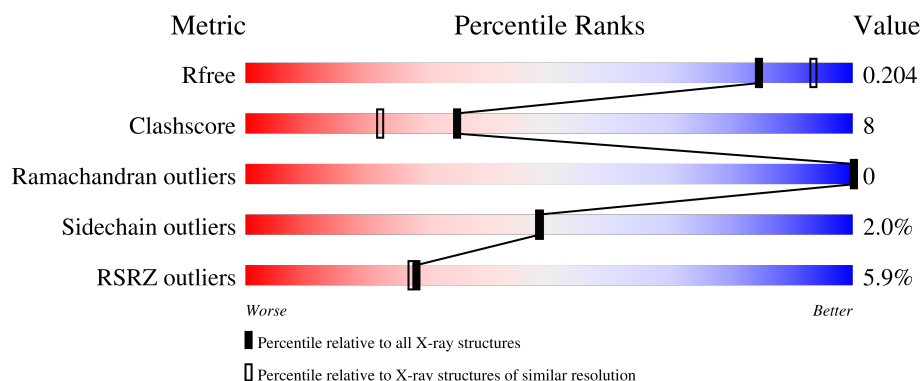
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

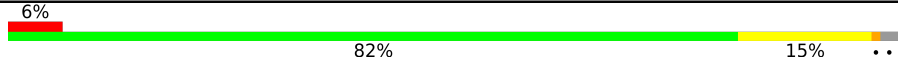
The reported resolution of this entry is 2.01 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	448	

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	GOL	A	504	-	-	X	-

2 Entry composition [i](#)

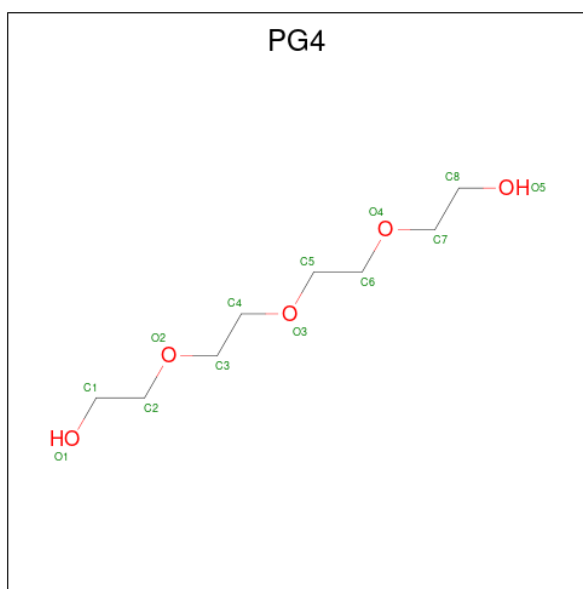
There are 4 unique types of molecules in this entry. The entry contains 3743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hydroxycinnamoyl-CoA:shikimate hydroxycinnamoyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3364	2142	599	605	18			

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

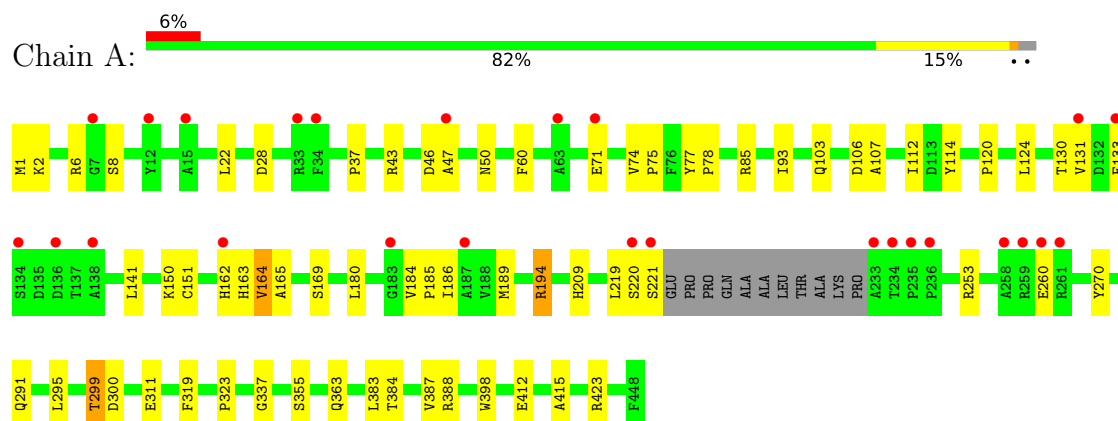
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	334	Total	O	0	0
			334	334		

3 Residue-property plots

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: Hydroxycinnamoyl-CoA:shikimate hydroxycinnamoyl transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	135.95Å 135.95Å 64.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.50 – 2.01 44.50 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.50-2.01) 97.7 (44.50-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.182 , 0.207 0.182 , 0.204	Depositor DCC
R_{free} test set	2004 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, PG4

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	0/3455	0.75	4/4704 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	107	ALA	CA-C-N	6.25	125.99	119.05
1	A	107	ALA	C-N-CA	6.25	125.99	119.05
1	A	363	GLN	CA-C-N	5.49	125.01	119.19
1	A	363	GLN	C-N-CA	5.49	125.01	119.19

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	3364	0	3304	46	0
2	A	39	0	54	10	0
3	A	6	0	8	4	0
4	A	334	0	0	7	0
All	All	3743	0	3366	51	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 8.

All (51) 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:270:TYR:HB2	3:A:504:GOL:H2	1.44	0.99
1:A:300:ASP:H	2:A:502:PG4:H81	1.23	0.99
1:A:219:LEU:H	1:A:291:GLN:HE22	1.15	0.92
2:A:501:PG4:H21	2:A:501:PG4:H51	1.53	0.91
1:A:388:ARG:HH12	2:A:502:PG4:H21	1.38	0.86
1:A:164:VAL:O	1:A:194:ARG:NH2	2.18	0.76
1:A:71:GLU:HG2	1:A:180:LEU:HD13	1.73	0.70
1:A:131:VAL:HB	1:A:133:PHE:CZ	2.26	0.70
1:A:300:ASP:N	2:A:502:PG4:H81	2.03	0.69
1:A:299:THR:HB	1:A:319:PHE:O	1.94	0.67
1:A:2:LYS:O	4:A:760:HOH:O	2.13	0.66
1:A:74:VAL:HB	1:A:75:PRO:HD3	1.76	0.66
1:A:253:ARG:NE	4:A:849:HOH:O	2.14	0.62
1:A:209:HIS:HE1	1:A:355:SER:OG	1.86	0.59
1:A:1:MET:HE3	1:A:114:TYR:CD2	2.38	0.58
1:A:6:ARG:HD3	1:A:106:ASP:OD2	2.06	0.56
1:A:28:ASP:O	1:A:163:HIS:HD2	1.90	0.55
1:A:300:ASP:H	2:A:502:PG4:C8	2.08	0.55
1:A:219:LEU:H	1:A:291:GLN:NE2	1.96	0.54
1:A:46:ASP:O	1:A:47:ALA:HB3	2.08	0.54
1:A:85:ARG:HD2	4:A:723:HOH:O	2.07	0.54
1:A:130:THR:HG22	4:A:917:HOH:O	2.10	0.51
1:A:387:VAL:HB	3:A:504:GOL:H31	1.92	0.51
1:A:8:SER:CB	1:A:103:GLN:HG2	2.41	0.50
1:A:120:PRO:HA	1:A:124:LEU:HD12	1.94	0.50
1:A:37:PRO:HD2	2:A:501:PG4:H42	1.94	0.50
1:A:219:LEU:N	1:A:291:GLN:HE22	1.95	0.50
1:A:22:LEU:HB3	1:A:93:ILE:HB	1.95	0.49
2:A:501:PG4:H21	2:A:501:PG4:C5	2.34	0.49
1:A:186:ILE:HB	1:A:189:MET:CE	2.43	0.48
1:A:141:LEU:HD13	1:A:164:VAL:CG1	2.45	0.47
1:A:165:ALA:HB1	1:A:169:SER:HB2	1.97	0.47
1:A:60:PHE:HA	1:A:398:TRP:CZ3	2.50	0.46
1:A:295:LEU:HB3	1:A:323:PRO:HG2	1.98	0.46
1:A:383:LEU:HD23	1:A:415:ALA:HB3	1.99	0.45
1:A:43:ARG:HG2	1:A:112:ILE:HD11	2.00	0.44
1:A:423:ARG:HA	4:A:851:HOH:O	2.17	0.44
1:A:184:VAL:CG1	1:A:185:PRO:HD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:503:PG4:H81	2:A:503:PG4:H62	1.85	0.44
1:A:384:THR:HG21	2:A:503:PG4:H21	1.99	0.43
1:A:388:ARG:CZ	3:A:504:GOL:O3	2.67	0.43
1:A:220:SER:O	1:A:221:SER:C	2.62	0.43
1:A:8:SER:HB3	1:A:103:GLN:HG2	2.01	0.42
1:A:150:LYS:O	1:A:151:CYS:HB2	2.19	0.42
1:A:141:LEU:HD13	1:A:164:VAL:HG12	2.02	0.42
1:A:46:ASP:CG	1:A:50:ASN:HB2	2.44	0.42
3:A:504:GOL:O2	4:A:852:HOH:O	1.87	0.41
1:A:186:ILE:HB	1:A:189:MET:HE1	2.02	0.41
1:A:337:GLY:HA3	4:A:641:HOH:O	2.21	0.40
1:A:77:TYR:N	1:A:78:PRO:CD	2.85	0.40
2:A:503:PG4:H32	2:A:503:PG4:H52	1.82	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	433/448 (97%)	421 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	344/352 (98%)	337 (98%)	7 (2%)	48	48

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

Mol	Chain	Res	Type
1	A	162	HIS
1	A	164	VAL
1	A	194	ARG
1	A	260	GLU
1	A	299	THR
1	A	311	GLU
1	A	412	GLU

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	103	GLN
1	A	162	HIS
1	A	163	HIS
1	A	209	HIS
1	A	291	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	PG4	A	501	-	12,12,12	0.56	0	11,11,11	1.76	3 (27%)
2	PG4	A	503	-	12,12,12	0.68	0	11,11,11	1.32	0
2	PG4	A	502	-	12,12,12	0.64	0	11,11,11	1.49	0
3	GOL	A	504	-	5,5,5	0.32	0	5,5,5	0.77	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
2	PG4	A	501	-	-	3/10/10/10	-
2	PG4	A	503	-	-	6/10/10/10	-
2	PG4	A	502	-	-	9/10/10/10	-
3	GOL	A	504	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PG4	O4-C7-C8	2.11	119.43	110.11
2	A	501	PG4	O3-C4-C3	2.04	119.64	110.35
2	A	501	PG4	O4-C6-C5	2.02	119.56	110.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	O1-C1-C2-C3
2	A	503	PG4	C1-C2-O2-C3
2	A	503	PG4	C3-C4-O3-C5
2	A	501	PG4	O3-C5-C6-O4
2	A	502	PG4	O1-C1-C2-O2
2	A	503	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
2	A	502	PG4	C5-C6-O4-C7
2	A	502	PG4	O3-C5-C6-O4
2	A	503	PG4	O3-C5-C6-O4
2	A	502	PG4	C8-C7-O4-C6
3	A	504	GOL	O1-C1-C2-O2
2	A	502	PG4	O4-C7-C8-O5
2	A	501	PG4	C3-C4-O3-C5
2	A	502	PG4	C1-C2-O2-C3
2	A	502	PG4	C6-C5-O3-C4
2	A	503	PG4	C5-C6-O4-C7
2	A	501	PG4	C6-C5-O3-C4
2	A	502	PG4	C3-C4-O3-C5
2	A	503	PG4	C6-C5-O3-C4
2	A	502	PG4	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PG4	3	0
2	A	503	PG4	3	0
2	A	502	PG4	4	0
3	A	504	GOL	4	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	437/448 (97%)	0.16	26 (5%)	28 27	11, 29, 55, 86	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	SER	4.8
1	A	133	PHE	4.3
1	A	34	PHE	4.0
1	A	258	ALA	4.0
1	A	260	GLU	3.9
1	A	234	THR	3.7
1	A	183	GLY	3.5
1	A	259	ARG	3.4
1	A	236	PRO	3.3
1	A	233	ALA	3.2
1	A	47	ALA	3.1
1	A	235	PRO	3.1
1	A	7	GLY	3.0
1	A	131	VAL	3.0
1	A	261	ARG	2.9
1	A	134	SER	2.7
1	A	15	ALA	2.6
1	A	33	ARG	2.6
1	A	12	TYR	2.4
1	A	221	SER	2.4
1	A	162	HIS	2.3
1	A	138	ALA	2.3
1	A	71	GLU	2.2
1	A	136	ASP	2.1
1	A	187	ALA	2.1
1	A	63	ALA	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
2	PG4	A	501	13/13	0.67	0.22	43,49,61,64	0
2	PG4	A	503	13/13	0.78	0.18	37,44,50,50	0
2	PG4	A	502	13/13	0.79	0.17	37,45,52,62	0
3	GOL	A	504	6/6	0.79	0.18	31,35,38,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.