Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 06:17 PM EDT

PDB ID	:	1K7D
Title	:	Penicillin Acylase with Phenyl Proprionic Acid
Authors	:	Hensgens, C.M.H.; Keizer, E.; Snijder, H.J.; Dijkstra, B.W.
Deposited on	:	2001-10-19
Resolution	:	2.15 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:

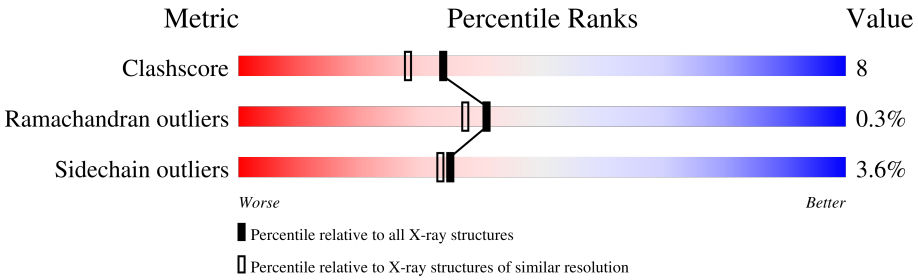
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	85% 11%
2	B	557	82% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6403 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 Penicillin Acylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1657	1058	278	313	8	0	0	0

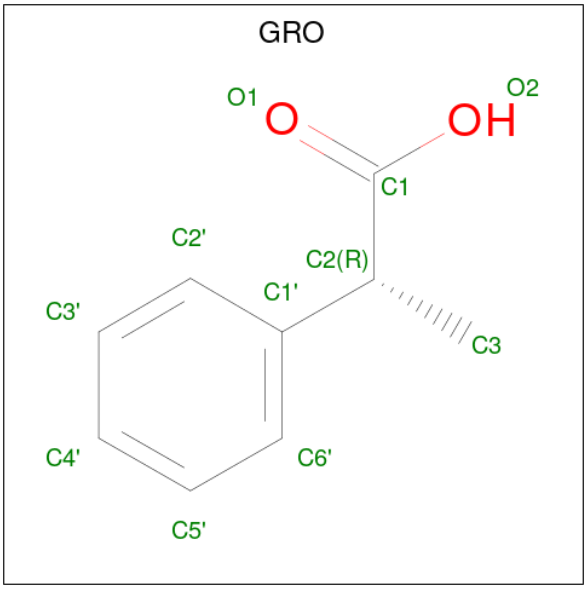
- Molecule 2 is a protein called penicillin Acylase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	557	4415	2805	766	834	10	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	B	1	1	1	0	0

- Molecule 4 is R-2-PHENYL-PROPRIONIC ACID (three-letter code: GRO) (formula: $C_9H_{10}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 11 9 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0
5	B	217	Total O 217 217	0	0

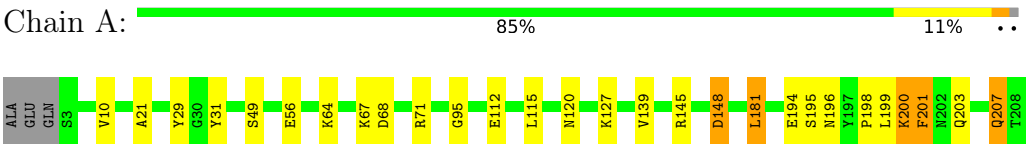
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

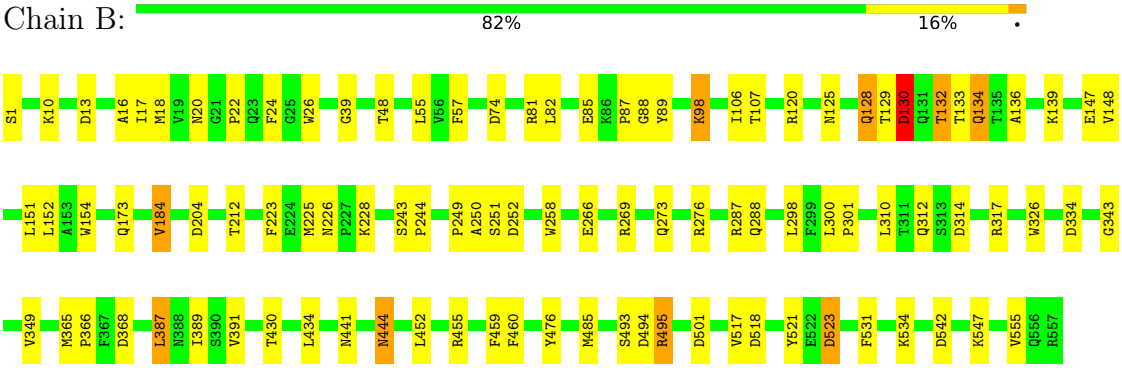
• Molecule 1: Penicillin Acylase alpha subunit

Chain A:



• Molecule 2: penicillin Acylase beta subunit

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.33Å 64.55Å 64.35Å 72.54° 73.29° 73.58°	Depositor
Resolution (Å)	30.15 – 2.15	Depositor
% Data completeness (in resolution range)	91.2 (30.15-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.182 , 0.216	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GRO

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	0.74	0/1699	0.87	2/2305 (0.1%)
2	B	0.76	0/4541	0.91	13/6192 (0.2%)
All	All	0.76	0/6240	0.90	15/8497 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	523	ASP	CB-CG-OD2	7.44	125.00	118.30
2	B	334	ASP	CB-CG-OD2	7.38	124.94	118.30
2	B	518	ASP	CB-CG-OD2	7.31	124.88	118.30
2	B	455	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	B	542	ASP	CB-CG-OD2	6.51	124.16	118.30
2	B	130	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	148	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	68	ASP	CB-CG-OD2	6.12	123.81	118.30
2	B	455	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	B	13	ASP	CB-CG-OD2	5.53	123.28	118.30
2	B	494	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	555	VAL	CB-CA-C	-5.17	101.58	111.40
2	B	252	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	184	VAL	CB-CA-C	-5.08	101.74	111.40
2	B	74	ASP	CB-CG-OD2	5.02	122.81	118.30

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	1657	0	1604	36	0
2	B	4415	0	4242	86	3
3	B	1	0	0	0	0
4	B	11	0	10	2	0
5	A	102	0	0	5	3
5	B	217	0	0	11	0
All	All	6403	0	5856	101	3

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 (101) 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)
2:B:128:GLN:O	5:B:984:HOH:O	1.69	1.11
2:B:128:GLN:OE1	5:B:1025:HOH:O	1.77	1.02
1:A:200:LYS:O	1:A:201:PHE:CD2	2.14	1.01
1:A:120:ASN:ND2	5:A:1034:HOH:O	1.98	0.96
1:A:181:LEU:HD22	1:A:203:GLN:HB3	1.48	0.94
1:A:207:GLN:HE22	2:B:204:ASP:H	1.07	0.94
2:B:128:GLN:CD	5:B:1025:HOH:O	2.06	0.93
2:B:128:GLN:C	5:B:984:HOH:O	2.03	0.89
1:A:71:ARG:CZ	2:B:128:GLN:HG3	2.03	0.87
1:A:200:LYS:O	1:A:201:PHE:CG	2.29	0.86
1:A:67:LYS:HG2	2:B:106:ILE:HD11	1.65	0.78
2:B:151:LEU:HG	5:B:851:HOH:O	1.85	0.77
2:B:132:THR:HG22	2:B:134:GLN:H	1.50	0.77
2:B:444:ASN:C	2:B:444:ASN:HD22	1.92	0.71
1:A:201:PHE:CE2	2:B:249:PRO:HG3	2.25	0.71
2:B:501:ASP:OD1	2:B:534:LYS:HE2	1.92	0.70
1:A:196:ASN:O	5:A:1116:HOH:O	2.11	0.69
1:A:67:LYS:HG2	2:B:106:ILE:CD1	2.23	0.68
1:A:181:LEU:CD2	1:A:203:GLN:HB3	2.23	0.68
1:A:10:VAL:HG13	2:B:547:LYS:HG3	1.76	0.67
2:B:493:SER:OG	2:B:495:ARG:HD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:THR:CG2	2:B:134:GLN:HE21	2.11	0.64
2:B:132:THR:CG2	2:B:134:GLN:HG2	2.27	0.64
1:A:71:ARG:NE	2:B:128:GLN:HG3	2.12	0.64
1:A:196:ASN:O	1:A:198:PRO:HD3	1.98	0.63
2:B:1:SER:CB	4:B:601:GRO:HO2	2.11	0.63
1:A:71:ARG:NH1	2:B:128:GLN:HG3	2.15	0.60
2:B:120:ARG:HH11	2:B:125:ASN:ND2	2.01	0.58
1:A:10:VAL:CG1	2:B:547:LYS:HG3	2.33	0.58
2:B:132:THR:HG21	2:B:134:GLN:HG2	1.87	0.57
2:B:22:PRO:HG3	2:B:57:PHE:CZ	2.40	0.57
2:B:132:THR:CG2	2:B:134:GLN:NE2	2.68	0.57
2:B:444:ASN:C	2:B:444:ASN:ND2	2.58	0.57
1:A:207:GLN:NE2	2:B:204:ASP:H	1.90	0.56
2:B:132:THR:HG23	2:B:134:GLN:NE2	2.20	0.56
2:B:18:MET:O	2:B:485:MET:HA	2.06	0.56
2:B:517:VAL:HG13	2:B:521:TYR:CB	2.36	0.56
2:B:132:THR:HG23	2:B:134:GLN:HE21	1.72	0.55
1:A:56:GLU:HG2	2:B:107:THR:HB	1.90	0.54
2:B:148:VAL:O	2:B:152:LEU:HD23	2.08	0.54
2:B:129:THR:HG22	2:B:130:ASP:N	2.25	0.51
2:B:317:ARG:HG3	2:B:317:ARG:HH11	1.76	0.50
2:B:517:VAL:HG13	2:B:521:TYR:CG	2.46	0.50
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.47	0.50
2:B:129:THR:HG22	2:B:130:ASP:CG	2.32	0.50
1:A:71:ARG:CD	2:B:128:GLN:HG3	2.42	0.49
2:B:132:THR:HG22	2:B:134:GLN:HG2	1.94	0.49
2:B:287:ARG:HA	2:B:531:PHE:CE1	2.48	0.49
1:A:199:LEU:HG	2:B:225:MET:CE	2.42	0.49
2:B:317:ARG:HG3	2:B:317:ARG:NH1	2.27	0.49
1:A:145:ARG:HD2	2:B:459:PHE:CE1	2.48	0.49
1:A:71:ARG:NE	5:A:827:HOH:O	2.46	0.48
2:B:1:SER:OG	4:B:601:GRO:HC2'	2.13	0.48
2:B:300:LEU:HB3	2:B:301:PRO:HD3	1.96	0.48
2:B:523:ASP:OD1	2:B:523:ASP:N	2.47	0.47
2:B:128:GLN:CG	5:B:1025:HOH:O	2.54	0.47
2:B:365:MET:HE2	5:B:892:HOH:O	2.14	0.47
2:B:365:MET:HE2	5:B:959:HOH:O	2.14	0.47
1:A:199:LEU:HG	2:B:225:MET:HE1	1.97	0.47
2:B:132:THR:CG2	2:B:133:THR:N	2.77	0.47
1:A:71:ARG:CZ	2:B:128:GLN:CG	2.85	0.46
1:A:21:ALA:O	2:B:39:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:THR:HG22	2:B:434:LEU:HD12	1.98	0.46
2:B:349:VAL:HB	2:B:430:THR:HG23	1.96	0.45
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.98	0.45
2:B:85:GLU:C	2:B:87:PRO:HD3	2.37	0.45
2:B:120:ARG:HH11	2:B:125:ASN:HD21	1.64	0.45
1:A:49:SER:HB3	2:B:460:PHE:CD1	2.52	0.45
2:B:89:TYR:CE2	2:B:98:LYS:HB2	2.52	0.44
1:A:194:GLU:O	1:A:195:SER:HB3	2.17	0.44
1:A:29:TYR:HA	1:A:95:GLY:O	2.16	0.44
1:A:115:LEU:HD23	1:A:120:ASN:OD1	2.18	0.44
2:B:287:ARG:NH1	2:B:288:GLN:NE2	2.65	0.44
2:B:266:GLU:OE1	2:B:269:ARG:NH2	2.51	0.43
2:B:132:THR:HG22	2:B:134:GLN:N	2.26	0.43
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.45	0.43
1:A:145:ARG:HD2	2:B:459:PHE:CZ	2.53	0.43
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.54	0.42
2:B:22:PRO:HG3	2:B:57:PHE:CE1	2.54	0.42
2:B:128:GLN:HE21	2:B:128:GLN:HB3	1.73	0.42
2:B:310:LEU:HD22	2:B:314:ASP:OD2	2.20	0.42
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.55	0.42
2:B:365:MET:CE	5:B:892:HOH:O	2.66	0.42
1:A:64:LYS:HG3	5:A:1038:HOH:O	2.20	0.42
1:A:115:LEU:CD2	1:A:120:ASN:OD1	2.68	0.42
2:B:128:GLN:HG2	5:B:1025:HOH:O	2.17	0.41
1:A:127:LYS:NZ	5:A:1046:HOH:O	2.36	0.41
2:B:10:LYS:HE2	5:B:924:HOH:O	2.20	0.41
2:B:16:ALA:C	2:B:17:ILE:HG13	2.41	0.41
2:B:48:THR:HB	2:B:55:LEU:HA	2.03	0.41
2:B:243:SER:HA	2:B:244:PRO:HD3	1.91	0.41
2:B:298:LEU:HD11	2:B:389:ILE:HD13	2.01	0.41
1:A:139:VAL:HG22	2:B:147:GLU:HB3	2.01	0.41
1:A:200:LYS:HE3	1:A:200:LYS:HB2	1.42	0.41
2:B:88:GLY:O	2:B:98:LYS:HE2	2.20	0.41
2:B:366:PRO:HA	2:B:368:ASP:OD1	2.20	0.41
2:B:269:ARG:O	2:B:273:GLN:HB2	2.21	0.40
2:B:365:MET:HA	2:B:366:PRO:HA	1.80	0.40
2:B:26:TRP:CE2	2:B:452:LEU:HD11	2.55	0.40
2:B:223:PHE:HA	2:B:226:ASN:OD1	2.22	0.40
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ARG:CZ	5:A:1100:HOH:O[1_556]	1.66	0.54
2:B:276:ARG:NH2	5:A:1100:HOH:O[1_556]	1.77	0.43
2:B:276:ARG:NH1	5:A:1100:HOH:O[1_556]	1.89	0.31

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	204/209 (98%)	194 (95%)	9 (4%)	1 (0%)	29	22
2	B	555/557 (100%)	541 (98%)	13 (2%)	1 (0%)	47	46
All	All	759/766 (99%)	735 (97%)	22 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	PHE
2	B	251	SER

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	178/180 (99%)	173 (97%)	5 (3%)	43	44
2	B	460/460 (100%)	442 (96%)	18 (4%)	32	30
All	All	638/640 (100%)	615 (96%)	23 (4%)	35	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	TYR
1	A	112	GLU
1	A	181	LEU
1	A	200	LYS
1	A	207	GLN
2	B	20	ASN
2	B	81	ARG
2	B	98	LYS
2	B	128	GLN
2	B	130	ASP
2	B	132	THR
2	B	134	GLN
2	B	154	TRP
2	B	173	GLN
2	B	184	VAL
2	B	212	THR
2	B	228	LYS
2	B	312	GLN
2	B	387	LEU
2	B	391	VAL
2	B	441	ASN
2	B	444	ASN
2	B	495	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
2	B	93	ASN
2	B	125	ASN
2	B	128	GLN
2	B	134	GLN
2	B	288	GLN
2	B	312	GLN
2	B	348	ASN
2	B	401	GLN
2	B	440	ASN
2	B	441	ASN
2	B	444	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 monosaccharides in this entry.

5.6 Ligand geometry

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	GRO	B	601	2	11,11,11	2.38	3 (27%)	14,14,14	0.73	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	GRO	B	601	2	-	3/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	GRO	O1-C1	6.13	1.40	1.22
4	B	601	GRO	O2-C1	3.81	1.43	1.30
4	B	601	GRO	C1'-C2	-3.07	1.47	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	GRO	O2-C1-C2-C3
4	B	601	GRO	O1-C1-C2-C3
4	B	601	GRO	O2-C1-C2-C1'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	GRO	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.