Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 07:32 PM EDT

PDB ID	:	1K5S
Title	:	PENICILLIN ACYLASE, MUTANT COMPLEXED WITH PPA
Authors	:	Hensgens, C.M.H.; Keizer, E.; Snijder, H.J.; Dijkstra, B.W.
Deposited on	:	2001-10-12
Resolution	:	2.43 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 (i) 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 (i)) were used in the production of this report:

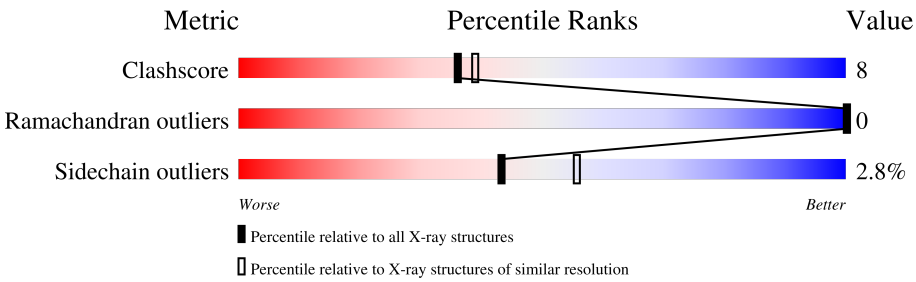
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.43 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	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)

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% 12% • •
2	B	557	80% 18% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6439 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 G 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 G ACYLASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	557	4410	2800	766	834	10	0	0	0

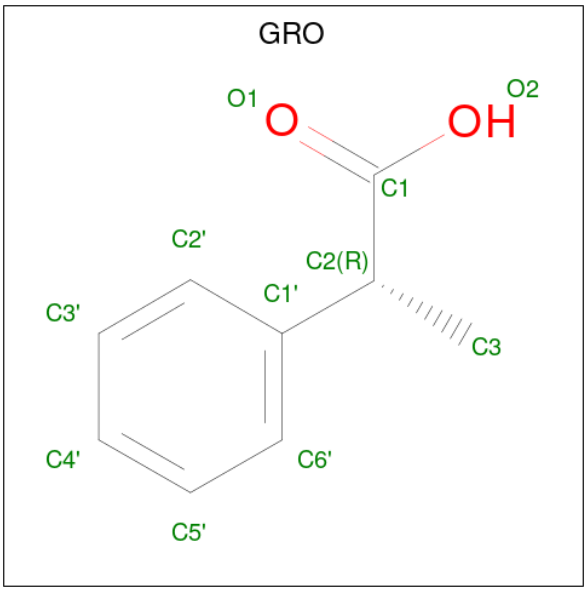
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	PHE	engineered mutation	UNP P06875
B	148	LEU	VAL	engineered mutation	UNP P06875

- 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	98	Total O 98 98	0	0
5	B	262	Total O 262 262	0	0

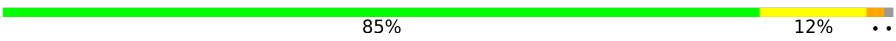
3 Residue-property plots (i)

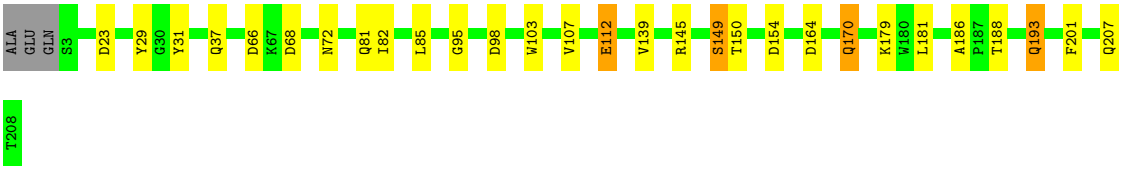
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 G ACYLASE ALPHA SUBUNIT

Chain A:





• Molecule 2: PENICILLIN G 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	50.82Å 64.36Å 64.75Å 72.89° 74.01° 73.55°	Depositor
Resolution (Å)	30.00 – 2.43	Depositor
% Data completeness (in resolution range)	96.2 (30.00-2.43)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS, REFMAC 5.0	Depositor
R, R_{free}	0.173 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6439	wwPDB-VP
Average B, all atoms ($Å^2$)	18.0	wwPDB-VP

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: 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	0.41	0/1699	0.71	6/2305 (0.3%)
2	B	0.46	3/4535 (0.1%)	0.75	15/6184 (0.2%)
All	All	0.44	3/6234 (0.0%)	0.74	21/8489 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	557	ARG	C-OXT	-8.10	1.07	1.23
2	B	165	GLU	CD-OE2	7.09	1.33	1.25
2	B	557	ARG	C-O	5.27	1.33	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	542	ASP	CB-CG-OD2	6.55	124.20	118.30
2	B	518	ASP	CB-CG-OD2	6.25	123.93	118.30
2	B	403	ASP	CB-CG-OD2	6.25	123.93	118.30
2	B	381	ASP	CB-CG-OD2	6.18	123.86	118.30
2	B	523	ASP	CB-CG-OD2	6.13	123.82	118.30
2	B	130	ASP	CB-CG-OD2	6.02	123.72	118.30
2	B	494	ASP	CB-CG-OD2	5.87	123.58	118.30
2	B	74	ASP	CB-CG-OD2	5.86	123.57	118.30
2	B	13	ASP	CB-CG-OD2	5.71	123.44	118.30
2	B	557	ARG	CA-C-O	-5.64	108.25	120.10
1	A	98	ASP	CB-CG-OD2	5.40	123.16	118.30
2	B	43	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	154	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	280	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	68	ASP	CB-CG-OD2	5.23	123.00	118.30
2	B	73	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	327	ASP	CB-CG-OD2	5.08	122.88	118.30
2	B	334	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	23	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	164	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	66	ASP	CB-CG-OD2	5.02	122.82	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	23	0
2	B	4410	0	4240	84	0
3	B	1	0	0	0	0
4	B	11	0	9	1	0
5	A	98	0	0	1	0
5	B	262	0	0	7	0
All	All	6439	0	5853	95	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 (95) 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:132:THR:HG22	2:B:134:GLN:H	1.07	1.19
2:B:129:THR:HG22	2:B:130:ASP:H	1.35	0.92
2:B:132:THR:HG22	2:B:134:GLN:N	1.86	0.90
2:B:129:THR:HG22	2:B:130:ASP:N	1.90	0.85
2:B:1:SER:HB3	2:B:22:PRO:HA	1.57	0.85
1:A:193:GLN:HE21	1:A:193:GLN:H	1.26	0.83
1:A:181:LEU:HD21	1:A:201:PHE:HB2	1.63	0.81
2:B:132:THR:CG2	2:B:134:GLN:H	1.92	0.80
2:B:59:HIS:HD2	2:B:61:GLY:H	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:HH11	2:B:125:ASN:ND2	1.81	0.78
2:B:132:THR:HG21	2:B:134:GLN:HG2	1.67	0.77
1:A:82:ILE:HG13	2:B:148:LEU:HD11	1.66	0.75
2:B:129:THR:CG2	2:B:130:ASP:H	1.99	0.75
1:A:181:LEU:CD2	1:A:201:PHE:HB2	2.21	0.71
1:A:72:ASN:HD21	2:B:139:LYS:NZ	1.92	0.66
2:B:132:THR:CG2	2:B:134:GLN:HG2	2.29	0.61
2:B:526:LYS:HA	2:B:526:LYS:HE2	1.81	0.61
1:A:112:GLU:H	1:A:112:GLU:CD	2.06	0.59
2:B:114:GLU:OE1	5:B:719:HOH:O	2.17	0.58
1:A:72:ASN:HD21	2:B:139:LYS:HZ1	1.53	0.57
2:B:132:THR:CG2	2:B:133:THR:N	2.66	0.57
2:B:156:HIS:HD2	5:B:634:HOH:O	1.89	0.56
2:B:318:GLN:NE2	5:B:675:HOH:O	2.10	0.56
2:B:477:GLN:HE21	2:B:479:ARG:HD3	1.71	0.56
2:B:59:HIS:HD2	2:B:61:GLY:N	2.02	0.55
2:B:471:ARG:NH2	2:B:522:GLU:OE1	2.40	0.55
2:B:457:ASN:HD22	2:B:463:PRO:HA	1.72	0.55
1:A:170:GLN:HB2	5:A:299:HOH:O	2.07	0.55
2:B:468:GLU:HG2	5:B:855:HOH:O	2.08	0.54
2:B:18:MET:O	2:B:485:MET:HA	2.06	0.54
2:B:387:LEU:HD22	2:B:476:TYR:HE2	1.73	0.54
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.91	0.53
2:B:88:GLY:O	2:B:99:MET:HG3	2.07	0.53
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.42	0.53
2:B:303:LEU:HD21	2:B:350:TRP:CE2	2.44	0.52
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.44	0.52
2:B:151:LEU:HD23	2:B:151:LEU:C	2.30	0.52
2:B:26:TRP:CE2	2:B:452:LEU:HD11	2.44	0.52
1:A:145:ARG:HD3	2:B:459:PHE:CE1	2.46	0.50
1:A:81:GLN:HB3	2:B:148:LEU:HD12	1.93	0.50
2:B:246:LYS:O	2:B:247:ASP:HB2	2.12	0.50
1:A:179:LYS:O	1:A:179:LYS:HG3	2.12	0.49
2:B:457:ASN:ND2	2:B:463:PRO:HA	2.29	0.48
2:B:120:ARG:HH11	2:B:125:ASN:HD21	1.60	0.48
1:A:82:ILE:HG13	2:B:148:LEU:CD1	2.41	0.48
2:B:120:ARG:NH1	2:B:125:ASN:ND2	2.57	0.48
2:B:59:HIS:CD2	2:B:61:GLY:H	2.20	0.48
2:B:35:ILE:HG13	2:B:36:GLY:N	2.29	0.47
2:B:67:SER:HA	2:B:178:ASN:O	2.13	0.47
1:A:207:GLN:HA	2:B:215:TRP:CZ2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:ASN:OD1	2:B:460:PHE:HB2	2.15	0.47
2:B:166:TRP:CH2	2:B:179:TRP:HB3	2.50	0.47
2:B:142:ALA:HB2	2:B:197:PRO:HD3	1.95	0.46
1:A:72:ASN:ND2	2:B:139:LYS:NZ	2.62	0.46
2:B:132:THR:HG22	2:B:133:THR:N	2.29	0.46
2:B:27:TYR:OH	2:B:459:PHE:HB3	2.15	0.46
2:B:22:PRO:HG3	2:B:57:PHE:CZ	2.51	0.46
2:B:369:LYS:HE3	2:B:369:LYS:HB3	1.84	0.45
2:B:479:ARG:NH1	2:B:528:TYR:O	2.47	0.45
2:B:261:ALA:O	2:B:394:LYS:HE2	2.17	0.45
2:B:132:THR:HG23	2:B:134:GLN:NE2	2.31	0.45
2:B:359:VAL:HG22	2:B:413:LEU:HD13	1.97	0.45
2:B:454:PHE:HB2	2:B:471:ARG:HB2	2.00	0.44
1:A:37:GLN:HG2	1:A:103:TRP:CE2	2.52	0.44
2:B:358:THR:HB	2:B:413:LEU:HB3	1.98	0.44
1:A:103:TRP:O	1:A:107:VAL:HG23	2.18	0.44
2:B:489:SER:N	2:B:490:PRO:CD	2.81	0.43
1:A:149:SER:HB3	2:B:253:LEU:HD11	2.00	0.43
1:A:29:TYR:HA	1:A:95:GLY:O	2.18	0.43
2:B:419:GLN:NE2	5:B:835:HOH:O	2.46	0.43
2:B:163:TRP:O	2:B:167:THR:HG23	2.19	0.43
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.00	0.43
2:B:90:TYR:CD2	2:B:99:MET:HG2	2.54	0.43
2:B:161:LYS:HA	2:B:161:LYS:HD3	1.75	0.43
1:A:193:GLN:HE21	1:A:193:GLN:N	2.06	0.42
2:B:349:VAL:HB	2:B:430:THR:HG23	2.02	0.42
2:B:300:LEU:N	2:B:301:PRO:CD	2.82	0.42
2:B:436:LYS:HD2	5:B:857:HOH:O	2.20	0.42
1:A:150:THR:HA	2:B:252:ASP:OD1	2.20	0.42
2:B:316:ARG:NH1	2:B:424:LEU:HB3	2.34	0.42
2:B:176:THR:O	2:B:176:THR:HG23	2.19	0.42
2:B:526:LYS:HE2	2:B:526:LYS:CA	2.46	0.42
1:A:139:VAL:HG22	2:B:147:GLU:HB3	2.01	0.41
2:B:64:SER:HB3	2:B:486:ILE:HG21	2.02	0.41
2:B:129:THR:CG2	2:B:130:ASP:N	2.59	0.41
2:B:99:MET:HE2	2:B:119:TRP:HB3	2.01	0.41
2:B:368:ASP:OD1	2:B:368:ASP:N	2.53	0.41
2:B:477:GLN:NE2	2:B:479:ARG:HH11	2.19	0.41
1:A:85:LEU:HD22	2:B:152:LEU:HD11	2.03	0.40
1:A:186:ALA:O	1:A:188:THR:HG23	2.20	0.40
2:B:99:MET:CE	2:B:119:TRP:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:TYR:HD2	2:B:99:MET:HG2	1.85	0.40
2:B:156:HIS:CD2	5:B:634:HOH:O	2.69	0.40
2:B:1:SER:OG	4:B:601:GRO:O2	2.32	0.40
2:B:300:LEU:HB3	2:B:301:PRO:HD3	2.04	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	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
2	B	555/557 (100%)	543 (98%)	12 (2%)	0	100	100
All	All	759/766 (99%)	741 (98%)	18 (2%)	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	178/180 (99%)	173 (97%)	5 (3%)	43	56
2	B	459/459 (100%)	446 (97%)	13 (3%)	43	56
All	All	637/639 (100%)	619 (97%)	18 (3%)	43	56

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	TYR
1	A	112	GLU
1	A	149	SER
1	A	170	GLN
1	A	193	GLN
2	B	1	SER
2	B	20	ASN
2	B	128	GLN
2	B	130	ASP
2	B	134	GLN
2	B	154	TRP
2	B	173	GLN
2	B	387	LEU
2	B	432	GLU
2	B	459	PHE
2	B	471	ARG
2	B	495	ARG
2	B	534	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	120	ASN
1	A	193	GLN
2	B	59	HIS
2	B	110	ASN
2	B	125	ASN
2	B	134	GLN
2	B	156	HIS
2	B	273	GLN
2	B	292	GLN
2	B	304	GLN
2	B	312	GLN
2	B	333	ASN
2	B	348	ASN
2	B	419	GLN
2	B	457	ASN
2	B	477	GLN
2	B	556	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 monosaccharides 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	GRO	B	601	-	11,11,11	1.02	2 (18%)	14,14,14	0.98	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	-	-	4/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	GRO	O2-C1	-2.27	1.23	1.30
4	B	601	GRO	C1'-C2	-2.12	1.49	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.