wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 01:27 am GMT

PDB ID	:	1OK2
Title	:	Decay accelerating factor (CD55): the structure of an intact human complement regulator.
Authors	:	Lukacik, P.; Roversi, P.; White, J.; Esser, D.; Smith, G.P.; Billington, J.; Williams, P.A.; Rudd, P.M.; Wormald, M.R.; Crispin, M.D.M.; Radcliffe, C.M.; Dwek, R.A.; Evans, D.J.; Morgan, B.P.; Smith, R.A.G.; Lea, S.M.
Deposited on	:	2003-07-16
Resolution	:	2.50 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 (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:

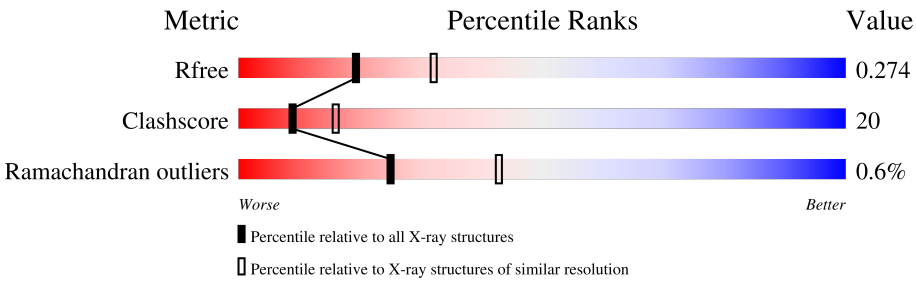
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)

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%

Mol	Chain	Length	Quality of chain
1	A	254	71% 27% ··
1	B	254	68% 31%

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
2	ACT	A	1255	-	-	X	-
2	ACT	A	1256	-	-	X	-
2	ACT	B	1255	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	1256	-	-	X	-
4	GOL	A	1258	-	X	-	-
4	GOL	A	1259	-	X	-	-
4	GOL	A	1260	-	X	-	-
4	GOL	A	1261	-	X	-	-
4	GOL	A	1262	-	X	-	-
4	GOL	B	1258	-	X	-	-
4	GOL	B	1259	-	X	-	-
4	GOL	B	1260	-	X	-	-
4	GOL	B	1261	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4285 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.

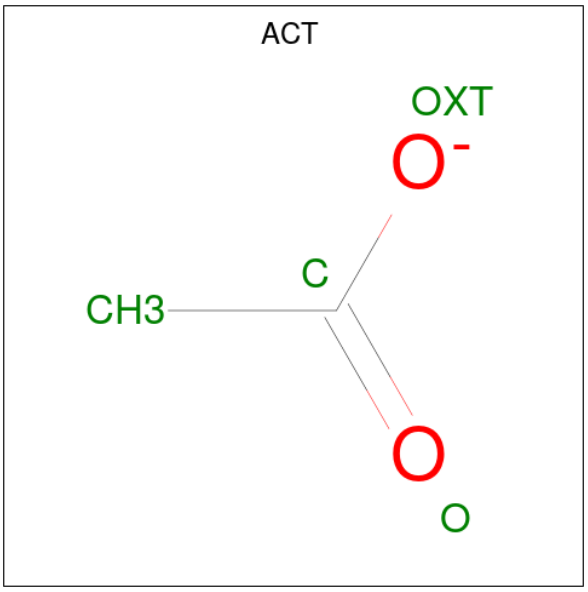
- Molecule 1 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	1969	1234	330	386	19	0	0	0
1	B	253	1961	1229	329	385	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ILE	THR	SEE REMARK 999	UNP P08174
B	48	ILE	THR	SEE REMARK 999	UNP P08174

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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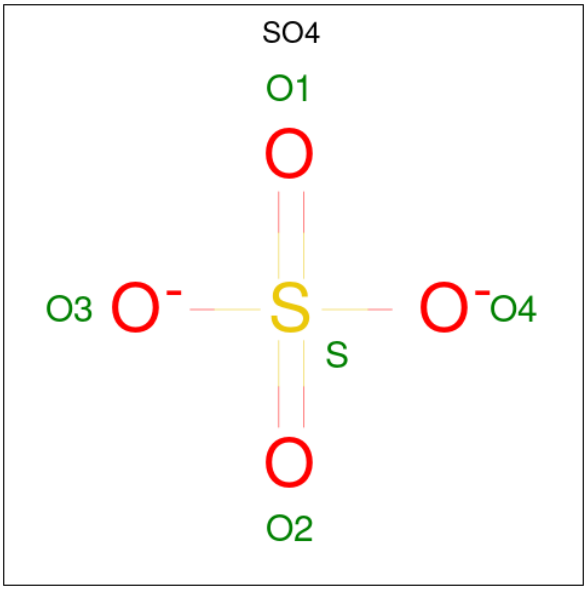
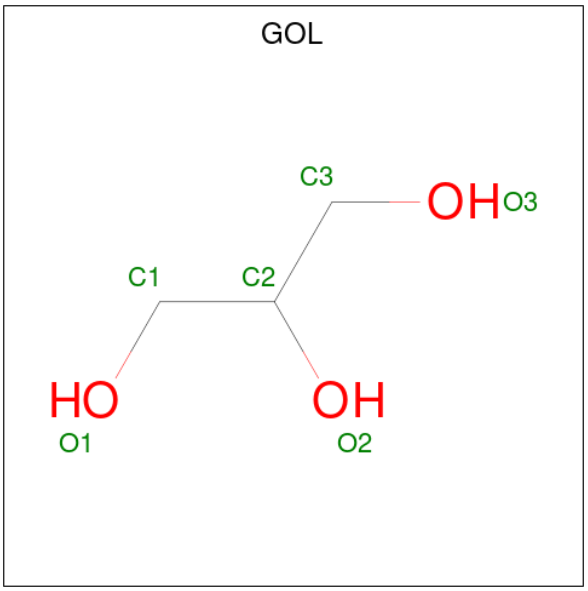
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0

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



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

- Molecule 5 is water.

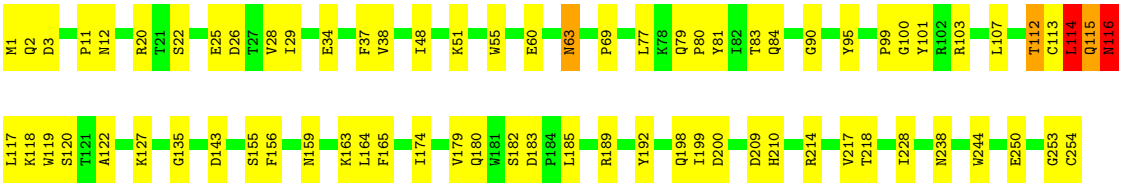
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	133	133	133	0	0
			Total	O		
5	B	142	142	142	0	0

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.

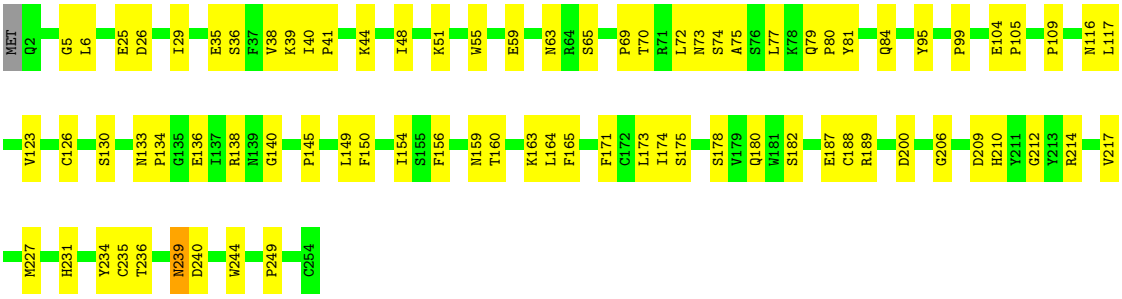
• Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain A:



• Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.58Å 55.62Å 61.53Å 86.56° 84.44° 64.22°	Depositor
Resolution (Å)	19.00 – 2.50 18.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.00-2.50) 93.7 (18.77-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.49Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.229 , (Not available) 0.225 , 0.274	Depositor DCC
R_{free} test set	931 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 21.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	4285	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, ACT

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	0.68	9/2022 (0.4%)	0.68	7/2749 (0.3%)
1	B	0.35	0/2014	0.51	1/2739 (0.0%)
All	All	0.54	9/4036 (0.2%)	0.60	8/5488 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLN	C-O	10.79	1.43	1.23
1	A	115	GLN	CA-C	-9.23	1.28	1.52
1	A	113	CYS	N-CA	9.02	1.64	1.46
1	A	116	ASN	CB-CG	-8.89	1.30	1.51
1	A	116	ASN	N-CA	-8.79	1.28	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	GLN	CB-CA-C	-10.04	90.32	110.40
1	A	116	ASN	CB-CA-C	8.71	127.82	110.40
1	A	113	CYS	CB-CA-C	-7.91	94.58	110.40
1	A	115	GLN	C-N-CA	6.05	136.82	121.70
1	A	115	GLN	O-C-N	-5.93	113.21	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	116	ASN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	LEU	Mainchain
1	A	115	GLN	Mainchain,Peptide
1	A	63	ASN	Mainchain,Peptide

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	1969	0	1867	78	3
1	B	1961	0	1855	82	2
2	A	8	0	6	8	0
2	B	8	0	6	9	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	30	0	20	3	0
4	B	24	0	16	1	1
5	A	133	0	0	12	1
5	B	142	0	0	15	1
All	All	4285	0	3770	158	4

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 20.

The worst 5 of 158 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:114:LEU:HB3	1:A:116:ASN:OD1	1.15	1.23
1:A:114:LEU:CB	1:A:116:ASN:OD1	1.93	1.15
1:B:26:ASP:HA	1:B:48:ILE:HD11	1.47	0.97
1:B:70:THR:O	5:B:2048:HOH:O	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:N	1:A:118:LYS:O	2.05	0.90

All (4) 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)
1:A:90:GLY:O	1:B:5:GLY:CA[1_486]	1.98	0.22
1:A:25:GLU:OE2	4:B:1258:GOL:O3[1_476]	2.09	0.11
1:A:90:GLY:O	1:B:6:LEU:N[1_486]	2.15	0.05
5:A:2003:HOH:O	5:B:2060:HOH:O[1_386]	2.15	0.05

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	252/254 (99%)	238 (94%)	12 (5%)	2 (1%)	19 35
1	B	251/254 (99%)	238 (95%)	12 (5%)	1 (0%)	34 54
All	All	503/508 (99%)	476 (95%)	24 (5%)	3 (1%)	25 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	116	ASN
1	B	109	PRO

5.3.2 Protein sidechains (i)

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

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)

15 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	$\#\|Z\| > 2$
3	SO4	B	1257	-	4,4,4	0.42	0	6,6,6	0.76	0
4	GOL	A	1260	-	5,5,5	4.54	5 (100%)	5,5,5	5.73	3 (60%)
4	GOL	B	1261	-	5,5,5	4.50	5 (100%)	5,5,5	5.73	3 (60%)
2	ACT	B	1255	-	3,3,3	1.14	0	3,3,3	0.79	0
3	SO4	A	1257	-	4,4,4	0.31	0	6,6,6	0.76	0
4	GOL	A	1259	-	5,5,5	4.53	5 (100%)	5,5,5	5.70	3 (60%)
4	GOL	A	1261	-	5,5,5	4.48	5 (100%)	5,5,5	5.73	3 (60%)
4	GOL	A	1258	-	5,5,5	4.54	5 (100%)	5,5,5	5.67	3 (60%)
4	GOL	B	1258	-	5,5,5	4.51	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	B	1260	-	5,5,5	4.50	5 (100%)	5,5,5	5.73	3 (60%)
2	ACT	B	1256	-	3,3,3	1.21	1 (33%)	3,3,3	0.77	0
2	ACT	A	1256	-	3,3,3	1.28	1 (33%)	3,3,3	0.80	0
2	ACT	A	1255	-	3,3,3	1.19	0	3,3,3	0.71	0
4	GOL	A	1262	-	5,5,5	4.46	5 (100%)	5,5,5	5.71	3 (60%)
4	GOL	B	1259	-	5,5,5	4.53	5 (100%)	5,5,5	5.72	3 (60%)

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	1260	-	-	2/4/4/4	-
4	GOL	B	1261	-	-	2/4/4/4	-
4	GOL	A	1259	-	-	3/4/4/4	-
4	GOL	A	1261	-	-	2/4/4/4	-
4	GOL	A	1258	-	-	2/4/4/4	-
4	GOL	B	1258	-	-	2/4/4/4	-
4	GOL	B	1260	-	-	3/4/4/4	-
4	GOL	A	1262	-	-	3/4/4/4	-
4	GOL	B	1259	-	-	3/4/4/4	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1260	GOL	C3-C2	-7.57	1.20	1.51
4	A	1259	GOL	C3-C2	-7.45	1.21	1.51
4	B	1258	GOL	C3-C2	-7.42	1.21	1.51
4	B	1259	GOL	C3-C2	-7.42	1.21	1.51
4	A	1258	GOL	C3-C2	-7.42	1.21	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1260	GOL	O3-C3-C2	10.51	160.60	110.20
4	B	1261	GOL	O3-C3-C2	10.48	160.46	110.20
4	B	1258	GOL	O3-C3-C2	10.48	160.44	110.20
4	A	1261	GOL	O3-C3-C2	10.47	160.39	110.20
4	A	1262	GOL	O3-C3-C2	10.46	160.36	110.20

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1259	GOL	O1-C1-C2-C3
4	A	1259	GOL	O2-C2-C3-O3
4	A	1260	GOL	O1-C1-C2-C3
4	A	1261	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1261	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1260	GOL	2	0
2	B	1255	ACT	3	0
4	A	1261	GOL	1	0
4	B	1258	GOL	0	1
2	B	1256	ACT	6	0
2	A	1256	ACT	6	0
2	A	1255	ACT	2	0
4	B	1259	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.