



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:48 AM UTC

PDB ID : 5MCN / pdb_00005mcn
Title : Radiation damage to GH7 Family Cellobiohydrolase from Daphnia pulex: Dose (DWD) 22.7 MGy
Authors : Bury, C.S.; McGeehan, J.E.; Ebrahim, A.; Garman, E.F.
Deposited on : 2016-11-10
Resolution : 2.00 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

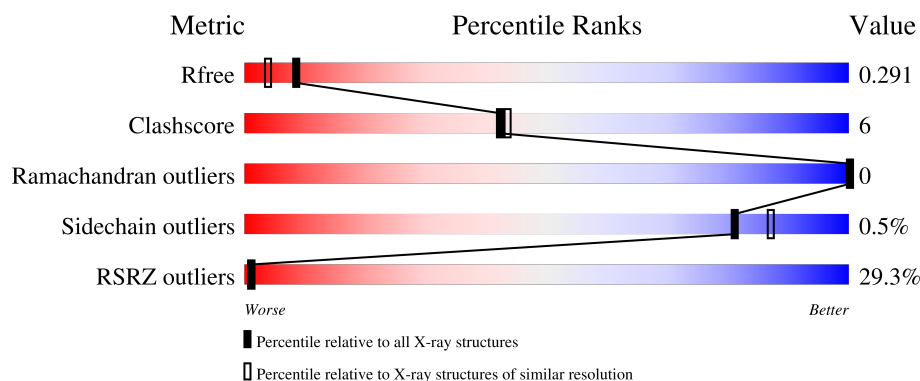
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	445	23% 97% ..
1	B	445	35% 85% 14% .

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	GOL	B	501	-	-	-	X

2 Entry composition [i](#)

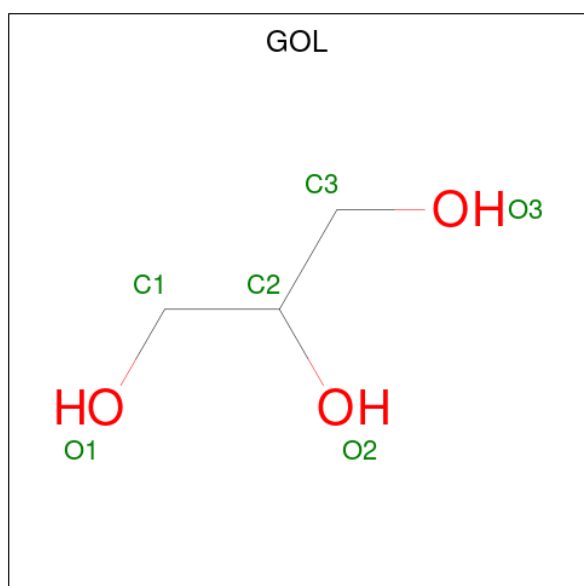
There are 4 unique types of molecules in this entry. The entry contains 7298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cellobiohydrolase CHBI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3353	2082	566	676	29			
1	B	441	Total	C	N	O	S	0	0	0
			3347	2079	565	674	29			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

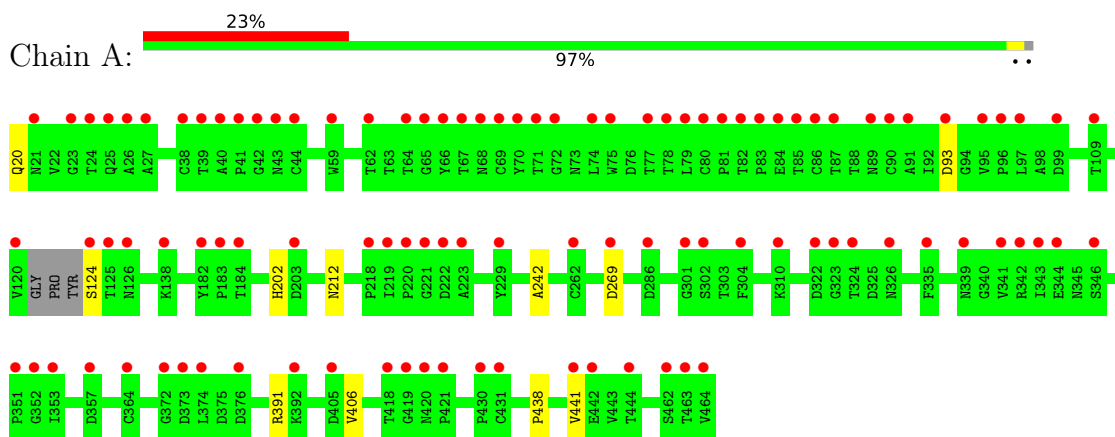
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	340	Total	O	0	0
			340	340		
4	B	235	Total	O	0	0
			235	235		

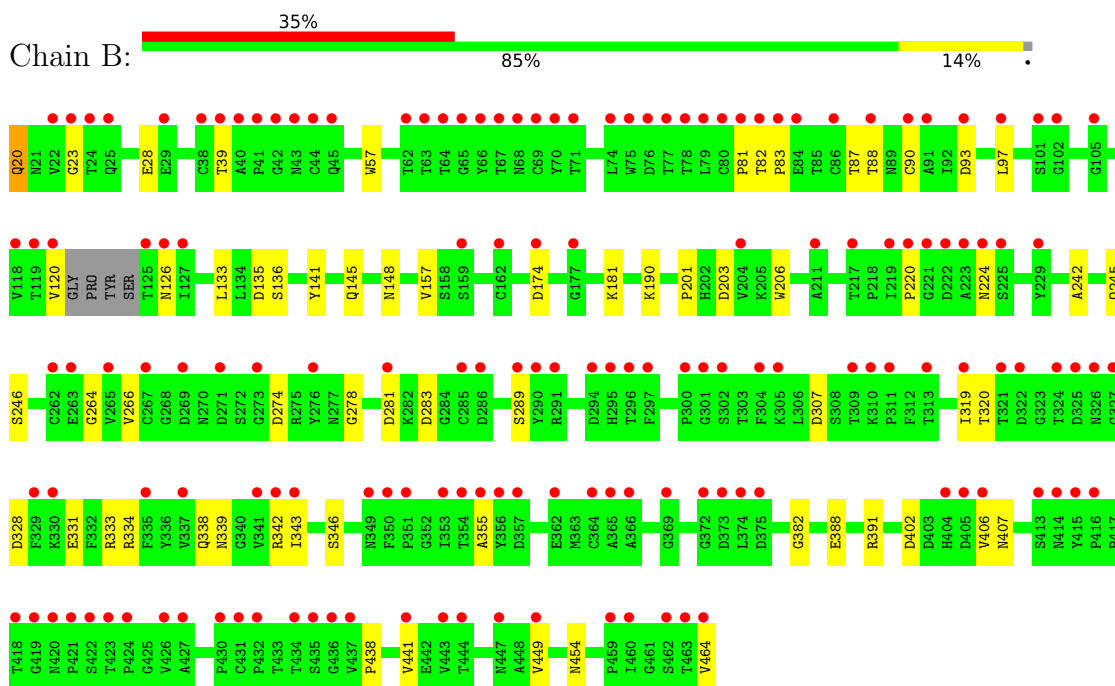
3 Residue-property plots

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: Cellobiohydrolase CHBI



• Molecule 1: Cellobiohydrolase CHBI



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.77Å 46.84Å 174.92Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	83.08 – 2.00 83.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (83.08-2.00) 99.4 (83.08-2.00)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.262 , 0.284 0.269 , 0.291	Depositor DCC
R_{free} test set	3285 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7298	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: SO4, GOL, PCA

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	0.52	0/3427	0.72	1/4667 (0.0%)
1	B	0.50	0/3421	0.72	1/4659 (0.0%)
All	All	0.51	0/6848	0.72	2/9326 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ALA	N-CA-C	6.04	117.70	108.52
1	B	242	ALA	N-CA-C	5.61	117.62	108.76

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	3353	0	3114	6	0
1	B	3347	0	3109	75	0
2	A	6	0	8	0	0
2	B	12	0	16	3	0
3	B	5	0	0	0	0
4	A	340	0	0	2	0
4	B	235	0	0	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7298	0	6247	81	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 6.

All (81) 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:B:449:VAL:O	4:B:601:HOH:O	1.84	0.94
1:B:334:ARG:O	4:B:602:HOH:O	1.84	0.94
1:B:388:GLU:OE2	4:B:603:HOH:O	1.89	0.89
1:B:20:PCA:OE	4:B:604:HOH:O	1.90	0.89
1:B:23:GLY:O	4:B:605:HOH:O	1.91	0.88
1:B:281:ASP:OD1	4:B:606:HOH:O	1.93	0.87
1:B:97:LEU:O	4:B:607:HOH:O	1.93	0.84
1:B:407:ASN:O	4:B:608:HOH:O	1.95	0.84
1:B:454:ASN:O	4:B:609:HOH:O	1.95	0.84
1:B:220:PRO:O	4:B:610:HOH:O	1.97	0.82
1:B:87:THR:O	4:B:611:HOH:O	1.98	0.82
1:B:339:ASN:O	4:B:612:HOH:O	1.99	0.81
1:B:331:GLU:OE1	4:B:613:HOH:O	1.99	0.79
1:B:338:GLN:OE1	4:B:615:HOH:O	2.01	0.79
1:B:39:THR:O	4:B:617:HOH:O	2.02	0.78
1:B:342:ARG:O	4:B:616:HOH:O	2.01	0.78
1:B:174:ASP:OD1	4:B:619:HOH:O	2.03	0.76
1:B:320:THR:O	4:B:618:HOH:O	2.03	0.76
1:B:319:ILE:HG23	2:B:501:GOL:H11	1.68	0.75
1:B:333:ARG:HA	4:B:642:HOH:O	1.88	0.74
1:B:28:GLU:OE2	4:B:620:HOH:O	2.06	0.73
1:B:289:SER:HA	4:B:682:HOH:O	1.89	0.72
1:B:245:GLN:O	4:B:621:HOH:O	2.09	0.70
1:B:224:ASN:HB2	4:B:660:HOH:O	1.93	0.68
1:B:264:GLY:O	4:B:622:HOH:O	2.12	0.68
1:B:441:VAL:HG12	4:B:722:HOH:O	1.95	0.66
1:B:90:CYS:O	4:B:611:HOH:O	2.13	0.66
1:B:346:SER:HB2	4:B:644:HOH:O	1.95	0.66
1:B:148:ASN:OD1	4:B:625:HOH:O	2.14	0.65
1:B:81:PRO:O	4:B:626:HOH:O	2.14	0.65
1:B:328:ASP:OD2	4:B:624:HOH:O	2.13	0.64
1:B:83:PRO:HB3	4:B:681:HOH:O	1.97	0.64
1:B:28:GLU:HG3	4:B:674:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:NH2	4:A:607:HOH:O	2.32	0.61
1:B:20:PCA:O	4:B:629:HOH:O	2.15	0.60
1:B:88:THR:OG1	4:B:631:HOH:O	2.17	0.59
1:B:136:SER:OG	4:B:628:HOH:O	2.15	0.59
1:B:307:ASP:HB2	4:B:745:HOH:O	2.02	0.58
1:B:319:ILE:CG2	2:B:501:GOL:H11	2.33	0.58
1:B:206:TRP:HD1	4:B:702:HOH:O	1.88	0.57
1:B:319:ILE:HG23	2:B:501:GOL:C1	2.35	0.56
1:B:283:ASP:O	4:B:632:HOH:O	2.17	0.56
1:B:145:GLN:HB3	4:B:703:HOH:O	2.06	0.55
1:B:334:ARG:N	4:B:642:HOH:O	2.25	0.54
1:B:203:ASP:OD1	4:B:633:HOH:O	2.17	0.54
1:B:206:TRP:HB2	4:B:738:HOH:O	2.08	0.53
1:B:157:VAL:N	4:B:623:HOH:O	2.12	0.53
1:A:202:HIS:HE1	1:A:269:ASP:OD1	1.92	0.52
1:B:57:TRP:HD1	1:B:126:ASN:HD21	1.57	0.52
1:B:28:GLU:CG	4:B:674:HOH:O	2.54	0.52
1:B:246:SER:HA	4:B:650:HOH:O	2.10	0.51
1:B:278:GLY:HA3	4:B:735:HOH:O	2.10	0.51
1:B:133:LEU:O	4:B:635:HOH:O	2.19	0.51
1:B:57:TRP:CD1	1:B:126:ASN:HD21	2.30	0.50
1:B:333:ARG:CA	4:B:642:HOH:O	2.54	0.49
1:B:28:GLU:CD	4:B:620:HOH:O	2.55	0.49
1:B:343:ILE:HA	4:B:630:HOH:O	2.12	0.49
1:B:190:LYS:HG3	4:B:759:HOH:O	2.13	0.49
1:B:201:PRO:HB3	4:B:828:HOH:O	2.12	0.48
1:B:441:VAL:CG1	4:B:722:HOH:O	2.58	0.48
1:B:406:VAL:HG12	1:B:406:VAL:O	2.14	0.47
1:A:406:VAL:HG12	1:A:406:VAL:O	2.13	0.47
1:B:181:LYS:NZ	4:B:678:HOH:O	2.47	0.47
1:B:355:ALA:O	4:B:637:HOH:O	2.21	0.46
1:B:342:ARG:HB3	4:B:616:HOH:O	2.18	0.44
1:B:141:TYR:HB3	4:B:635:HOH:O	2.18	0.43
1:B:120:VAL:O	1:B:120:VAL:HG23	2.20	0.42
1:B:441:VAL:HA	4:B:779:HOH:O	2.19	0.42
1:A:202:HIS:CE1	1:A:269:ASP:OD1	2.71	0.42
1:B:438:PRO:HA	1:B:441:VAL:HG22	2.02	0.42
1:B:283:ASP:HB3	4:B:632:HOH:O	2.19	0.42
1:B:274:ASP:HA	4:B:662:HOH:O	2.19	0.41
1:B:135:ASP:HB2	4:B:634:HOH:O	2.20	0.41
1:B:283:ASP:HB2	4:B:651:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLY:HA2	4:B:670:HOH:O	2.21	0.41
1:B:391:ARG:HA	4:B:703:HOH:O	2.21	0.41
1:B:402:ASP:HB2	4:B:653:HOH:O	2.20	0.41
1:A:212:ASN:HA	4:A:681:HOH:O	2.20	0.40
1:B:266:VAL:HA	4:B:789:HOH:O	2.22	0.40
1:A:438:PRO:HA	1:A:441:VAL:HG22	2.04	0.40
1:B:82:THR:CA	4:B:646:HOH:O	2.70	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	438/445 (98%)	432 (99%)	6 (1%)	0	100	100
1	B	437/445 (98%)	431 (99%)	6 (1%)	0	100	100
All	All	875/890 (98%)	863 (99%)	12 (1%)	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	365/367 (100%)	363 (100%)	2 (0%)	81	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	364/367 (99%)	362 (100%)	2 (0%)	81	87
All	All	729/734 (99%)	725 (100%)	4 (0%)	81	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASP
1	A	124	SER
1	B	93	ASP
1	B	464	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	202	HIS
1	A	259	GLN
1	A	326	ASN
1	A	447	ASN
1	B	126	ASN
1	B	259	GLN
1	B	339	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	PCA	B	20	1	7,8,9	0.57	0	9,10,12	1.53	2 (22%)
1	PCA	A	20	1	7,8,9	0.53	0	9,10,12	1.49	2 (22%)

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
1	PCA	B	20	1	-	0/0/11/13	0/1/1/1
1	PCA	A	20	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	PCA	CB-CA-C	-3.27	108.17	112.66
1	A	20	PCA	CB-CA-C	-3.03	108.51	112.66
1	B	20	PCA	OE-CD-CG	-2.22	122.76	126.72
1	A	20	PCA	OE-CD-CG	-2.17	122.84	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	20	PCA	2	0

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	$\# Z > 2$
3	SO4	B	503	-	4,4,4	0.42	0	6,6,6	0.07	0
2	GOL	A	501	-	5,5,5	0.36	0	5,5,5	0.32	0
2	GOL	B	501	-	5,5,5	0.31	0	5,5,5	0.46	0
2	GOL	B	502	-	5,5,5	0.33	0	5,5,5	0.27	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	GOL	A	501	-	-	2/4/4/4	-
2	GOL	B	501	-	-	1/4/4/4	-
2	GOL	B	502	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	B	502	GOL	C1-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	B	501	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	GOL	3	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	441/445 (99%)	1.38	103 (23%) 2 2	13, 26, 40, 49	0
1	B	440/445 (98%)	1.74	155 (35%) 1 1	16, 32, 46, 57	0
All	All	881/890 (98%)	1.56	258 (29%) 1 1	13, 29, 44, 57	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	VAL	6.7
1	B	364	CYS	6.6
1	A	44	CYS	6.1
1	A	26	ALA	5.4
1	A	364	CYS	5.0
1	B	419	GLY	4.9
1	B	44	CYS	4.8
1	A	66	TYR	4.7
1	B	374	LEU	4.6
1	B	101	SER	4.6
1	A	419	GLY	4.6
1	A	40	ALA	4.5
1	B	356	TYR	4.4
1	B	41	PRO	4.3
1	B	302	SER	4.2
1	A	79	LEU	4.2
1	B	125	THR	4.1
1	B	423	THR	4.1
1	B	335	PHE	4.1
1	B	45	GLN	4.1
1	A	23	GLY	4.0
1	B	343	ILE	4.0
1	B	40	ALA	4.0
1	A	120	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	3.9
1	A	65	GLY	3.8
1	A	80	CYS	3.8
1	A	43	ASN	3.8
1	B	74	LEU	3.8
1	A	262	CYS	3.7
1	B	64	THR	3.7
1	A	72	GLY	3.7
1	B	267	CYS	3.7
1	A	183	PRO	3.7
1	B	23	GLY	3.7
1	A	222	ASP	3.7
1	B	38	CYS	3.6
1	B	80	CYS	3.6
1	A	392	LYS	3.6
1	B	223	ALA	3.6
1	B	79	LEU	3.6
1	B	24	THR	3.6
1	A	41	PRO	3.6
1	B	432	PRO	3.6
1	B	221	GLY	3.6
1	B	324	THR	3.5
1	B	350	PHE	3.5
1	B	420	ASN	3.5
1	A	42	GLY	3.5
1	B	406	VAL	3.5
1	B	464	VAL	3.5
1	B	63	THR	3.5
1	B	427	ALA	3.5
1	B	224	ASN	3.4
1	B	322	ASP	3.4
1	B	362	GLU	3.4
1	A	462	SER	3.4
1	B	422	SER	3.4
1	A	69	CYS	3.3
1	A	87	THR	3.3
1	B	66	TYR	3.3
1	B	337	VAL	3.2
1	A	124	SER	3.2
1	A	352	GLY	3.2
1	B	421	PRO	3.2
1	B	353	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	77	THR	3.2
1	B	262	CYS	3.2
1	A	405	ASP	3.2
1	A	62	THR	3.2
1	B	355	ALA	3.1
1	B	462	SER	3.1
1	A	372	GLY	3.1
1	B	375	ASP	3.1
1	A	82	THR	3.1
1	B	67	THR	3.1
1	A	74	LEU	3.1
1	B	217	THR	3.0
1	A	38	CYS	3.0
1	A	353	ILE	3.0
1	A	81	PRO	3.0
1	A	77	THR	3.0
1	B	297	PHE	3.0
1	A	341	VAL	3.0
1	B	418	THR	3.0
1	A	374	LEU	2.9
1	B	426	VAL	2.9
1	A	24	THR	2.9
1	B	78	THR	2.9
1	B	415	TYR	2.9
1	A	91	ALA	2.9
1	B	326	ASN	2.9
1	B	295	HIS	2.9
1	A	464	VAL	2.9
1	A	39	THR	2.9
1	A	67	THR	2.9
1	A	219	ILE	2.9
1	B	290	TYR	2.9
1	B	329	PHE	2.9
1	B	222	ASP	2.8
1	B	405	ASP	2.8
1	A	342	ARG	2.8
1	A	431	CYS	2.8
1	B	354	THR	2.8
1	B	463	THR	2.8
1	A	184	THR	2.8
1	A	420	ASN	2.8
1	B	84	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	351	PRO	2.8
1	B	310	LYS	2.8
1	B	413	SER	2.8
1	B	25	GLN	2.8
1	A	323	GLY	2.8
1	A	203	ASP	2.7
1	A	64	THR	2.7
1	A	86	CYS	2.7
1	A	93	ASP	2.7
1	A	310	LYS	2.7
1	B	68	ASN	2.7
1	A	95	VAL	2.7
1	B	271	ASP	2.7
1	B	75	TRP	2.7
1	A	78	THR	2.7
1	A	84	GLU	2.7
1	B	416	PRO	2.7
1	B	225	SER	2.7
1	B	441	VAL	2.7
1	A	322	ASP	2.7
1	B	281	ASP	2.6
1	B	357	ASP	2.6
1	B	65	GLY	2.6
1	B	436	GLY	2.6
1	A	71	THR	2.6
1	A	109	THR	2.6
1	A	125	THR	2.6
1	B	39	THR	2.6
1	B	447	ASN	2.6
1	B	341	VAL	2.6
1	B	86	CYS	2.6
1	B	126	ASN	2.6
1	A	59	TRP	2.6
1	B	119	THR	2.6
1	B	162	CYS	2.6
1	B	330	LYS	2.6
1	A	357	ASP	2.6
1	B	304	PHE	2.5
1	B	43	ASN	2.5
1	B	414	ASN	2.5
1	B	424	PRO	2.5
1	A	97	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	441	VAL	2.5
1	B	127	ILE	2.5
1	B	219	ILE	2.5
1	B	301	GLY	2.5
1	A	68	ASN	2.5
1	B	93	ASP	2.5
1	A	25	GLN	2.5
1	B	71	THR	2.5
1	B	42	GLY	2.5
1	B	327	GLY	2.5
1	A	126	ASN	2.5
1	A	229	TYR	2.5
1	B	76	ASP	2.5
1	B	269	ASP	2.5
1	B	349	ASN	2.5
1	B	265	VAL	2.4
1	B	373	ASP	2.4
1	B	69	CYS	2.4
1	B	319	ILE	2.4
1	B	435	SER	2.4
1	B	444	THR	2.4
1	A	421	PRO	2.4
1	B	342	ARG	2.4
1	A	75	TRP	2.4
1	A	90	CYS	2.4
1	A	324	THR	2.4
1	B	211	ALA	2.4
1	B	369	GLY	2.4
1	B	229	TYR	2.3
1	A	344	GLU	2.3
1	A	99	ASP	2.3
1	B	286	ASP	2.3
1	B	460	ILE	2.3
1	B	118	VAL	2.3
1	B	443	VAL	2.3
1	A	220	PRO	2.3
1	B	311	PRO	2.3
1	B	91	ALA	2.3
1	B	273	GLY	2.3
1	A	304	PHE	2.3
1	B	263	GLU	2.3
1	A	351	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	444	THR	2.3
1	A	463	THR	2.3
1	B	431	CYS	2.3
1	A	70	TYR	2.3
1	B	70	TYR	2.3
1	B	294	ASP	2.3
1	B	289	SER	2.3
1	A	85	THR	2.3
1	B	62	THR	2.3
1	B	81	PRO	2.3
1	A	326	ASN	2.3
1	B	365	ALA	2.3
1	A	301	GLY	2.3
1	A	182	TYR	2.3
1	A	218	PRO	2.2
1	B	204	VAL	2.2
1	B	305	LYS	2.2
1	B	102	GLY	2.2
1	B	372	GLY	2.2
1	A	442	GLU	2.2
1	B	404	HIS	2.2
1	A	21	ASN	2.2
1	B	88	THR	2.2
1	B	459	PRO	2.2
1	A	286	ASP	2.2
1	A	373	ASP	2.2
1	B	276	TYR	2.2
1	A	346	SER	2.2
1	A	339	ASN	2.2
1	A	335	PHE	2.2
1	B	313	THR	2.2
1	B	174	ASP	2.2
1	B	22	VAL	2.2
1	A	83	PRO	2.1
1	B	296	THR	2.2
1	B	366	ALA	2.1
1	B	291	ARG	2.1
1	A	302	SER	2.1
1	B	159	SER	2.1
1	A	269	ASP	2.1
1	A	96	PRO	2.1
1	B	300	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	309	THR	2.1
1	A	343	ILE	2.1
1	B	177	GLY	2.1
1	A	223	ALA	2.1
1	B	321	THR	2.1
1	B	434	THR	2.1
1	B	105	GLY	2.1
1	B	437	VAL	2.1
1	A	138	LYS	2.1
1	B	29	GLU	2.1
1	A	418	THR	2.1
1	A	430	PRO	2.1
1	B	220	PRO	2.1
1	A	221	GLY	2.1
1	A	89	ASN	2.0
1	A	376	ASP	2.0
1	B	90	CYS	2.0
1	B	325	ASP	2.0
1	B	83	PRO	2.0
1	B	449	VAL	2.0
1	A	27	ALA	2.0
1	B	285	CYS	2.0
1	B	82	THR	2.0
1	B	430	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PCA	B	20	8/9	0.84	0.12	20,23,27,28	0
1	PCA	A	20	8/9	0.88	0.12	28,29,30,32	0

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(Å ²)	Q<0.9
2	GOL	B	501	6/6	0.34	0.47	55,66,68,69	0
2	GOL	B	502	6/6	0.50	0.27	45,54,57,59	0
3	SO4	B	503	5/5	0.67	0.20	68,70,80,84	0
2	GOL	A	501	6/6	0.68	0.24	34,36,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.