



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 08:17 AM UTC

PDB ID : 4CBO / pdb_00004cbo
Title : Crystal structure of Complement Factor D mutant R202A after ensemble refinement
Authors : Forneris, F.; Burnley, B.T.; Gros, P.
Deposited on : 2013-10-15
Resolution : 1.80 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	:	FAILED
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

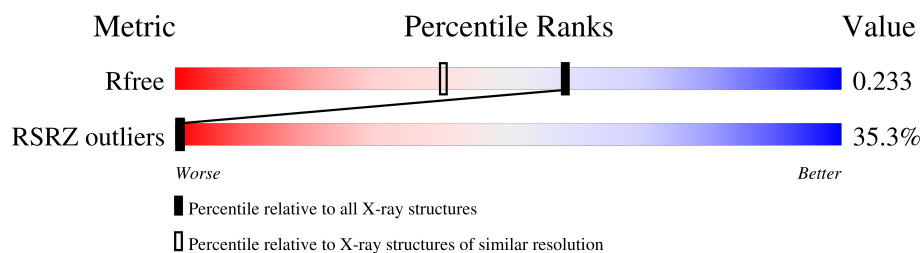
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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	17-A	1000	-	X	-	-
2	GOL	21-A	1000	-	X	-	-
2	GOL	28-A	1000	-	X	-	-
2	GOL	29-A	1000	-	X	-	-
2	GOL	54-A	1000	-	X	-	-
2	GOL	64-A	1000	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 546299 atoms, of which 263032 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 FACTOR D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	2-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	3-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	4-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	5-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	6-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	7-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	8-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	9-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	10-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	11-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	12-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	13-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	14-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	15-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	16-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	18-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	19-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	20-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	21-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	22-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	23-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	24-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	25-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	26-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	27-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	28-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	29-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	30-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	31-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	32-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	33-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	34-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	35-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	36-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	37-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	39-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	40-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	41-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	42-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	43-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	44-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	45-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	46-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	47-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	48-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	49-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	50-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	51-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	52-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	53-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	54-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	55-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	56-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	57-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	58-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	60-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	61-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	62-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	63-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	64-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	65-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	66-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	1-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	2-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	3-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	4-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	5-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	6-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	7-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	8-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	9-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	10-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	11-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	12-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	13-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	14-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	15-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	16-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	17-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	18-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	19-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	20-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	21-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	22-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	23-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	24-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	25-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	26-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	27-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	28-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	29-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	30-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	31-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	32-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	33-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	34-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	35-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	36-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	37-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	38-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	39-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	40-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	41-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	42-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	43-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	44-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	45-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	46-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	47-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	48-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	49-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	50-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	51-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	52-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	53-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	54-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	55-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	56-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	57-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	58-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	59-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	60-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	61-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	62-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	63-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	64-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	65-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	66-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	ARG	engineered mutation	UNP P00746
B	202	ALA	ARG	engineered mutation	UNP P00746

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	2-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	3-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	4-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	5-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	6-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	7-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	8-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	9-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	10-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	11-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	12-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	13-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	14-A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	15-A	1	Total 14	C 3	H 8	O 3	0	0
2	16-A	1	Total 14	C 3	H 8	O 3	0	0
2	17-A	1	Total 14	C 3	H 8	O 3	0	0
2	18-A	1	Total 14	C 3	H 8	O 3	0	0
2	19-A	1	Total 14	C 3	H 8	O 3	0	0
2	20-A	1	Total 14	C 3	H 8	O 3	0	0
2	21-A	1	Total 14	C 3	H 8	O 3	0	0
2	22-A	1	Total 14	C 3	H 8	O 3	0	0
2	23-A	1	Total 14	C 3	H 8	O 3	0	0
2	24-A	1	Total 14	C 3	H 8	O 3	0	0
2	25-A	1	Total 14	C 3	H 8	O 3	0	0
2	26-A	1	Total 14	C 3	H 8	O 3	0	0
2	27-A	1	Total 14	C 3	H 8	O 3	0	0
2	28-A	1	Total 14	C 3	H 8	O 3	0	0
2	29-A	1	Total 14	C 3	H 8	O 3	0	0
2	30-A	1	Total 14	C 3	H 8	O 3	0	0
2	31-A	1	Total 14	C 3	H 8	O 3	0	0
2	32-A	1	Total 14	C 3	H 8	O 3	0	0
2	33-A	1	Total 14	C 3	H 8	O 3	0	0
2	34-A	1	Total 14	C 3	H 8	O 3	0	0
2	35-A	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	36-A	1	Total 14	C 3	H 8	O 3	0	0
2	37-A	1	Total 14	C 3	H 8	O 3	0	0
2	38-A	1	Total 14	C 3	H 8	O 3	0	0
2	39-A	1	Total 14	C 3	H 8	O 3	0	0
2	40-A	1	Total 14	C 3	H 8	O 3	0	0
2	41-A	1	Total 14	C 3	H 8	O 3	0	0
2	42-A	1	Total 14	C 3	H 8	O 3	0	0
2	43-A	1	Total 14	C 3	H 8	O 3	0	0
2	44-A	1	Total 14	C 3	H 8	O 3	0	0
2	45-A	1	Total 14	C 3	H 8	O 3	0	0
2	46-A	1	Total 14	C 3	H 8	O 3	0	0
2	47-A	1	Total 14	C 3	H 8	O 3	0	0
2	48-A	1	Total 14	C 3	H 8	O 3	0	0
2	49-A	1	Total 14	C 3	H 8	O 3	0	0
2	50-A	1	Total 14	C 3	H 8	O 3	0	0
2	51-A	1	Total 14	C 3	H 8	O 3	0	0
2	52-A	1	Total 14	C 3	H 8	O 3	0	0
2	53-A	1	Total 14	C 3	H 8	O 3	0	0
2	54-A	1	Total 14	C 3	H 8	O 3	0	0
2	55-A	1	Total 14	C 3	H 8	O 3	0	0
2	56-A	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	57-A	1	Total 14	C 3	H 8	O 3	0	0
2	58-A	1	Total 14	C 3	H 8	O 3	0	0
2	59-A	1	Total 14	C 3	H 8	O 3	0	0
2	60-A	1	Total 14	C 3	H 8	O 3	0	0
2	61-A	1	Total 14	C 3	H 8	O 3	0	0
2	62-A	1	Total 14	C 3	H 8	O 3	0	0
2	63-A	1	Total 14	C 3	H 8	O 3	0	0
2	64-A	1	Total 14	C 3	H 8	O 3	0	0
2	65-A	1	Total 14	C 3	H 8	O 3	0	0
2	66-A	1	Total 14	C 3	H 8	O 3	0	0
2	67-A	1	Total 14	C 3	H 8	O 3	0	0
2	68-A	1	Total 14	C 3	H 8	O 3	0	0
2	69-A	1	Total 14	C 3	H 8	O 3	0	0
2	70-A	1	Total 14	C 3	H 8	O 3	0	0
2	71-A	1	Total 14	C 3	H 8	O 3	0	0
2	72-A	1	Total 14	C 3	H 8	O 3	0	0
2	73-A	1	Total 14	C 3	H 8	O 3	0	0
2	74-A	1	Total 14	C 3	H 8	O 3	0	0
2	75-A	1	Total 14	C 3	H 8	O 3	0	0
2	76-A	1	Total 14	C 3	H 8	O 3	0	0
2	77-A	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	2-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	3-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	4-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	5-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	6-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	7-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	8-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	9-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	10-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	11-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	12-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	13-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	14-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	15-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	16-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	17-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	18-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	19-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	20-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	21-B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	22-B	1	Total 14	C 3	H 8	O 3	0	0
2	23-B	1	Total 14	C 3	H 8	O 3	0	0
2	24-B	1	Total 14	C 3	H 8	O 3	0	0
2	25-B	1	Total 14	C 3	H 8	O 3	0	0
2	26-B	1	Total 14	C 3	H 8	O 3	0	0
2	27-B	1	Total 14	C 3	H 8	O 3	0	0
2	28-B	1	Total 14	C 3	H 8	O 3	0	0
2	29-B	1	Total 14	C 3	H 8	O 3	0	0
2	30-B	1	Total 14	C 3	H 8	O 3	0	0
2	31-B	1	Total 14	C 3	H 8	O 3	0	0
2	32-B	1	Total 14	C 3	H 8	O 3	0	0
2	33-B	1	Total 14	C 3	H 8	O 3	0	0
2	34-B	1	Total 14	C 3	H 8	O 3	0	0
2	35-B	1	Total 14	C 3	H 8	O 3	0	0
2	36-B	1	Total 14	C 3	H 8	O 3	0	0
2	37-B	1	Total 14	C 3	H 8	O 3	0	0
2	38-B	1	Total 14	C 3	H 8	O 3	0	0
2	39-B	1	Total 14	C 3	H 8	O 3	0	0
2	40-B	1	Total 14	C 3	H 8	O 3	0	0
2	41-B	1	Total 14	C 3	H 8	O 3	0	0
2	42-B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	43-B	1	Total 14	C 3	H 8	O 3	0	0
2	44-B	1	Total 14	C 3	H 8	O 3	0	0
2	45-B	1	Total 14	C 3	H 8	O 3	0	0
2	46-B	1	Total 14	C 3	H 8	O 3	0	0
2	47-B	1	Total 14	C 3	H 8	O 3	0	0
2	48-B	1	Total 14	C 3	H 8	O 3	0	0
2	49-B	1	Total 14	C 3	H 8	O 3	0	0
2	50-B	1	Total 14	C 3	H 8	O 3	0	0
2	51-B	1	Total 14	C 3	H 8	O 3	0	0
2	52-B	1	Total 14	C 3	H 8	O 3	0	0
2	53-B	1	Total 14	C 3	H 8	O 3	0	0
2	54-B	1	Total 14	C 3	H 8	O 3	0	0
2	55-B	1	Total 14	C 3	H 8	O 3	0	0
2	56-B	1	Total 14	C 3	H 8	O 3	0	0
2	57-B	1	Total 14	C 3	H 8	O 3	0	0
2	58-B	1	Total 14	C 3	H 8	O 3	0	0
2	59-B	1	Total 14	C 3	H 8	O 3	0	0
2	60-B	1	Total 14	C 3	H 8	O 3	0	0
2	61-B	1	Total 14	C 3	H 8	O 3	0	0
2	62-B	1	Total 14	C 3	H 8	O 3	0	0
2	63-B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	64-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	65-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	66-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	67-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	68-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	69-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	70-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	71-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	72-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	73-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	74-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	75-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	76-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	77-B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	148	Total	O	0	0
			148	148		
3	2-A	139	Total	O	0	0
			139	139		
3	3-A	142	Total	O	0	0
			142	142		
3	4-A	129	Total	O	0	0
			129	129		
3	5-A	128	Total	O	0	1
			129	129		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	6-A	135	Total 136	O 136	0	1
3	7-A	134	Total 134	O 134	0	0
3	8-A	136	Total 136	O 136	0	0
3	9-A	138	Total 138	O 138	0	0
3	10-A	135	Total 135	O 135	0	0
3	11-A	123	Total 123	O 123	0	0
3	12-A	145	Total 145	O 145	0	0
3	13-A	164	Total 165	O 165	0	1
3	14-A	157	Total 157	O 157	0	0
3	15-A	142	Total 142	O 142	0	0
3	16-A	135	Total 135	O 135	0	0
3	17-A	142	Total 142	O 142	0	0
3	18-A	147	Total 147	O 147	0	0
3	19-A	127	Total 127	O 127	0	0
3	20-A	131	Total 131	O 131	0	0
3	21-A	144	Total 144	O 144	0	0
3	22-A	142	Total 143	O 143	0	1
3	23-A	142	Total 142	O 142	0	0
3	24-A	127	Total 127	O 127	0	0
3	25-A	136	Total 137	O 137	0	1
3	26-A	144	Total 145	O 145	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	27-A	139	Total 139	O 139	0	0
3	28-A	136	Total 137	O 137	0	1
3	29-A	134	Total 135	O 135	0	1
3	30-A	149	Total 149	O 149	0	0
3	31-A	146	Total 146	O 146	0	0
3	32-A	135	Total 135	O 135	0	0
3	33-A	133	Total 133	O 133	0	0
3	34-A	139	Total 139	O 139	0	0
3	35-A	125	Total 125	O 125	0	0
3	36-A	130	Total 130	O 130	0	0
3	37-A	138	Total 138	O 138	0	0
3	38-A	133	Total 134	O 134	0	1
3	39-A	130	Total 130	O 130	0	0
3	40-A	127	Total 128	O 128	0	1
3	41-A	139	Total 139	O 139	0	0
3	42-A	128	Total 128	O 128	0	0
3	43-A	154	Total 155	O 155	0	1
3	44-A	143	Total 143	O 143	0	0
3	45-A	140	Total 140	O 140	0	0
3	46-A	131	Total 131	O 131	0	0
3	47-A	127	Total 127	O 127	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	48-A	141	Total 141	O 141	0	0
3	49-A	121	Total 121	O 121	0	0
3	50-A	138	Total 139	O 139	0	1
3	51-A	137	Total 137	O 137	0	0
3	52-A	145	Total 145	O 145	0	0
3	53-A	141	Total 141	O 141	0	0
3	54-A	137	Total 137	O 137	0	0
3	55-A	135	Total 136	O 136	0	1
3	56-A	152	Total 153	O 153	0	1
3	57-A	124	Total 124	O 124	0	0
3	58-A	133	Total 133	O 133	0	0
3	59-A	142	Total 143	O 143	0	1
3	60-A	132	Total 132	O 132	0	0
3	61-A	138	Total 138	O 138	0	0
3	62-A	136	Total 137	O 137	0	1
3	63-A	151	Total 151	O 151	0	0
3	64-A	142	Total 142	O 142	0	0
3	65-A	148	Total 149	O 149	0	1
3	66-A	135	Total 135	O 135	0	0
3	67-A	143	Total 143	O 143	0	0
3	68-A	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	69-A	131	Total 131	O 131	0	0
3	70-A	136	Total 136	O 136	0	0
3	71-A	137	Total 138	O 138	0	1
3	72-A	135	Total 135	O 135	0	0
3	73-A	134	Total 134	O 134	0	0
3	74-A	153	Total 153	O 153	0	0
3	75-A	147	Total 147	O 147	0	0
3	76-A	145	Total 145	O 145	0	0
3	77-A	131	Total 131	O 131	0	0
3	1-B	113	Total 113	O 113	0	0
3	2-B	122	Total 122	O 122	0	0
3	3-B	96	Total 96	O 96	0	0
3	4-B	108	Total 108	O 108	0	0
3	5-B	109	Total 109	O 109	0	0
3	6-B	111	Total 111	O 111	0	0
3	7-B	111	Total 111	O 111	0	0
3	8-B	104	Total 104	O 104	0	0
3	9-B	118	Total 119	O 119	0	1
3	10-B	117	Total 117	O 117	0	0
3	11-B	118	Total 118	O 118	0	0
3	12-B	114	Total 115	O 115	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	13-B	109	Total 109	O 109	0	0
3	14-B	115	Total 115	O 115	0	0
3	15-B	113	Total 113	O 113	0	0
3	16-B	117	Total 117	O 117	0	0
3	17-B	121	Total 122	O 122	0	1
3	18-B	111	Total 111	O 111	0	0
3	19-B	117	Total 117	O 117	0	0
3	20-B	122	Total 123	O 123	0	1
3	21-B	103	Total 103	O 103	0	0
3	22-B	122	Total 122	O 122	0	0
3	23-B	113	Total 113	O 113	0	0
3	24-B	116	Total 116	O 116	0	0
3	25-B	120	Total 120	O 120	0	0
3	26-B	114	Total 114	O 114	0	0
3	27-B	114	Total 114	O 114	0	0
3	28-B	123	Total 123	O 123	0	0
3	29-B	132	Total 132	O 132	0	0
3	30-B	115	Total 115	O 115	0	0
3	31-B	117	Total 117	O 117	0	0
3	32-B	127	Total 127	O 127	0	0
3	33-B	119	Total 119	O 119	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	34-B	109	Total 109	O 109	0	0
3	35-B	102	Total 102	O 102	0	0
3	36-B	119	Total 120	O 120	0	1
3	37-B	110	Total 110	O 110	0	0
3	38-B	118	Total 118	O 118	0	0
3	39-B	112	Total 112	O 112	0	0
3	40-B	118	Total 118	O 118	0	0
3	41-B	106	Total 106	O 106	0	0
3	42-B	123	Total 124	O 124	0	1
3	43-B	125	Total 125	O 125	0	0
3	44-B	118	Total 118	O 118	0	0
3	45-B	108	Total 108	O 108	0	0
3	46-B	105	Total 105	O 105	0	0
3	47-B	117	Total 118	O 118	0	1
3	48-B	128	Total 129	O 129	0	1
3	49-B	109	Total 109	O 109	0	0
3	50-B	111	Total 111	O 111	0	0
3	51-B	130	Total 131	O 131	0	1
3	52-B	119	Total 119	O 119	0	0
3	53-B	113	Total 113	O 113	0	0
3	54-B	109	Total 109	O 109	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	55-B	120	Total 120	O 120	0	0
3	56-B	127	Total 127	O 127	0	0
3	57-B	122	Total 122	O 122	0	0
3	58-B	121	Total 122	O 122	0	1
3	59-B	117	Total 117	O 117	0	0
3	60-B	116	Total 116	O 116	0	0
3	61-B	118	Total 119	O 119	0	1
3	62-B	121	Total 121	O 121	0	0
3	63-B	122	Total 123	O 123	0	1
3	64-B	121	Total 121	O 121	0	0
3	65-B	128	Total 128	O 128	0	0
3	66-B	112	Total 112	O 112	0	0
3	67-B	124	Total 125	O 125	0	1
3	68-B	126	Total 126	O 126	0	0
3	69-B	112	Total 112	O 112	0	0
3	70-B	122	Total 123	O 123	0	1
3	71-B	122	Total 122	O 122	0	0
3	72-B	121	Total 121	O 121	0	0
3	73-B	131	Total 132	O 132	0	1
3	74-B	113	Total 113	O 113	0	0
3	75-B	111	Total 111	O 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	76-B	105	Total 105	O 105	0	0
3	77-B	119	Total 119	O 119	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.14Å 67.31Å 133.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 1.80 47.33 – 1.80	Depositor Estimate
% Data completeness (in resolution range)	98.7 (47.33-1.80) 98.7 (47.33-1.80)	Depositor Estimate
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1259)	Depositor
R, R_{free}	0.163 , 0.212 0.176 , 0.233	Depositor Depositor
R_{free} test set	1857 reflections (5.00%)	wwPDB
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 33.7	Estimate
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	Estimate
Total number of atoms	546299	wwPDB
Average B, all atoms (Å ²)	26.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.92% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

154 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	GOL	71-A	1000	-	5,5,5	0.46	0	5,5,5	1.34	1 (20%)
2	GOL	64-A	1000	-	5,5,5	0.71	0	5,5,5	1.87	2 (40%)
2	GOL	21-B	1000	-	5,5,5	0.24	0	5,5,5	0.31	0
2	GOL	14-B	1000	-	5,5,5	0.25	0	5,5,5	0.49	0
2	GOL	5-B	1000	-	5,5,5	0.24	0	5,5,5	0.27	0
2	GOL	67-B	1000	-	5,5,5	0.20	0	5,5,5	0.50	0
2	GOL	3-B	1000	-	5,5,5	0.24	0	5,5,5	0.29	0
2	GOL	54-A	1000	-	5,5,5	0.47	0	5,5,5	1.68	2 (40%)
2	GOL	25-B	1000	-	5,5,5	0.24	0	5,5,5	0.39	0
2	GOL	47-B	1000	-	5,5,5	0.18	0	5,5,5	0.37	0
2	GOL	60-B	1000	-	5,5,5	0.25	0	5,5,5	0.47	0
2	GOL	35-B	1000	-	5,5,5	0.21	0	5,5,5	0.34	0
2	GOL	42-B	1000	-	5,5,5	0.29	0	5,5,5	0.30	0
2	GOL	43-B	1000	-	5,5,5	0.24	0	5,5,5	0.29	0
2	GOL	41-A	1000	-	5,5,5	0.39	0	5,5,5	2.00	1 (20%)
2	GOL	34-B	1000	-	5,5,5	0.28	0	5,5,5	0.29	0
2	GOL	40-B	1000	-	5,5,5	0.22	0	5,5,5	0.39	0
2	GOL	9-B	1000	-	5,5,5	0.23	0	5,5,5	0.35	0
2	GOL	28-B	1000	-	5,5,5	0.24	0	5,5,5	0.42	0
2	GOL	12-B	1000	-	5,5,5	0.20	0	5,5,5	0.33	0
2	GOL	8-B	1000	-	5,5,5	0.23	0	5,5,5	0.40	0
2	GOL	32-B	1000	-	5,5,5	0.27	0	5,5,5	0.35	0
2	GOL	37-B	1000	-	5,5,5	0.25	0	5,5,5	0.34	0
2	GOL	33-B	1000	-	5,5,5	0.22	0	5,5,5	0.31	0
2	GOL	5-A	1000	-	5,5,5	0.43	0	5,5,5	1.51	0
2	GOL	22-A	1000	-	5,5,5	0.41	0	5,5,5	1.68	2 (40%)
2	GOL	12-A	1000	-	5,5,5	0.45	0	5,5,5	1.63	1 (20%)
2	GOL	30-B	1000	-	5,5,5	0.36	0	5,5,5	0.35	0
2	GOL	26-A	1000	-	5,5,5	0.48	0	5,5,5	1.33	0
2	GOL	17-B	1000	-	5,5,5	0.23	0	5,5,5	0.44	0
2	GOL	49-A	1000	-	5,5,5	0.49	0	5,5,5	1.89	2 (40%)
2	GOL	63-A	1000	-	5,5,5	0.47	0	5,5,5	0.37	0
2	GOL	75-A	1000	-	5,5,5	0.44	0	5,5,5	1.57	1 (20%)
2	GOL	70-A	1000	-	5,5,5	0.39	0	5,5,5	0.88	0
2	GOL	47-A	1000	-	5,5,5	0.71	0	5,5,5	0.69	0
2	GOL	57-B	1000	-	5,5,5	0.26	0	5,5,5	0.47	0
2	GOL	59-A	1000	-	5,5,5	0.37	0	5,5,5	1.43	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	50-A	1000	-	5,5,5	0.47	0	5,5,5	1.49	0
2	GOL	51-B	1000	-	5,5,5	0.25	0	5,5,5	0.48	0
2	GOL	42-A	1000	-	5,5,5	0.73	0	5,5,5	1.26	0
2	GOL	50-B	1000	-	5,5,5	0.25	0	5,5,5	0.51	0
2	GOL	19-A	1000	-	5,5,5	0.46	0	5,5,5	1.64	1 (20%)
2	GOL	72-A	1000	-	5,5,5	0.46	0	5,5,5	1.55	0
2	GOL	48-B	1000	-	5,5,5	0.22	0	5,5,5	0.53	0
2	GOL	75-B	1000	-	5,5,5	0.26	0	5,5,5	0.61	0
2	GOL	24-A	1000	-	5,5,5	0.50	0	5,5,5	0.53	0
2	GOL	27-B	1000	-	5,5,5	0.25	0	5,5,5	0.37	0
2	GOL	56-B	1000	-	5,5,5	0.28	0	5,5,5	0.47	0
2	GOL	3-A	1000	-	5,5,5	0.52	0	5,5,5	1.37	0
2	GOL	16-B	1000	-	5,5,5	0.22	0	5,5,5	0.44	0
2	GOL	1-A	1000	-	5,5,5	0.42	0	5,5,5	0.43	0
2	GOL	48-A	1000	-	5,5,5	0.45	0	5,5,5	1.72	1 (20%)
2	GOL	28-A	1000	-	5,5,5	0.56	0	5,5,5	1.74	2 (40%)
2	GOL	7-B	1000	-	5,5,5	0.23	0	5,5,5	0.27	0
2	GOL	61-A	1000	-	5,5,5	0.37	0	5,5,5	1.11	0
2	GOL	13-A	1000	-	5,5,5	0.85	0	5,5,5	1.08	0
2	GOL	66-A	1000	-	5,5,5	0.46	0	5,5,5	1.23	1 (20%)
2	GOL	8-A	1000	-	5,5,5	0.35	0	5,5,5	1.40	0
2	GOL	10-B	1000	-	5,5,5	0.24	0	5,5,5	0.39	0
2	GOL	9-A	1000	-	5,5,5	0.39	0	5,5,5	0.53	0
2	GOL	24-B	1000	-	5,5,5	0.24	0	5,5,5	0.33	0
2	GOL	2-B	1000	-	5,5,5	0.30	0	5,5,5	0.34	0
2	GOL	52-A	1000	-	5,5,5	0.64	0	5,5,5	1.62	1 (20%)
2	GOL	34-A	1000	-	5,5,5	0.63	0	5,5,5	1.46	1 (20%)
2	GOL	53-A	1000	-	5,5,5	0.43	0	5,5,5	1.56	1 (20%)
2	GOL	27-A	1000	-	5,5,5	0.53	0	5,5,5	1.60	1 (20%)
2	GOL	25-A	1000	-	5,5,5	0.35	0	5,5,5	1.29	1 (20%)
2	GOL	37-A	1000	-	5,5,5	0.61	0	5,5,5	1.61	0
2	GOL	33-A	1000	-	5,5,5	0.61	0	5,5,5	0.96	0
2	GOL	69-A	1000	-	5,5,5	0.34	0	5,5,5	1.20	0
2	GOL	29-B	1000	-	5,5,5	0.23	0	5,5,5	0.54	0
2	GOL	68-B	1000	-	5,5,5	0.20	0	5,5,5	0.47	0
2	GOL	4-B	1000	-	5,5,5	0.23	0	5,5,5	0.36	0
2	GOL	15-B	1000	-	5,5,5	0.20	0	5,5,5	0.41	0
2	GOL	40-A	1000	-	5,5,5	0.68	0	5,5,5	0.38	0
2	GOL	19-B	1000	-	5,5,5	0.27	0	5,5,5	0.39	0
2	GOL	22-B	1000	-	5,5,5	0.23	0	5,5,5	0.41	0
2	GOL	61-B	1000	-	5,5,5	0.23	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	30-A	1000	-	5,5,5	0.49	0	5,5,5	1.70	1 (20%)
2	GOL	57-A	1000	-	5,5,5	0.40	0	5,5,5	1.24	0
2	GOL	68-A	1000	-	5,5,5	0.55	0	5,5,5	1.54	0
2	GOL	56-A	1000	-	5,5,5	0.50	0	5,5,5	0.48	0
2	GOL	6-B	1000	-	5,5,5	0.20	0	5,5,5	0.26	0
2	GOL	45-B	1000	-	5,5,5	0.24	0	5,5,5	0.39	0
2	GOL	36-A	1000	-	5,5,5	0.44	0	5,5,5	1.06	0
2	GOL	16-A	1000	-	5,5,5	0.32	0	5,5,5	1.62	1 (20%)
2	GOL	51-A	1000	-	5,5,5	0.52	0	5,5,5	1.63	1 (20%)
2	GOL	13-B	1000	-	5,5,5	0.19	0	5,5,5	0.38	0
2	GOL	20-A	1000	-	5,5,5	0.37	0	5,5,5	1.55	1 (20%)
2	GOL	55-B	1000	-	5,5,5	0.25	0	5,5,5	0.46	0
2	GOL	77-B	1000	-	5,5,5	0.22	0	5,5,5	0.55	0
2	GOL	43-A	1000	-	5,5,5	0.35	0	5,5,5	1.33	1 (20%)
2	GOL	67-A	1000	-	5,5,5	0.59	0	5,5,5	0.25	0
2	GOL	29-A	1000	-	5,5,5	0.49	0	5,5,5	1.90	2 (40%)
2	GOL	18-B	1000	-	5,5,5	0.25	0	5,5,5	0.39	0
2	GOL	63-B	1000	-	5,5,5	0.22	0	5,5,5	0.43	0
2	GOL	11-A	1000	-	5,5,5	0.39	0	5,5,5	0.67	0
2	GOL	77-A	1000	-	5,5,5	0.48	0	5,5,5	1.22	0
2	GOL	10-A	1000	-	5,5,5	0.34	0	5,5,5	1.36	1 (20%)
2	GOL	62-B	1000	-	5,5,5	0.22	0	5,5,5	0.48	0
2	GOL	73-A	1000	-	5,5,5	0.33	0	5,5,5	1.38	1 (20%)
2	GOL	36-B	1000	-	5,5,5	0.24	0	5,5,5	0.34	0
2	GOL	39-A	1000	-	5,5,5	0.83	0	5,5,5	0.51	0
2	GOL	35-A	1000	-	5,5,5	0.63	0	5,5,5	1.62	1 (20%)
2	GOL	31-A	1000	-	5,5,5	0.93	0	5,5,5	1.02	0
2	GOL	69-B	1000	-	5,5,5	0.19	0	5,5,5	0.49	0
2	GOL	46-A	1000	-	5,5,5	0.38	0	5,5,5	1.32	1 (20%)
2	GOL	49-B	1000	-	5,5,5	0.22	0	5,5,5	0.60	0
2	GOL	18-A	1000	-	5,5,5	0.56	0	5,5,5	1.64	1 (20%)
2	GOL	21-A	1000	-	5,5,5	0.62	0	5,5,5	1.87	2 (40%)
2	GOL	6-A	1000	-	5,5,5	0.42	0	5,5,5	1.41	0
2	GOL	74-B	1000	-	5,5,5	0.29	0	5,5,5	0.53	0
2	GOL	26-B	1000	-	5,5,5	0.25	0	5,5,5	0.44	0
2	GOL	15-A	1000	-	5,5,5	0.51	0	5,5,5	0.73	0
2	GOL	32-A	1000	-	5,5,5	0.35	0	5,5,5	0.28	0
2	GOL	76-B	1000	-	5,5,5	0.21	0	5,5,5	0.68	0
2	GOL	45-A	1000	-	5,5,5	0.82	0	5,5,5	0.98	0
2	GOL	58-A	1000	-	5,5,5	0.50	0	5,5,5	1.58	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	74-A	1000	-	5,5,5	0.44	0	5,5,5	1.65	2 (40%)
2	GOL	73-B	1000	-	5,5,5	0.28	0	5,5,5	0.59	0
2	GOL	1-B	1000	-	5,5,5	0.24	0	5,5,5	0.26	0
2	GOL	7-A	1000	-	5,5,5	0.42	0	5,5,5	1.58	0
2	GOL	71-B	1000	-	5,5,5	0.26	0	5,5,5	0.59	0
2	GOL	4-A	1000	-	5,5,5	0.47	0	5,5,5	1.58	0
2	GOL	70-B	1000	-	5,5,5	0.20	0	5,5,5	0.53	0
2	GOL	38-A	1000	-	5,5,5	0.41	0	5,5,5	1.06	0
2	GOL	20-B	1000	-	5,5,5	0.27	0	5,5,5	0.37	0
2	GOL	53-B	1000	-	5,5,5	0.25	0	5,5,5	0.58	0
2	GOL	65-A	1000	-	5,5,5	0.55	0	5,5,5	1.59	1 (20%)
2	GOL	66-B	1000	-	5,5,5	0.20	0	5,5,5	0.59	0
2	GOL	17-A	1000	-	5,5,5	0.67	0	5,5,5	1.80	2 (40%)
2	GOL	60-A	1000	-	5,5,5	0.46	0	5,5,5	1.00	0
2	GOL	58-B	1000	-	5,5,5	0.22	0	5,5,5	0.55	0
2	GOL	65-B	1000	-	5,5,5	0.18	0	5,5,5	0.62	0
2	GOL	2-A	1000	-	5,5,5	0.36	0	5,5,5	1.53	1 (20%)
2	GOL	31-B	1000	-	5,5,5	0.26	0	5,5,5	0.33	0
2	GOL	54-B	1000	-	5,5,5	0.23	0	5,5,5	0.53	0
2	GOL	72-B	1000	-	5,5,5	0.25	0	5,5,5	0.44	0
2	GOL	11-B	1000	-	5,5,5	0.21	0	5,5,5	0.35	0
2	GOL	52-B	1000	-	5,5,5	0.25	0	5,5,5	0.57	0
2	GOL	14-A	1000	-	5,5,5	0.31	0	5,5,5	1.67	1 (20%)
2	GOL	44-B	1000	-	5,5,5	0.28	0	5,5,5	0.47	0
2	GOL	39-B	1000	-	5,5,5	0.27	0	5,5,5	0.33	0
2	GOL	23-A	1000	-	5,5,5	0.59	0	5,5,5	1.01	0
2	GOL	46-B	1000	-	5,5,5	0.24	0	5,5,5	0.35	0
2	GOL	76-A	1000	-	5,5,5	0.54	0	5,5,5	1.53	1 (20%)
2	GOL	62-A	1000	-	5,5,5	0.51	0	5,5,5	0.32	0
2	GOL	23-B	1000	-	5,5,5	0.26	0	5,5,5	0.33	0
2	GOL	59-B	1000	-	5,5,5	0.21	0	5,5,5	0.52	0
2	GOL	41-B	1000	-	5,5,5	0.22	0	5,5,5	0.53	0
2	GOL	64-B	1000	-	5,5,5	0.18	0	5,5,5	0.48	0
2	GOL	55-A	1000	-	5,5,5	0.41	0	5,5,5	1.63	1 (20%)
2	GOL	38-B	1000	-	5,5,5	0.26	0	5,5,5	0.57	0
2	GOL	44-A	1000	-	5,5,5	0.47	0	5,5,5	0.51	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	71-A	1000	-	-	4/4/4/4	-
2	GOL	64-A	1000	-	-	4/4/4/4	-
2	GOL	21-B	1000	-	-	2/4/4/4	-
2	GOL	14-B	1000	-	-	2/4/4/4	-
2	GOL	5-B	1000	-	-	0/4/4/4	-
2	GOL	67-B	1000	-	-	2/4/4/4	-
2	GOL	3-B	1000	-	-	2/4/4/4	-
2	GOL	54-A	1000	-	-	4/4/4/4	-
2	GOL	25-B	1000	-	-	2/4/4/4	-
2	GOL	47-B	1000	-	-	2/4/4/4	-
2	GOL	60-B	1000	-	-	2/4/4/4	-
2	GOL	35-B	1000	-	-	2/4/4/4	-
2	GOL	42-B	1000	-	-	2/4/4/4	-
2	GOL	43-B	1000	-	-	0/4/4/4	-
2	GOL	41-A	1000	-	-	1/4/4/4	-
2	GOL	34-B	1000	-	-	0/4/4/4	-
2	GOL	40-B	1000	-	-	0/4/4/4	-
2	GOL	9-B	1000	-	-	0/4/4/4	-
2	GOL	28-B	1000	-	-	2/4/4/4	-
2	GOL	12-B	1000	-	-	0/4/4/4	-
2	GOL	8-B	1000	-	-	1/4/4/4	-
2	GOL	32-B	1000	-	-	0/4/4/4	-
2	GOL	37-B	1000	-	-	0/4/4/4	-
2	GOL	33-B	1000	-	-	0/4/4/4	-
2	GOL	5-A	1000	-	-	4/4/4/4	-
2	GOL	22-A	1000	-	-	3/4/4/4	-
2	GOL	12-A	1000	-	-	2/4/4/4	-
2	GOL	30-B	1000	-	-	2/4/4/4	-
2	GOL	26-A	1000	-	-	3/4/4/4	-
2	GOL	17-B	1000	-	-	0/4/4/4	-
2	GOL	49-A	1000	-	-	3/4/4/4	-
2	GOL	63-A	1000	-	-	0/4/4/4	-
2	GOL	75-A	1000	-	-	3/4/4/4	-
2	GOL	70-A	1000	-	-	0/4/4/4	-
2	GOL	47-A	1000	-	-	0/4/4/4	-
2	GOL	57-B	1000	-	-	0/4/4/4	-
2	GOL	59-A	1000	-	-	3/4/4/4	-
2	GOL	50-A	1000	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	51-B	1000	-	-	0/4/4/4	-
2	GOL	42-A	1000	-	-	0/4/4/4	-
2	GOL	50-B	1000	-	-	0/4/4/4	-
2	GOL	19-A	1000	-	-	4/4/4/4	-
2	GOL	72-A	1000	-	-	4/4/4/4	-
2	GOL	48-B	1000	-	-	2/4/4/4	-
2	GOL	75-B	1000	-	-	2/4/4/4	-
2	GOL	24-A	1000	-	-	0/4/4/4	-
2	GOL	27-B	1000	-	-	2/4/4/4	-
2	GOL	56-B	1000	-	-	0/4/4/4	-
2	GOL	3-A	1000	-	-	4/4/4/4	-
2	GOL	16-B	1000	-	-	2/4/4/4	-
2	GOL	1-A	1000	-	-	0/4/4/4	-
2	GOL	48-A	1000	-	-	0/4/4/4	-
2	GOL	28-A	1000	-	-	4/4/4/4	-
2	GOL	7-B	1000	-	-	1/4/4/4	-
2	GOL	61-A	1000	-	-	3/4/4/4	-
2	GOL	13-A	1000	-	-	0/4/4/4	-
2	GOL	66-A	1000	-	-	2/4/4/4	-
2	GOL	8-A	1000	-	-	3/4/4/4	-
2	GOL	10-B	1000	-	-	2/4/4/4	-
2	GOL	9-A	1000	-	-	0/4/4/4	-
2	GOL	24-B	1000	-	-	2/4/4/4	-
2	GOL	2-B	1000	-	-	2/4/4/4	-
2	GOL	52-A	1000	-	-	4/4/4/4	-
2	GOL	34-A	1000	-	-	4/4/4/4	-
2	GOL	53-A	1000	-	-	4/4/4/4	-
2	GOL	27-A	1000	-	-	3/4/4/4	-
2	GOL	25-A	1000	-	-	2/4/4/4	-
2	GOL	37-A	1000	-	-	4/4/4/4	-
2	GOL	33-A	1000	-	-	2/4/4/4	-
2	GOL	69-A	1000	-	-	2/4/4/4	-
2	GOL	29-B	1000	-	-	2/4/4/4	-
2	GOL	68-B	1000	-	-	0/4/4/4	-
2	GOL	4-B	1000	-	-	2/4/4/4	-
2	GOL	15-B	1000	-	-	0/4/4/4	-
2	GOL	40-A	1000	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	19-B	1000	-	-	2/4/4/4	-
2	GOL	22-B	1000	-	-	0/4/4/4	-
2	GOL	61-B	1000	-	-	2/4/4/4	-
2	GOL	30-A	1000	-	-	4/4/4/4	-
2	GOL	57-A	1000	-	-	0/4/4/4	-
2	GOL	68-A	1000	-	-	0/4/4/4	-
2	GOL	56-A	1000	-	-	0/4/4/4	-
2	GOL	6-B	1000	-	-	1/4/4/4	-
2	GOL	45-B	1000	-	-	2/4/4/4	-
2	GOL	36-A	1000	-	-	1/4/4/4	-
2	GOL	16-A	1000	-	-	0/4/4/4	-
2	GOL	51-A	1000	-	-	4/4/4/4	-
2	GOL	13-B	1000	-	-	0/4/4/4	-
2	GOL	20-A	1000	-	-	3/4/4/4	-
2	GOL	55-B	1000	-	-	0/4/4/4	-
2	GOL	77-B	1000	-	-	2/4/4/4	-
2	GOL	43-A	1000	-	-	2/4/4/4	-
2	GOL	67-A	1000	-	-	0/4/4/4	-
2	GOL	29-A	1000	-	-	4/4/4/4	-
2	GOL	18-B	1000	-	-	0/4/4/4	-
2	GOL	63-B	1000	-	-	2/4/4/4	-
2	GOL	11-A	1000	-	-	2/4/4/4	-
2	GOL	77-A	1000	-	-	2/4/4/4	-
2	GOL	10-A	1000	-	-	2/4/4/4	-
2	GOL	62-B	1000	-	-	2/4/4/4	-
2	GOL	73-A	1000	-	-	3/4/4/4	-
2	GOL	36-B	1000	-	-	0/4/4/4	-
2	GOL	39-A	1000	-	-	3/4/4/4	-
2	GOL	35-A	1000	-	-	4/4/4/4	-
2	GOL	31-A	1000	-	-	3/4/4/4	-
2	GOL	69-B	1000	-	-	2/4/4/4	-
2	GOL	46-A	1000	-	-	0/4/4/4	-
2	GOL	49-B	1000	-	-	0/4/4/4	-
2	GOL	18-A	1000	-	-	4/4/4/4	-
2	GOL	21-A	1000	-	-	4/4/4/4	-
2	GOL	6-A	1000	-	-	4/4/4/4	-
2	GOL	74-B	1000	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	26-B	1000	-	-	0/4/4/4	-
2	GOL	15-A	1000	-	-	0/4/4/4	-
2	GOL	32-A	1000	-	-	0/4/4/4	-
2	GOL	76-B	1000	-	-	2/4/4/4	-
2	GOL	45-A	1000	-	-	0/4/4/4	-
2	GOL	58-A	1000	-	-	4/4/4/4	-
2	GOL	74-A	1000	-	-	3/4/4/4	-
2	GOL	73-B	1000	-	-	2/4/4/4	-
2	GOL	1-B	1000	-	-	0/4/4/4	-
2	GOL	7-A	1000	-	-	4/4/4/4	-
2	GOL	71-B	1000	-	-	2/4/4/4	-
2	GOL	4-A	1000	-	-	4/4/4/4	-
2	GOL	70-B	1000	-	-	0/4/4/4	-
2	GOL	38-A	1000	-	-	1/4/4/4	-
2	GOL	20-B	1000	-	-	2/4/4/4	-
2	GOL	53-B	1000	-	-	2/4/4/4	-
2	GOL	65-A	1000	-	-	4/4/4/4	-
2	GOL	66-B	1000	-	-	0/4/4/4	-
2	GOL	17-A	1000	-	-	4/4/4/4	-
2	GOL	60-A	1000	-	-	2/4/4/4	-
2	GOL	58-B	1000	-	-	0/4/4/4	-
2	GOL	65-B	1000	-	-	2/4/4/4	-
2	GOL	2-A	1000	-	-	1/4/4/4	-
2	GOL	31-B	1000	-	-	0/4/4/4	-
2	GOL	54-B	1000	-	-	0/4/4/4	-
2	GOL	72-B	1000	-	-	0/4/4/4	-
2	GOL	11-B	1000	-	-	0/4/4/4	-
2	GOL	52-B	1000	-	-	0/4/4/4	-
2	GOL	14-A	1000	-	-	2/4/4/4	-
2	GOL	44-B	1000	-	-	2/4/4/4	-
2	GOL	39-B	1000	-	-	0/4/4/4	-
2	GOL	23-A	1000	-	-	2/4/4/4	-
2	GOL	46-B	1000	-	-	1/4/4/4	-
2	GOL	76-A	1000	-	-	4/4/4/4	-
2	GOL	62-A	1000	-	-	0/4/4/4	-
2	GOL	23-B	1000	-	-	0/4/4/4	-
2	GOL	59-B	1000	-	-	2/4/4/4	-
2	GOL	41-B	1000	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	64-B	1000	-	-	0/4/4/4	-
2	GOL	55-A	1000	-	-	4/4/4/4	-
2	GOL	38-B	1000	-	-	2/4/4/4	-
2	GOL	44-A	1000	-	-	0/4/4/4	-

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	41-A	1000	GOL	O2-C2-C1	-3.39	95.16	109.18
2	64-A	1000	GOL	O1-C1-C2	3.11	124.39	110.38
2	48-A	1000	GOL	O2-C2-C1	-3.02	96.67	109.18
2	49-A	1000	GOL	O2-C2-C1	3.01	121.66	109.18
2	16-A	1000	GOL	O2-C2-C1	-2.95	96.95	109.18
2	12-A	1000	GOL	O2-C2-C1	-2.95	96.98	109.18
2	2-A	1000	GOL	O2-C2-C1	-2.57	98.53	109.18
2	29-A	1000	GOL	O2-C2-C1	2.48	119.44	109.18
2	21-A	1000	GOL	C3-C2-C1	2.45	120.78	111.80
2	46-A	1000	GOL	O2-C2-C1	-2.38	99.32	109.18
2	17-A	1000	GOL	O2-C2-C1	2.38	119.02	109.18
2	25-A	1000	GOL	O2-C2-C1	-2.35	99.46	109.18
2	75-A	1000	GOL	O2-C2-C1	2.35	118.89	109.18
2	10-A	1000	GOL	O2-C2-C1	-2.33	99.55	109.18
2	17-A	1000	GOL	O1-C1-C2	2.31	120.76	110.38
2	14-A	1000	GOL	O2-C2-C1	-2.29	99.68	109.18
2	30-A	1000	GOL	O2-C2-C1	2.27	118.58	109.18
2	19-A	1000	GOL	O2-C2-C1	2.25	118.51	109.18
2	65-A	1000	GOL	O2-C2-C1	2.25	118.48	109.18
2	49-A	1000	GOL	O1-C1-C2	2.25	120.49	110.38
2	54-A	1000	GOL	O2-C2-C1	2.21	118.33	109.18
2	21-A	1000	GOL	O2-C2-C1	2.21	118.33	109.18
2	20-A	1000	GOL	O2-C2-C1	2.20	118.31	109.18
2	35-A	1000	GOL	O2-C2-C1	2.18	118.21	109.18
2	22-A	1000	GOL	O2-C2-C1	2.17	118.15	109.18
2	76-A	1000	GOL	O2-C2-C1	2.16	118.10	109.18
2	58-A	1000	GOL	O2-C2-C1	2.15	118.08	109.18
2	28-A	1000	GOL	O2-C2-C1	2.15	118.08	109.18
2	55-A	1000	GOL	O2-C2-C1	2.15	118.07	109.18
2	66-A	1000	GOL	O2-C2-C1	2.14	118.03	109.18
2	29-A	1000	GOL	C3-C2-C1	2.14	119.63	111.80
2	43-A	1000	GOL	O2-C2-C1	-2.13	100.35	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	74-A	1000	GOL	C3-C2-C1	2.12	119.58	111.80
2	27-A	1000	GOL	O2-C2-C1	2.11	117.91	109.18
2	22-A	1000	GOL	C3-C2-C1	2.11	119.52	111.80
2	51-A	1000	GOL	O2-C2-C1	2.10	117.89	109.18
2	18-A	1000	GOL	O2-C2-C1	2.10	117.87	109.18
2	53-A	1000	GOL	O2-C2-C1	2.10	117.86	109.18
2	28-A	1000	GOL	C3-C2-C1	2.09	119.47	111.80
2	52-A	1000	GOL	O2-C2-C1	2.08	117.80	109.18
2	71-A	1000	GOL	O2-C2-C1	2.05	117.67	109.18
2	34-A	1000	GOL	O2-C2-C1	2.05	117.67	109.18
2	54-A	1000	GOL	C3-C2-C1	2.04	119.28	111.80
2	64-A	1000	GOL	O2-C2-C1	2.04	117.61	109.18
2	59-A	1000	GOL	O2-C2-C1	2.02	117.55	109.18
2	73-A	1000	GOL	O2-C2-C1	2.01	117.51	109.18
2	74-A	1000	GOL	O2-C2-C1	2.01	117.50	109.18

There are no chirality outliers.

All (255) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3-A	1000	GOL	O1-C1-C2-O2
2	3-A	1000	GOL	O1-C1-C2-C3
2	3-A	1000	GOL	C1-C2-C3-O3
2	4-A	1000	GOL	O1-C1-C2-C3
2	4-A	1000	GOL	C1-C2-C3-O3
2	5-A	1000	GOL	O1-C1-C2-C3
2	5-A	1000	GOL	C1-C2-C3-O3
2	5-A	1000	GOL	O2-C2-C3-O3
2	6-A	1000	GOL	O1-C1-C2-C3
2	7-A	1000	GOL	O1-C1-C2-C3
2	7-A	1000	GOL	C1-C2-C3-O3
2	8-A	1000	GOL	O1-C1-C2-C3
2	17-A	1000	GOL	O1-C1-C2-C3
2	17-A	1000	GOL	C1-C2-C3-O3
2	18-A	1000	GOL	O1-C1-C2-C3
2	18-A	1000	GOL	C1-C2-C3-O3
2	19-A	1000	GOL	O1-C1-C2-C3
2	19-A	1000	GOL	C1-C2-C3-O3
2	20-A	1000	GOL	O1-C1-C2-C3
2	21-A	1000	GOL	O1-C1-C2-C3
2	21-A	1000	GOL	C1-C2-C3-O3
2	22-A	1000	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	22-A	1000	GOL	C1-C2-C3-O3
2	23-A	1000	GOL	C1-C2-C3-O3
2	26-A	1000	GOL	O1-C1-C2-C3
2	27-A	1000	GOL	C1-C2-C3-O3
2	28-A	1000	GOL	O1-C1-C2-C3
2	29-A	1000	GOL	O1-C1-C2-C3
2	29-A	1000	GOL	C1-C2-C3-O3
2	30-A	1000	GOL	O1-C1-C2-C3
2	30-A	1000	GOL	C1-C2-C3-O3
2	34-A	1000	GOL	O1-C1-C2-C3
2	34-A	1000	GOL	C1-C2-C3-O3
2	35-A	1000	GOL	C1-C2-C3-O3
2	37-A	1000	GOL	O1-C1-C2-C3
2	37-A	1000	GOL	O2-C2-C3-O3
2	49-A	1000	GOL	O1-C1-C2-C3
2	50-A	1000	GOL	O1-C1-C2-C3
2	50-A	1000	GOL	C1-C2-C3-O3
2	51-A	1000	GOL	O1-C1-C2-C3
2	51-A	1000	GOL	C1-C2-C3-O3
2	52-A	1000	GOL	O1-C1-C2-C3
2	53-A	1000	GOL	C1-C2-C3-O3
2	54-A	1000	GOL	O1-C1-C2-C3
2	54-A	1000	GOL	C1-C2-C3-O3
2	55-A	1000	GOL	O1-C1-C2-C3
2	55-A	1000	GOL	C1-C2-C3-O3
2	58-A	1000	GOL	O1-C1-C2-C3
2	58-A	1000	GOL	C1-C2-C3-O3
2	59-A	1000	GOL	O1-C1-C2-C3
2	60-A	1000	GOL	C1-C2-C3-O3
2	61-A	1000	GOL	O1-C1-C2-C3
2	64-A	1000	GOL	O1-C1-C2-C3
2	64-A	1000	GOL	C1-C2-C3-O3
2	65-A	1000	GOL	O1-C1-C2-O2
2	65-A	1000	GOL	O1-C1-C2-C3
2	65-A	1000	GOL	C1-C2-C3-O3
2	71-A	1000	GOL	O1-C1-C2-O2
2	71-A	1000	GOL	O1-C1-C2-C3
2	71-A	1000	GOL	C1-C2-C3-O3
2	72-A	1000	GOL	O1-C1-C2-C3
2	72-A	1000	GOL	C1-C2-C3-O3
2	73-A	1000	GOL	O1-C1-C2-C3
2	74-A	1000	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	75-A	1000	GOL	O1-C1-C2-C3
2	75-A	1000	GOL	C1-C2-C3-O3
2	76-A	1000	GOL	O1-C1-C2-C3
2	76-A	1000	GOL	C1-C2-C3-O3
2	77-A	1000	GOL	C1-C2-C3-O3
2	14-B	1000	GOL	O1-C1-C2-O2
2	44-B	1000	GOL	O1-C1-C2-C3
2	61-B	1000	GOL	O1-C1-C2-C3
2	75-B	1000	GOL	O1-C1-C2-C3
2	4-A	1000	GOL	O1-C1-C2-O2
2	4-A	1000	GOL	O2-C2-C3-O3
2	5-A	1000	GOL	O1-C1-C2-O2
2	6-A	1000	GOL	O2-C2-C3-O3
2	7-A	1000	GOL	O1-C1-C2-O2
2	18-A	1000	GOL	O1-C1-C2-O2
2	19-A	1000	GOL	O1-C1-C2-O2
2	28-A	1000	GOL	O1-C1-C2-O2
2	34-A	1000	GOL	O1-C1-C2-O2
2	35-A	1000	GOL	O1-C1-C2-O2
2	37-A	1000	GOL	O1-C1-C2-O2
2	50-A	1000	GOL	O1-C1-C2-O2
2	51-A	1000	GOL	O1-C1-C2-O2
2	52-A	1000	GOL	O1-C1-C2-O2
2	53-A	1000	GOL	O1-C1-C2-O2
2	54-A	1000	GOL	O2-C2-C3-O3
2	58-A	1000	GOL	O1-C1-C2-O2
2	65-A	1000	GOL	O2-C2-C3-O3
2	72-A	1000	GOL	O1-C1-C2-O2
2	76-A	1000	GOL	O1-C1-C2-O2
2	2-B	1000	GOL	O1-C1-C2-O2
2	38-B	1000	GOL	O1-C1-C2-O2
2	6-A	1000	GOL	C1-C2-C3-O3
2	8-A	1000	GOL	C1-C2-C3-O3
2	10-A	1000	GOL	C1-C2-C3-O3
2	12-A	1000	GOL	C1-C2-C3-O3
2	20-A	1000	GOL	C1-C2-C3-O3
2	25-A	1000	GOL	C1-C2-C3-O3
2	28-A	1000	GOL	C1-C2-C3-O3
2	31-A	1000	GOL	C1-C2-C3-O3
2	33-A	1000	GOL	C1-C2-C3-O3
2	35-A	1000	GOL	O1-C1-C2-C3
2	36-A	1000	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	37-A	1000	GOL	C1-C2-C3-O3
2	38-A	1000	GOL	C1-C2-C3-O3
2	39-A	1000	GOL	C1-C2-C3-O3
2	43-A	1000	GOL	C1-C2-C3-O3
2	49-A	1000	GOL	C1-C2-C3-O3
2	52-A	1000	GOL	C1-C2-C3-O3
2	53-A	1000	GOL	O1-C1-C2-C3
2	66-A	1000	GOL	O1-C1-C2-C3
2	69-A	1000	GOL	C1-C2-C3-O3
2	73-A	1000	GOL	C1-C2-C3-O3
2	74-A	1000	GOL	C1-C2-C3-O3
2	2-B	1000	GOL	O1-C1-C2-C3
2	4-B	1000	GOL	O1-C1-C2-C3
2	10-B	1000	GOL	O1-C1-C2-C3
2	14-B	1000	GOL	O1-C1-C2-C3
2	16-B	1000	GOL	O1-C1-C2-C3
2	19-B	1000	GOL	O1-C1-C2-C3
2	20-B	1000	GOL	O1-C1-C2-C3
2	21-B	1000	GOL	O1-C1-C2-C3
2	25-B	1000	GOL	O1-C1-C2-C3
2	27-B	1000	GOL	O1-C1-C2-C3
2	28-B	1000	GOL	O1-C1-C2-C3
2	29-B	1000	GOL	O1-C1-C2-C3
2	30-B	1000	GOL	O1-C1-C2-C3
2	38-B	1000	GOL	O1-C1-C2-C3
2	41-B	1000	GOL	O1-C1-C2-C3
2	45-B	1000	GOL	O1-C1-C2-C3
2	53-B	1000	GOL	O1-C1-C2-C3
2	59-B	1000	GOL	O1-C1-C2-C3
2	60-B	1000	GOL	O1-C1-C2-C3
2	65-B	1000	GOL	O1-C1-C2-C3
2	69-B	1000	GOL	O1-C1-C2-C3
2	71-B	1000	GOL	O1-C1-C2-C3
2	73-B	1000	GOL	O1-C1-C2-C3
2	74-B	1000	GOL	O1-C1-C2-C3
2	76-B	1000	GOL	O1-C1-C2-C3
2	77-B	1000	GOL	O1-C1-C2-C3
2	3-A	1000	GOL	O2-C2-C3-O3
2	6-A	1000	GOL	O1-C1-C2-O2
2	7-A	1000	GOL	O2-C2-C3-O3
2	8-A	1000	GOL	O1-C1-C2-O2
2	12-A	1000	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	17-A	1000	GOL	O1-C1-C2-O2
2	20-A	1000	GOL	O1-C1-C2-O2
2	21-A	1000	GOL	O1-C1-C2-O2
2	21-A	1000	GOL	O2-C2-C3-O3
2	23-A	1000	GOL	O2-C2-C3-O3
2	26-A	1000	GOL	O1-C1-C2-O2
2	27-A	1000	GOL	O2-C2-C3-O3
2	28-A	1000	GOL	O2-C2-C3-O3
2	29-A	1000	GOL	O1-C1-C2-O2
2	29-A	1000	GOL	O2-C2-C3-O3
2	30-A	1000	GOL	O1-C1-C2-O2
2	31-A	1000	GOL	O2-C2-C3-O3
2	35-A	1000	GOL	O2-C2-C3-O3
2	49-A	1000	GOL	O1-C1-C2-O2
2	51-A	1000	GOL	O2-C2-C3-O3
2	52-A	1000	GOL	O2-C2-C3-O3
2	53-A	1000	GOL	O2-C2-C3-O3
2	54-A	1000	GOL	O1-C1-C2-O2
2	55-A	1000	GOL	O1-C1-C2-O2
2	61-A	1000	GOL	O2-C2-C3-O3
2	64-A	1000	GOL	O1-C1-C2-O2
2	71-A	1000	GOL	O2-C2-C3-O3
2	75-A	1000	GOL	O1-C1-C2-O2
2	29-B	1000	GOL	O1-C1-C2-O2
2	30-B	1000	GOL	O1-C1-C2-O2
2	74-B	1000	GOL	O1-C1-C2-O2
2	10-A	1000	GOL	O2-C2-C3-O3
2	22-A	1000	GOL	O1-C1-C2-O2
2	27-A	1000	GOL	O1-C1-C2-O2
2	30-A	1000	GOL	O2-C2-C3-O3
2	33-A	1000	GOL	O2-C2-C3-O3
2	58-A	1000	GOL	O2-C2-C3-O3
2	59-A	1000	GOL	O1-C1-C2-O2
2	60-A	1000	GOL	O2-C2-C3-O3
2	73-A	1000	GOL	O1-C1-C2-O2
2	74-A	1000	GOL	O1-C1-C2-O2
2	28-B	1000	GOL	O1-C1-C2-O2
2	60-B	1000	GOL	O1-C1-C2-O2
2	25-A	1000	GOL	O2-C2-C3-O3
2	43-A	1000	GOL	O2-C2-C3-O3
2	50-A	1000	GOL	O2-C2-C3-O3
2	66-A	1000	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	69-A	1000	GOL	O2-C2-C3-O3
2	72-A	1000	GOL	O2-C2-C3-O3
2	44-B	1000	GOL	O1-C1-C2-O2
2	61-B	1000	GOL	O1-C1-C2-O2
2	71-B	1000	GOL	O1-C1-C2-O2
2	73-B	1000	GOL	O1-C1-C2-O2
2	75-B	1000	GOL	O1-C1-C2-O2
2	31-A	1000	GOL	O1-C1-C2-O2
2	39-A	1000	GOL	O2-C2-C3-O3
2	59-A	1000	GOL	C1-C2-C3-O3
2	3-B	1000	GOL	O1-C1-C2-C3
2	63-B	1000	GOL	O1-C1-C2-C3
2	18-A	1000	GOL	O2-C2-C3-O3
2	39-A	1000	GOL	O1-C1-C2-O2
2	76-B	1000	GOL	O1-C1-C2-O2
2	2-A	1000	GOL	O1-C1-C2-O2
2	17-A	1000	GOL	O2-C2-C3-O3
2	55-A	1000	GOL	O2-C2-C3-O3
2	64-A	1000	GOL	O2-C2-C3-O3
2	76-A	1000	GOL	O2-C2-C3-O3
2	10-B	1000	GOL	O1-C1-C2-O2
2	19-B	1000	GOL	O1-C1-C2-O2
2	25-B	1000	GOL	O1-C1-C2-O2
2	41-B	1000	GOL	O1-C1-C2-O2
2	45-B	1000	GOL	O1-C1-C2-O2
2	65-B	1000	GOL	O1-C1-C2-O2
2	11-A	1000	GOL	C1-C2-C3-O3
2	14-A	1000	GOL	C1-C2-C3-O3
2	61-A	1000	GOL	C1-C2-C3-O3
2	24-B	1000	GOL	O1-C1-C2-C3
2	35-B	1000	GOL	O1-C1-C2-C3
2	62-B	1000	GOL	O1-C1-C2-C3
2	41-A	1000	GOL	O1-C1-C2-O2
2	26-A	1000	GOL	C1-C2-C3-O3
2	42-B	1000	GOL	O1-C1-C2-C3
2	46-B	1000	GOL	O1-C1-C2-C3
2	47-B	1000	GOL	O1-C1-C2-C3
2	67-B	1000	GOL	O1-C1-C2-C3
2	77-A	1000	GOL	O2-C2-C3-O3
2	4-B	1000	GOL	O1-C1-C2-O2
2	20-B	1000	GOL	O1-C1-C2-O2
2	27-B	1000	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	53-B	1000	GOL	O1-C1-C2-O2
2	59-B	1000	GOL	O1-C1-C2-O2
2	63-B	1000	GOL	O1-C1-C2-O2
2	77-B	1000	GOL	O1-C1-C2-O2
2	11-A	1000	GOL	O2-C2-C3-O3
2	34-A	1000	GOL	O2-C2-C3-O3
2	3-B	1000	GOL	O1-C1-C2-O2
2	16-B	1000	GOL	O1-C1-C2-O2
2	21-B	1000	GOL	O1-C1-C2-O2
2	24-B	1000	GOL	O1-C1-C2-O2
2	35-B	1000	GOL	O1-C1-C2-O2
2	47-B	1000	GOL	O1-C1-C2-O2
2	62-B	1000	GOL	O1-C1-C2-O2
2	67-B	1000	GOL	O1-C1-C2-O2
2	69-B	1000	GOL	O1-C1-C2-O2
2	6-B	1000	GOL	O1-C1-C2-C3
2	8-B	1000	GOL	O1-C1-C2-C3
2	48-B	1000	GOL	O1-C1-C2-C3
2	14-A	1000	GOL	O2-C2-C3-O3
2	7-B	1000	GOL	O1-C1-C2-C3
2	19-A	1000	GOL	O2-C2-C3-O3
2	42-B	1000	GOL	O1-C1-C2-O2
2	48-B	1000	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	1-A	228/228 (100%)	2.17	74 (32%) ⓘ ⓘ	0, 0, 0, 1	228 (100%)
1	1-B	228/228 (100%)	2.04	87 (38%) ⓘ ⓘ	0, 0, 0, 1	228 (100%)
1	2-A	0/228	-	-	-	-
1	2-B	0/228	-	-	-	-
1	3-A	0/228	-	-	-	-
1	3-B	0/228	-	-	-	-
1	4-A	0/228	-	-	-	-
1	4-B	0/228	-	-	-	-
1	5-A	0/228	-	-	-	-
1	5-B	0/228	-	-	-	-
1	6-A	0/228	-	-	-	-
1	6-B	0/228	-	-	-	-
1	7-A	0/228	-	-	-	-
1	7-B	0/228	-	-	-	-
1	8-A	0/228	-	-	-	-
1	8-B	0/228	-	-	-	-
1	9-A	0/228	-	-	-	-
1	9-B	0/228	-	-	-	-
1	10-A	0/228	-	-	-	-
1	10-B	0/228	-	-	-	-
1	11-A	0/228	-	-	-	-
1	11-B	0/228	-	-	-	-
1	12-A	0/228	-	-	-	-
1	12-B	0/228	-	-	-	-
1	13-A	0/228	-	-	-	-
1	13-B	0/228	-	-	-	-
1	14-A	0/228	-	-	-	-
1	14-B	0/228	-	-	-	-
1	15-A	0/228	-	-	-	-
1	15-B	0/228	-	-	-	-
1	16-A	0/228	-	-	-	-
1	16-B	0/228	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	17-A	0/228	-	-	-	-
1	17-B	0/228	-	-	-	-
1	18-A	0/228	-	-	-	-
1	18-B	0/228	-	-	-	-
1	19-A	0/228	-	-	-	-
1	19-B	0/228	-	-	-	-
1	20-A	0/228	-	-	-	-
1	20-B	0/228	-	-	-	-
1	21-A	0/228	-	-	-	-
1	21-B	0/228	-	-	-	-
1	22-A	0/228	-	-	-	-
1	22-B	0/228	-	-	-	-
1	23-A	0/228	-	-	-	-
1	23-B	0/228	-	-	-	-
1	24-A	0/228	-	-	-	-
1	24-B	0/228	-	-	-	-
1	25-A	0/228	-	-	-	-
1	25-B	0/228	-	-	-	-
1	26-A	0/228	-	-	-	-
1	26-B	0/228	-	-	-	-
1	27-A	0/228	-	-	-	-
1	27-B	0/228	-	-	-	-
1	28-A	0/228	-	-	-	-
1	28-B	0/228	-	-	-	-
1	29-A	0/228	-	-	-	-
1	29-B	0/228	-	-	-	-
1	30-A	0/228	-	-	-	-
1	30-B	0/228	-	-	-	-
1	31-A	0/228	-	-	-	-
1	31-B	0/228	-	-	-	-
1	32-A	0/228	-	-	-	-
1	32-B	0/228	-	-	-	-
1	33-A	0/228	-	-	-	-
1	33-B	0/228	-	-	-	-
1	34-A	0/228	-	-	-	-
1	34-B	0/228	-	-	-	-
1	35-A	0/228	-	-	-	-
1	35-B	0/228	-	-	-	-
1	36-A	0/228	-	-	-	-
1	36-B	0/228	-	-	-	-
1	37-A	0/228	-	-	-	-
1	37-B	0/228	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	38-A	0/228	-	-	-	-
1	38-B	0/228	-	-	-	-
1	39-A	0/228	-	-	-	-
1	39-B	0/228	-	-	-	-
1	40-A	0/228	-	-	-	-
1	40-B	0/228	-	-	-	-
1	41-A	0/228	-	-	-	-
1	41-B	0/228	-	-	-	-
1	42-A	0/228	-	-	-	-
1	42-B	0/228	-	-	-	-
1	43-A	0/228	-	-	-	-
1	43-B	0/228	-	-	-	-
1	44-A	0/228	-	-	-	-
1	44-B	0/228	-	-	-	-
1	45-A	0/228	-	-	-	-
1	45-B	0/228	-	-	-	-
1	46-A	0/228	-	-	-	-
1	46-B	0/228	-	-	-	-
1	47-A	0/228	-	-	-	-
1	47-B	0/228	-	-	-	-
1	48-A	0/228	-	-	-	-
1	48-B	0/228	-	-	-	-
1	49-A	0/228	-	-	-	-
1	49-B	0/228	-	-	-	-
1	50-A	0/228	-	-	-	-
1	50-B	0/228	-	-	-	-
1	51-A	0/228	-	-	-	-
1	51-B	0/228	-	-	-	-
1	52-A	0/228	-	-	-	-
1	52-B	0/228	-	-	-	-
1	53-A	0/228	-	-	-	-
1	53-B	0/228	-	-	-	-
1	54-A	0/228	-	-	-	-
1	54-B	0/228	-	-	-	-
1	55-A	0/228	-	-	-	-
1	55-B	0/228	-	-	-	-
1	56-A	0/228	-	-	-	-
1	56-B	0/228	-	-	-	-
1	57-A	0/228	-	-	-	-
1	57-B	0/228	-	-	-	-
1	58-A	0/228	-	-	-	-
1	58-B	0/228	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	59-A	0/228	-	-	-	-
1	59-B	0/228	-	-	-	-
1	60-A	0/228	-	-	-	-
1	60-B	0/228	-	-	-	-
1	61-A	0/228	-	-	-	-
1	61-B	0/228	-	-	-	-
1	62-A	0/228	-	-	-	-
1	62-B	0/228	-	-	-	-
1	63-A	0/228	-	-	-	-
1	63-B	0/228	-	-	-	-
1	64-A	0/228	-	-	-	-
1	64-B	0/228	-	-	-	-
1	65-A	0/228	-	-	-	-
1	65-B	0/228	-	-	-	-
1	66-A	0/228	-	-	-	-
1	66-B	0/228	-	-	-	-
1	67-A	0/228	-	-	-	-
1	67-B	0/228	-	-	-	-
1	68-A	0/228	-	-	-	-
1	68-B	0/228	-	-	-	-
1	69-A	0/228	-	-	-	-
1	69-B	0/228	-	-	-	-
1	70-A	0/228	-	-	-	-
1	70-B	0/228	-	-	-	-
1	71-A	0/228	-	-	-	-
1	71-B	0/228	-	-	-	-
1	72-A	0/228	-	-	-	-
1	72-B	0/228	-	-	-	-
1	73-A	0/228	-	-	-	-
1	73-B	0/228	-	-	-	-
1	74-A	0/228	-	-	-	-
1	74-B	0/228	-	-	-	-
1	75-A	0/228	-	-	-	-
1	75-B	0/228	-	-	-	-
1	76-A	0/228	-	-	-	-
1	76-B	0/228	-	-	-	-
1	77-A	0/228	-	-	-	-
1	77-B	0/228	-	-	-	-
All	All	456/35112 (1%)	2.10	161 (35%) 1 1	0, 0, 0, 1	456 (100%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	178	SER	11.0
1	1-A	135	GLY	10.8
1	1-A	206	ASN	10.3
1	1-A	130	ILE	8.7
1	1-A	46	ALA	8.5
1	1-A	129	GLY	8.4
1	1-A	205	GLY	8.3
1	1-A	203	VAL	8.3
1	1-A	133	HIS	8.0
1	1-A	181	GLY	7.8
1	1-A	134	ALA	7.6
1	1-A	2	LEU	7.5
1	1-B	46	ALA	7.5
1	1-B	228	ALA	7.5
1	1-B	204	CYS	7.4
1	1-A	200	GLY	7.4
1	1-A	179	CYS	7.3
1	1-B	200	GLY	7.3
1	1-A	131	VAL	7.2
1	1-A	204	CYS	7.1
1	1-B	199	SER	6.9
1	1-A	137	ARG	6.6
1	1-A	132	ASN	6.4
1	1-B	227	LEU	6.3
1	1-A	208	LYS	6.1
1	1-A	202	ALA	6.0
1	1-A	207	ARG	6.0
1	1-B	45	ASP	6.0
1	1-A	47	ALA	5.9
1	1-A	175	ARG	5.8
1	1-A	182	ASP	5.8
1	1-A	3	GLY	5.8
1	1-A	228	ALA	5.7
1	1-B	79	PRO	5.7
1	1-B	154	CYS	5.7
1	1-A	176	ARG	5.6
1	1-A	43	LEU	5.6
1	1-B	86	ILE	5.4
1	1-B	48	ASP	5.3
1	1-A	201	SER	5.3
1	1-B	50	LYS	5.2
1	1-B	226	VAL	5.2
1	1-B	201	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	48	ASP	5.0
1	1-A	136	ARG	5.0
1	1-B	47	ALA	5.0
1	1-A	177	ASP	4.9
1	1-B	203	VAL	4.8
1	1-A	1	ILE	4.8
1	1-A	199	SER	4.7
1	1-B	167	ARG	4.6
1	1-A	172	GLU	4.6
1	1-A	115	ARG	4.6
1	1-A	198	THR	4.5
1	1-B	150	ASP	4.5
1	1-B	43	LEU	4.4
1	1-A	174	ASN	4.4
1	1-B	73	LEU	4.3
1	1-B	84	ASP	4.2
1	1-B	49	GLY	4.1
1	1-B	202	ALA	4.1
1	1-B	85	THR	4.0
1	1-B	136	ARG	4.0
1	1-A	173	SER	4.0
1	1-B	44	GLU	3.9
1	1-B	133	HIS	3.9
1	1-B	176	ARG	3.9
1	1-A	209	LYS	3.8
1	1-B	134	ALA	3.8
1	1-B	152	ALA	3.8
1	1-A	5	ARG	3.8
1	1-B	62	GLN	3.8
1	1-B	42	CYS	3.7
1	1-B	162	GLY	3.7
1	1-A	85	THR	3.6
1	1-A	68	ARG	3.6
1	1-B	72	VAL	3.5
1	1-A	98	LYS	3.5
1	1-B	110	TRP	3.5
1	1-A	45	ASP	3.5
1	1-B	163	ALA	3.4
1	1-B	170	CYS	3.4
1	1-B	208	LYS	3.4
1	1-B	219	TYR	3.3
1	1-B	22	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	25	LEU	3.3
1	1-A	50	LYS	3.3
1	1-A	158	THR	3.3
1	1-A	138	PRO	3.3
1	1-B	206	ASN	3.3
1	1-B	198	THR	3.3
1	1-A	4	GLY	3.3
1	1-B	98	LYS	3.3
1	1-A	84	ASP	3.3
1	1-A	112	ARG	3.2
1	1-A	86	ILE	3.2
1	1-B	158	THR	3.2
1	1-B	21	ASN	3.2
1	1-B	149	LEU	3.2
1	1-A	157	ARG	3.1
1	1-B	174	ASN	3.1
1	1-B	115	ARG	3.1
1	1-B	223	ILE	3.1
1	1-B	76	VAL	3.1
1	1-B	157	ARG	3.0
1	1-A	100	THR	2.9
1	1-B	97	GLU	2.9
1	1-B	68	ARG	2.9
1	1-A	44	GLU	2.9
1	1-B	165	THR	2.9
1	1-B	175	ARG	2.9
1	1-B	180	LYS	2.9
1	1-A	69	LEU	2.9
1	1-B	40	ALA	2.8
1	1-B	137	ARG	2.7
1	1-A	32	ALA	2.7
1	1-B	212	ILE	2.7
1	1-A	166	GLU	2.7
1	1-B	160	HIS	2.7
1	1-A	49	GLY	2.7
1	1-B	80	ASP	2.7
1	1-B	92	LEU	2.7
1	1-A	82	GLN	2.6
1	1-B	225	SER	2.6
1	1-B	18	VAL	2.6
1	1-A	62	GLN	2.6
1	1-B	5	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-B	209	LYS	2.6
1	1-A	41	HIS	2.5
1	1-A	8	GLU	2.5
1	1-B	164	ILE	2.5
1	1-B	51	VAL	2.5
1	1-A	180	LYS	2.5
1	1-B	74	ARG	2.5
1	1-B	20	LEU	2.4
1	1-B	118	ALA	2.4
1	1-B	116	ASP	2.4
1	1-A	152	ALA	2.4
1	1-B	207	ARG	2.4
1	1-B	113	VAL	2.4
1	1-B	205	GLY	2.4
1	1-B	83	PRO	2.4
1	1-A	183	SER	2.3
1	1-B	106	ARG	2.3
1	1-B	35	TRP	2.3
1	1-B	168	LEU	2.3
1	1-A	221	ALA	2.3
1	1-A	20	LEU	2.3
1	1-A	162	GLY	2.2
1	1-B	11	ALA	2.2
1	1-A	159	HIS	2.2
1	1-A	146	LEU	2.2
1	1-A	210	PRO	2.2
1	1-B	130	ILE	2.1
1	1-B	96	SER	2.1
1	1-B	82	GLN	2.1
1	1-B	222	TRP	2.1
1	1-B	153	THR	2.0
1	1-B	159	HIS	2.0
1	1-A	83	PRO	2.0
1	1-B	156	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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	GOL	1-A	1000	6/6	0.75	0.14	18,19,20,21	14
2	GOL	2-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	3-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	4-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	5-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	6-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	7-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	8-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	9-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	10-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	11-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	12-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	13-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	14-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	15-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	16-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	17-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	18-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	19-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	20-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	21-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	22-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	23-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	24-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	25-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	26-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	27-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	28-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	29-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	30-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	31-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	32-A	1000	6/6	-	-	18,19,20,21	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	33-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	34-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	35-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	36-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	37-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	38-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	39-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	40-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	41-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	42-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	43-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	44-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	45-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	46-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	47-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	48-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	49-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	50-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	51-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	52-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	53-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	54-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	55-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	56-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	57-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	58-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	59-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	60-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	61-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	62-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	63-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	64-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	65-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	66-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	67-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	68-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	69-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	70-A	1000	6/6	-	-	18,19,21,21	14
2	GOL	71-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	72-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	73-A	1000	6/6	-	-	18,19,20,20	14
2	GOL	74-A	1000	6/6	-	-	18,19,20,20	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	75-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	76-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	77-A	1000	6/6	-	-	18,19,20,21	14
2	GOL	1-B	1000	6/6	0.88	0.12	30,32,36,38	14
2	GOL	2-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	3-B	1000	6/6	-	-	31,32,37,38	14
2	GOL	4-B	1000	6/6	-	-	31,33,37,38	14
2	GOL	5-B	1000	6/6	-	-	31,32,37,38	14
2	GOL	6-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	7-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	8-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	9-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	10-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	11-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	12-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	13-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	14-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	15-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	16-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	17-B	1000	6/6	-	-	31,32,37,38	14
2	GOL	18-B	1000	6/6	-	-	31,32,37,38	14
2	GOL	19-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	20-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	21-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	22-B	1000	6/6	-	-	31,32,37,38	14
2	GOL	23-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	24-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	25-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	26-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	27-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	28-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	29-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	30-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	31-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	32-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	33-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	34-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	35-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	36-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	37-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	38-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	39-B	1000	6/6	-	-	29,32,36,38	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	40-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	41-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	42-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	43-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	44-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	45-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	46-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	47-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	48-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	49-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	50-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	51-B	1000	6/6	-	-	29,33,37,38	14
2	GOL	52-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	53-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	54-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	55-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	56-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	57-B	1000	6/6	-	-	29,32,36,38	14
2	GOL	58-B	1000	6/6	-	-	29,32,37,38	14
2	GOL	59-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	60-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	61-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	62-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	63-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	64-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	65-B	1000	6/6	-	-	30,32,36,38	14
2	GOL	66-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	67-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	68-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	69-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	70-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	71-B	1000	6/6	-	-	31,33,37,38	14
2	GOL	72-B	1000	6/6	-	-	31,33,37,38	14
2	GOL	73-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	74-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	75-B	1000	6/6	-	-	30,32,37,38	14
2	GOL	76-B	1000	6/6	-	-	30,33,37,38	14
2	GOL	77-B	1000	6/6	-	-	30,33,37,38	14

5.5 Other polymers ⓘ

There are no such residues in this entry.