wwPDB X-ray Structure Validation Summary Report (i)

Dec 14, 2023 – 03:37 am GMT

PDB ID	:	4CBO
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 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:

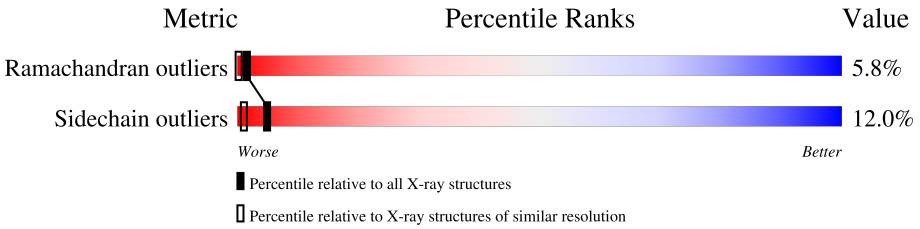
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline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

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 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))
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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	29-A	1000	-	X	-	-

2 Entry composition (i)

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	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	4-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	5-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	6-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	7-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	8-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	9-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	10-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	11-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	12-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	13-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	14-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	15-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	16-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	17-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	18-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	19-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	20-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	21-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	22-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	23-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	24-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	25-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	26-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	27-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	28-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	29-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	30-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	31-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	32-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	33-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	34-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	35-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	36-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	37-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	38-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	39-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	40-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	41-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	42-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	43-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	44-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	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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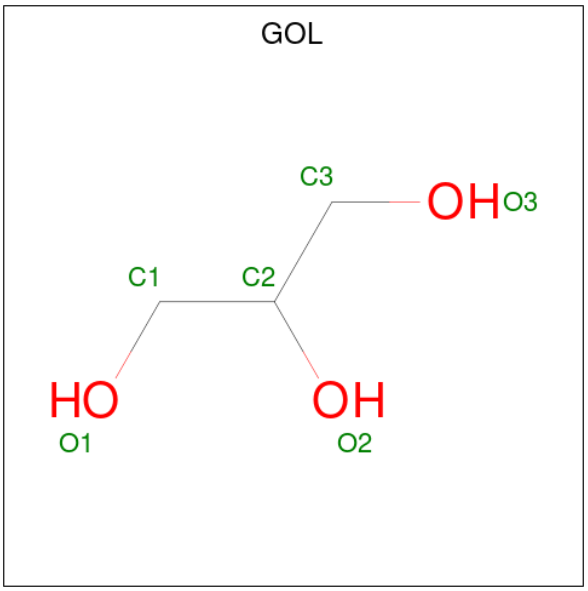
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	66-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

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

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

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

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

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

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

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

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

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

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

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Deposito
Cell constants a, b, c, α, β, γ	44.14Å 67.31Å 133.14Å 90.00° 90.00° 90.00°	Deposito
Resolution (Å)	47.33 – 1.80	Deposito
% Data completeness (in resolution range)	98.7 (47.33-1.80)	Deposito
R_{merge}	0.14	Deposito
R_{sym}	(Not available)	Deposito
$< I/\sigma(I) >$ [1]	2.04 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1259)	Deposito
R, R_{free}	0.163 , 0.212	Deposito
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.319	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	546299	wwPDB-V
Average B, all atoms (Å^2)	26.0	wwPDB-V

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.*

[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.

4 Model quality (i)

4.1 Standard geometry (i)

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

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	1-A	0.72	0/1741	1.01	5/2370 (0.2%)
1	1-B	0.58	0/1741	0.75	2/2370 (0.1%)
1	2-A	0.77	2/1741 (0.1%)	0.97	2/2370 (0.1%)
1	2-B	0.60	1/1741 (0.1%)	0.82	1/2370 (0.0%)
1	3-A	0.80	1/1741 (0.1%)	0.98	5/2370 (0.2%)
1	3-B	0.54	0/1741	0.79	0/2370
1	4-A	0.79	3/1741 (0.2%)	1.02	7/2370 (0.3%)
1	4-B	0.56	0/1741	0.77	1/2370 (0.0%)
1	5-A	0.77	2/1741 (0.1%)	1.00	8/2370 (0.3%)
1	5-B	0.59	0/1741	0.78	1/2370 (0.0%)
1	6-A	0.74	1/1741 (0.1%)	0.99	3/2370 (0.1%)
1	6-B	0.61	0/1741	0.77	1/2370 (0.0%)
1	7-A	0.74	1/1741 (0.1%)	0.98	7/2370 (0.3%)
1	7-B	0.58	1/1741 (0.1%)	0.82	2/2370 (0.1%)
1	8-A	0.72	0/1741	1.00	6/2370 (0.3%)
1	8-B	0.58	0/1741	0.79	2/2370 (0.1%)
1	9-A	0.76	1/1741 (0.1%)	0.97	6/2370 (0.3%)
1	9-B	0.60	1/1741 (0.1%)	0.81	2/2370 (0.1%)
1	10-A	0.78	5/1741 (0.3%)	1.05	7/2370 (0.3%)
1	10-B	0.59	1/1741 (0.1%)	0.79	0/2370
1	11-A	0.74	2/1741 (0.1%)	1.03	8/2370 (0.3%)
1	11-B	0.62	0/1741	0.80	3/2370 (0.1%)
1	12-A	0.74	1/1741 (0.1%)	1.00	11/2370 (0.5%)
1	12-B	0.59	0/1741	0.80	0/2370
1	13-A	0.75	0/1741	1.00	9/2370 (0.4%)
1	13-B	0.60	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	14-A	0.73	1/1741 (0.1%)	0.97	6/2370 (0.3%)
1	14-B	0.59	0/1741	0.84	1/2370 (0.0%)
1	15-A	0.70	0/1741	0.96	2/2370 (0.1%)
1	15-B	0.61	0/1741	0.82	2/2370 (0.1%)
1	16-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	16-B	0.62	0/1741	0.81	0/2370

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	17-A	0.77	1/1741 (0.1%)	1.01	4/2370 (0.2%)
1	17-B	0.62	0/1741	0.83	1/2370 (0.0%)
1	18-A	0.73	2/1741 (0.1%)	0.92	3/2370 (0.1%)
1	18-B	0.60	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	19-A	0.67	0/1741	0.89	2/2370 (0.1%)
1	19-B	0.62	1/1741 (0.1%)	0.82	0/2370
1	20-A	0.79	2/1741 (0.1%)	0.97	3/2370 (0.1%)
1	20-B	0.69	3/1741 (0.2%)	0.82	1/2370 (0.0%)
1	21-A	0.71	0/1741	0.87	2/2370 (0.1%)
1	21-B	0.57	0/1741	0.76	0/2370
1	22-A	0.75	0/1741	1.02	11/2370 (0.5%)
1	22-B	0.65	1/1741 (0.1%)	0.89	5/2370 (0.2%)
1	23-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	23-B	0.66	1/1741 (0.1%)	0.81	1/2370 (0.0%)
1	24-A	0.83	4/1741 (0.2%)	1.10	9/2370 (0.4%)
1	24-B	0.68	2/1741 (0.1%)	0.83	1/2370 (0.0%)
1	25-A	0.78	0/1741	0.98	4/2370 (0.2%)
1	25-B	0.62	0/1741	0.80	0/2370
1	26-A	0.75	1/1741 (0.1%)	0.98	5/2370 (0.2%)
1	26-B	0.63	0/1741	0.83	1/2370 (0.0%)
1	27-A	0.74	0/1741	0.99	4/2370 (0.2%)
1	27-B	0.58	0/1741	0.78	0/2370
1	28-A	0.83	4/1741 (0.2%)	1.10	12/2370 (0.5%)
1	28-B	0.57	1/1741 (0.1%)	0.77	1/2370 (0.0%)
1	29-A	0.75	1/1741 (0.1%)	0.98	4/2370 (0.2%)
1	29-B	0.57	0/1741	0.77	2/2370 (0.1%)
1	30-A	0.73	0/1741	1.00	5/2370 (0.2%)
1	30-B	0.63	0/1741	0.82	1/2370 (0.0%)
1	31-A	0.73	1/1741 (0.1%)	0.96	4/2370 (0.2%)
1	31-B	0.55	0/1741	0.76	0/2370
1	32-A	0.73	1/1741 (0.1%)	0.92	3/2370 (0.1%)
1	32-B	0.56	0/1741	0.82	5/2370 (0.2%)
1	33-A	0.76	1/1741 (0.1%)	1.00	8/2370 (0.3%)
1	33-B	0.58	0/1741	0.75	0/2370
1	34-A	0.80	5/1741 (0.3%)	0.98	6/2370 (0.3%)
1	34-B	0.59	0/1741	0.78	0/2370
1	35-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	35-B	0.60	1/1741 (0.1%)	0.80	0/2370
1	36-A	0.75	1/1741 (0.1%)	0.99	8/2370 (0.3%)
1	36-B	0.60	0/1741	0.82	2/2370 (0.1%)
1	37-A	0.71	0/1741	0.98	8/2370 (0.3%)
1	37-B	0.61	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	38-A	0.75	1/1741 (0.1%)	0.97	8/2370 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	38-B	0.62	1/1741 (0.1%)	0.84	3/2370 (0.1%)
1	39-A	0.73	0/1741	0.98	7/2370 (0.3%)
1	39-B	0.57	0/1741	0.77	2/2370 (0.1%)
1	40-A	0.71	1/1741 (0.1%)	0.91	2/2370 (0.1%)
1	40-B	0.58	0/1741	0.80	4/2370 (0.2%)
1	41-A	0.76	1/1741 (0.1%)	1.15	7/2370 (0.3%)
1	41-B	0.61	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	42-A	0.81	2/1741 (0.1%)	1.09	11/2370 (0.5%)
1	42-B	0.59	0/1741	0.82	1/2370 (0.0%)
1	43-A	0.78	1/1741 (0.1%)	0.98	4/2370 (0.2%)
1	43-B	0.58	0/1741	0.78	2/2370 (0.1%)
1	44-A	0.77	1/1741 (0.1%)	1.10	14/2370 (0.6%)
1	44-B	0.55	0/1741	0.78	1/2370 (0.0%)
1	45-A	0.73	0/1741	0.94	2/2370 (0.1%)
1	45-B	0.76	3/1741 (0.2%)	0.81	2/2370 (0.1%)
1	46-A	0.73	0/1741	1.01	9/2370 (0.4%)
1	46-B	0.57	0/1741	0.78	1/2370 (0.0%)
1	47-A	0.78	0/1741	0.99	5/2370 (0.2%)
1	47-B	0.60	0/1741	0.79	1/2370 (0.0%)
1	48-A	0.70	0/1741	0.97	5/2370 (0.2%)
1	48-B	0.60	1/1741 (0.1%)	0.80	0/2370
1	49-A	0.74	0/1741	1.04	9/2370 (0.4%)
1	49-B	0.61	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	50-A	0.75	1/1741 (0.1%)	0.94	6/2370 (0.3%)
1	50-B	0.59	0/1741	0.77	3/2370 (0.1%)
1	51-A	0.76	0/1741	0.99	4/2370 (0.2%)
1	51-B	0.61	1/1741 (0.1%)	0.82	3/2370 (0.1%)
1	52-A	0.75	2/1741 (0.1%)	0.97	5/2370 (0.2%)
1	52-B	0.63	1/1741 (0.1%)	0.82	4/2370 (0.2%)
1	53-A	0.79	0/1741	0.96	4/2370 (0.2%)
1	53-B	0.58	1/1741 (0.1%)	0.77	2/2370 (0.1%)
1	54-A	0.74	1/1741 (0.1%)	0.99	6/2370 (0.3%)
1	54-B	0.63	0/1741	0.81	2/2370 (0.1%)
1	55-A	0.72	1/1741 (0.1%)	1.01	6/2370 (0.3%)
1	55-B	0.58	0/1741	0.80	0/2370
1	56-A	0.74	0/1741	0.91	1/2370 (0.0%)
1	56-B	0.68	1/1741 (0.1%)	0.78	0/2370
1	57-A	0.72	0/1741	1.01	7/2370 (0.3%)
1	57-B	0.62	1/1741 (0.1%)	0.81	1/2370 (0.0%)
1	58-A	0.71	0/1741	0.98	5/2370 (0.2%)
1	58-B	0.60	1/1741 (0.1%)	0.84	2/2370 (0.1%)
1	59-A	0.72	1/1741 (0.1%)	0.90	2/2370 (0.1%)
1	59-B	0.64	3/1741 (0.2%)	0.81	2/2370 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	60-A	0.69	0/1741	0.89	3/2370 (0.1%)
1	60-B	0.63	3/1741 (0.2%)	0.81	0/2370
1	61-A	0.71	1/1741 (0.1%)	0.93	3/2370 (0.1%)
1	61-B	0.58	1/1741 (0.1%)	0.77	0/2370
1	62-A	0.71	0/1741	0.98	6/2370 (0.3%)
1	62-B	0.62	1/1741 (0.1%)	0.80	2/2370 (0.1%)
1	63-A	0.79	3/1741 (0.2%)	1.03	8/2370 (0.3%)
1	63-B	0.60	0/1741	0.84	2/2370 (0.1%)
1	64-A	0.73	0/1741	0.97	8/2370 (0.3%)
1	64-B	0.61	0/1741	0.79	2/2370 (0.1%)
1	65-A	0.72	1/1741 (0.1%)	0.94	4/2370 (0.2%)
1	65-B	0.66	1/1741 (0.1%)	0.82	3/2370 (0.1%)
1	66-A	0.73	1/1741 (0.1%)	0.89	3/2370 (0.1%)
1	66-B	0.60	1/1741 (0.1%)	0.78	1/2370 (0.0%)
1	67-A	0.76	1/1741 (0.1%)	0.95	5/2370 (0.2%)
1	67-B	0.59	1/1741 (0.1%)	0.79	2/2370 (0.1%)
1	68-A	0.79	2/1741 (0.1%)	1.01	6/2370 (0.3%)
1	68-B	0.58	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	69-A	0.79	3/1741 (0.2%)	0.95	6/2370 (0.3%)
1	69-B	0.57	0/1741	0.78	0/2370
1	70-A	0.80	4/1741 (0.2%)	0.98	4/2370 (0.2%)
1	70-B	0.64	0/1741	0.82	1/2370 (0.0%)
1	71-A	0.78	3/1741 (0.2%)	1.05	8/2370 (0.3%)
1	71-B	0.59	1/1741 (0.1%)	0.77	0/2370
1	72-A	0.75	0/1741	1.00	5/2370 (0.2%)
1	72-B	0.65	1/1741 (0.1%)	0.83	1/2370 (0.0%)
1	73-A	0.80	1/1741 (0.1%)	1.00	7/2370 (0.3%)
1	73-B	0.60	0/1741	0.78	1/2370 (0.0%)
1	74-A	0.79	2/1741 (0.1%)	1.06	8/2370 (0.3%)
1	74-B	0.66	3/1741 (0.2%)	0.78	1/2370 (0.0%)
1	75-A	0.70	0/1741	0.92	3/2370 (0.1%)
1	75-B	0.59	0/1741	0.77	0/2370
1	76-A	0.77	1/1741 (0.1%)	0.92	2/2370 (0.1%)
1	76-B	0.62	2/1741 (0.1%)	0.77	1/2370 (0.0%)
1	77-A	0.75	1/1741 (0.1%)	0.93	4/2370 (0.2%)
1	77-B	0.61	3/1741 (0.2%)	0.72	0/2370
All	All	0.68	133/268114 (0.0%)	0.90	535/364980 (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	1-A	0	6
1	1-B	0	2
1	2-A	0	5
1	2-B	0	2
1	3-A	0	4
1	3-B	0	1
1	4-A	0	5
1	4-B	0	3
1	5-A	0	4
1	6-A	0	6
1	6-B	0	2
1	7-A	0	6
1	7-B	0	2
1	8-A	0	9
1	8-B	0	1
1	9-A	0	5
1	9-B	0	2
1	10-A	0	9
1	10-B	0	2
1	11-A	0	6
1	11-B	0	4
1	12-A	0	2
1	12-B	0	1
1	13-A	0	4
1	13-B	0	1
1	14-A	0	4
1	14-B	0	1
1	15-A	0	3
1	15-B	0	2
1	16-A	0	5
1	16-B	0	1
1	17-A	0	5
1	17-B	0	5
1	18-A	0	5
1	18-B	0	1
1	19-A	0	6
1	19-B	0	1
1	20-A	0	5
1	20-B	0	3
1	21-A	0	2
1	21-B	0	2
1	22-A	0	8
1	22-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	23-A	0	3
1	24-A	0	6
1	25-A	0	2
1	26-A	0	4
1	26-B	0	2
1	27-A	0	4
1	27-B	0	2
1	28-A	0	4
1	28-B	0	1
1	29-A	0	4
1	29-B	0	1
1	30-A	0	3
1	30-B	0	1
1	31-A	0	5
1	31-B	0	1
1	32-A	0	10
1	32-B	0	1
1	33-A	0	8
1	34-A	0	4
1	35-A	0	4
1	35-B	0	2
1	36-A	0	3
1	36-B	0	1
1	37-A	0	7
1	37-B	0	1
1	38-A	0	5
1	38-B	0	1
1	39-A	0	5
1	40-A	0	5
1	40-B	0	1
1	41-A	0	6
1	42-A	0	6
1	43-A	0	5
1	43-B	0	3
1	44-A	0	7
1	44-B	0	4
1	45-A	0	5
1	45-B	0	1
1	46-A	0	8
1	46-B	0	1
1	47-A	0	5
1	47-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	48-A	0	9
1	48-B	0	2
1	49-A	0	5
1	49-B	0	1
1	50-A	0	6
1	51-A	0	7
1	51-B	0	1
1	52-A	0	7
1	53-A	0	3
1	53-B	0	1
1	54-A	0	3
1	54-B	0	4
1	55-A	0	7
1	56-A	0	1
1	57-A	0	7
1	58-A	0	5
1	58-B	0	7
1	59-A	0	4
1	60-A	0	2
1	61-B	0	1
1	62-A	0	2
1	63-A	0	3
1	63-B	0	2
1	64-A	0	6
1	64-B	0	1
1	65-A	0	4
1	65-B	0	1
1	66-A	0	9
1	66-B	0	1
1	67-A	0	9
1	67-B	0	1
1	68-A	0	3
1	69-A	0	7
1	69-B	0	2
1	70-A	0	6
1	70-B	0	3
1	71-A	0	3
1	71-B	0	2
1	72-A	0	7
1	73-A	0	4
1	73-B	0	1
1	74-A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	74-B	0	1
1	75-A	0	5
1	75-B	0	1
1	76-A	0	2
1	77-A	0	2
1	77-B	0	2
All	All	0	485

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	56-B	204	CYS	CB-SG	13.21	2.04	1.82
1	45-B	97	GLU	CG-CD	-12.87	1.32	1.51
1	20-A	97	GLU	CB-CG	-12.81	1.27	1.52
1	65-B	179	CYS	CB-SG	12.24	2.03	1.82
1	23-B	179	CYS	CB-SG	10.94	2.00	1.82

The worst 5 of 535 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	41-A	115	ARG	NE-CZ-NH2	-18.51	111.04	120.30
1	41-A	215	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	24-A	137	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	74-A	215	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	41-A	215	ARG	NE-CZ-NH2	-14.54	113.03	120.30

There are no chirality outliers.

5 of 485 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	1	ILE	Peptide
1	1-A	131	VAL	Peptide
1	1-A	137	ARG	Peptide
1	1-A	178	SER	Peptide
1	1-A	49	GLY	Peptide

4.2 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	1-A	1706	1700	1690	0	0
1	1-B	1706	1700	1690	0	0
1	2-A	1706	1700	1690	0	0
1	2-B	1706	1700	1690	0	0
1	3-A	1706	1700	1690	0	0
1	3-B	1706	1700	1690	0	0
1	4-A	1706	1700	1690	0	0
1	4-B	1706	1700	1690	0	0
1	5-A	1706	1700	1690	0	0
1	5-B	1706	1700	1690	0	0
1	6-A	1706	1700	1690	0	0
1	6-B	1706	1700	1690	0	0
1	7-A	1706	1700	1690	0	0
1	7-B	1706	1700	1690	0	0
1	8-A	1706	1700	1690	0	0
1	8-B	1706	1700	1690	0	0
1	9-A	1706	1700	1690	0	0
1	9-B	1706	1700	1690	0	0
1	10-A	1706	1700	1690	0	0
1	10-B	1706	1700	1690	0	0
1	11-A	1706	1700	1690	0	0
1	11-B	1706	1700	1690	0	0
1	12-A	1706	1700	1690	0	0
1	12-B	1706	1700	1690	0	0
1	13-A	1706	1700	1690	0	0
1	13-B	1706	1700	1690	0	0
1	14-A	1706	1700	1690	0	0
1	14-B	1706	1700	1690	0	0
1	15-A	1706	1700	1690	0	0
1	15-B	1706	1700	1690	0	0
1	16-A	1706	1700	1690	0	0
1	16-B	1706	1700	1690	0	0
1	17-A	1706	1700	1690	0	0
1	17-B	1706	1700	1690	0	0
1	18-A	1706	1700	1690	0	0
1	18-B	1706	1700	1690	0	0
1	19-A	1706	1700	1690	0	0
1	19-B	1706	1700	1690	0	0
1	20-A	1706	1700	1690	0	0
1	20-B	1706	1700	1690	0	0
1	21-A	1706	1700	1690	0	0
1	21-B	1706	1700	1690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	22-A	1706	1700	1690	0	0
1	22-B	1706	1700	1690	0	0
1	23-A	1706	1700	1690	0	0
1	23-B	1706	1700	1690	0	0
1	24-A	1706	1700	1690	0	0
1	24-B	1706	1700	1690	0	0
1	25-A	1706	1700	1690	0	0
1	25-B	1706	1700	1690	0	0
1	26-A	1706	1700	1690	0	0
1	26-B	1706	1700	1690	0	0
1	27-A	1706	1700	1690	0	0
1	27-B	1706	1700	1690	0	0
1	28-A	1706	1700	1690	0	0
1	28-B	1706	1700	1690	0	0
1	29-A	1706	1700	1690	0	0
1	29-B	1706	1700	1690	0	0
1	30-A	1706	1700	1690	0	0
1	30-B	1706	1700	1690	0	0
1	31-A	1706	1700	1690	0	0
1	31-B	1706	1700	1690	0	0
1	32-A	1706	1700	1690	0	0
1	32-B	1706	1700	1690	0	0
1	33-A	1706	1700	1690	0	0
1	33-B	1706	1700	1690	0	0
1	34-A	1706	1700	1690	0	0
1	34-B	1706	1700	1690	0	0
1	35-A	1706	1700	1690	0	0
1	35-B	1706	1700	1690	0	0
1	36-A	1706	1700	1690	0	0
1	36-B	1706	1700	1690	0	0
1	37-A	1706	1700	1690	0	0
1	37-B	1706	1700	1690	0	0
1	38-A	1706	1700	1690	0	0
1	38-B	1706	1700	1690	0	0
1	39-A	1706	1700	1690	0	0
1	39-B	1706	1700	1690	0	0
1	40-A	1706	1700	1690	0	0
1	40-B	1706	1700	1690	0	0
1	41-A	1706	1700	1690	0	0
1	41-B	1706	1700	1690	0	0
1	42-A	1706	1700	1690	0	0
1	42-B	1706	1700	1690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	43-A	1706	1700	1690	0	0
1	43-B	1706	1700	1690	0	0
1	44-A	1706	1700	1690	0	0
1	44-B	1706	1700	1690	0	0
1	45-A	1706	1700	1690	0	0
1	45-B	1706	1700	1690	0	0
1	46-A	1706	1700	1690	0	0
1	46-B	1706	1700	1690	0	0
1	47-A	1706	1700	1690	0	0
1	47-B	1706	1700	1690	0	0
1	48-A	1706	1700	1690	0	0
1	48-B	1706	1700	1690	0	0
1	49-A	1706	1700	1690	0	0
1	49-B	1706	1700	1690	0	0
1	50-A	1706	1700	1690	0	0
1	50-B	1706	1700	1690	0	0
1	51-A	1706	1700	1690	0	0
1	51-B	1706	1700	1690	0	0
1	52-A	1706	1700	1690	0	0
1	52-B	1706	1700	1690	0	0
1	53-A	1706	1700	1690	0	0
1	53-B	1706	1700	1690	0	0
1	54-A	1706	1700	1690	0	0
1	54-B	1706	1700	1690	0	0
1	55-A	1706	1700	1690	0	0
1	55-B	1706	1700	1690	0	0
1	56-A	1706	1700	1690	0	0
1	56-B	1706	1700	1690	0	0
1	57-A	1706	1700	1690	0	0
1	57-B	1706	1700	1690	0	0
1	58-A	1706	1700	1690	0	0
1	58-B	1706	1700	1690	0	0
1	59-A	1706	1700	1690	0	0
1	59-B	1706	1700	1690	0	0
1	60-A	1706	1700	1690	0	0
1	60-B	1706	1700	1690	0	0
1	61-A	1706	1700	1690	0	0
1	61-B	1706	1700	1690	0	0
1	62-A	1706	1700	1690	0	0
1	62-B	1706	1700	1690	0	0
1	63-A	1706	1700	1690	0	0
1	63-B	1706	1700	1690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	64-A	1706	1700	1690	0	0
1	64-B	1706	1700	1690	0	0
1	65-A	1706	1700	1690	0	0
1	65-B	1706	1700	1690	0	0
1	66-A	1706	1700	1690	0	0
1	66-B	1706	1700	1690	0	0
1	67-A	1706	1700	1690	0	0
1	67-B	1706	1700	1690	0	0
1	68-A	1706	1700	1690	0	0
1	68-B	1706	1700	1690	0	0
1	69-A	1706	1700	1690	0	0
1	69-B	1706	1700	1690	0	0
1	70-A	1706	1700	1690	0	0
1	70-B	1706	1700	1690	0	0
1	71-A	1706	1700	1690	0	0
1	71-B	1706	1700	1690	0	0
1	72-A	1706	1700	1690	0	0
1	72-B	1706	1700	1690	0	0
1	73-A	1706	1700	1690	0	0
1	73-B	1706	1700	1690	0	0
1	74-A	1706	1700	1690	0	0
1	74-B	1706	1700	1690	0	0
1	75-A	1706	1700	1690	0	0
1	75-B	1706	1700	1690	0	0
1	76-A	1706	1700	1690	0	0
1	76-B	1706	1700	1690	0	0
1	77-A	1706	1700	1690	0	0
1	77-B	1706	1700	1690	0	0
2	1-A	6	8	8	0	0
2	1-B	6	8	8	0	0
2	2-A	6	8	8	0	0
2	2-B	6	8	8	0	0
2	3-A	6	8	8	0	0
2	3-B	6	8	8	0	0
2	4-A	6	8	8	0	0
2	4-B	6	8	8	0	0
2	5-A	6	8	8	0	0
2	5-B	6	8	8	0	0
2	6-A	6	8	8	0	0
2	6-B	6	8	8	0	0
2	7-A	6	8	8	0	0
2	7-B	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8-A	6	8	8	0	0
2	8-B	6	8	8	0	0
2	9-A	6	8	8	0	0
2	9-B	6	8	8	0	0
2	10-A	6	8	8	0	0
2	10-B	6	8	8	0	0
2	11-A	6	8	8	0	0
2	11-B	6	8	8	0	0
2	12-A	6	8	8	0	0
2	12-B	6	8	8	0	0
2	13-A	6	8	8	0	0
2	13-B	6	8	8	0	0
2	14-A	6	8	8	0	0
2	14-B	6	8	8	0	0
2	15-A	6	8	8	0	0
2	15-B	6	8	8	0	0
2	16-A	6	8	8	0	0
2	16-B	6	8	8	0	0
2	17-A	6	8	8	0	0
2	17-B	6	8	8	0	0
2	18-A	6	8	8	0	0
2	18-B	6	8	8	0	0
2	19-A	6	8	8	0	0
2	19-B	6	8	8	0	0
2	20-A	6	8	8	0	0
2	20-B	6	8	8	0	0
2	21-A	6	8	8	0	0
2	21-B	6	8	8	0	0
2	22-A	6	8	8	0	0
2	22-B	6	8	8	0	0
2	23-A	6	8	8	0	0
2	23-B	6	8	8	0	0
2	24-A	6	8	8	0	0
2	24-B	6	8	8	0	0
2	25-A	6	8	8	0	0
2	25-B	6	8	8	0	0
2	26-A	6	8	8	0	0
2	26-B	6	8	8	0	0
2	27-A	6	8	8	0	0
2	27-B	6	8	8	0	0
2	28-A	6	8	8	0	0
2	28-B	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	29-A	6	8	8	0	0
2	29-B	6	8	8	0	0
2	30-A	6	8	8	0	0
2	30-B	6	8	8	0	0
2	31-A	6	8	8	0	0
2	31-B	6	8	8	0	0
2	32-A	6	8	8	0	0
2	32-B	6	8	8	0	0
2	33-A	6	8	8	0	0
2	33-B	6	8	8	0	0
2	34-A	6	8	8	0	0
2	34-B	6	8	8	0	0
2	35-A	6	8	8	0	0
2	35-B	6	8	8	0	0
2	36-A	6	8	8	0	0
2	36-B	6	8	8	0	0
2	37-A	6	8	8	0	0
2	37-B	6	8	8	0	0
2	38-A	6	8	8	0	0
2	38-B	6	8	8	0	0
2	39-A	6	8	8	0	0
2	39-B	6	8	8	0	0
2	40-A	6	8	8	0	0
2	40-B	6	8	8	0	0
2	41-A	6	8	8	0	0
2	41-B	6	8	8	0	0
2	42-A	6	8	8	0	0
2	42-B	6	8	8	0	0
2	43-A	6	8	8	0	0
2	43-B	6	8	8	0	0
2	44-A	6	8	8	0	0
2	44-B	6	8	8	0	0
2	45-A	6	8	8	0	0
2	45-B	6	8	8	0	0
2	46-A	6	8	8	0	0
2	46-B	6	8	8	0	0
2	47-A	6	8	8	0	0
2	47-B	6	8	8	0	0
2	48-A	6	8	8	0	0
2	48-B	6	8	8	0	0
2	49-A	6	8	8	0	0
2	49-B	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	50-A	6	8	8	0	0
2	50-B	6	8	8	0	0
2	51-A	6	8	8	0	0
2	51-B	6	8	8	0	0
2	52-A	6	8	8	0	0
2	52-B	6	8	8	0	0
2	53-A	6	8	8	0	0
2	53-B	6	8	8	0	0
2	54-A	6	8	8	0	0
2	54-B	6	8	8	0	0
2	55-A	6	8	8	0	0
2	55-B	6	8	8	0	0
2	56-A	6	8	8	0	0
2	56-B	6	8	8	0	0
2	57-A	6	8	8	0	0
2	57-B	6	8	8	0	0
2	58-A	6	8	8	0	0
2	58-B	6	8	8	0	0
2	59-A	6	8	8	0	0
2	59-B	6	8	8	0	0
2	60-A	6	8	8	0	0
2	60-B	6	8	8	0	0
2	61-A	6	8	8	0	0
2	61-B	6	8	8	0	0
2	62-A	6	8	8	0	0
2	62-B	6	8	8	0	0
2	63-A	6	8	8	0	0
2	63-B	6	8	8	0	0
2	64-A	6	8	8	0	0
2	64-B	6	8	8	0	0
2	65-A	6	8	8	0	0
2	65-B	6	8	8	0	0
2	66-A	6	8	8	0	0
2	66-B	6	8	8	0	0
2	67-A	6	8	8	0	0
2	67-B	6	8	8	0	0
2	68-A	6	8	8	0	0
2	68-B	6	8	8	0	0
2	69-A	6	8	8	0	0
2	69-B	6	8	8	0	0
2	70-A	6	8	8	0	0
2	70-B	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	71-A	6	8	8	0	0
2	71-B	6	8	8	0	0
2	72-A	6	8	8	0	0
2	72-B	6	8	8	0	0
2	73-A	6	8	8	0	0
2	73-B	6	8	8	0	0
2	74-A	6	8	8	0	0
2	74-B	6	8	8	0	0
2	75-A	6	8	8	0	0
2	75-B	6	8	8	0	0
2	76-A	6	8	8	0	0
2	76-B	6	8	8	0	0
2	77-A	6	8	8	0	0
2	77-B	6	8	8	0	0
3	1-A	148	0	0	0	0
3	1-B	113	0	0	0	0
3	2-A	139	0	0	0	0
3	2-B	122	0	0	0	0
3	3-A	142	0	0	0	0
3	3-B	96	0	0	0	0
3	4-A	129	0	0	0	0
3	4-B	108	0	0	0	0
3	5-A	129	0	0	0	0
3	5-B	109	0	0	0	0
3	6-A	136	0	0	0	0
3	6-B	111	0	0	0	0
3	7-A	134	0	0	0	0
3	7-B	111	0	0	0	0
3	8-A	136	0	0	0	0
3	8-B	104	0	0	0	0
3	9-A	138	0	0	0	0
3	9-B	119	0	0	0	0
3	10-A	135	0	0	0	0
3	10-B	117	0	0	0	0
3	11-A	123	0	0	0	0
3	11-B	118	0	0	0	0
3	12-A	145	0	0	0	0
3	12-B	115	0	0	0	0
3	13-A	165	0	0	0	0
3	13-B	109	0	0	0	0
3	14-A	157	0	0	0	0
3	14-B	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	15-A	142	0	0	0	0
3	15-B	113	0	0	0	0
3	16-A	135	0	0	0	0
3	16-B	117	0	0	0	0
3	17-A	142	0	0	0	0
3	17-B	122	0	0	0	0
3	18-A	147	0	0	0	0
3	18-B	111	0	0	0	0
3	19-A	127	0	0	0	0
3	19-B	117	0	0	0	0
3	20-A	131	0	0	0	0
3	20-B	123	0	0	0	0
3	21-A	144	0	0	0	0
3	21-B	103	0	0	0	0
3	22-A	143	0	0	0	0
3	22-B	122	0	0	0	0
3	23-A	142	0	0	0	0
3	23-B	113	0	0	0	0
3	24-A	127	0	0	0	0
3	24-B	116	0	0	0	0
3	25-A	137	0	0	0	0
3	25-B	120	0	0	0	0
3	26-A	145	0	0	0	0
3	26-B	114	0	0	0	0
3	27-A	139	0	0	0	0
3	27-B	114	0	0	0	0
3	28-A	137	0	0	0	0
3	28-B	123	0	0	0	0
3	29-A	135	0	0	0	0
3	29-B	132	0	0	0	0
3	30-A	149	0	0	0	0
3	30-B	115	0	0	0	0
3	31-A	146	0	0	0	0
3	31-B	117	0	0	0	0
3	32-A	135	0	0	0	0
3	32-B	127	0	0	0	0
3	33-A	133	0	0	0	0
3	33-B	119	0	0	0	0
3	34-A	139	0	0	0	0
3	34-B	109	0	0	0	0
3	35-A	125	0	0	0	0
3	35-B	102	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	36-A	130	0	0	0	0
3	36-B	120	0	0	0	0
3	37-A	138	0	0	0	0
3	37-B	110	0	0	0	0
3	38-A	134	0	0	0	0
3	38-B	118	0	0	0	0
3	39-A	130	0	0	0	0
3	39-B	112	0	0	0	0
3	40-A	128	0	0	0	0
3	40-B	118	0	0	0	0
3	41-A	139	0	0	0	0
3	41-B	106	0	0	0	0
3	42-A	128	0	0	0	0
3	42-B	124	0	0	0	0
3	43-A	155	0	0	0	0
3	43-B	125	0	0	0	0
3	44-A	143	0	0	0	0
3	44-B	118	0	0	0	0
3	45-A	140	0	0	0	0
3	45-B	108	0	0	0	0
3	46-A	131	0	0	0	0
3	46-B	105	0	0	0	0
3	47-A	127	0	0	0	0
3	47-B	118	0	0	0	0
3	48-A	141	0	0	0	0
3	48-B	129	0	0	0	0
3	49-A	121	0	0	0	0
3	49-B	109	0	0	0	0
3	50-A	139	0	0	0	0
3	50-B	111	0	0	0	0
3	51-A	137	0	0	0	0
3	51-B	131	0	0	0	0
3	52-A	145	0	0	0	0
3	52-B	119	0	0	0	0
3	53-A	141	0	0	0	0
3	53-B	113	0	0	0	0
3	54-A	137	0	0	0	0
3	54-B	109	0	0	0	0
3	55-A	136	0	0	0	0
3	55-B	120	0	0	0	0
3	56-A	153	0	0	0	0
3	56-B	127	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	57-A	124	0	0	0	0
3	57-B	122	0	0	0	0
3	58-A	133	0	0	0	0
3	58-B	122	0	0	0	0
3	59-A	143	0	0	0	0
3	59-B	117	0	0	0	0
3	60-A	132	0	0	0	0
3	60-B	116	0	0	0	0
3	61-A	138	0	0	0	0
3	61-B	119	0	0	0	0
3	62-A	137	0	0	0	0
3	62-B	121	0	0	0	0
3	63-A	151	0	0	0	0
3	63-B	123	0	0	0	0
3	64-A	142	0	0	0	0
3	64-B	121	0	0	0	0
3	65-A	149	0	0	0	0
3	65-B	128	0	0	0	0
3	66-A	135	0	0	0	0
3	66-B	112	0	0	0	0
3	67-A	143	0	0	0	0
3	67-B	125	0	0	0	0
3	68-A	137	0	0	0	0
3	68-B	126	0	0	0	0
3	69-A	131	0	0	0	0
3	69-B	112	0	0	0	0
3	70-A	136	0	0	0	0
3	70-B	123	0	0	0	0
3	71-A	138	0	0	0	0
3	71-B	122	0	0	0	0
3	72-A	135	0	0	0	0
3	72-B	121	0	0	0	0
3	73-A	134	0	0	0	0
3	73-B	132	0	0	0	0
3	74-A	153	0	0	0	0
3	74-B	113	0	0	0	0
3	75-A	147	0	0	0	0
3	75-B	111	0	0	0	0
3	76-A	145	0	0	0	0
3	76-B	105	0	0	0	0
3	77-A	131	0	0	0	0
3	77-B	119	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	283267	263032	261492	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	1-A	226/228 (99%)	191 (84%)	19 (8%)	16 (7%)	1	0
1	1-B	226/228 (99%)	203 (90%)	15 (7%)	8 (4%)	3	0
1	2-A	226/228 (99%)	184 (81%)	15 (7%)	27 (12%)	0	0
1	2-B	226/228 (99%)	197 (87%)	18 (8%)	11 (5%)	2	0
1	3-A	226/228 (99%)	184 (81%)	27 (12%)	15 (7%)	1	0
1	3-B	226/228 (99%)	204 (90%)	13 (6%)	9 (4%)	3	0
1	4-A	226/228 (99%)	181 (80%)	23 (10%)	22 (10%)	0	0
1	4-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	5-A	226/228 (99%)	187 (83%)	24 (11%)	15 (7%)	1	0
1	5-B	226/228 (99%)	198 (88%)	24 (11%)	4 (2%)	8	2
1	6-A	226/228 (99%)	185 (82%)	26 (12%)	15 (7%)	1	0
1	6-B	226/228 (99%)	201 (89%)	18 (8%)	7 (3%)	4	0
1	7-A	226/228 (99%)	180 (80%)	21 (9%)	25 (11%)	0	0
1	7-B	226/228 (99%)	204 (90%)	18 (8%)	4 (2%)	8	2
1	8-A	226/228 (99%)	185 (82%)	18 (8%)	23 (10%)	0	0
1	8-B	226/228 (99%)	202 (89%)	16 (7%)	8 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	226/228 (99%)	186 (82%)	20 (9%)	20 (9%)	1	0
1	9-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
1	10-A	226/228 (99%)	176 (78%)	28 (12%)	22 (10%)	0	0
1	10-B	226/228 (99%)	203 (90%)	19 (8%)	4 (2%)	8	2
1	11-A	226/228 (99%)	185 (82%)	25 (11%)	16 (7%)	1	0
1	11-B	226/228 (99%)	205 (91%)	15 (7%)	6 (3%)	5	1
1	12-A	226/228 (99%)	182 (80%)	21 (9%)	23 (10%)	0	0
1	12-B	226/228 (99%)	197 (87%)	15 (7%)	14 (6%)	1	0
1	13-A	226/228 (99%)	191 (84%)	17 (8%)	18 (8%)	1	0
1	13-B	226/228 (99%)	199 (88%)	20 (9%)	7 (3%)	4	0
1	14-A	226/228 (99%)	193 (85%)	11 (5%)	22 (10%)	0	0
1	14-B	226/228 (99%)	206 (91%)	14 (6%)	6 (3%)	5	1
1	15-A	226/228 (99%)	181 (80%)	21 (9%)	24 (11%)	0	0
1	15-B	226/228 (99%)	200 (88%)	20 (9%)	6 (3%)	5	1
1	16-A	226/228 (99%)	186 (82%)	20 (9%)	20 (9%)	1	0
1	16-B	226/228 (99%)	198 (88%)	18 (8%)	10 (4%)	2	0
1	17-A	226/228 (99%)	189 (84%)	14 (6%)	23 (10%)	0	0
1	17-B	226/228 (99%)	187 (83%)	26 (12%)	13 (6%)	1	0
1	18-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	18-B	226/228 (99%)	200 (88%)	17 (8%)	9 (4%)	3	0
1	19-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	19-B	226/228 (99%)	198 (88%)	17 (8%)	11 (5%)	2	0
1	20-A	226/228 (99%)	190 (84%)	25 (11%)	11 (5%)	2	0
1	20-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
1	21-A	226/228 (99%)	189 (84%)	25 (11%)	12 (5%)	2	0
1	21-B	226/228 (99%)	200 (88%)	16 (7%)	10 (4%)	2	0
1	22-A	226/228 (99%)	189 (84%)	20 (9%)	17 (8%)	1	0
1	22-B	226/228 (99%)	198 (88%)	16 (7%)	12 (5%)	2	0
1	23-A	226/228 (99%)	189 (84%)	21 (9%)	16 (7%)	1	0
1	23-B	226/228 (99%)	200 (88%)	16 (7%)	10 (4%)	2	0
1	24-A	226/228 (99%)	183 (81%)	26 (12%)	17 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	24-B	226/228 (99%)	202 (89%)	18 (8%)	6 (3%)	5	1
1	25-A	226/228 (99%)	188 (83%)	25 (11%)	13 (6%)	1	0
1	25-B	226/228 (99%)	202 (89%)	18 (8%)	6 (3%)	5	1
1	26-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	26-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
1	27-A	226/228 (99%)	184 (81%)	20 (9%)	22 (10%)	0	0
1	27-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	28-A	226/228 (99%)	183 (81%)	24 (11%)	19 (8%)	1	0
1	28-B	226/228 (99%)	198 (88%)	17 (8%)	11 (5%)	2	0
1	29-A	226/228 (99%)	187 (83%)	27 (12%)	12 (5%)	2	0
1	29-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	4	0
1	30-A	226/228 (99%)	195 (86%)	21 (9%)	10 (4%)	2	0
1	30-B	226/228 (99%)	201 (89%)	17 (8%)	8 (4%)	3	0
1	31-A	226/228 (99%)	185 (82%)	22 (10%)	19 (8%)	1	0
1	31-B	226/228 (99%)	207 (92%)	9 (4%)	10 (4%)	2	0
1	32-A	226/228 (99%)	188 (83%)	21 (9%)	17 (8%)	1	0
1	32-B	226/228 (99%)	202 (89%)	15 (7%)	9 (4%)	3	0
1	33-A	226/228 (99%)	193 (85%)	20 (9%)	13 (6%)	1	0
1	33-B	226/228 (99%)	203 (90%)	13 (6%)	10 (4%)	2	0
1	34-A	226/228 (99%)	189 (84%)	23 (10%)	14 (6%)	1	0
1	34-B	226/228 (99%)	198 (88%)	18 (8%)	10 (4%)	2	0
1	35-A	226/228 (99%)	188 (83%)	25 (11%)	13 (6%)	1	0
1	35-B	226/228 (99%)	201 (89%)	15 (7%)	10 (4%)	2	0
1	36-A	226/228 (99%)	186 (82%)	22 (10%)	18 (8%)	1	0
1	36-B	226/228 (99%)	206 (91%)	11 (5%)	9 (4%)	3	0
1	37-A	226/228 (99%)	181 (80%)	23 (10%)	22 (10%)	0	0
1	37-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	3	0
1	38-A	226/228 (99%)	183 (81%)	22 (10%)	21 (9%)	0	0
1	38-B	226/228 (99%)	200 (88%)	17 (8%)	9 (4%)	3	0
1	39-A	226/228 (99%)	190 (84%)	18 (8%)	18 (8%)	1	0
1	39-B	226/228 (99%)	196 (87%)	22 (10%)	8 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	40-A	226/228 (99%)	186 (82%)	28 (12%)	12 (5%)	2	0
1	40-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	41-A	226/228 (99%)	185 (82%)	16 (7%)	25 (11%)	0	0
1	41-B	226/228 (99%)	201 (89%)	19 (8%)	6 (3%)	5	1
1	42-A	226/228 (99%)	186 (82%)	19 (8%)	21 (9%)	0	0
1	42-B	226/228 (99%)	199 (88%)	23 (10%)	4 (2%)	8	2
1	43-A	226/228 (99%)	189 (84%)	20 (9%)	17 (8%)	1	0
1	43-B	226/228 (99%)	197 (87%)	20 (9%)	9 (4%)	3	0
1	44-A	226/228 (99%)	184 (81%)	24 (11%)	18 (8%)	1	0
1	44-B	226/228 (99%)	204 (90%)	13 (6%)	9 (4%)	3	0
1	45-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	45-B	226/228 (99%)	203 (90%)	14 (6%)	9 (4%)	3	0
1	46-A	226/228 (99%)	182 (80%)	27 (12%)	17 (8%)	1	0
1	46-B	226/228 (99%)	198 (88%)	15 (7%)	13 (6%)	1	0
1	47-A	226/228 (99%)	182 (80%)	22 (10%)	22 (10%)	0	0
1	47-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	48-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	48-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	4	0
1	49-A	226/228 (99%)	181 (80%)	25 (11%)	20 (9%)	1	0
1	49-B	226/228 (99%)	201 (89%)	16 (7%)	9 (4%)	3	0
1	50-A	226/228 (99%)	185 (82%)	22 (10%)	19 (8%)	1	0
1	50-B	226/228 (99%)	196 (87%)	22 (10%)	8 (4%)	3	0
1	51-A	226/228 (99%)	190 (84%)	17 (8%)	19 (8%)	1	0
1	51-B	226/228 (99%)	195 (86%)	20 (9%)	11 (5%)	2	0
1	52-A	226/228 (99%)	182 (80%)	26 (12%)	18 (8%)	1	0
1	52-B	226/228 (99%)	206 (91%)	13 (6%)	7 (3%)	4	0
1	53-A	226/228 (99%)	185 (82%)	28 (12%)	13 (6%)	1	0
1	53-B	226/228 (99%)	204 (90%)	14 (6%)	8 (4%)	3	0
1	54-A	226/228 (99%)	188 (83%)	21 (9%)	17 (8%)	1	0
1	54-B	226/228 (99%)	200 (88%)	19 (8%)	7 (3%)	4	0
1	55-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	55-B	226/228 (99%)	197 (87%)	18 (8%)	11 (5%)	2	0
1	56-A	226/228 (99%)	191 (84%)	23 (10%)	12 (5%)	2	0
1	56-B	226/228 (99%)	199 (88%)	19 (8%)	8 (4%)	3	0
1	57-A	226/228 (99%)	184 (81%)	19 (8%)	23 (10%)	0	0
1	57-B	226/228 (99%)	195 (86%)	23 (10%)	8 (4%)	3	0
1	58-A	226/228 (99%)	189 (84%)	16 (7%)	21 (9%)	0	0
1	58-B	226/228 (99%)	201 (89%)	11 (5%)	14 (6%)	1	0
1	59-A	226/228 (99%)	193 (85%)	14 (6%)	19 (8%)	1	0
1	59-B	226/228 (99%)	199 (88%)	19 (8%)	8 (4%)	3	0
1	60-A	226/228 (99%)	186 (82%)	23 (10%)	17 (8%)	1	0
1	60-B	226/228 (99%)	197 (87%)	16 (7%)	13 (6%)	1	0
1	61-A	226/228 (99%)	177 (78%)	28 (12%)	21 (9%)	0	0
1	61-B	226/228 (99%)	203 (90%)	10 (4%)	13 (6%)	1	0
1	62-A	226/228 (99%)	187 (83%)	22 (10%)	17 (8%)	1	0
1	62-B	226/228 (99%)	202 (89%)	17 (8%)	7 (3%)	4	0
1	63-A	226/228 (99%)	186 (82%)	24 (11%)	16 (7%)	1	0
1	63-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	3	0
1	64-A	226/228 (99%)	183 (81%)	20 (9%)	23 (10%)	0	0
1	64-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	65-A	226/228 (99%)	187 (83%)	22 (10%)	17 (8%)	1	0
1	65-B	226/228 (99%)	198 (88%)	21 (9%)	7 (3%)	4	0
1	66-A	226/228 (99%)	192 (85%)	21 (9%)	13 (6%)	1	0
1	66-B	226/228 (99%)	202 (89%)	16 (7%)	8 (4%)	3	0
1	67-A	226/228 (99%)	185 (82%)	24 (11%)	17 (8%)	1	0
1	67-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	68-A	226/228 (99%)	179 (79%)	23 (10%)	24 (11%)	0	0
1	68-B	226/228 (99%)	202 (89%)	14 (6%)	10 (4%)	2	0
1	69-A	226/228 (99%)	184 (81%)	28 (12%)	14 (6%)	1	0
1	69-B	226/228 (99%)	195 (86%)	18 (8%)	13 (6%)	1	0
1	70-A	226/228 (99%)	186 (82%)	24 (11%)	16 (7%)	1	0
1	70-B	226/228 (99%)	202 (89%)	14 (6%)	10 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	71-A	226/228 (99%)	184 (81%)	27 (12%)	15 (7%)	1 0
1	71-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	4 0
1	72-A	226/228 (99%)	183 (81%)	30 (13%)	13 (6%)	1 0
1	72-B	226/228 (99%)	207 (92%)	14 (6%)	5 (2%)	6 1
1	73-A	226/228 (99%)	185 (82%)	21 (9%)	20 (9%)	1 0
1	73-B	226/228 (99%)	203 (90%)	18 (8%)	5 (2%)	6 1
1	74-A	226/228 (99%)	187 (83%)	20 (9%)	19 (8%)	1 0
1	74-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	3 0
1	75-A	226/228 (99%)	185 (82%)	23 (10%)	18 (8%)	1 0
1	75-B	226/228 (99%)	200 (88%)	23 (10%)	3 (1%)	12 3
1	76-A	226/228 (99%)	190 (84%)	19 (8%)	17 (8%)	1 0
1	76-B	226/228 (99%)	207 (92%)	13 (6%)	6 (3%)	5 1
1	77-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1 0
1	77-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2 0
All	All	34804/35112 (99%)	29722 (85%)	3047 (9%)	2035 (6%)	1 0

5 of 2035 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	45	ASP
1	1-A	131	VAL
1	1-A	134	ALA
1	1-A	180	LYS
1	1-A	206	ASN

4.3.2 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	1-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	1-B	181/181 (100%)	166 (92%)	15 (8%)	11 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	2-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	2-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	3-A	181/181 (100%)	153 (84%)	28 (16%)	2 0
1	3-B	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	4-A	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	4-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	5-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	5-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	6-A	181/181 (100%)	152 (84%)	29 (16%)	2 0
1	6-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	7-A	181/181 (100%)	154 (85%)	27 (15%)	3 0
1	7-B	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	8-A	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	8-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	9-A	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	9-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	10-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	10-B	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	11-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	11-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	12-A	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	12-B	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	13-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	13-B	181/181 (100%)	167 (92%)	14 (8%)	13 4
1	14-A	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	14-B	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	15-A	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	15-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	16-A	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	16-B	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	17-A	181/181 (100%)	150 (83%)	31 (17%)	2 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	17-B	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	18-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	18-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	19-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	19-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	20-A	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	20-B	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	21-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	21-B	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	22-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	22-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	23-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	23-B	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	24-A	181/181 (100%)	149 (82%)	32 (18%)	2	0
1	24-B	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	25-A	181/181 (100%)	150 (83%)	31 (17%)	2	0
1	25-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	26-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	26-B	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	27-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	27-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	28-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	28-B	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	29-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	29-B	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	30-A	181/181 (100%)	152 (84%)	29 (16%)	2	0
1	30-B	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	31-A	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	31-B	181/181 (100%)	167 (92%)	14 (8%)	13	4
1	32-A	181/181 (100%)	151 (83%)	30 (17%)	2	0
1	32-B	181/181 (100%)	160 (88%)	21 (12%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	33-A	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	33-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	34-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	34-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	35-A	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	35-B	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	36-A	181/181 (100%)	154 (85%)	27 (15%)	3 0
1	36-B	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	37-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	37-B	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	38-A	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	38-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	39-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	39-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	40-A	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	40-B	181/181 (100%)	167 (92%)	14 (8%)	13 4
1	41-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	41-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	42-A	181/181 (100%)	153 (84%)	28 (16%)	2 0
1	42-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	43-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	43-B	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	44-A	181/181 (100%)	147 (81%)	34 (19%)	1 0
1	44-B	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	45-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	45-B	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	46-A	181/181 (100%)	146 (81%)	35 (19%)	1 0
1	46-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	47-A	181/181 (100%)	153 (84%)	28 (16%)	2 0
1	47-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	48-A	181/181 (100%)	154 (85%)	27 (15%)	3 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	48-B	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	49-A	181/181 (100%)	153 (84%)	28 (16%)	2 0
1	49-B	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	50-A	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	50-B	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	51-A	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	51-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	52-A	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	52-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	53-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	53-B	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	54-A	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	54-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	55-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	55-B	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	56-A	181/181 (100%)	151 (83%)	30 (17%)	2 0
1	56-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	57-A	181/181 (100%)	154 (85%)	27 (15%)	3 0
1	57-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	58-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	58-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	59-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	59-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	60-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	60-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	61-A	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	61-B	181/181 (100%)	153 (84%)	28 (16%)	2 0
1	62-A	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	62-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	63-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	63-B	181/181 (100%)	168 (93%)	13 (7%)	14 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	64-A	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	64-B	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	65-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	65-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	66-A	181/181 (100%)	150 (83%)	31 (17%)	2 0
1	66-B	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	67-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	67-B	181/181 (100%)	169 (93%)	12 (7%)	16 5
1	68-A	181/181 (100%)	152 (84%)	29 (16%)	2 0
1	68-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	69-A	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	69-B	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	70-A	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	70-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	71-A	181/181 (100%)	154 (85%)	27 (15%)	3 0
1	71-B	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	72-A	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	72-B	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	73-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	73-B	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	74-A	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	74-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	75-A	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	75-B	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	76-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	76-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	77-A	181/181 (100%)	162 (90%)	19 (10%)	7 1
1	77-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
All	All	27874/27874 (100%)	24533 (88%)	3341 (12%)	5 1

5 of 3341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	43-A	199	SER
1	53-A	115	ARG
1	74-A	183	SER
1	44-B	29	VAL
1	43-A	180	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides 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	58-B	1000	-	5,5,5	0.22	0	5,5,5	0.53	0
2	GOL	18-B	1000	-	5,5,5	0.25	0	5,5,5	0.38	0
2	GOL	1-B	1000	-	5,5,5	0.24	0	5,5,5	0.25	0
2	GOL	18-A	1000	-	5,5,5	0.54	0	5,5,5	1.56	0
2	GOL	43-A	1000	-	5,5,5	0.34	0	5,5,5	1.25	0
2	GOL	42-A	1000	-	5,5,5	0.69	0	5,5,5	1.19	0
2	GOL	13-A	1000	-	5,5,5	0.81	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	44-B	1000	-	5,5,5	0.28	0	5,5,5	0.45	0
2	GOL	22-A	1000	-	5,5,5	0.39	0	5,5,5	1.60	2 (40%)
2	GOL	63-B	1000	-	5,5,5	0.21	0	5,5,5	0.41	0
2	GOL	2-B	1000	-	5,5,5	0.29	0	5,5,5	0.34	0
2	GOL	23-B	1000	-	5,5,5	0.26	0	5,5,5	0.33	0
2	GOL	33-B	1000	-	5,5,5	0.22	0	5,5,5	0.30	0
2	GOL	4-A	1000	-	5,5,5	0.45	0	5,5,5	1.51	0
2	GOL	59-A	1000	-	5,5,5	0.36	0	5,5,5	1.37	0
2	GOL	16-B	1000	-	5,5,5	0.21	0	5,5,5	0.42	0
2	GOL	9-A	1000	-	5,5,5	0.38	0	5,5,5	0.51	0
2	GOL	47-A	1000	-	5,5,5	0.67	0	5,5,5	0.66	0
2	GOL	40-B	1000	-	5,5,5	0.22	0	5,5,5	0.37	0
2	GOL	6-B	1000	-	5,5,5	0.20	0	5,5,5	0.26	0
2	GOL	42-B	1000	-	5,5,5	0.29	0	5,5,5	0.30	0
2	GOL	5-A	1000	-	5,5,5	0.41	0	5,5,5	1.45	0
2	GOL	53-A	1000	-	5,5,5	0.41	0	5,5,5	1.49	0
2	GOL	7-B	1000	-	5,5,5	0.23	0	5,5,5	0.27	0
2	GOL	11-B	1000	-	5,5,5	0.21	0	5,5,5	0.34	0
2	GOL	25-B	1000	-	5,5,5	0.24	0	5,5,5	0.37	0
2	GOL	38-B	1000	-	5,5,5	0.26	0	5,5,5	0.54	0
2	GOL	19-A	1000	-	5,5,5	0.45	0	5,5,5	1.56	1 (20%)
2	GOL	4-B	1000	-	5,5,5	0.22	0	5,5,5	0.35	0
2	GOL	39-B	1000	-	5,5,5	0.27	0	5,5,5	0.32	0
2	GOL	27-B	1000	-	5,5,5	0.25	0	5,5,5	0.35	0
2	GOL	54-A	1000	-	5,5,5	0.45	0	5,5,5	1.61	1 (20%)
2	GOL	16-A	1000	-	5,5,5	0.31	0	5,5,5	1.53	1 (20%)
2	GOL	8-B	1000	-	5,5,5	0.23	0	5,5,5	0.39	0
2	GOL	24-B	1000	-	5,5,5	0.23	0	5,5,5	0.33	0
2	GOL	1-A	1000	-	5,5,5	0.40	0	5,5,5	0.40	0
2	GOL	14-B	1000	-	5,5,5	0.25	0	5,5,5	0.47	0
2	GOL	30-B	1000	-	5,5,5	0.35	0	5,5,5	0.35	0
2	GOL	10-B	1000	-	5,5,5	0.23	0	5,5,5	0.38	0
2	GOL	3-B	1000	-	5,5,5	0.23	0	5,5,5	0.29	0
2	GOL	57-A	1000	-	5,5,5	0.38	0	5,5,5	1.17	0
2	GOL	35-B	1000	-	5,5,5	0.21	0	5,5,5	0.33	0
2	GOL	44-A	1000	-	5,5,5	0.45	0	5,5,5	0.49	0
2	GOL	60-B	1000	-	5,5,5	0.24	0	5,5,5	0.45	0
2	GOL	37-A	1000	-	5,5,5	0.59	0	5,5,5	1.53	0
2	GOL	19-B	1000	-	5,5,5	0.26	0	5,5,5	0.38	0
2	GOL	15-B	1000	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	28-A	1000	-	5,5,5	0.53	0	5,5,5	1.66	1 (20%)
2	GOL	8-A	1000	-	5,5,5	0.34	0	5,5,5	1.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	9-B	1000	-	5,5,5	0.23	0	5,5,5	0.34	0
2	GOL	52-A	1000	-	5,5,5	0.61	0	5,5,5	1.55	0
2	GOL	50-B	1000	-	5,5,5	0.25	0	5,5,5	0.48	0
2	GOL	2-A	1000	-	5,5,5	0.34	0	5,5,5	1.44	1 (20%)
2	GOL	3-A	1000	-	5,5,5	0.49	0	5,5,5	1.31	0
2	GOL	22-B	1000	-	5,5,5	0.23	0	5,5,5	0.39	0
2	GOL	55-B	1000	-	5,5,5	0.25	0	5,5,5	0.43	0
2	GOL	59-B	1000	-	5,5,5	0.20	0	5,5,5	0.49	0
2	GOL	37-B	1000	-	5,5,5	0.25	0	5,5,5	0.33	0
2	GOL	49-B	1000	-	5,5,5	0.22	0	5,5,5	0.56	0
2	GOL	17-B	1000	-	5,5,5	0.22	0	5,5,5	0.42	0
2	GOL	28-B	1000	-	5,5,5	0.24	0	5,5,5	0.41	0
2	GOL	23-A	1000	-	5,5,5	0.56	0	5,5,5	0.97	0
2	GOL	20-A	1000	-	5,5,5	0.36	0	5,5,5	1.48	1 (20%)
2	GOL	34-A	1000	-	5,5,5	0.61	0	5,5,5	1.40	0
2	GOL	52-B	1000	-	5,5,5	0.25	0	5,5,5	0.53	0
2	GOL	13-B	1000	-	5,5,5	0.19	0	5,5,5	0.37	0
2	GOL	32-B	1000	-	5,5,5	0.27	0	5,5,5	0.34	0
2	GOL	14-A	1000	-	5,5,5	0.29	0	5,5,5	1.57	1 (20%)
2	GOL	39-A	1000	-	5,5,5	0.80	0	5,5,5	0.50	0
2	GOL	58-A	1000	-	5,5,5	0.48	0	5,5,5	1.51	1 (20%)
2	GOL	12-A	1000	-	5,5,5	0.44	0	5,5,5	1.53	1 (20%)
2	GOL	6-A	1000	-	5,5,5	0.40	0	5,5,5	1.35	0
2	GOL	38-A	1000	-	5,5,5	0.39	0	5,5,5	1.02	0
2	GOL	7-A	1000	-	5,5,5	0.40	0	5,5,5	1.51	0
2	GOL	24-A	1000	-	5,5,5	0.48	0	5,5,5	0.51	0
2	GOL	48-A	1000	-	5,5,5	0.43	0	5,5,5	1.62	1 (20%)
2	GOL	29-A	1000	-	5,5,5	0.47	0	5,5,5	1.80	2 (40%)
2	GOL	54-B	1000	-	5,5,5	0.23	0	5,5,5	0.50	0
2	GOL	11-A	1000	-	5,5,5	0.38	0	5,5,5	0.62	0
2	GOL	47-B	1000	-	5,5,5	0.18	0	5,5,5	0.35	0
2	GOL	10-A	1000	-	5,5,5	0.33	0	5,5,5	1.28	1 (20%)
2	GOL	12-B	1000	-	5,5,5	0.19	0	5,5,5	0.33	0
2	GOL	27-A	1000	-	5,5,5	0.50	0	5,5,5	1.53	0
2	GOL	57-B	1000	-	5,5,5	0.26	0	5,5,5	0.45	0
2	GOL	29-B	1000	-	5,5,5	0.23	0	5,5,5	0.51	0
2	GOL	34-B	1000	-	5,5,5	0.28	0	5,5,5	0.28	0
2	GOL	15-A	1000	-	5,5,5	0.49	0	5,5,5	0.69	0
2	GOL	17-A	1000	-	5,5,5	0.63	0	5,5,5	1.71	2 (40%)
2	GOL	5-B	1000	-	5,5,5	0.23	0	5,5,5	0.27	0
2	GOL	48-B	1000	-	5,5,5	0.22	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	49-A	1000	-	5,5,5	0.47	0	5,5,5	1.79	2 (40%)
2	GOL	33-A	1000	-	5,5,5	0.60	0	5,5,5	0.90	0
2	GOL	53-B	1000	-	5,5,5	0.25	0	5,5,5	0.55	0
2	GOL	32-A	1000	-	5,5,5	0.34	0	5,5,5	0.27	0
2	GOL	45-B	1000	-	5,5,5	0.24	0	5,5,5	0.37	0
2	GOL	43-B	1000	-	5,5,5	0.24	0	5,5,5	0.29	0
2	GOL	20-B	1000	-	5,5,5	0.27	0	5,5,5	0.35	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	58-B	1000	-	-	0/4/4/4	-
2	GOL	18-B	1000	-	-	0/4/4/4	-
2	GOL	1-B	1000	-	-	0/4/4/4	-
2	GOL	18-A	1000	-	-	4/4/4/4	-
2	GOL	43-A	1000	-	-	2/4/4/4	-
2	GOL	42-A	1000	-	-	0/4/4/4	-
2	GOL	13-A	1000	-	-	0/4/4/4	-
2	GOL	44-B	1000	-	-	2/4/4/4	-
2	GOL	22-A	1000	-	-	3/4/4/4	-
2	GOL	63-B	1000	-	-	2/4/4/4	-
2	GOL	2-B	1000	-	-	2/4/4/4	-
2	GOL	23-B	1000	-	-	0/4/4/4	-
2	GOL	33-B	1000	-	-	0/4/4/4	-
2	GOL	4-A	1000	-	-	4/4/4/4	-
2	GOL	59-A	1000	-	-	3/4/4/4	-
2	GOL	16-B	1000	-	-	2/4/4/4	-
2	GOL	9-A	1000	-	-	0/4/4/4	-
2	GOL	47-A	1000	-	-	0/4/4/4	-
2	GOL	40-B	1000	-	-	0/4/4/4	-
2	GOL	6-B	1000	-	-	1/4/4/4	-
2	GOL	42-B	1000	-	-	1/4/4/4	-
2	GOL	5-A	1000	-	-	4/4/4/4	-
2	GOL	53-A	1000	-	-	4/4/4/4	-
2	GOL	7-B	1000	-	-	0/4/4/4	-
2	GOL	11-B	1000	-	-	0/4/4/4	-
2	GOL	25-B	1000	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	38-B	1000	-	-	2/4/4/4	-
2	GOL	19-A	1000	-	-	3/4/4/4	-
2	GOL	4-B	1000	-	-	2/4/4/4	-
2	GOL	39-B	1000	-	-	0/4/4/4	-
2	GOL	27-B	1000	-	-	2/4/4/4	-
2	GOL	54-A	1000	-	-	4/4/4/4	-
2	GOL	16-A	1000	-	-	0/4/4/4	-
2	GOL	8-B	1000	-	-	1/4/4/4	-
2	GOL	24-B	1000	-	-	2/4/4/4	-
2	GOL	1-A	1000	-	-	0/4/4/4	-
2	GOL	14-B	1000	-	-	2/4/4/4	-
2	GOL	30-B	1000	-	-	2/4/4/4	-
2	GOL	10-B	1000	-	-	2/4/4/4	-
2	GOL	3-B	1000	-	-	2/4/4/4	-
2	GOL	57-A	1000	-	-	0/4/4/4	-
2	GOL	35-B	1000	-	-	2/4/4/4	-
2	GOL	44-A	1000	-	-	0/4/4/4	-
2	GOL	60-B	1000	-	-	2/4/4/4	-
2	GOL	37-A	1000	-	-	4/4/4/4	-
2	GOL	19-B	1000	-	-	2/4/4/4	-
2	GOL	15-B	1000	-	-	0/4/4/4	-
2	GOL	28-A	1000	-	-	4/4/4/4	-
2	GOL	8-A	1000	-	-	3/4/4/4	-
2	GOL	9-B	1000	-	-	0/4/4/4	-
2	GOL	52-A	1000	-	-	4/4/4/4	-
2	GOL	50-B	1000	-	-	0/4/4/4	-
2	GOL	2-A	1000	-	-	1/4/4/4	-
2	GOL	3-A	1000	-	-	4/4/4/4	-
2	GOL	22-B	1000	-	-	0/4/4/4	-
2	GOL	55-B	1000	-	-	0/4/4/4	-
2	GOL	59-B	1000	-	-	2/4/4/4	-
2	GOL	37-B	1000	-	-	0/4/4/4	-
2	GOL	49-B	1000	-	-	0/4/4/4	-
2	GOL	17-B	1000	-	-	0/4/4/4	-
2	GOL	28-B	1000	-	-	2/4/4/4	-
2	GOL	23-A	1000	-	-	2/4/4/4	-
2	GOL	20-A	1000	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	34-A	1000	-	-	4/4/4/4	-
2	GOL	52-B	1000	-	-	0/4/4/4	-
2	GOL	13-B	1000	-	-	0/4/4/4	-
2	GOL	32-B	1000	-	-	0/4/4/4	-
2	GOL	14-A	1000	-	-	2/4/4/4	-
2	GOL	39-A	1000	-	-	3/4/4/4	-
2	GOL	58-A	1000	-	-	4/4/4/4	-
2	GOL	12-A	1000	-	-	2/4/4/4	-
2	GOL	6-A	1000	-	-	4/4/4/4	-
2	GOL	38-A	1000	-	-	1/4/4/4	-
2	GOL	7-A	1000	-	-	4/4/4/4	-
2	GOL	24-A	1000	-	-	0/4/4/4	-
2	GOL	48-A	1000	-	-	0/4/4/4	-
2	GOL	29-A	1000	-	-	4/4/4/4	-
2	GOL	54-B	1000	-	-	0/4/4/4	-
2	GOL	11-A	1000	-	-	2/4/4/4	-
2	GOL	47-B	1000	-	-	2/4/4/4	-
2	GOL	10-A	1000	-	-	2/4/4/4	-
2	GOL	12-B	1000	-	-	0/4/4/4	-
2	GOL	27-A	1000	-	-	3/4/4/4	-
2	GOL	57-B	1000	-	-	0/4/4/4	-
2	GOL	29-B	1000	-	-	2/4/4/4	-
2	GOL	34-B	1000	-	-	0/4/4/4	-
2	GOL	15-A	1000	-	-	0/4/4/4	-
2	GOL	17-A	1000	-	-	4/4/4/4	-
2	GOL	5-B	1000	-	-	0/4/4/4	-
2	GOL	48-B	1000	-	-	1/4/4/4	-
2	GOL	49-A	1000	-	-	3/4/4/4	-
2	GOL	33-A	1000	-	-	2/4/4/4	-
2	GOL	53-B	1000	-	-	2/4/4/4	-
2	GOL	32-A	1000	-	-	0/4/4/4	-
2	GOL	45-B	1000	-	-	2/4/4/4	-
2	GOL	43-B	1000	-	-	0/4/4/4	-
2	GOL	20-B	1000	-	-	2/4/4/4	-

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	49-A	1000	GOL	O2-C2-C1	2.85	121.66	109.12
2	48-A	1000	GOL	O2-C2-C1	-2.83	96.67	109.12
2	16-A	1000	GOL	O2-C2-C1	-2.76	96.95	109.12
2	12-A	1000	GOL	O2-C2-C1	-2.76	96.98	109.12
2	2-A	1000	GOL	O2-C2-C1	-2.41	98.53	109.12

There are no chirality outliers.

5 of 150 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

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

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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