



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:19 PM GMT

PDB ID : 2D6B
Title : Novel Bromate Species trapped within a Protein Crystal
Authors : Ondracek, J.; Mesters, J.R.
Deposited on : 2005-11-10
Resolution : 1.25 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

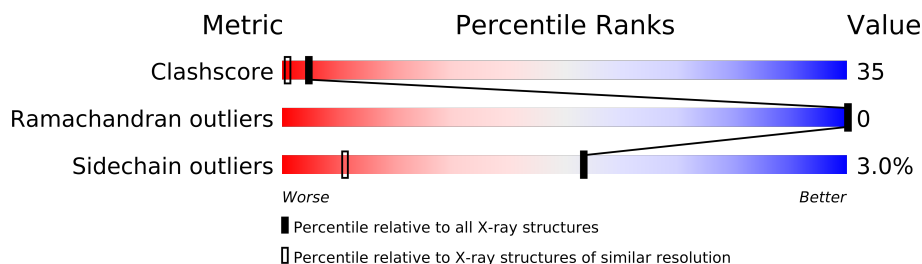
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1125 (1.30-1.22)
Ramachandran outliers	78287	1075 (1.30-1.22)
Sidechain outliers	78261	1073 (1.30-1.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	129	
1	10-A	129	
1	2-A	129	
1	3-A	129	
1	4-A	129	
1	5-A	129	
1	6-A	129	
1	7-A	129	
1	8-A	129	
1	9-A	129	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13393 atoms, of which 0 are hydrogen and 0 are deuterium.

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 lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	2-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	3-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	4-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	5-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	6-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	7-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	8-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	9-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			
1	10-A	129	Total	C	N	O	S	0	6	0
			1014	621	195	188	10			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-A	2	Total	Cl	0	0
			2	2		
2	4-A	2	Total	Cl	0	0
			2	2		
2	5-A	2	Total	Cl	0	0
			2	2		
2	8-A	2	Total	Cl	0	0
			2	2		

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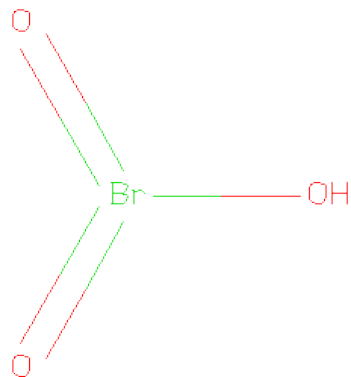
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	2	Total 2	Cl 2	0	0
2	6-A	2	Total 2	Cl 2	0	0
2	2-A	2	Total 2	Cl 2	0	0
2	10-A	2	Total 2	Cl 2	0	0
2	9-A	2	Total 2	Cl 2	0	0
2	7-A	2	Total 2	Cl 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	3-A	1	Total 1	Na 1	0	0
3	4-A	1	Total 1	Na 1	0	0
3	5-A	1	Total 1	Na 1	0	0
3	8-A	1	Total 1	Na 1	0	0
3	1-A	1	Total 1	Na 1	0	0
3	6-A	1	Total 1	Na 1	0	0
3	2-A	1	Total 1	Na 1	0	0
3	10-A	1	Total 1	Na 1	0	0
3	9-A	1	Total 1	Na 1	0	0
3	7-A	1	Total 1	Na 1	0	0

- Molecule 4 is BROMIC ACID (three-letter code: 202) (formula: BrHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	Br	O	0	0
			4	1	3		
4	1-A	1	Total	Br	O	0	0
			4	1	3		
4	1-A	1	Total	Br	O	0	0
			4	1	3		
4	1-A	1	Total	Br	O	0	0
			3	1	2		
4	1-A	1	Total	Br	O	0	0
			2	1	1		
4	1-A	1	Total	Br	O	0	0
			3	1	2		
4	1-A	1	Total	Br	O	0	0
			2	1	1		
4	1-A	1	Total	Br	O	0	0
			2	1	1		
4	1-A	1	Total	Br	O	0	0
			2	1	1		
4	2-A	1	Total	Br	O	0	0
			4	1	3		
4	2-A	1	Total	Br	O	0	0
			4	1	3		
4	2-A	1	Total	Br	O	0	0
			4	1	3		
4	2-A	1	Total	Br	O	0	0
			3	1	2		
4	2-A	1	Total	Br	O	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	2-A	1	Total 3	Br 1	O 2	0	0
4	2-A	1	Total 2	Br 1	O 1	0	0
4	2-A	1	Total 2	Br 1	O 1	0	0
4	2-A	1	Total 2	Br 1	O 1	0	0
4	3-A	1	Total 4	Br 1	O 3	0	0
4	3-A	1	Total 4	Br 1	O 3	0	0
4	3-A	1	Total 4	Br 1	O 3	0	0
4	3-A	1	Total 3	Br 1	O 2	0	0
4	3-A	1	Total 2	Br 1	O 1	0	0
4	3-A	1	Total 3	Br 1	O 2	0	0
4	3-A	1	Total 2	Br 1	O 1	0	0
4	3-A	1	Total 2	Br 1	O 1	0	0
4	3-A	1	Total 2	Br 1	O 1	0	0
4	3-A	1	Total 2	Br 1	O 1	0	0
4	4-A	1	Total 4	Br 1	O 3	0	0
4	4-A	1	Total 4	Br 1	O 3	0	0
4	4-A	1	Total 4	Br 1	O 3	0	0
4	4-A	1	Total 3	Br 1	O 2	0	0
4	4-A	1	Total 2	Br 1	O 1	0	0
4	4-A	1	Total 3	Br 1	O 2	0	0
4	4-A	1	Total 2	Br 1	O 1	0	0
4	4-A	1	Total 2	Br 1	O 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	4-A	1	Total 2	Br 1	O 1	0	0
4	5-A	1	Total 4	Br 1	O 3	0	0
4	5-A	1	Total 4	Br 1	O 3	0	0
4	5-A	1	Total 4	Br 1	O 3	0	0
4	5-A	1	Total 3	Br 1	O 2	0	0
4	5-A	1	Total 2	Br 1	O 1	0	0
4	5-A	1	Total 3	Br 1	O 2	0	0
4	5-A	1	Total 2	Br 1	O 1	0	0
4	5-A	1	Total 2	Br 1	O 1	0	0
4	5-A	1	Total 2	Br 1	O 1	0	0
4	6-A	1	Total 4	Br 1	O 3	0	0
4	6-A	1	Total 4	Br 1	O 3	0	0
4	6-A	1	Total 4	Br 1	O 3	0	0
4	6-A	1	Total 3	Br 1	O 2	0	0
4	6-A	1	Total 2	Br 1	O 1	0	0
4	6-A	1	Total 3	Br 1	O 2	0	0
4	6-A	1	Total 2	Br 1	O 1	0	0
4	6-A	1	Total 2	Br 1	O 1	0	0
4	6-A	1	Total 2	Br 1	O 1	0	0
4	7-A	1	Total 4	Br 1	O 3	0	0
4	7-A	1	Total 4	Br 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	7-A	1	Total 4	Br 1	O 3	0	0
4	7-A	1	Total 3	Br 1	O 2	0	0
4	7-A	1	Total 2	Br 1	O 1	0	0
4	7-A	1	Total 3	Br 1	O 2	0	0
4	7-A	1	Total 2	Br 1	O 1	0	0
4	7-A	1	Total 2	Br 1	O 1	0	0
4	7-A	1	Total 2	Br 1	O 1	0	0
4	8-A	1	Total 4	Br 1	O 3	0	0
4	8-A	1	Total 4	Br 1	O 3	0	0
4	8-A	1	Total 4	Br 1	O 3	0	0
4	8-A	1	Total 3	Br 1	O 2	0	0
4	8-A	1	Total 2	Br 1	O 1	0	0
4	8-A	1	Total 3	Br 1	O 2	0	0
4	8-A	1	Total 2	Br 1	O 1	0	0
4	8-A	1	Total 2	Br 1	O 1	0	0
4	8-A	1	Total 2	Br 1	O 1	0	0
4	9-A	1	Total 4	Br 1	O 3	0	0
4	9-A	1	Total 4	Br 1	O 3	0	0
4	9-A	1	Total 4	Br 1	O 3	0	0
4	9-A	1	Total 3	Br 1	O 2	0	0
4	9-A	1	Total 2	Br 1	O 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	9-A	1	Total 3	Br 1	O 2	0	0
4	9-A	1	Total 2	Br 1	O 1	0	0
4	9-A	1	Total 2	Br 1	O 1	0	0
4	9-A	1	Total 2	Br 1	O 1	0	0
4	10-A	1	Total 4	Br 1	O 3	0	0
4	10-A	1	Total 4	Br 1	O 3	0	0
4	10-A	1	Total 4	Br 1	O 3	0	0
4	10-A	1	Total 3	Br 1	O 2	0	0
4	10-A	1	Total 2	Br 1	O 1	0	0
4	10-A	1	Total 3	Br 1	O 2	0	0
4	10-A	1	Total 2	Br 1	O 1	0	0
4	10-A	1	Total 2	Br 1	O 1	0	0
4	10-A	1	Total 2	Br 1	O 1	0	0
4	10-A	1	Total 2	Br 1	O 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	298	Total 298	O 298	0	0
5	2-A	303	Total 303	O 303	0	0
5	3-A	302	Total 302	O 302	0	0
5	4-A	293	Total 293	O 293	0	0
5	5-A	307	Total 307	O 307	0	0
5	6-A	292	Total 292	O 292	0	0

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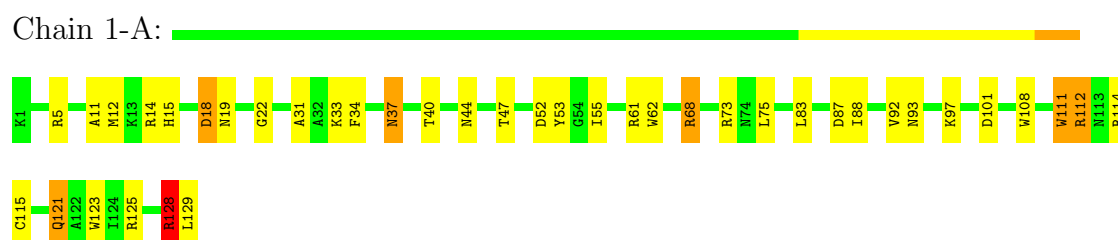
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	7-A	291	Total 291	O 291	0	0
5	8-A	292	Total 292	O 292	0	0
5	9-A	290	Total 290	O 290	0	0
5	10-A	295	Total 295	O 295	0	0

3 Residue-property plots

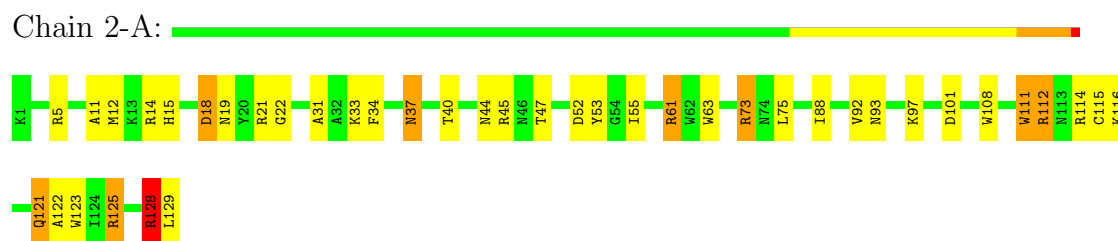
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

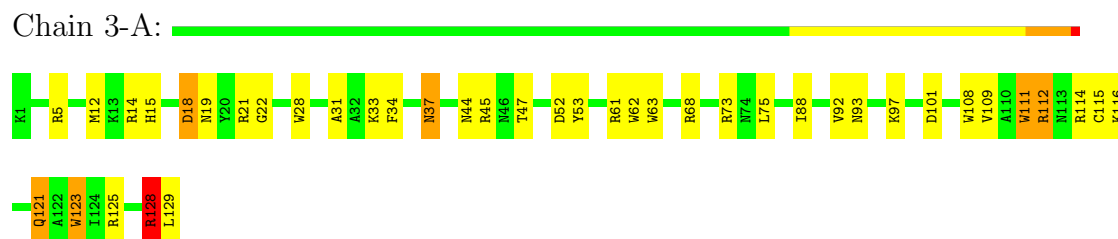
- Molecule 1: lysozyme C



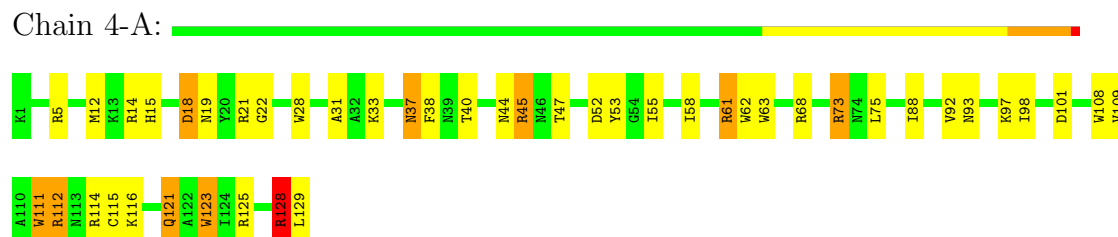
- Molecule 1: lysozyme C



- Molecule 1: lysozyme C

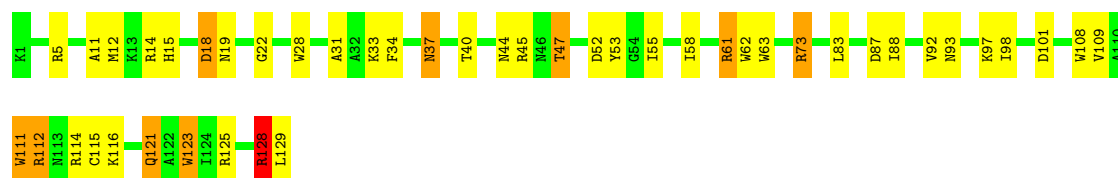


- Molecule 1: lysozyme C



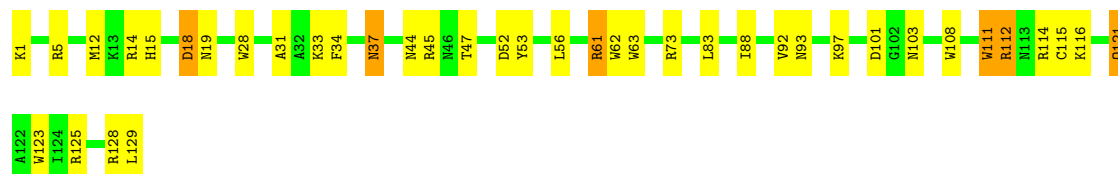
- Molecule 1: lysozyme C

Chain 5-A: 



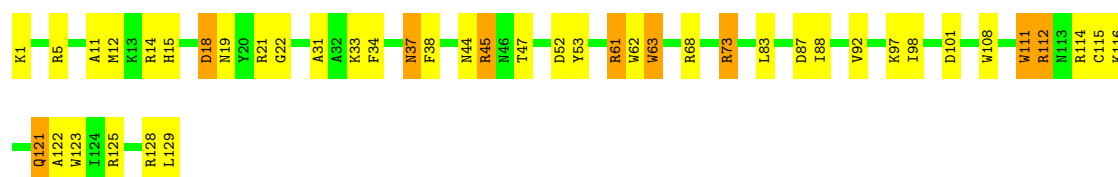
- Molecule 1: lysozyme C

Chain 6-A: 



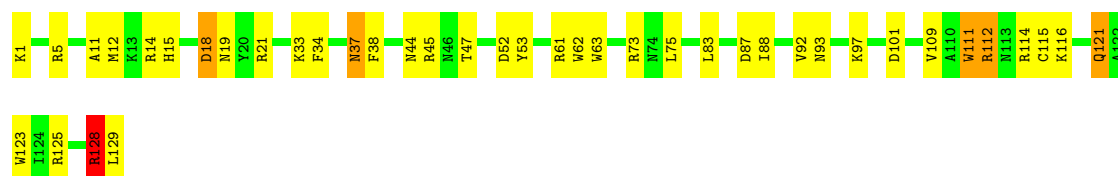
- Molecule 1: lysozyme C

Chain 7-A: 



- Molecule 1: lysozyme C

Chain 8-A: 



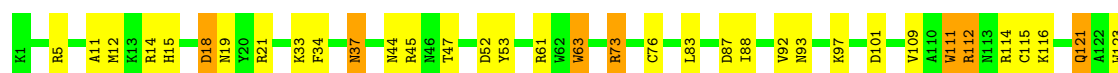
- Molecule 1: lysozyme C

Chain 9-A: 



- Molecule 1: lysozyme C

Chain 10-A: 





4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.21Å 77.21Å 38.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.25	Depositor
% Data completeness (in resolution range)	95.2 (8.00-1.25)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.58 (at 1.25Å)	Xtriage
Refinement program	HIPHOP, SHELXL	Depositor
R, R_{free}	0.178 , 0.213	Depositor
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.275	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60602 reflections	Xtriage
Total number of atoms	13393	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 202, CL

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	1.02	0/1069	1.81	21/1442 (1.5%)
1	2-A	1.01	0/1069	1.85	28/1442 (1.9%)
1	3-A	1.01	0/1069	1.83	25/1442 (1.7%)
1	4-A	0.99	0/1069	1.82	24/1442 (1.7%)
1	5-A	1.01	0/1069	1.81	28/1442 (1.9%)
1	6-A	1.01	0/1069	1.84	23/1442 (1.6%)
1	7-A	1.01	0/1069	1.83	26/1442 (1.8%)
1	8-A	1.02	0/1069	1.80	28/1442 (1.9%)
1	9-A	1.02	0/1069	1.81	25/1442 (1.7%)
1	10-A	1.03	0/1069	1.81	24/1442 (1.7%)
All	All	1.01	0/10690	1.82	252/14420 (1.7%)

There are no bond length outliers.

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	18	ASP	CB-CG-OD2	-18.07	102.04	118.30
1	7-A	18	ASP	CB-CG-OD2	-17.93	102.17	118.30
1	9-A	18	ASP	CB-CG-OD2	-17.30	102.73	118.30
1	1-A	18	ASP	CB-CG-OD2	-16.92	103.07	118.30
1	2-A	18	ASP	CB-CG-OD2	-16.87	103.12	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1014	0	975	73	2
1	2-A	1014	0	975	59	1
1	3-A	1014	0	975	67	3
1	4-A	1014	0	975	67	2
1	5-A	1014	0	975	69	2
1	6-A	1014	0	975	60	2
1	7-A	1014	0	975	62	3
1	8-A	1014	0	975	62	3
1	9-A	1014	0	975	65	2
1	10-A	1014	0	975	59	1
2	1-A	2	0	0	0	0
2	2-A	2	0	0	0	0
2	3-A	2	0	0	0	0
2	4-A	2	0	0	0	0
2	5-A	2	0	0	0	0
2	6-A	2	0	0	0	0
2	7-A	2	0	0	0	0
2	8-A	2	0	0	0	0
2	9-A	2	0	0	0	0
2	10-A	2	0	0	0	0
3	1-A	1	0	0	0	0
3	2-A	1	0	0	0	0
3	3-A	1	0	0	0	0
3	4-A	1	0	0	0	0
3	5-A	1	0	0	0	0
3	6-A	1	0	0	0	0
3	7-A	1	0	0	0	0
3	8-A	1	0	0	0	0
3	9-A	1	0	0	0	0
3	10-A	1	0	0	0	0
4	1-A	26	0	0	4	0
4	2-A	26	0	0	4	0
4	3-A	26	0	0	7	0
4	4-A	26	0	0	5	0
4	5-A	26	0	0	7	0
4	6-A	26	0	0	7	0
4	7-A	26	0	0	9	0
4	8-A	26	0	0	5	0
4	9-A	26	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	10-A	26	0	0	8	1
5	1-A	298	0	0	59	5
5	2-A	303	0	0	43	3
5	3-A	302	0	0	55	4
5	4-A	293	0	0	53	5
5	5-A	307	0	0	54	5
5	6-A	292	0	0	51	6
5	7-A	291	0	0	52	8
5	8-A	292	0	0	49	4
5	9-A	290	0	0	50	3
5	10-A	295	0	0	46	5
All	All	13393	0	9750	705	59

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 705 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:137:202:BR	4:A:137:202:O1	1.15	1.68
4:A:137:202:BR	4:A:137:202:O1	1.07	1.60
4:A:137:202:BR	4:A:137:202:O1	1.03	1.58
4:A:137:202:BR	4:A:137:202:O1	1.04	1.57
4:A:137:202:BR	4:A:137:202:O1	1.03	1.56

The worst 5 of 59 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:LEU:OXT	1:A:129:LEU:OXT[8_555]	1.56	0.64
1:A:129:LEU:OXT	1:A:129:LEU:OXT[8_555]	1.61	0.59
1:A:129:LEU:OXT	1:A:129:LEU:OXT[8_555]	1.64	0.56
1:A:129:LEU:OXT	1:A:129:LEU:OXT[8_555]	1.65	0.55
1:A:129:LEU:OXT	1:A:129:LEU:OXT[8_555]	1.67	0.53

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	132/129 (102%)	128 (97%)	4 (3%)	0	100	100
1	2-A	132/129 (102%)	129 (98%)	3 (2%)	0	100	100
1	3-A	132/129 (102%)	128 (97%)	4 (3%)	0	100	100
1	4-A	132/129 (102%)	130 (98%)	2 (2%)	0	100	100
1	5-A	132/129 (102%)	130 (98%)	2 (2%)	0	100	100
1	6-A	132/129 (102%)	130 (98%)	2 (2%)	0	100	100
1	7-A	132/129 (102%)	130 (98%)	2 (2%)	0	100	100
1	8-A	132/129 (102%)	129 (98%)	3 (2%)	0	100	100
1	9-A	132/129 (102%)	129 (98%)	3 (2%)	0	100	100
1	10-A	132/129 (102%)	129 (98%)	3 (2%)	0	100	100
All	All	1320/1290 (102%)	1292 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	111/105 (106%)	108 (97%)	3 (3%)	57	14
1	2-A	111/105 (106%)	108 (97%)	3 (3%)	57	14
1	3-A	111/105 (106%)	108 (97%)	3 (3%)	57	14
1	4-A	111/105 (106%)	107 (96%)	4 (4%)	47	8
1	5-A	111/105 (106%)	107 (96%)	4 (4%)	47	8
1	6-A	111/105 (106%)	109 (98%)	2 (2%)	71	30
1	7-A	111/105 (106%)	109 (98%)	2 (2%)	71	30
1	8-A	111/105 (106%)	108 (97%)	3 (3%)	57	14
1	9-A	111/105 (106%)	108 (97%)	3 (3%)	57	14
1	10-A	111/105 (106%)	107 (96%)	4 (4%)	47	8
All	All	1110/1050 (106%)	1079 (97%)	31 (3%)	53	13

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-A	73	ARG
1	6-A	37	ASN
1	10-A	73	ARG
1	5-A	121	GLN
1	6-A	121	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	5-A	46	ASN
1	6-A	46	ASN
1	10-A	37	ASN
1	5-A	121	GLN
1	6-A	93	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 120 ligands modelled in this entry, 30 are monoatomic - leaving 90 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	202	1-A	131	-	2,3,3	0.66	0	1,3,3	0.54	0
4	202	1-A	132	-	2,3,3	0.82	0	1,3,3	0.51	0
4	202	1-A	133	-	2,3,3	4.61	2 (100%)	1,3,3	1.57	0
4	202	1-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	1-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	1-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	1-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	1-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	1-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	10-A	131	-	2,3,3	0.74	0	1,3,3	0.55	0
4	202	10-A	132	-	2,3,3	1.11	0	1,3,3	0.49	0
4	202	10-A	133	-	2,3,3	4.84	2 (100%)	1,3,3	1.53	0
4	202	10-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	10-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	10-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	10-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	10-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	10-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	2-A	131	-	2,3,3	0.54	0	1,3,3	0.58	0
4	202	2-A	132	-	2,3,3	1.09	0	1,3,3	0.50	0
4	202	2-A	133	-	2,3,3	2.81	1 (50%)	1,3,3	1.68	0
4	202	2-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	2-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	2-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	2-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	2-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	2-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	3-A	131	-	2,3,3	0.37	0	1,3,3	0.42	0
4	202	3-A	132	-	2,3,3	0.77	0	1,3,3	0.59	0
4	202	3-A	133	-	2,3,3	3.14	2 (100%)	1,3,3	1.81	0
4	202	3-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	3-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	3-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	3-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	3-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	3-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	4-A	131	-	2,3,3	0.44	0	1,3,3	0.43	0
4	202	4-A	132	-	2,3,3	0.82	0	1,3,3	0.58	0
4	202	4-A	133	-	2,3,3	2.86	2 (100%)	1,3,3	1.73	0
4	202	4-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	4-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	4-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	202	4-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	4-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	4-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	5-A	131	-	2,3,3	0.54	0	1,3,3	0.41	0
4	202	5-A	132	-	2,3,3	0.87	0	1,3,3	0.54	0
4	202	5-A	133	-	2,3,3	3.71	2 (100%)	1,3,3	1.89	0
4	202	5-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	5-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	5-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	5-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	5-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	5-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	6-A	131	-	2,3,3	0.79	0	1,3,3	0.62	0
4	202	6-A	132	-	2,3,3	1.11	0	1,3,3	0.57	0
4	202	6-A	133	-	2,3,3	4.68	2 (100%)	1,3,3	1.36	0
4	202	6-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	6-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	6-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	6-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	6-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	6-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	7-A	131	-	2,3,3	0.74	0	1,3,3	0.62	0
4	202	7-A	132	-	2,3,3	0.85	0	1,3,3	0.60	0
4	202	7-A	133	-	2,3,3	3.55	2 (100%)	1,3,3	1.36	0
4	202	7-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	7-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	7-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	7-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	7-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	7-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	8-A	131	-	2,3,3	0.64	0	1,3,3	0.57	0
4	202	8-A	132	-	2,3,3	0.94	0	1,3,3	0.56	0
4	202	8-A	133	-	2,3,3	3.22	1 (50%)	1,3,3	1.52	0
4	202	8-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	8-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	8-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	8-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	8-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	8-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	9-A	131	-	2,3,3	0.95	0	1,3,3	0.49	0
4	202	9-A	132	-	2,3,3	1.01	0	1,3,3	0.51	0
4	202	9-A	133	-	2,3,3	4.61	2 (100%)	1,3,3	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	202	9-A	134	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	9-A	135	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	9-A	136	-	0,2,3	0.00	-	0,1,3	0.00	-
4	202	9-A	137	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	9-A	138	-	0,1,3	0.00	-	0,0,3	0.00	-
4	202	9-A	139	-	0,1,3	0.00	-	0,0,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	202	1-A	131	-	-	0/0/0/0	0/0/0/0
4	202	1-A	132	-	-	0/0/0/0	0/0/0/0
4	202	1-A	133	-	-	0/0/0/0	0/0/0/0
4	202	1-A	134	-	-	0/0/0/0	0/0/0/0
4	202	1-A	135	-	-	0/0/0/0	0/0/0/0
4	202	1-A	136	-	-	0/0/0/0	0/0/0/0
4	202	1-A	137	-	-	0/0/0/0	0/0/0/0
4	202	1-A	138	-	-	0/0/0/0	0/0/0/0
4	202	1-A	139	-	-	0/0/0/0	0/0/0/0
4	202	10-A	131	-	-	0/0/0/0	0/0/0/0
4	202	10-A	132	-	-	0/0/0/0	0/0/0/0
4	202	10-A	133	-	-	0/0/0/0	0/0/0/0
4	202	10-A	134	-	-	0/0/0/0	0/0/0/0
4	202	10-A	135	-	-	0/0/0/0	0/0/0/0
4	202	10-A	136	-	-	0/0/0/0	0/0/0/0
4	202	10-A	137	-	-	0/0/0/0	0/0/0/0
4	202	10-A	138	-	-	0/0/0/0	0/0/0/0
4	202	10-A	139	-	-	0/0/0/0	0/0/0/0
4	202	2-A	131	-	-	0/0/0/0	0/0/0/0
4	202	2-A	132	-	-	0/0/0/0	0/0/0/0
4	202	2-A	133	-	-	0/0/0/0	0/0/0/0
4	202	2-A	134	-	-	0/0/0/0	0/0/0/0
4	202	2-A	135	-	-	0/0/0/0	0/0/0/0
4	202	2-A	136	-	-	0/0/0/0	0/0/0/0
4	202	2-A	137	-	-	0/0/0/0	0/0/0/0
4	202	2-A	138	-	-	0/0/0/0	0/0/0/0
4	202	2-A	139	-	-	0/0/0/0	0/0/0/0
4	202	3-A	131	-	-	0/0/0/0	0/0/0/0
4	202	3-A	132	-	-	0/0/0/0	0/0/0/0
4	202	3-A	133	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	202	3-A	134	-	-	0/0/0/0	0/0/0/0
4	202	3-A	135	-	-	0/0/0/0	0/0/0/0
4	202	3-A	136	-	-	0/0/0/0	0/0/0/0
4	202	3-A	137	-	-	0/0/0/0	0/0/0/0
4	202	3-A	138	-	-	0/0/0/0	0/0/0/0
4	202	3-A	139	-	-	0/0/0/0	0/0/0/0
4	202	4-A	131	-	-	0/0/0/0	0/0/0/0
4	202	4-A	132	-	-	0/0/0/0	0/0/0/0
4	202	4-A	133	-	-	0/0/0/0	0/0/0/0
4	202	4-A	134	-	-	0/0/0/0	0/0/0/0
4	202	4-A	135	-	-	0/0/0/0	0/0/0/0
4	202	4-A	136	-	-	0/0/0/0	0/0/0/0
4	202	4-A	137	-	-	0/0/0/0	0/0/0/0
4	202	4-A	138	-	-	0/0/0/0	0/0/0/0
4	202	4-A	139	-	-	0/0/0/0	0/0/0/0
4	202	5-A	131	-	-	0/0/0/0	0/0/0/0
4	202	5-A	132	-	-	0/0/0/0	0/0/0/0
4	202	5-A	133	-	-	0/0/0/0	0/0/0/0
4	202	5-A	134	-	-	0/0/0/0	0/0/0/0
4	202	5-A	135	-	-	0/0/0/0	0/0/0/0
4	202	5-A	136	-	-	0/0/0/0	0/0/0/0
4	202	5-A	137	-	-	0/0/0/0	0/0/0/0
4	202	5-A	138	-	-	0/0/0/0	0/0/0/0
4	202	5-A	139	-	-	0/0/0/0	0/0/0/0
4	202	6-A	131	-	-	0/0/0/0	0/0/0/0
4	202	6-A	132	-	-	0/0/0/0	0/0/0/0
4	202	6-A	133	-	-	0/0/0/0	0/0/0/0
4	202	6-A	134	-	-	0/0/0/0	0/0/0/0
4	202	6-A	135	-	-	0/0/0/0	0/0/0/0
4	202	6-A	136	-	-	0/0/0/0	0/0/0/0
4	202	6-A	137	-	-	0/0/0/0	0/0/0/0
4	202	6-A	138	-	-	0/0/0/0	0/0/0/0
4	202	6-A	139	-	-	0/0/0/0	0/0/0/0
4	202	7-A	131	-	-	0/0/0/0	0/0/0/0
4	202	7-A	132	-	-	0/0/0/0	0/0/0/0
4	202	7-A	133	-	-	0/0/0/0	0/0/0/0
4	202	7-A	134	-	-	0/0/0/0	0/0/0/0
4	202	7-A	135	-	-	0/0/0/0	0/0/0/0
4	202	7-A	136	-	-	0/0/0/0	0/0/0/0
4	202	7-A	137	-	-	0/0/0/0	0/0/0/0
4	202	7-A	138	-	-	0/0/0/0	0/0/0/0
4	202	7-A	139	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	202	8-A	131	-	-	0/0/0/0	0/0/0/0
4	202	8-A	132	-	-	0/0/0/0	0/0/0/0
4	202	8-A	133	-	-	0/0/0/0	0/0/0/0
4	202	8-A	134	-	-	0/0/0/0	0/0/0/0
4	202	8-A	135	-	-	0/0/0/0	0/0/0/0
4	202	8-A	136	-	-	0/0/0/0	0/0/0/0
4	202	8-A	137	-	-	0/0/0/0	0/0/0/0
4	202	8-A	138	-	-	0/0/0/0	0/0/0/0
4	202	8-A	139	-	-	0/0/0/0	0/0/0/0
4	202	9-A	131	-	-	0/0/0/0	0/0/0/0
4	202	9-A	132	-	-	0/0/0/0	0/0/0/0
4	202	9-A	133	-	-	0/0/0/0	0/0/0/0
4	202	9-A	134	-	-	0/0/0/0	0/0/0/0
4	202	9-A	135	-	-	0/0/0/0	0/0/0/0
4	202	9-A	136	-	-	0/0/0/0	0/0/0/0
4	202	9-A	137	-	-	0/0/0/0	0/0/0/0
4	202	9-A	138	-	-	0/0/0/0	0/0/0/0
4	202	9-A	139	-	-	0/0/0/0	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9-A	133	202	BR-O3	6.19	2.06	1.63
4	10-A	133	202	BR-O3	6.16	2.06	1.63
4	6-A	133	202	BR-O3	5.79	2.03	1.63
4	1-A	133	202	BR-O3	5.72	2.03	1.63
4	7-A	133	202	BR-O3	4.48	1.94	1.63

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.