



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:08 PM GMT

PDB ID : 1S8C  
Title : Crystal structure of human heme oxygenase in a complex with biliverdine  
Authors : Lad, L.; Friedman, J.; Li, H.; Bhaskar, B.; Ortiz de Montellano, P.R.; Poulos, T.L.  
Deposited on : 2004-02-02  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

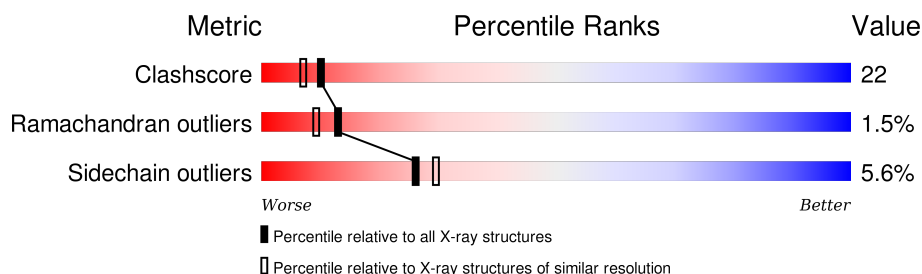
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	233	
1	B	233	
1	C	233	
1	D	233	

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	BLA	A	400	-	-	X	-

## 2 Entry composition [i](#)

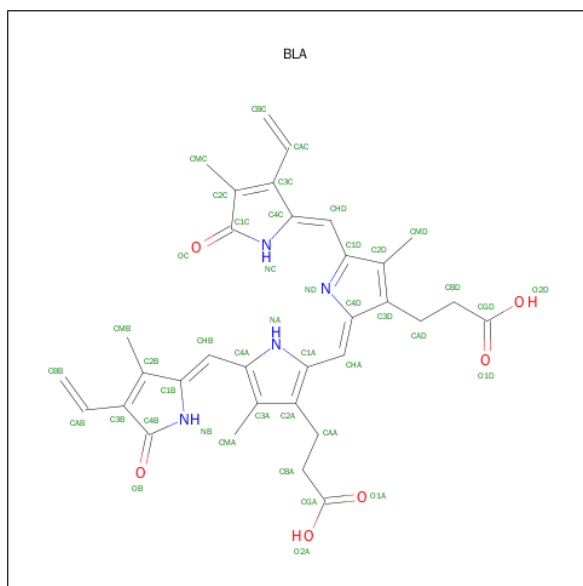
There are 3 unique types of molecules in this entry. The entry contains 7341 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heme oxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	10	0	0
			1745	1121	299	320	5			
1	B	214	Total	C	N	O	S	11	0	0
			1745	1121	299	320	5			
1	C	214	Total	C	N	O	S	8	0	0
			1745	1121	299	320	5			
1	D	213	Total	C	N	O	S	7	0	0
			1738	1116	298	319	5			

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	1	0
			43	33	4	6		

- Molecule 3 is water.

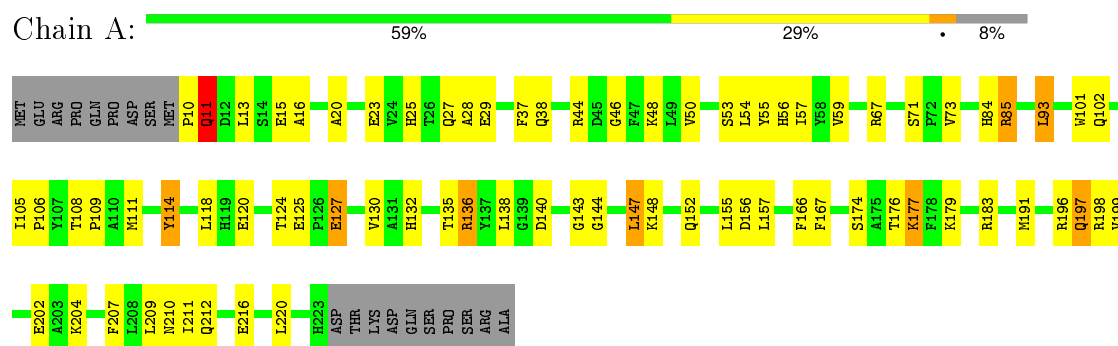
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total 103	O 103	0	0
3	B	76	Total 76	O 76	0	0
3	C	111	Total 111	O 111	0	0
3	D	35	Total 35	O 35	0	0

### 3 Residue-property plots [i](#)

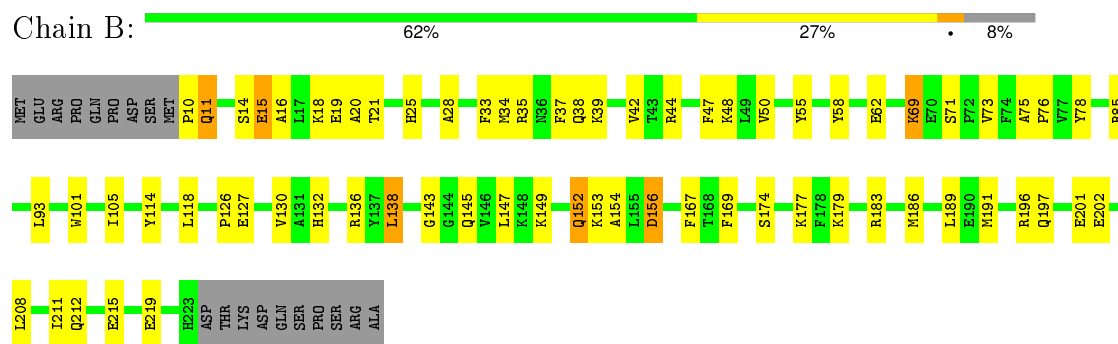
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 was not executed.

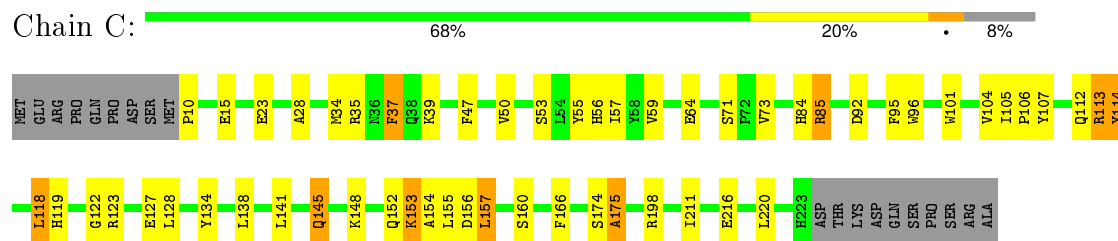
- Molecule 1: Heme oxygenase 1



- Molecule 1: Heme oxygenase 1

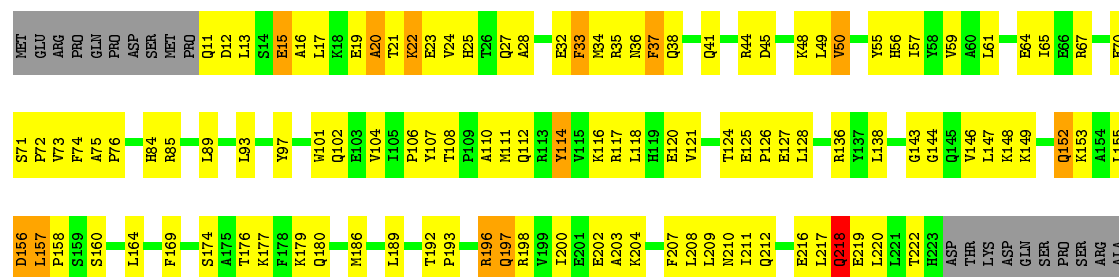


- Molecule 1: Heme oxygenase 1



- Molecule 1: Heme oxygenase 1

Chain D:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.41 Å   56.46 Å   109.75 Å 90.00°   100.39°   90.00°	Depositor
Resolution (Å)	50.00 – 2.19	Depositor
% Data completeness (in resolution range)	86.5 (50.00-2.19)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.240 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/1786	0.57	0/2414
1	B	0.34	0/1786	0.55	0/2414
1	C	0.36	0/1786	0.57	0/2414
1	D	0.32	0/1778	0.57	0/2403
All	All	0.35	0/7136	0.56	0/9645

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	0	1738	84	0
1	B	1745	0	1738	49	0
1	C	1745	0	1738	53	0
1	D	1738	0	1730	112	0
2	A	43	0	32	33	0
3	A	103	0	0	11	0
3	B	76	0	0	3	0
3	C	111	0	0	5	0
3	D	35	0	0	2	0
All	All	7341	0	6976	305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:HA	1:A:111:MET:HE3	1.25	1.13
2:A:400:BLA:HHA	2:A:400:BLA:HBA2	1.14	1.08
1:D:136:ARG:HH12	1:D:210:ASN:HD21	1.01	0.93
2:A:400:BLA:CHA	2:A:400:BLA:HBA2	1.89	0.93
1:A:136:ARG:HH12	1:A:210:ASN:HD21	1.07	0.92
1:D:138:LEU:HD12	1:D:179:LYS:HG2	1.51	0.92
1:D:143:GLY:O	1:D:146:VAL:HG12	1.73	0.89
1:C:119:HIS:HB3	1:C:123:ARG:HE	1.40	0.87
1:B:35:ARG:HG2	1:B:39:LYS:HE2	1.61	0.83
1:A:53:SER:CA	1:A:111:MET:HE3	2.09	0.82
1:D:153:LYS:H	1:D:153:LYS:HD2	1.44	0.81
1:A:136:ARG:HA	2:A:400:BLA:HAB	1.61	0.80
1:D:197:GLN:H	1:D:197:GLN:HE21	1.29	0.80
1:A:144:GLY:HA2	2:A:400:BLA:O1D	1.82	0.80
1:C:39:LYS:HE2	3:C:316:HOH:O	1.79	0.80
1:C:47:PHE:O	1:C:50:VAL:HG22	1.82	0.78
1:C:153:LYS:HD2	1:C:154:ALA:N	1.99	0.77
1:A:136:ARG:HG2	2:A:400:BLA:HAB	1.67	0.77
1:D:196:ARG:O	1:D:200:ILE:HD13	1.86	0.75
1:D:148:LYS:O	1:D:152:GLN:HG2	1.86	0.74
1:A:53:SER:HA	1:A:111:MET:CE	2.12	0.74
1:A:44:ARG:HD3	1:A:155:LEU:HD22	1.70	0.74
1:D:20:ALA:HB1	1:D:204:LYS:HE2	1.70	0.74
1:A:130:VAL:HG13	3:A:403:HOH:O	1.88	0.74
1:C:160:SER:O	1:D:164:LEU:HD12	1.86	0.73
1:C:128:LEU:HD11	1:C:198:ARG:NH1	2.02	0.73
1:B:10:PRO:O	1:B:11:GLN:HB3	1.90	0.71
1:C:128:LEU:HD11	1:C:198:ARG:HH12	1.56	0.70
1:D:218:GLN:O	1:D:222:THR:HG23	1.92	0.70
1:B:19:GLU:HG3	1:B:20:ALA:N	2.03	0.70
1:D:136:ARG:NH1	1:D:210:ASN:HD21	1.84	0.70
1:B:34:MET:O	1:B:38:GLN:HG2	1.91	0.70
1:D:89:LEU:O	1:D:93:LEU:HD13	1.92	0.69
1:D:186:MET:O	1:D:189:LEU:HB2	1.92	0.69
1:D:127:GLU:CD	1:D:127:GLU:H	1.94	0.69
1:A:136:ARG:NH1	1:A:210:ASN:HD21	1.88	0.69
1:A:136:ARG:NH1	2:A:400:BLA:HMC2	2.07	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ARG:HH12	1:D:210:ASN:ND2	1.84	0.69
1:D:208:LEU:O	1:D:212:GLN:HG3	1.93	0.69
1:D:128:LEU:HD11	1:D:198:ARG:HD3	1.74	0.68
1:B:138:LEU:HD13	1:B:179:LYS:HG3	1.74	0.68
1:B:130:VAL:HG23	3:B:268:HOH:O	1.94	0.67
2:A:400:BLA:CBA	3:A:451:HOH:O	2.41	0.67
1:D:128:LEU:HD21	1:D:198:ARG:HD2	1.76	0.67
1:B:143:GLY:O	1:B:147:LEU:HD23	1.94	0.67
1:D:153:LYS:HD2	1:D:153:LYS:N	2.09	0.67
2:A:400:BLA:HBA2	3:A:451:HOH:O	1.95	0.66
1:C:155:LEU:O	1:C:156:ASP:HB2	1.95	0.66
1:A:144:GLY:CA	2:A:400:BLA:O1D	2.43	0.66
1:D:85:ARG:HD3	1:D:169:PHE:CE2	2.30	0.65
1:A:10:PRO:HD2	1:A:16:ALA:HA	1.77	0.65
1:A:136:ARG:HH12	1:A:210:ASN:ND2	1.90	0.65
1:D:176:THR:O	1:D:180:GLN:HG3	1.97	0.65
1:D:101:TRP:HA	1:D:104:VAL:HG12	1.78	0.65
1:A:56:HIS:ND1	1:A:111:MET:CE	2.60	0.65
1:D:17:LEU:HD22	1:D:203:ALA:HB2	1.76	0.65
1:B:19:GLU:HG3	1:B:20:ALA:H	1.61	0.65
1:A:120:GLU:O	1:A:124:THR:HG22	1.97	0.64
1:D:197:GLN:H	1:D:197:GLN:NE2	1.96	0.64
1:D:152:GLN:HB2	1:D:153:LYS:HD2	1.80	0.64
1:D:16:ALA:HB1	1:D:200:ILE:CG1	2.27	0.64
1:D:196:ARG:HB3	1:D:197:GLN:NE2	2.12	0.64
1:D:27:GLN:HE21	1:D:211:ILE:HD13	1.62	0.64
1:C:84:HIS:HD2	3:C:241:HOH:O	1.80	0.64
1:A:209:LEU:O	1:A:212:GLN:HG3	1.97	0.64
1:A:16:ALA:HB2	1:A:196:ARG:HH22	1.63	0.64
1:D:149:LYS:HD3	1:D:153:LYS:NZ	2.13	0.63
1:A:44:ARG:O	1:A:48:LYS:HG3	1.99	0.63
1:B:28:ALA:HA	1:B:211:ILE:HG12	1.80	0.63
1:D:128:LEU:HD11	1:D:198:ARG:CD	2.29	0.63
1:D:216:GLU:O	1:D:220:LEU:HD23	1.99	0.62
1:A:56:HIS:ND1	1:A:111:MET:HE2	2.14	0.62
1:C:85:ARG:HG2	1:C:166:PHE:CE1	2.34	0.62
1:C:39:LYS:HD2	1:C:39:LYS:N	2.15	0.61
1:A:38:GLN:NE2	2:A:400:BLA:O1A	2.32	0.61
1:C:174:SER:O	1:C:175:ALA:HB2	2.00	0.61
1:A:210:ASN:ND2	2:A:400:BLA:HMC3	2.15	0.61
1:D:138:LEU:HD22	1:D:138:LEU:N	2.16	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:CD2	2:A:400:BLA:HMB2	2.36	0.61
1:C:10:PRO:HG2	1:C:15:GLU:HG2	1.81	0.61
1:A:71:SER:OG	1:A:73:VAL:HG22	1.99	0.61
1:D:13:LEU:O	1:D:16:ALA:HB3	2.01	0.61
1:A:124:THR:HG23	1:A:125:GLU:HG3	1.83	0.61
1:D:27:GLN:NE2	1:D:211:ILE:HD13	2.16	0.61
1:D:28:ALA:HA	1:D:211:ILE:HG12	1.82	0.61
1:A:147:LEU:HD13	2:A:400:BLA:HAD2	1.84	0.60
1:D:23:GLU:HG2	1:D:24:VAL:N	2.16	0.60
1:C:56:HIS:HD2	3:C:309:HOH:O	1.85	0.60
1:C:113:ARG:HH11	1:C:113:ARG:HB3	1.65	0.60
1:D:192:THR:OG1	1:D:193:PRO:HD2	2.01	0.60
1:A:176:THR:HG23	3:A:492:HOH:O	2.00	0.60
1:A:174:SER:OG	1:A:177:LYS:HD3	2.01	0.60
1:D:125:GLU:OE2	1:D:198:ARG:HD3	2.00	0.60
1:B:145:GLN:O	1:B:149:LYS:HG3	2.02	0.59
1:D:196:ARG:HB3	1:D:197:GLN:HE21	1.66	0.59
1:A:148:LYS:O	1:A:152:GLN:HG3	2.01	0.59
1:D:32:GLU:HB2	1:D:35:ARG:NH2	2.16	0.59
1:A:23:GLU:HG3	1:A:27:GLN:HE21	1.68	0.59
1:A:136:ARG:HH22	2:A:400:BLA:C1C	2.13	0.59
2:A:400:BLA:ND	2:A:400:BLA:NC	2.51	0.59
1:A:147:LEU:HD11	2:A:400:BLA:CGA	2.32	0.59
1:B:15:GLU:HA	1:B:18:LYS:HD3	1.85	0.58
1:D:70:GLU:HG2	3:D:263:HOH:O	2.01	0.58
1:B:73:VAL:HG11	1:B:127:GLU:HG3	1.84	0.58
1:D:16:ALA:O	1:D:200:ILE:HG13	2.03	0.58
1:C:141:LEU:HD13	1:C:141:LEU:C	2.24	0.57
1:D:116:LYS:O	1:D:120:GLU:HG3	2.04	0.57
1:B:47:PHE:O	1:B:50:VAL:HG22	2.05	0.57
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.86	0.57
1:B:208:LEU:O	1:B:212:GLN:HG3	2.04	0.57
1:A:85:ARG:HG2	1:A:166:PHE:CE1	2.40	0.57
1:A:84:HIS:HD2	3:A:430:HOH:O	1.87	0.57
1:C:35:ARG:O	1:C:39:LYS:HD3	2.04	0.57
1:B:42:VAL:HB	3:B:283:HOH:O	2.05	0.57
1:D:196:ARG:HG2	1:D:196:ARG:HH11	1.71	0.56
1:C:55:TYR:O	1:C:59:VAL:HG23	2.05	0.56
1:D:15:GLU:N	1:D:15:GLU:OE1	2.38	0.56
1:B:197:GLN:O	1:B:201:GLU:HG2	2.06	0.56
1:B:35:ARG:CG	1:B:39:LYS:HE2	2.35	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:SER:OG	1:C:73:VAL:HG22	2.05	0.56
1:B:179:LYS:HB2	1:B:179:LYS:NZ	2.21	0.56
1:D:21:THR:HA	1:D:24:VAL:HG22	1.88	0.56
1:A:143:GLY:O	1:A:147:LEU:HD12	2.06	0.55
1:D:157:LEU:HD12	1:D:157:LEU:N	2.21	0.55
1:D:107:TYR:CE2	1:D:112:GLN:HG2	2.42	0.55
1:A:197:GLN:HG2	3:A:449:HOH:O	2.06	0.55
1:C:160:SER:HA	1:D:152:GLN:HE22	1.71	0.55
1:D:84:HIS:O	1:D:85:ARG:HD2	2.07	0.54
1:A:136:ARG:CA	2:A:400:BLA:HAB	2.33	0.54
1:A:136:ARG:NH2	2:A:400:BLA:OC	2.29	0.54
1:A:108:THR:HB	1:A:109:PRO:HD2	1.89	0.54
1:D:75:ALA:HB3	1:D:76:PRO:HD3	1.88	0.54
1:A:210:ASN:ND2	2:A:400:BLA:OC	2.40	0.54
1:D:56:HIS:HE1	1:D:106:PRO:O	1.91	0.54
1:D:20:ALA:H	1:D:22:LYS:HG3	1.71	0.54
1:B:58:TYR:O	1:B:62:GLU:HG3	2.07	0.54
2:A:400:BLA:CBA	2:A:400:BLA:CHA	2.70	0.53
1:A:67:ARG:HH11	1:A:67:ARG:HG3	1.71	0.53
1:B:215:GLU:O	1:B:219:GLU:HG3	2.08	0.53
1:A:56:HIS:HD2	3:A:466:HOH:O	1.92	0.53
1:A:56:HIS:ND1	1:A:111:MET:HE1	2.23	0.53
1:A:57:ILE:HD12	2:A:400:BLA:HMC1	1.90	0.53
1:D:203:ALA:O	1:D:207:PHE:HD1	1.90	0.53
1:B:189:LEU:HD23	1:B:191:MET:CE	2.38	0.53
1:A:166:PHE:CE2	2:A:400:BLA:O2D	2.62	0.53
1:A:132:HIS:HE1	1:A:202:GLU:OE2	1.92	0.53
1:D:114:TYR:O	1:D:118:LEU:HD13	2.08	0.53
1:A:11:GLN:HA	1:A:11:GLN:OE1	2.08	0.53
1:D:36:ASN:HB3	1:D:41:GLN:HB3	1.91	0.53
1:B:14:SER:O	1:B:18:LYS:HG3	2.08	0.52
1:D:64:GLU:OE1	1:D:67:ARG:HD2	2.08	0.52
1:B:71:SER:OG	1:B:73:VAL:HG22	2.10	0.52
1:A:55:TYR:HB2	1:A:93:LEU:HD21	1.91	0.52
1:C:113:ARG:NH1	1:C:113:ARG:HB3	2.24	0.52
1:A:10:PRO:CD	1:A:16:ALA:HA	2.39	0.52
1:D:196:ARG:HD3	1:D:200:ILE:HD13	1.92	0.52
1:D:197:GLN:N	1:D:197:GLN:HE21	2.03	0.52
1:C:174:SER:O	1:C:175:ALA:CB	2.58	0.52
1:A:127:GLU:H	1:A:127:GLU:CD	2.11	0.52
1:D:44:ARG:HD3	1:D:155:LEU:HD22	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:O	1:B:25:HIS:HB2	2.10	0.51
1:A:101:TRP:O	1:A:105:ILE:HG23	2.10	0.51
1:D:216:GLU:HA	1:D:219:GLU:HB3	1.90	0.51
1:D:19:GLU:O	1:D:20:ALA:HB2	2.11	0.51
1:D:21:THR:O	1:D:25:HIS:HB2	2.11	0.51
1:B:44:ARG:HH12	1:B:48:LYS:NZ	2.09	0.51
1:C:138:LEU:N	1:C:138:LEU:HD22	2.26	0.50
1:C:107:TYR:CZ	1:C:112:GLN:HG2	2.46	0.50
1:C:148:LYS:O	1:C:152:GLN:HG3	2.12	0.49
1:D:125:GLU:N	1:D:126:PRO:HD3	2.28	0.49
2:A:400:BLA:HAA2	3:A:442:HOH:O	2.12	0.49
1:C:134:TYR:HA	1:C:138:LEU:HD23	1.95	0.49
1:B:127:GLU:CD	1:B:127:GLU:H	2.16	0.49
1:C:28:ALA:HA	1:C:211:ILE:HG12	1.95	0.49
1:D:138:LEU:H	1:D:138:LEU:HD22	1.77	0.48
1:B:10:PRO:O	1:B:11:GLN:CB	2.58	0.48
1:A:157:LEU:H	1:A:157:LEU:HD12	1.78	0.48
1:A:25:HIS:O	1:A:29:GLU:HG3	2.14	0.48
1:D:149:LYS:HD3	1:D:153:LYS:HZ2	1.77	0.48
1:A:136:ARG:HA	2:A:400:BLA:CAB	2.38	0.48
1:A:155:LEU:HB2	1:A:157:LEU:CD1	2.44	0.48
1:A:136:ARG:HG2	2:A:400:BLA:CAB	2.40	0.48
1:A:167:PHE:CE1	2:A:400:BLA:HMD1	2.49	0.47
1:D:21:THR:HA	1:D:24:VAL:CG2	2.43	0.47
1:C:113:ARG:HH11	1:C:113:ARG:CB	2.27	0.47
1:B:35:ARG:O	1:B:39:LYS:HG3	2.15	0.47
1:C:155:LEU:HG	3:C:247:HOH:O	2.14	0.47
1:A:10:PRO:HG2	1:A:16:ALA:HA	1.97	0.47
1:A:197:GLN:HE22	1:A:198:ARG:HG2	1.80	0.47
1:C:138:LEU:H	1:C:138:LEU:HD22	1.80	0.47
1:D:108:THR:HG23	1:D:111:MET:HE3	1.96	0.47
1:A:16:ALA:HB2	1:A:196:ARG:NH2	2.29	0.47
1:D:102:GLN:HB2	3:D:266:HOH:O	2.14	0.47
1:C:152:GLN:HA	1:C:157:LEU:HD23	1.96	0.46
1:A:15:GLU:HA	1:A:15:GLU:OE1	2.15	0.46
1:D:44:ARG:NH2	1:D:156:ASP:O	2.49	0.46
1:B:132:HIS:HD2	3:B:300:HOH:O	1.98	0.46
1:A:20:ALA:O	1:A:204:LYS:HE2	2.16	0.46
1:D:146:VAL:HG13	1:D:147:LEU:N	2.30	0.46
1:B:101:TRP:O	1:B:105:ILE:HG23	2.15	0.46
1:A:56:HIS:HE1	1:A:106:PRO:O	1.99	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HG2	1:B:127:GLU:OE2	2.15	0.46
1:C:53:SER:O	1:C:57:ILE:HG13	2.15	0.46
1:D:101:TRP:HA	1:D:104:VAL:CG1	2.44	0.46
1:C:101:TRP:O	1:C:105:ILE:HG23	2.15	0.46
1:D:193:PRO:O	1:D:197:GLN:NE2	2.49	0.46
1:C:156:ASP:O	1:C:157:LEU:C	2.54	0.45
1:A:85:ARG:HG2	1:A:166:PHE:CD1	2.51	0.45
1:D:33:PHE:HZ	1:D:50:VAL:HG22	1.82	0.45
1:B:132:HIS:HE1	1:B:202:GLU:OE2	1.99	0.45
1:A:140:ASP:O	2:A:400:BLA:O1D	2.35	0.45
1:D:138:LEU:H	1:D:138:LEU:CD2	2.30	0.45
1:C:141:LEU:HD13	1:C:141:LEU:O	2.16	0.45
1:B:47:PHE:HZ	1:B:167:PHE:HE2	1.64	0.45
1:D:16:ALA:HB2	1:D:196:ARG:NH2	2.32	0.45
1:B:69:LYS:HE3	1:B:78:TYR:CE2	2.51	0.45
1:D:200:ILE:HD12	1:D:200:ILE:N	2.32	0.45
1:A:46:GLY:O	1:A:50:VAL:HG13	2.17	0.45
1:D:22:LYS:H	1:D:22:LYS:HG3	1.49	0.44
1:D:138:LEU:N	1:D:138:LEU:CD2	2.80	0.44
1:A:136:ARG:NH1	2:A:400:BLA:CMC	2.78	0.44
1:B:149:LYS:O	1:B:153:LYS:NZ	2.51	0.44
1:D:71:SER:OG	1:D:73:VAL:HG22	2.18	0.44
1:D:27:GLN:HE21	1:D:211:ILE:HG21	1.82	0.44
1:D:174:SER:CB	1:D:177:LYS:HD2	2.48	0.44
1:D:196:ARG:HG2	1:D:196:ARG:NH1	2.33	0.44
1:D:84:HIS:C	1:D:85:ARG:HD2	2.38	0.44
1:D:44:ARG:HD3	1:D:155:LEU:HB2	1.99	0.44
1:D:153:LYS:CD	1:D:153:LYS:H	2.24	0.44
1:A:108:THR:HG21	1:A:220:LEU:HD11	1.99	0.44
1:B:174:SER:OG	1:B:177:LYS:HG2	2.18	0.44
1:D:32:GLU:O	1:D:33:PHE:HB2	2.18	0.43
1:A:28:ALA:HA	1:A:211:ILE:HG12	2.00	0.43
1:A:57:ILE:CD1	2:A:400:BLA:HMC1	2.48	0.43
1:D:16:ALA:HB1	1:D:200:ILE:HG13	1.96	0.43
1:C:96:TRP:CZ2	1:C:157:LEU:HD11	2.53	0.43
1:D:65:ILE:HG23	1:D:74:PHE:CE2	2.53	0.43
1:B:183:ARG:HA	1:B:186:MET:HG2	2.00	0.43
2:A:400:BLA:HHA	3:A:451:HOH:O	2.18	0.43
1:D:124:THR:C	1:D:126:PRO:HD3	2.39	0.43
1:A:55:TYR:O	1:A:59:VAL:HG23	2.18	0.43
1:C:113:ARG:HG3	1:C:114:TYR:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PHE:HE2	1:B:50:VAL:CG1	2.31	0.43
1:B:85:ARG:HD2	1:B:169:PHE:CZ	2.53	0.43
1:C:216:GLU:O	1:C:220:LEU:HG	2.19	0.43
1:D:32:GLU:HB3	1:D:218:GLN:HE21	1.82	0.43
1:C:35:ARG:O	1:C:39:LYS:CD	2.65	0.43
1:A:10:PRO:HG2	1:A:15:GLU:C	2.39	0.43
1:D:104:VAL:O	1:D:104:VAL:HG22	2.19	0.43
1:B:145:GLN:C	1:B:149:LYS:HE3	2.39	0.43
1:A:167:PHE:HE1	2:A:400:BLA:HAD1	1.84	0.42
1:C:37:PHE:O	1:C:37:PHE:HD1	2.02	0.42
1:D:17:LEU:CD2	1:D:200:ILE:HA	2.49	0.42
1:C:85:ARG:HG2	1:C:166:PHE:CD1	2.54	0.42
1:B:33:PHE:CE2	1:B:50:VAL:CG1	3.02	0.42
1:D:71:SER:HA	1:D:72:PRO:HD3	1.91	0.42
1:A:135:THR:O	2:A:400:BLA:OB	2.37	0.42
1:C:56:HIS:HE1	1:C:106:PRO:O	2.02	0.42
1:C:145:GLN:OE1	1:C:145:GLN:N	2.53	0.42
1:D:57:ILE:HG21	1:D:136:ARG:HD2	2.02	0.42
1:B:16:ALA:HB2	1:B:196:ARG:NH2	2.35	0.42
1:B:33:PHE:HE2	1:B:50:VAL:HG11	1.84	0.42
1:C:101:TRP:HA	1:C:104:VAL:HG12	2.02	0.42
1:C:23:GLU:HB3	3:C:285:HOH:O	2.19	0.42
1:D:149:LYS:HD3	1:D:153:LYS:HZ3	1.83	0.42
1:A:156:ASP:O	1:A:156:ASP:OD1	2.37	0.42
1:C:127:GLU:CD	1:C:127:GLU:H	2.23	0.42
1:B:152:GLN:HG2	1:B:152:GLN:H	1.47	0.42
1:D:117:ARG:O	1:D:121:VAL:HG23	2.20	0.42
1:A:157:LEU:N	1:A:157:LEU:HD12	2.35	0.42
1:D:217:LEU:O	1:D:218:GLN:CB	2.67	0.42
1:D:34:MET:CE	1:D:37:PHE:HB3	2.50	0.42
1:D:11:GLN:O	1:D:196:ARG:NH2	2.52	0.42
1:A:57:ILE:HD13	1:A:114:TYR:CE2	2.54	0.41
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.82	0.41
1:D:117:ARG:NH1	1:D:202:GLU:OE1	2.53	0.41
1:D:23:GLU:C	1:D:25:HIS:H	2.23	0.41
1:A:109:PRO:HG2	1:A:216:GLU:OE2	2.20	0.41
1:D:114:TYR:CD1	1:D:209:LEU:HD13	2.56	0.41
1:A:191:MET:CE	1:A:199:VAL:HG21	2.51	0.41
1:B:55:TYR:HB2	1:B:93:LEU:HD11	2.01	0.41
1:A:54:LEU:HD13	1:A:166:PHE:CZ	2.56	0.41
1:D:200:ILE:CD1	1:D:200:ILE:N	2.83	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ALA:HB3	1:D:216:GLU:OE1	2.21	0.41
1:A:132:HIS:O	1:A:136:ARG:HB2	2.20	0.41
1:A:10:PRO:CG	1:A:16:ALA:HA	2.50	0.41
1:D:146:VAL:CG1	1:D:147:LEU:N	2.84	0.41
1:D:207:PHE:O	1:D:211:ILE:HG13	2.21	0.41
1:A:183:ARG:HD3	3:A:429:HOH:O	2.19	0.41
1:C:64:GLU:OE1	1:C:122:GLY:HA3	2.21	0.41
1:D:44:ARG:HE	1:D:155:LEU:HB2	1.85	0.41
1:B:138:LEU:CD1	1:B:179:LYS:HG3	2.45	0.40
1:D:49:LEU:HD23	1:D:106:PRO:HG3	2.03	0.40
1:D:55:TYR:O	1:D:59:VAL:HG23	2.20	0.40
1:B:16:ALA:HB2	1:B:196:ARG:HH22	1.86	0.40
1:A:138:LEU:HG	1:A:179:LYS:HG2	2.02	0.40
1:D:48:LYS:HB3	1:D:97:TYR:OH	2.21	0.40
1:C:92:ASP:O	1:C:95:PHE:HB3	2.21	0.40
1:D:158:PRO:HG2	1:D:160:SER:OG	2.21	0.40
1:C:34:MET:HB2	1:C:34:MET:HE2	1.94	0.40
1:C:37:PHE:C	1:C:37:PHE:CD1	2.94	0.40
1:C:37:PHE:HD1	1:C:37:PHE:C	2.25	0.40
2:A:400:BLA:HBA1	3:A:451:HOH:O	2.16	0.40
1:C:10:PRO:CG	1:C:15:GLU:HG2	2.50	0.40
1:B:44:ARG:HH12	1:B:48:LYS:HZ2	1.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/233 (91%)	206 (97%)	5 (2%)	1 (0%)	34	35
1	B	212/233 (91%)	202 (95%)	7 (3%)	3 (1%)	14	10
1	C	212/233 (91%)	205 (97%)	5 (2%)	2 (1%)	21	19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	211/233 (91%)	189 (90%)	15 (7%)	7 (3%)	5	2
All	All	847/932 (91%)	802 (95%)	32 (4%)	13 (2%)	13	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	B	154	ALA
1	C	157	LEU
1	D	20	ALA
1	D	33	PHE
1	B	11	GLN
1	C	175	ALA
1	D	12	ASP
1	D	144	GLY
1	D	218	GLN
1	B	156	ASP
1	D	152	GLN
1	D	156	ASP

### 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	A	184/202 (91%)	171 (93%)	13 (7%)	18	19
1	B	184/202 (91%)	175 (95%)	9 (5%)	31	36
1	C	184/202 (91%)	177 (96%)	7 (4%)	40	49
1	D	183/202 (91%)	171 (93%)	12 (7%)	21	22
All	All	735/808 (91%)	694 (94%)	41 (6%)	26	29

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	13	LEU
1	A	37	PHE
1	A	85	ARG
1	A	93	LEU
1	A	102	GLN
1	A	114	TYR
1	A	118	LEU
1	A	127	GLU
1	A	136	ARG
1	A	147	LEU
1	A	177	LYS
1	A	197	GLN
1	B	15	GLU
1	B	37	PHE
1	B	69	LYS
1	B	114	TYR
1	B	118	LEU
1	B	136	ARG
1	B	138	LEU
1	B	152	GLN
1	B	156	ASP
1	C	37	PHE
1	C	85	ARG
1	C	113	ARG
1	C	114	TYR
1	C	118	LEU
1	C	145	GLN
1	C	153	LYS
1	D	15	GLU
1	D	22	LYS
1	D	37	PHE
1	D	38	GLN
1	D	45	ASP
1	D	50	VAL
1	D	61	LEU
1	D	114	TYR
1	D	157	LEU
1	D	196	ARG
1	D	197	GLN
1	D	218	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	68	ASN
1	A	84	HIS
1	A	102	GLN
1	A	132	HIS
1	A	152	GLN
1	A	180	GLN
1	A	197	GLN
1	A	210	ASN
1	B	36	ASN
1	B	41	GLN
1	B	56	HIS
1	B	68	ASN
1	B	91	GLN
1	B	102	GLN
1	B	132	HIS
1	B	171	ASN
1	B	212	GLN
1	C	11	GLN
1	C	27	GLN
1	C	30	ASN
1	C	36	ASN
1	C	41	GLN
1	C	56	HIS
1	C	84	HIS
1	C	102	GLN
1	C	132	HIS
1	C	171	ASN
1	C	180	GLN
1	D	11	GLN
1	D	27	GLN
1	D	41	GLN
1	D	56	HIS
1	D	68	ASN
1	D	152	GLN
1	D	197	GLN
1	D	210	ASN
1	D	212	GLN
1	D	218	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	BLA	A	400	-	35,46,46	2.51	8 (22%)	43,67,67	4.22	14 (32%)

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	BLA	A	400	-	-	0/22/74/74	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	BLA	C4B-NB	-2.97	1.31	1.37
2	A	400	BLA	C3B-C2B	2.29	1.41	1.36
2	A	400	BLA	C1B-NB	2.46	1.42	1.37
2	A	400	BLA	C1D-ND	2.72	1.43	1.37
2	A	400	BLA	C1B-C2B	2.77	1.50	1.45
2	A	400	BLA	CHB-C1B	2.79	1.40	1.34
2	A	400	BLA	CBC-CAC	3.33	1.46	1.30
2	A	400	BLA	CHA-C4D	11.89	1.45	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	BLA	CAA-C2A-C1A	-18.67	106.74	127.01
2	A	400	BLA	CHD-C1D-ND	-12.72	100.68	124.91
2	A	400	BLA	CHD-C4C-NC	-10.82	102.72	126.16
2	A	400	BLA	CHB-C1B-NB	-5.76	109.55	130.87
2	A	400	BLA	C1B-NB-C4B	-4.22	104.56	110.73
2	A	400	BLA	CHD-C1D-C2D	-3.36	116.68	124.88
2	A	400	BLA	OB-C4B-NB	-3.31	116.35	125.14
2	A	400	BLA	CHA-C4D-ND	-2.63	123.96	128.67
2	A	400	BLA	C4C-NC-C1C	-2.35	107.29	110.73
2	A	400	BLA	CBC-CAC-C3C	-2.07	116.51	127.01
2	A	400	BLA	CAD-CBD-CGD	-2.03	109.02	112.75
2	A	400	BLA	CMB-C2B-C1B	2.17	127.09	124.20
2	A	400	BLA	CAB-C3B-C2B	2.26	135.99	128.41
2	A	400	BLA	C4C-CHD-C1D	2.68	135.00	128.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	BLA	33	0

## 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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.