



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:28 AM 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 validation 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>

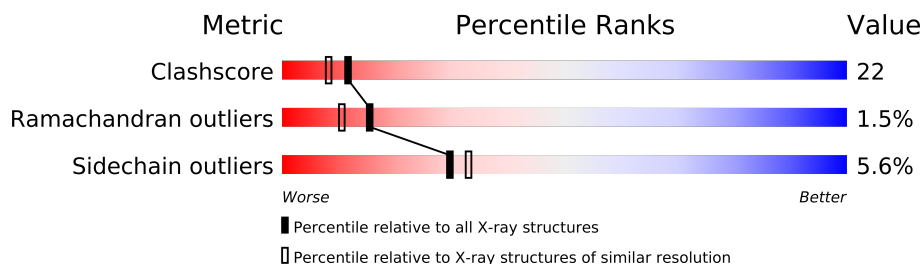
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (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 ≥ 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 was not executed.

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

2 Entry composition i

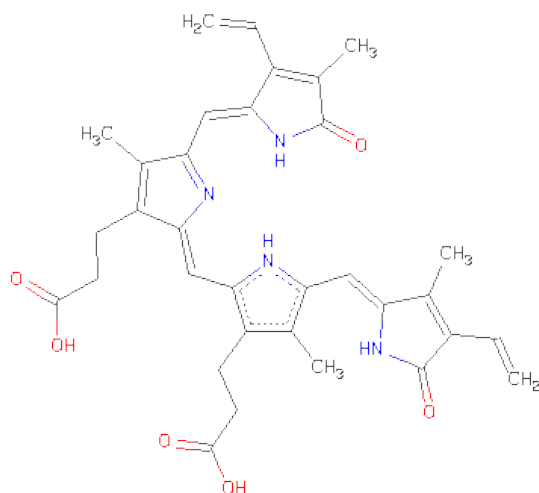
There are 3 unique types of molecules in this entry. The entry contains 7341 atoms, of which 0 are hydrogen and 0 are deuterium.

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 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.

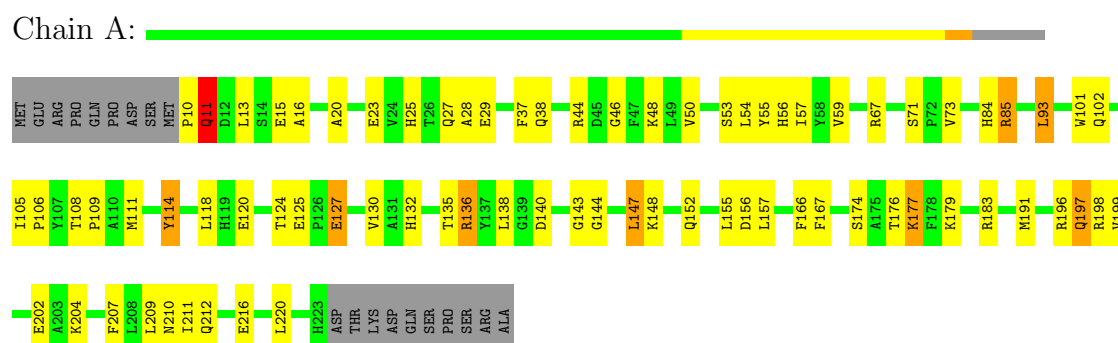
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total 103	O 103	0	0
3	B	76	Total 76	O 76	0	0
3	C	111	Total 111	O 111	0	0
3	D	35	Total 35	O 35	0	0

3 Residue-property plots

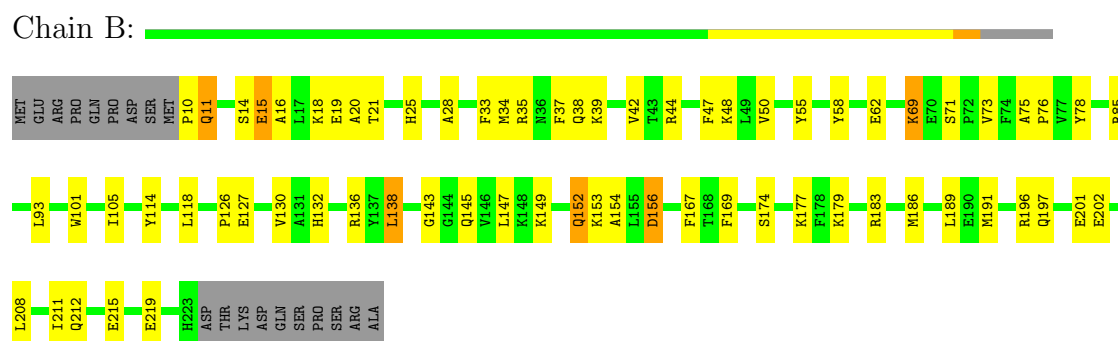
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

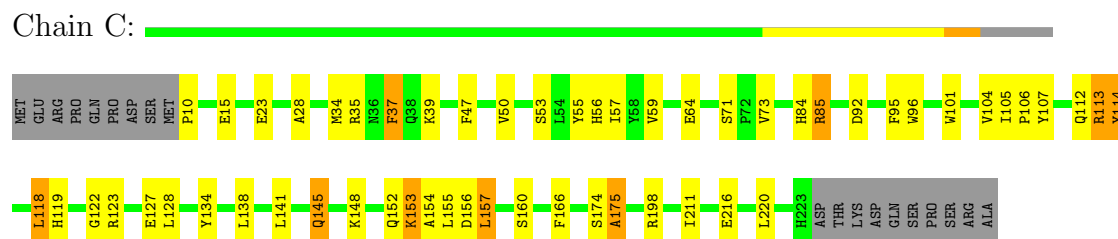
- Molecule 1: Heme oxygenase 1



- Molecule 1: Heme oxygenase 1



- Molecule 1: Heme oxygenase 1



- Molecule 1: Heme oxygenase 1



MET	GLU	ARG	PRO	GLN	PRO	ASP	SER	MET	PRO	Q11	D12	L13	S14	E15	A16	L17	K18	E19	A20	T21	K22	E23	V24	H25	T26	Q27	A28	E32	F33	K34	R35	N36	F37	Q38	Q41	R44	D45	K48	L49	V50	Y55	H56	I57	V58	V59	A60	L61	E64	I65	E66	R67	E70
S71	P72	V73	F74	A75	P76	H84	R85	L89	L93	Y97	W101	Q102	E103	V104	I105	P106	Y107	T108	P109	A110	M111	Q112	R113	Y114	V115	K116	R117	L118	H119	E120	V121	T124	E125	P126	E127	L128	R136	Y137	L138	G143	G144	Q145	V146	L147	K148	K149	Q152	K153	A154	L155		
D156	L157	P158	S159	S160	L164	F169	S174	A175	T176	K177	F178	K179	Q180	M186	L189	T192	P193	R196	Q197	R198	V199	I200	E201	E202	A203	K204	F207	L208	L209	N210	I211	Q212	E216	L217	Q218	E219	L220	L221	T222	H223	ASP	THR	LYS	ASP	GLN	SER	PRO	SER	ARG	ALA		

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, α , β , γ	77.41Å 56.46Å 109.75Å 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 ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	35	0	0	2	0
All	All	7341	0	6976	305	0

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 22.

All (305) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:35:ARG:CG	1:B:39:LYS:HE2	2.35	0.56
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

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:B:126:PRO:HG2	1:B:127:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	A	212/233 (91%)	206 (97%)	5 (2%)	1 (0%)	38	38
1	B	212/233 (91%)	202 (95%)	7 (3%)	3 (1%)	16	12
1	C	212/233 (91%)	205 (97%)	5 (2%)	2 (1%)	25	21
1	D	211/233 (91%)	189 (90%)	15 (7%)	7 (3%)	6	2
All	All	847/932 (91%)	802 (95%)	32 (4%)	13 (2%)	15	10

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%)	21	21
1	B	184/202 (91%)	175 (95%)	9 (5%)	35	40
1	C	184/202 (91%)	177 (96%)	7 (4%)	44	53
1	D	183/202 (91%)	171 (93%)	12 (7%)	24	25
All	All	735/808 (91%)	694 (94%)	41 (6%)	30	33

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

Mol	Chain	Res	Type
1	A	11	GLN
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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 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 ⓘ

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	-	46,46,46	3.19	11 (23%)	65,67,67	3.56	24 (36%)

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	-	-	0/26/74/74	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	BLA	CHA-C4D	15.32	1.45	1.35
2	A	400	BLA	O1A-CGA	10.83	1.60	1.22
2	A	400	BLA	C3C-C4C	3.46	1.52	1.45
2	A	400	BLA	CBC-CAC	3.38	1.46	1.29
2	A	400	BLA	C1A-C2A	3.29	1.50	1.42
2	A	400	BLA	C4B-NB	-2.94	1.31	1.37
2	A	400	BLA	C1B-C2B	2.75	1.50	1.45
2	A	400	BLA	C1D-ND	2.73	1.43	1.37
2	A	400	BLA	CHB-C1B	2.69	1.40	1.34
2	A	400	BLA	C3B-C2B	2.59	1.41	1.36
2	A	400	BLA	C1B-NB	2.42	1.42	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	BLA	CHD-C1D-ND	-12.77	100.68	124.99
2	A	400	BLA	O2A-CGA-O1A	-12.15	92.39	123.30
2	A	400	BLA	CHD-C4C-NC	-10.82	102.72	126.19
2	A	400	BLA	C3B-C4B-NB	8.99	114.78	106.66
2	A	400	BLA	CAA-C2A-C1A	-8.40	106.74	124.73
2	A	400	BLA	CHB-C1B-NB	-5.83	109.55	130.23
2	A	400	BLA	O1A-CGA-CBA	5.47	141.85	123.03
2	A	400	BLA	C4B-C3B-C2B	-4.47	102.25	107.97
2	A	400	BLA	C1B-NB-C4B	-4.37	104.56	110.74
2	A	400	BLA	CHD-C1D-C2D	-3.38	116.68	125.10
2	A	400	BLA	OB-C4B-NB	-3.36	116.35	125.12
2	A	400	BLA	C3B-C2B-C1B	-3.12	103.14	107.14
2	A	400	BLA	O2D-CGD-O1D	-2.95	115.80	123.30
2	A	400	BLA	C4C-CHD-C1D	2.76	135.00	128.13
2	A	400	BLA	CAB-C3B-C2B	2.72	135.99	128.75
2	A	400	BLA	C1A-C2A-C3A	-2.63	104.20	106.92
2	A	400	BLA	CHA-C4D-ND	-2.51	123.96	128.59
2	A	400	BLA	O2D-CGD-CBD	2.49	123.00	114.22
2	A	400	BLA	C4C-NC-C1C	-2.44	107.29	110.74
2	A	400	BLA	CAD-CBD-CGD	-2.43	109.02	113.53
2	A	400	BLA	CBD-CAD-C3D	-2.21	106.18	112.71
2	A	400	BLA	C2A-C1A-NA	2.20	110.42	106.79
2	A	400	BLA	CBC-CAC-C3C	-2.13	116.51	127.09
2	A	400	BLA	CMB-C2B-C1B	2.09	127.09	124.23

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 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.