



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:15 AM GMT

PDB ID : 3A18
Title : Crystal Structure of Aldoxime Dehydratase (OxdRE) in Complex with Butyraldoxime (soaked crystal)
Authors : Sawai, H.; Sugimoto, H.; Kato, Y.; Asano, Y.; Shiro, Y.; Aono, S.
Deposited on : 2009-03-26
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

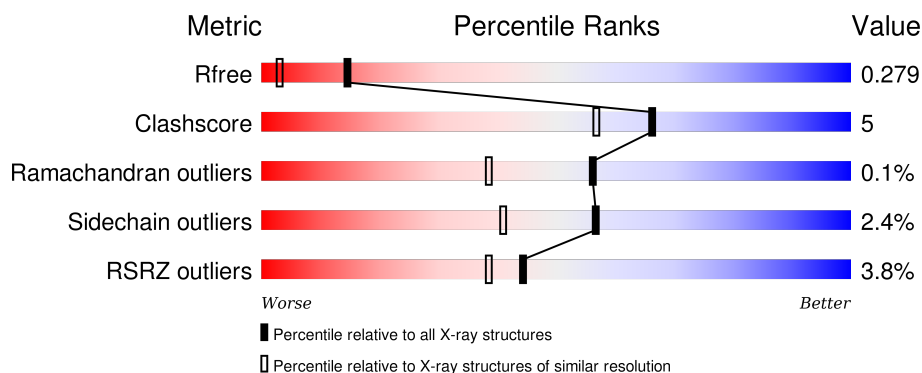
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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.

Mol	Chain	Length	Quality of chain
1	A	373	 3% 83% 10% • 5%
1	B	373	 2% 83% 10% • 5%
1	C	373	 5% 86% 8% • 5%
1	D	373	 4% 82% 12% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12589 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 Aldoxime dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	15	0
			2928	1848	515	553	12			
1	B	353	Total	C	N	O	S	0	4	0
			2843	1790	504	537	12			
1	C	353	Total	C	N	O	S	0	2	0
			2828	1779	500	537	12			
1	D	352	Total	C	N	O	S	0	16	0
			2926	1850	515	549	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
A	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
A	-17	SER	-	EXPRESSION TAG	UNP Q76K71
A	-16	SER	-	EXPRESSION TAG	UNP Q76K71
A	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-9	SER	-	EXPRESSION TAG	UNP Q76K71
A	-8	SER	-	EXPRESSION TAG	UNP Q76K71
A	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
A	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
A	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
A	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
A	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
A	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
A	-1	SER	-	EXPRESSION TAG	UNP Q76K71
A	0	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-19	MET	-	INITIATING METHIONINE	UNP Q76K71

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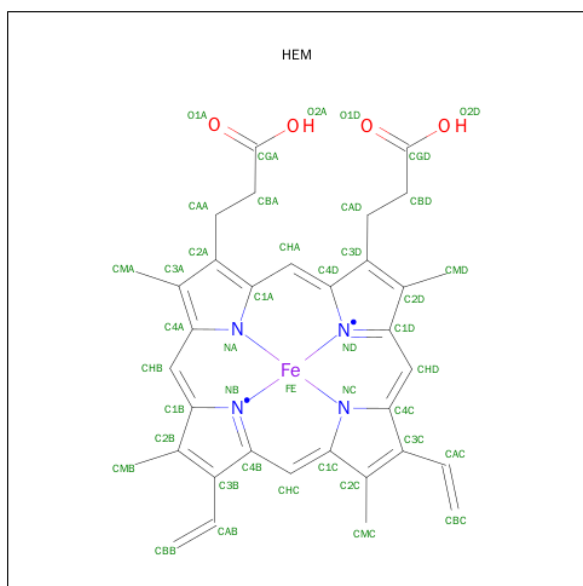
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
B	-17	SER	-	EXPRESSION TAG	UNP Q76K71
B	-16	SER	-	EXPRESSION TAG	UNP Q76K71
B	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-9	SER	-	EXPRESSION TAG	UNP Q76K71
B	-8	SER	-	EXPRESSION TAG	UNP Q76K71
B	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
B	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
B	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
B	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
B	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
B	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
B	-1	SER	-	EXPRESSION TAG	UNP Q76K71
B	0	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
C	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
C	-17	SER	-	EXPRESSION TAG	UNP Q76K71
C	-16	SER	-	EXPRESSION TAG	UNP Q76K71
C	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-9	SER	-	EXPRESSION TAG	UNP Q76K71
C	-8	SER	-	EXPRESSION TAG	UNP Q76K71
C	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
C	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
C	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
C	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
C	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
C	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
C	-1	SER	-	EXPRESSION TAG	UNP Q76K71
C	0	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
D	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
D	-17	SER	-	EXPRESSION TAG	UNP Q76K71

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q76K71
D	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-9	SER	-	EXPRESSION TAG	UNP Q76K71
D	-8	SER	-	EXPRESSION TAG	UNP Q76K71
D	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
D	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
D	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
D	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
D	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
D	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
D	-1	SER	-	EXPRESSION TAG	UNP Q76K71
D	0	HIS	-	EXPRESSION TAG	UNP Q76K71

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



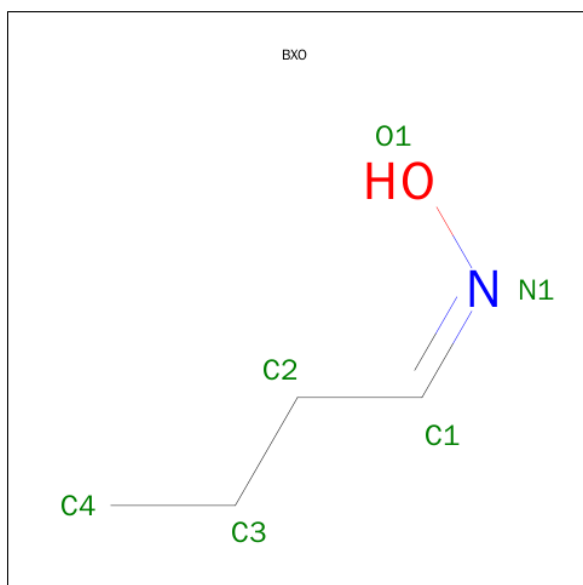
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (1Z)-BUTANAL OXIME (three-letter code: BXO) (formula: C₄H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	4	1	1		
3	B	1	Total	C	N	O	0	0
			6	4	1	1		
3	C	1	Total	C	N	O	0	0
			6	4	1	1		
3	D	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	238	Total	O	0	0
			238	238		
4	B	225	Total	O	0	0
			225	225		
4	C	214	Total	O	0	0
			214	214		

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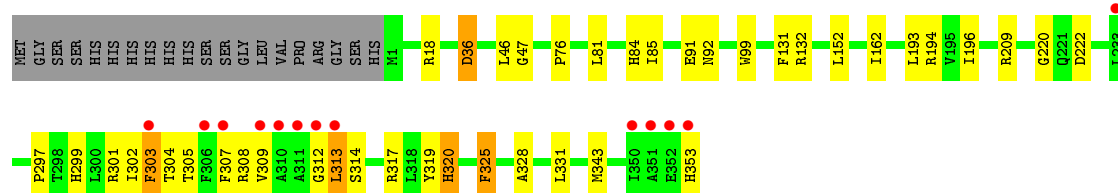
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	191	Total	O	0	0
			191	191		

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.

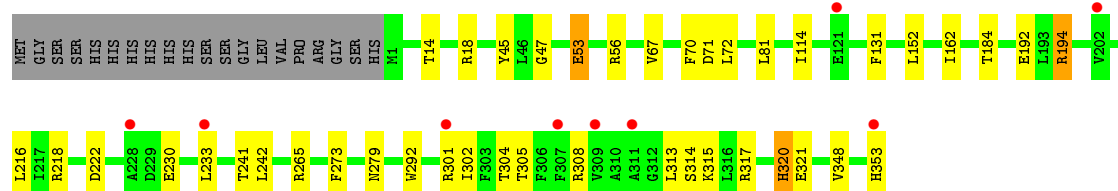
• Molecule 1: Aldoxime dehydratase

Chain A: 




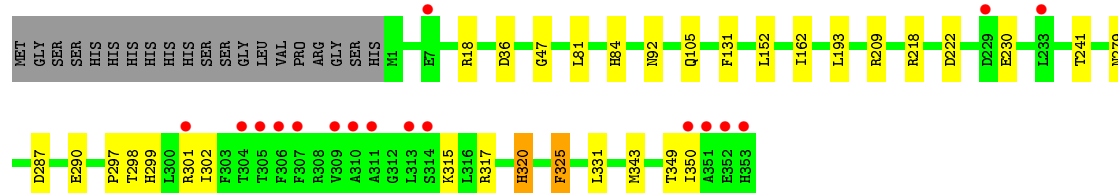
• Molecule 1: Aldoxime dehydratase

Chain B: 




• Molecule 1: Aldoxime dehydratase

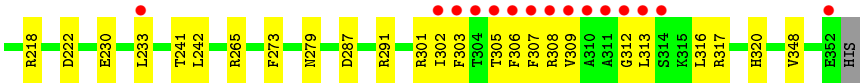
Chain C: 



• Molecule 1: Aldoxime dehydratase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 148.57Å 79.11Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	19.93 – 1.80 19.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.93-1.80) 98.8 (19.93-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.280 0.247 , 0.279	Depositor DCC
R_{free} test set	6625 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.5	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 132702 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12589	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	2/3017 (0.1%)	0.58	2/4103 (0.0%)
1	B	0.40	0/2932	0.56	0/3985
1	C	0.44	3/2911 (0.1%)	0.57	0/3959
1	D	0.40	0/3017	0.56	0/4103
All	All	0.42	5/11877 (0.0%)	0.57	2/16150 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	325	PHE	CE1-CZ	-5.51	1.26	1.37
1	A	325	PHE	CG-CD1	-5.34	1.30	1.38
1	C	325	PHE	CG-CD2	-5.29	1.30	1.38
1	C	325	PHE	CE2-CZ	-5.13	1.27	1.37
1	A	325	PHE	CE2-CZ	-5.04	1.27	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313[A]	LEU	C-N-CA	-5.68	107.50	121.70
1	A	313[B]	LEU	C-N-CA	-5.68	107.50	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2928	0	2764	36	0
1	B	2843	0	2691	30	0
1	C	2828	0	2663	18	0
1	D	2926	0	2779	41	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	6	0	9	0	0
3	B	6	0	9	0	0
3	C	6	0	9	0	0
3	D	6	0	9	0	0
4	A	238	0	0	0	0
4	B	225	0	0	2	0
4	C	214	0	0	3	0
4	D	191	0	0	0	0
All	All	12589	0	11053	111	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 5.

All (111) 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:C:241:THR:HG23	4:C:374:HOH:O	1.81	0.78
1:B:241:THR:HG22	1:B:301:ARG:HH21	1.48	0.77
1:A:36[B]:ASP:CG	1:D:194:ARG:HH21	1.89	0.75
1:D:241:THR:HG22	1:D:301:ARG:HH21	1.50	0.74
1:D:301:ARG:O	1:D:305[A]:THR:N	2.18	0.70
1:B:218[B]:ARG:HB2	1:B:321:GLU:HG2	1.74	0.69
1:B:301:ARG:O	1:B:304:THR:HB	1.93	0.69
1:D:105:GLN:HE21	1:D:105:GLN:C	1.96	0.68
1:B:45:TYR:OH	1:B:218[B]:ARG:HD2	1.94	0.67
1:A:303[A]:PHE:CE2	1:A:307[A]:PHE:CE1	2.83	0.66
1:B:241:THR:HG22	1:B:301:ARG:NH2	2.10	0.66
1:A:209:ARG:NH1	1:D:184:THR:HB	2.09	0.66
1:A:36[B]:ASP:OD2	1:D:209[B]:ARG:HD2	1.96	0.66
1:D:305[A]:THR:O	1:D:309[A]:VAL:HG22	1.96	0.66
1:B:241:THR:HG23	4:B:713:HOH:O	1.96	0.65
1:D:192:GLU:OE2	1:D:348:VAL:HG21	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302[A]:ILE:O	1:D:306[A]:PHE:HB2	1.97	0.64
1:A:36[B]:ASP:OD1	1:D:194:ARG:NH2	2.29	0.61
1:D:241:THR:HG22	1:D:301:ARG:NH2	2.14	0.60
1:D:242:LEU:HD13	2:D:354:HEM:HAB	1.85	0.59
1:B:302:ILE:HD12	2:B:354:HEM:C3B	2.38	0.59
1:A:305[A]:THR:O	1:A:309[A]:VAL:HG22	2.02	0.59
1:A:194:ARG:HD2	4:C:732:HOH:O	2.01	0.59
1:B:184:THR:HG22	4:B:641:HOH:O	2.03	0.59
1:C:152:LEU:HD21	1:C:162:ILE:HD13	1.85	0.58
1:B:302:ILE:HD12	2:B:354:HEM:C4B	2.38	0.58
1:A:209:ARG:NH2	1:D:184:THR:O	2.32	0.58
1:B:194:ARG:HB3	1:B:348:VAL:HG22	1.86	0.57
1:A:305[B]:THR:HG23	1:A:308[B]:ARG:HH21	1.69	0.56
1:D:48:VAL:HB	1:D:93[B]:LEU:HD13	1.85	0.56
1:C:222:ASP:HB3	1:C:317:ARG:HB2	1.87	0.55
1:A:152:LEU:HD21	1:A:162:ILE:HD13	1.88	0.55
1:A:222:ASP:HB3	1:A:317:ARG:HB2	1.88	0.55
1:A:209:ARG:HH12	1:D:184:THR:HB	1.71	0.55
1:B:192:GLU:OE2	1:B:348:VAL:HG21	2.07	0.54
1:D:222:ASP:HB3	1:D:317:ARG:HB2	1.89	0.54
1:D:302[A]:ILE:O	1:D:306[A]:PHE:CB	2.56	0.54
1:C:297:PRO:O	1:C:301:ARG:HB2	2.08	0.54
1:B:265:ARG:HG2	1:B:273:PHE:CD1	2.43	0.53
1:A:84:HIS:CE1	1:A:92:ASN:HB2	2.43	0.53
1:B:192:GLU:O	1:B:194:ARG:HG2	2.08	0.53
1:D:313[B]:LEU:HD11	1:D:316:LEU:HD23	1.91	0.53
1:C:18:ARG:HD2	1:D:18:ARG:HD2	1.91	0.52
1:A:36[B]:ASP:OD2	1:D:194:ARG:NH2	2.43	0.52
1:C:299:HIS:HA	1:C:302:ILE:HD12	1.92	0.52
1:B:222:ASP:HB3	1:B:317:ARG:HB2	1.90	0.52
1:A:18:ARG:HD2	1:B:18:ARG:HD2	1.91	0.52
1:A:297:PRO:O	1:A:301:ARG:HB2	2.10	0.52
1:B:305:THR:HA	1:B:308:ARG:HG2	1.94	0.50
1:C:84:HIS:CE1	1:C:92:ASN:HB2	2.47	0.49
1:A:85:ILE:HG12	1:A:91:GLU:HG2	1.94	0.49
1:C:298:THR:O	1:C:302:ILE:HG13	2.12	0.49
1:C:241:THR:HG22	1:C:301:ARG:CZ	2.43	0.49
1:A:196:ILE:HG21	1:D:14:THR:HG23	1.94	0.49
1:A:299:HIS:HA	1:A:302[A]:ILE:HD12	1.94	0.48
1:B:242:LEU:HD13	2:B:354:HEM:HAB	1.94	0.48
1:D:105:GLN:C	1:D:105:GLN:NE2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36[A]:ASP:OD2	1:D:209[A]:ARG:HD3	2.13	0.48
1:B:216:LEU:HG	1:B:218[B]:ARG:NE	2.29	0.48
1:C:302:ILE:HG23	2:C:354:HEM:HBB2	1.97	0.47
1:B:72:LEU:HD12	1:B:114:ILE:HD11	1.96	0.47
1:B:314:SER:OG	1:B:315[B]:LYS:HD2	2.14	0.47
1:B:53:GLU:OE1	1:B:56:ARG:NE	2.48	0.47
1:A:299:HIS:HA	1:A:302[B]:ILE:HD12	1.96	0.46
1:D:265:ARG:HG2	1:D:273:PHE:CD1	2.51	0.46
1:A:193:LEU:HD21	1:A:343:MET:HG3	1.97	0.46
1:C:279:ASN:OD1	2:C:354:HEM:HAC	2.16	0.45
1:A:320:HIS:CD2	1:A:320:HIS:C	2.89	0.45
1:B:152:LEU:HD21	1:B:162:ILE:HD13	1.97	0.45
1:B:67:VAL:O	1:B:70:PHE:HB2	2.17	0.45
1:C:209:ARG:HG3	4:C:679:HOH:O	2.17	0.45
1:D:152:LEU:HD21	1:D:162:ILE:HD13	1.98	0.45
1:D:230:GLU:HA	1:D:233:LEU:HD12	2.00	0.44
1:D:302[B]:ILE:HD12	2:D:354:HEM:C3B	2.52	0.44
1:D:218:ARG:HA	1:D:279:ASN:O	2.18	0.44
1:D:8:HIS:CE1	1:D:36:ASP:HA	2.53	0.44
1:A:209:ARG:CD	1:D:14:THR:HG21	2.48	0.43
1:D:67:VAL:O	1:D:70:PHE:HB2	2.18	0.43
1:A:305[B]:THR:O	1:A:309[B]:VAL:HG22	2.18	0.43
1:A:309[A]:VAL:O	1:A:313[A]:LEU:N	2.45	0.43
1:D:287:ASP:O	1:D:291:ARG:HG2	2.17	0.43
1:D:47:GLY:HA3	1:D:131:PHE:CZ	2.53	0.43
1:C:193:LEU:HD21	1:C:343:MET:HG3	2.01	0.43
1:B:218[A]:ARG:HB3	1:B:321:GLU:HG2	2.00	0.43
1:A:47:GLY:HA3	1:A:131:PHE:CZ	2.54	0.43
1:C:320:HIS:C	1:C:320:HIS:CD2	2.91	0.43
1:D:305[A]:THR:HG23	1:D:308[A]:ARG:HH21	1.84	0.43
1:A:302[A]:ILE:HG23	2:A:354:HEM:HBB2	2.01	0.43
1:B:230:GLU:HA	1:B:233:LEU:HD12	2.01	0.43
1:D:312[A]:GLY:O	1:D:313[A]:LEU:HD23	2.19	0.42
1:D:241:THR:OG1	1:D:302[B]:ILE:HG23	2.18	0.42
1:C:287:ASP:HA	1:C:290:GLU:OE1	2.19	0.42
1:D:303[B]:PHE:CZ	1:D:307[B]:PHE:CE1	3.07	0.42
1:D:72:LEU:HD12	1:D:114:ILE:HD11	2.02	0.42
1:A:36[A]:ASP:OD2	1:D:194:ARG:NH2	2.52	0.42
1:A:302[B]:ILE:HG23	2:A:354:HEM:HBB2	2.02	0.42
1:A:46:LEU:HD12	1:A:132:ARG:HG2	2.01	0.42
1:A:76:PRO:HD3	1:A:99:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302[A]:ILE:HD12	2:D:354:HEM:C3B	2.55	0.41
1:B:292:TRP:CZ3	2:B:354:HEM:HBC2	2.55	0.41
1:B:218[A]:ARG:HA	1:B:279:ASN:O	2.21	0.41
1:A:312[A]:GLY:O	1:A:313[A]:LEU:C	2.58	0.41
1:C:218:ARG:HA	1:C:279:ASN:O	2.21	0.41
1:B:47:GLY:HA3	1:B:131:PHE:CZ	2.55	0.41
1:C:47:GLY:HA3	1:C:131:PHE:CZ	2.55	0.41
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.96	0.41
1:B:320:HIS:C	1:B:320:HIS:CD2	2.94	0.41
1:A:209:ARG:NH1	1:A:328:ALA:HA	2.36	0.40
1:A:220:GLY:HA3	1:A:319:TYR:CE1	2.56	0.40
1:C:230:GLU:CD	1:C:315:LYS:H	2.25	0.40
1:A:36[B]:ASP:CG	1:D:194:ARG:NH2	2.66	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	366/373 (98%)	360 (98%)	5 (1%)	1 (0%)	46	29
1	B	355/373 (95%)	348 (98%)	7 (2%)	0	100	100
1	C	353/373 (95%)	344 (98%)	9 (2%)	0	100	100
1	D	366/373 (98%)	355 (97%)	11 (3%)	0	100	100
All	All	1440/1492 (96%)	1407 (98%)	32 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	SER

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	307/312 (98%)	296 (96%)	11 (4%)	42	24
1	B	299/312 (96%)	292 (98%)	7 (2%)	58	42
1	C	297/312 (95%)	288 (97%)	9 (3%)	48	31
1	D	307/312 (98%)	302 (98%)	5 (2%)	70	59
All	All	1210/1248 (97%)	1178 (97%)	32 (3%)	57	37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36[A]	ASP
1	A	36[B]	ASP
1	A	81	LEU
1	A	303[A]	PHE
1	A	303[B]	PHE
1	A	304[A]	THR
1	A	304[B]	THR
1	A	320	HIS
1	A	325	PHE
1	A	331	LEU
1	A	353	HIS
1	B	14	THR
1	B	53	GLU
1	B	71	ASP
1	B	81	LEU
1	B	194	ARG
1	B	320	HIS
1	B	353	HIS
1	C	36[A]	ASP
1	C	36[B]	ASP
1	C	81	LEU
1	C	105	GLN
1	C	320	HIS
1	C	325	PHE

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Mol	Chain	Res	Type
1	C	331	LEU
1	C	349	THR
1	C	350	ILE
1	D	14	THR
1	D	71	ASP
1	D	81	LEU
1	D	105	GLN
1	D	320	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	HIS
1	B	353	HIS
1	C	105	GLN
1	D	105	GLN
1	D	288	GLN

5.3.3 RNA [i](#)

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](#)

8 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	HEM	A	354	1,3	30,50,50	2.19	7 (23%)	24,82,82	2.46	10 (41%)
3	BXO	A	355	2	4,5,5	0.33	0	2,4,4	9.29	1 (50%)
2	HEM	B	354	1,3	30,50,50	2.12	7 (23%)	24,82,82	2.45	9 (37%)
3	BXO	B	355	2	4,5,5	0.17	0	2,4,4	8.30	1 (50%)
2	HEM	C	354	1,3	30,50,50	2.23	6 (20%)	24,82,82	2.45	9 (37%)
3	BXO	C	355	2	4,5,5	0.38	0	2,4,4	9.10	1 (50%)
2	HEM	D	354	1,3	30,50,50	2.10	7 (23%)	24,82,82	2.38	7 (29%)
3	BXO	D	355	2	4,5,5	0.22	0	2,4,4	8.52	1 (50%)

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	HEM	A	354	1,3	-	0/10/54/54	0/0/8/8
3	BXO	A	355	2	-	0/2/3/3	0/0/0/0
2	HEM	B	354	1,3	-	0/10/54/54	0/0/8/8
3	BXO	B	355	2	-	0/2/3/3	0/0/0/0
2	HEM	C	354	1,3	-	0/10/54/54	0/0/8/8
3	BXO	C	355	2	-	0/2/3/3	0/0/0/0
2	HEM	D	354	1,3	-	0/10/54/54	0/0/8/8
3	BXO	D	355	2	-	0/2/3/3	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	354	HEM	C3B-C4B	-7.42	1.45	1.51
2	C	354	HEM	C3B-C4B	-7.24	1.45	1.51
2	A	354	HEM	C3B-C4B	-7.21	1.45	1.51
2	D	354	HEM	C3B-C4B	-7.06	1.45	1.51
2	C	354	HEM	C3D-C4D	-5.59	1.44	1.51
2	A	354	HEM	C3D-C4D	-5.49	1.44	1.51
2	D	354	HEM	C3D-C4D	-5.26	1.44	1.51
2	B	354	HEM	C3D-C4D	-5.06	1.45	1.51
2	C	354	HEM	C2C-C1C	-4.12	1.44	1.52
2	A	354	HEM	C2C-C1C	-3.88	1.45	1.52
2	D	354	HEM	C2C-C1C	-3.83	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	354	HEM	C2C-C1C	-3.60	1.45	1.52
2	B	354	HEM	C2D-C1D	-2.20	1.44	1.51
2	A	354	HEM	C2D-C1D	-2.15	1.44	1.51
2	D	354	HEM	C2D-C1D	-2.04	1.45	1.51
2	B	354	HEM	C3B-CAB	2.00	1.55	1.51
2	D	354	HEM	CAA-C2A	2.02	1.55	1.52
2	A	354	HEM	FE-ND	2.03	2.08	1.97
2	C	354	HEM	C4C-NC	2.09	1.38	1.36
2	B	354	HEM	C3C-CAC	2.11	1.55	1.51
2	C	354	HEM	C1C-NC	2.14	1.38	1.36
2	D	354	HEM	C1C-NC	2.15	1.38	1.36
2	A	354	HEM	C3B-CAB	2.25	1.55	1.51
2	A	354	HEM	FE-NC	2.27	2.04	1.95
2	C	354	HEM	FE-NC	2.32	2.04	1.95
2	D	354	HEM	C3B-CAB	2.32	1.55	1.51
2	B	354	HEM	FE-NC	2.38	2.05	1.95

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	354	HEM	CBA-CAA-C2A	-4.70	104.10	112.53
2	D	354	HEM	CBA-CAA-C2A	-4.08	105.22	112.53
2	C	354	HEM	CBA-CAA-C2A	-3.61	106.05	112.53
2	A	354	HEM	CBA-CAA-C2A	-3.30	106.62	112.53
2	C	354	HEM	C3B-CAB-CBB	-2.79	120.17	124.46
2	A	354	HEM	C3B-CAB-CBB	-2.60	120.47	124.46
2	B	354	HEM	C3C-CAC-CBC	-2.39	120.79	124.46
2	A	354	HEM	C3C-CAC-CBC	-2.32	120.90	124.46
2	B	354	HEM	C2C-C1C-CHC	2.31	127.20	123.68
2	B	354	HEM	C2D-C3D-C4D	2.42	105.60	101.50
2	C	354	HEM	C2D-C3D-C4D	2.43	105.62	101.50
2	D	354	HEM	C2D-C3D-C4D	2.44	105.63	101.50
2	C	354	HEM	C3B-C4B-CHC	2.51	126.70	123.16
2	A	354	HEM	C3B-C4B-CHC	2.51	126.70	123.16
2	B	354	HEM	CMD-C2D-C3D	2.76	126.55	114.35
2	A	354	HEM	C2D-C3D-C4D	2.80	106.24	101.50
2	C	354	HEM	CMD-C2D-C3D	2.90	127.16	114.35
2	A	354	HEM	CMD-C2D-C3D	2.98	127.55	114.35
2	D	354	HEM	CMD-C2D-C3D	2.99	127.58	114.35
2	B	354	HEM	CMC-C2C-C3C	3.73	125.84	116.53
2	D	354	HEM	CMC-C2C-C3C	3.87	126.19	116.53
2	D	354	HEM	CAD-C3D-C4D	4.05	126.77	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	354	HEM	CMC-C2C-C3C	4.13	126.84	116.53
2	A	354	HEM	CMC-C2C-C3C	4.16	126.93	116.53
2	C	354	HEM	CAD-C3D-C4D	4.29	127.59	112.47
2	A	354	HEM	CAD-C3D-C4D	4.31	127.66	112.47
2	B	354	HEM	CAD-C3D-C2D	4.37	125.79	113.22
2	A	354	HEM	CMB-C2B-C3B	4.42	127.57	116.53
2	D	354	HEM	CMB-C2B-C3B	4.43	127.58	116.53
2	A	354	HEM	CAD-C3D-C2D	4.47	126.07	113.22
2	B	354	HEM	CAD-C3D-C4D	4.58	128.61	112.47
2	C	354	HEM	CMB-C2B-C3B	4.69	128.24	116.53
2	C	354	HEM	CAD-C3D-C2D	4.71	126.77	113.22
2	B	354	HEM	CMB-C2B-C3B	4.74	128.36	116.53
2	D	354	HEM	CAD-C3D-C2D	5.00	127.60	113.22
3	B	355	BXO	O1-N1-C1	11.73	122.96	111.69
3	D	355	BXO	O1-N1-C1	12.05	123.27	111.69
3	C	355	BXO	O1-N1-C1	12.87	124.06	111.69
3	A	355	BXO	O1-N1-C1	13.14	124.32	111.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	354	HEM	2	0
2	B	354	HEM	4	0
2	C	354	HEM	2	0
2	D	354	HEM	3	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	353/373 (94%)	0.02	13 (3%) 45 39	5, 9, 22, 31	0
1	B	353/373 (94%)	-0.03	9 (2%) 61 56	5, 9, 21, 27	0
1	C	353/373 (94%)	0.06	17 (4%) 34 28	5, 9, 22, 33	0
1	D	352/373 (94%)	0.09	15 (4%) 39 32	6, 10, 21, 28	0
All	All	1411/1492 (94%)	0.03	54 (3%) 44 38	5, 9, 21, 33	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	311[A]	ALA	12.0
1	A	353	HIS	8.9
1	C	353	HIS	7.8
1	A	311[A]	ALA	7.8
1	C	351	ALA	7.4
1	C	350	ILE	6.4
1	A	313[A]	LEU	5.9
1	D	312[A]	GLY	5.7
1	D	307[A]	PHE	5.5
1	D	313[A]	LEU	4.4
1	A	351	ALA	3.9
1	B	353	HIS	3.8
1	A	312[A]	GLY	3.7
1	B	233	LEU	3.7
1	C	301	ARG	3.7
1	A	310[A]	ALA	3.4
1	D	308[A]	ARG	3.4
1	C	310	ALA	3.1
1	D	310[A]	ALA	3.1
1	A	350	ILE	3.1
1	A	306[A]	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	121[A]	GLU	3.0
1	D	303[A]	PHE	3.0
1	C	309	VAL	3.0
1	D	306[A]	PHE	3.0
1	A	307[A]	PHE	3.0
1	D	233	LEU	3.0
1	D	304[A]	THR	2.9
1	A	352	GLU	2.9
1	C	305	THR	2.8
1	A	309[A]	VAL	2.8
1	D	309[A]	VAL	2.8
1	D	305[A]	THR	2.7
1	C	306	PHE	2.6
1	A	303[A]	PHE	2.6
1	A	233	LEU	2.6
1	B	311	ALA	2.6
1	C	352	GLU	2.5
1	C	7	GLU	2.5
1	B	307	PHE	2.5
1	C	233	LEU	2.4
1	C	311	ALA	2.4
1	D	352	GLU	2.3
1	C	313	LEU	2.3
1	D	314	SER	2.3
1	D	302[A]	ILE	2.3
1	C	314	SER	2.2
1	C	307	PHE	2.2
1	C	304	THR	2.2
1	B	202	VAL	2.2
1	B	309	VAL	2.2
1	B	228	ALA	2.1
1	C	229	ASP	2.0
1	B	301	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BXO	B	355	6/6	0.93	0.12	0.90	12,14,17,17	0
3	BXO	D	355	6/6	0.91	0.14	0.74	12,14,16,18	0
3	BXO	A	355	6/6	0.96	0.10	-0.18	8,11,15,15	0
2	HEM	B	354	43/43	0.97	0.09	-0.52	5,7,8,10	0
2	HEM	A	354	43/43	0.97	0.09	-0.53	5,7,10,10	0
2	HEM	C	354	43/43	0.98	0.08	-0.67	5,7,9,10	0
2	HEM	D	354	43/43	0.98	0.08	-0.72	5,8,9,11	0
3	BXO	C	355	6/6	0.96	0.09	-0.95	9,12,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.