



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:25 PM GMT

PDB ID : 3R9B
Title : Crystal structure of Mycobacterium smegmatis CYP164A2 in ligand free state
Authors : Agnew, C.R.J.; Warrilow, A.G.S.; Kelly, S.L.; Brady, R.L.
Deposited on : 2011-03-25
Resolution : 1.89 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

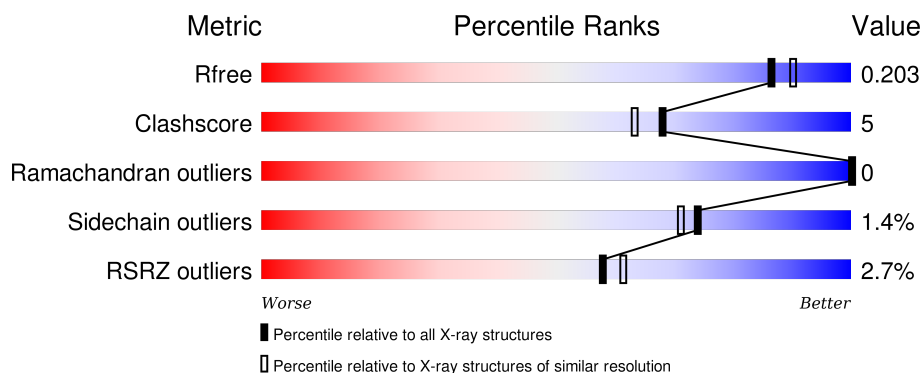
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	418	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	418	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	418	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>

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	HEM	A	501	-	-	-	X
2	HEM	B	501	-	-	-	X
2	HEM	C	501	-	-	-	X
3	PO4	A	503	-	-	-	X
3	PO4	C	503	-	-	-	X
4	EDO	A	504	-	-	-	X
4	EDO	A	505	-	-	-	X
4	EDO	A	508	-	-	-	X
4	EDO	B	504	-	-	-	X
4	EDO	B	506	-	-	-	X
4	EDO	C	504	-	-	-	X
4	EDO	C	505	-	-	-	X
4	EDO	C	506	-	-	-	X
4	EDO	C	507	-	-	-	X
4	EDO	C	508	-	-	X	X
4	EDO	C	510	-	-	-	X
7	D12	A	509	-	-	-	X
7	D12	B	509	-	-	-	X
7	D12	C	513	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9955 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 CYTOCHROME P450 164A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	19	2	0
			2998	1896	525	565	12			
1	B	391	Total	C	N	O	S	25	3	0
			3007	1902	529	564	12			
1	C	391	Total	C	N	O	S	39	1	0
			2992	1894	525	561	12			

There are 12 discrepancies between the modelled and reference sequences:

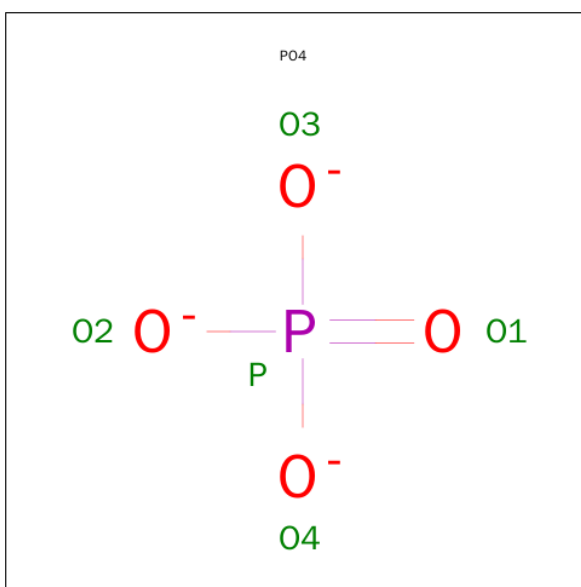
Chain	Residue	Modelled	Actual	Comment	Reference
A	415	HIS	-	EXPRESSION TAG	UNP A0R5U2
A	416	HIS	-	EXPRESSION TAG	UNP A0R5U2
A	417	HIS	-	EXPRESSION TAG	UNP A0R5U2
A	418	HIS	-	EXPRESSION TAG	UNP A0R5U2
B	415	HIS	-	EXPRESSION TAG	UNP A0R5U2
B	416	HIS	-	EXPRESSION TAG	UNP A0R5U2
B	417	HIS	-	EXPRESSION TAG	UNP A0R5U2
B	418	HIS	-	EXPRESSION TAG	UNP A0R5U2
C	415	HIS	-	EXPRESSION TAG	UNP A0R5U2
C	416	HIS	-	EXPRESSION TAG	UNP A0R5U2
C	417	HIS	-	EXPRESSION TAG	UNP A0R5U2
C	418	HIS	-	EXPRESSION TAG	UNP A0R5U2

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

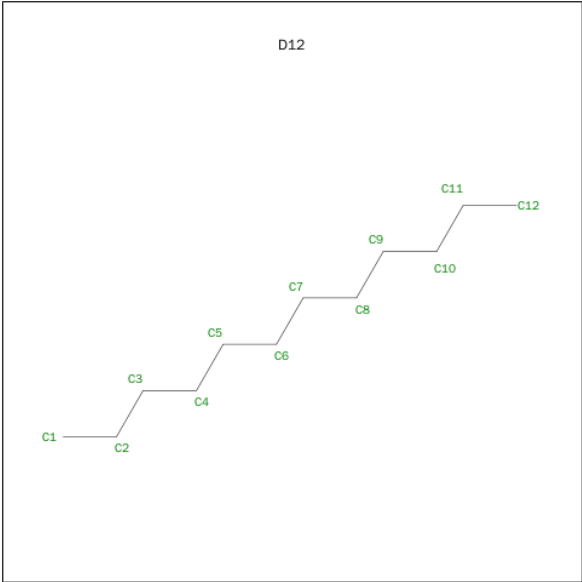
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 12 12	0	0
7	B	1	Total C 12 12	0	0
7	C	1	Total C 12 12	0	0

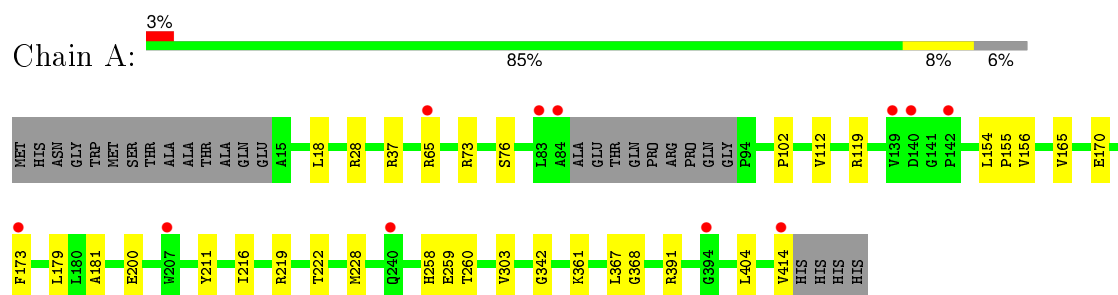
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	235	Total O 235 235	0	0
8	B	233	Total O 233 233	0	0
8	C	235	Total O 235 235	0	0

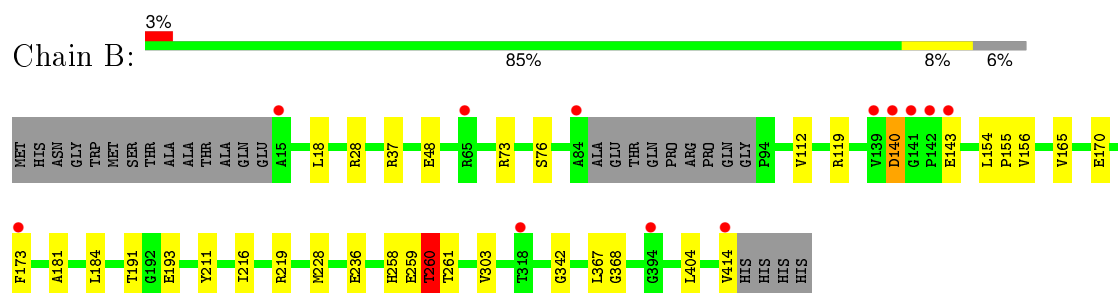
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

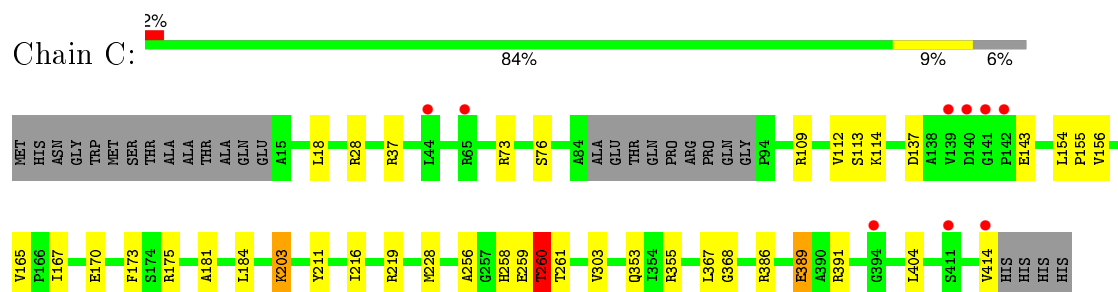
• Molecule 1: CYTOCHROME P450 164A2



• Molecule 1: CYTOCHROME P450 164A2



• Molecule 1: CYTOCHROME P450 164A2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.40Å 102.78Å 92.41Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	92.45 – 1.89 44.95 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (92.45-1.89) 99.5 (44.95-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.183 , 0.202 0.197 , 0.203	Depositor DCC
R_{free} test set	6616 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
Estimated twinning fraction	0.015 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.014 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.477 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.468 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.015 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 131604 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9955	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D12, NA, PO4, EDO, HEM, K

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	0.59	2/3063 (0.1%)	0.62	1/4170 (0.0%)
1	B	0.61	5/3075 (0.2%)	0.83	2/4185 (0.0%)
1	C	0.68	6/3054 (0.2%)	0.66	3/4158 (0.1%)
All	All	0.63	13/9192 (0.1%)	0.71	6/12513 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	143	GLU	CB-CG	-17.53	1.18	1.52
1	B	236[A]	GLU	CB-CG	-6.96	1.39	1.52
1	B	236[B]	GLU	CB-CG	-6.96	1.39	1.52
1	C	175	ARG	CG-CD	6.84	1.69	1.51
1	B	140	ASP	CB-CG	-6.73	1.37	1.51
1	A	391	ARG	CB-CG	6.60	1.70	1.52
1	A	260	THR	CB-CG2	-6.55	1.30	1.52
1	B	119	ARG	CB-CG	-6.13	1.35	1.52
1	C	389	GLU	CA-CB	-6.02	1.40	1.53
1	B	260	THR	CB-CG2	-5.86	1.33	1.52
1	C	167	ILE	CB-CG2	5.49	1.69	1.52
1	C	203	LYS	CG-CD	5.27	1.70	1.52
1	C	260	THR	CB-CG2	-5.20	1.35	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ASP	CB-CG-OD1	25.73	141.46	118.30
1	B	140	ASP	CB-CG-OD2	-24.43	96.31	118.30
1	A	260	THR	OG1-CB-CG2	-7.33	93.14	110.00
1	C	391	ARG	CB-CG-CD	5.96	127.09	111.60
1	C	167	ILE	CG1-CB-CG2	-5.81	98.62	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	THR	CA-CB-CG2	5.22	119.72	112.40

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	2998	0	3024	26	0
1	B	3007	0	3041	28	0
1	C	2992	0	3025	32	0
2	A	43	0	30	1	0
2	B	43	0	30	5	0
2	C	43	0	30	5	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	A	12	0	18	2	0
4	B	20	0	30	1	0
4	C	28	0	42	7	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	12	0	26	0	0
7	B	12	0	26	1	0
7	C	12	0	26	2	0
8	A	235	0	0	0	0
8	B	233	0	0	0	0
8	C	235	0	0	1	0
All	All	9955	0	9348	87	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 (87) 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:184:LEU:HD11	7:C:513:D12:H41	1.62	0.81
1:C:137:ASP:OD1	1:C:386:ARG:NH1	2.12	0.80
1:B:260:THR:HG23	2:B:501:HEM:HAB	1.75	0.69
1:B:173:PHE:HE1	1:B:211:TYR:CE2	2.13	0.67
1:A:173:PHE:HE1	1:A:211:TYR:CE2	2.13	0.67
1:C:173:PHE:HE1	1:C:211:TYR:CE2	2.12	0.67
1:A:342:GLY:H	4:A:504:EDO:H12	1.60	0.66
1:B:165:VAL:CG1	1:B:173:PHE:CZ	2.80	0.65
1:A:165:VAL:CG1	1:A:173:PHE:CZ	2.80	0.64
1:C:109:ARG:HE	4:C:508:EDO:H12	1.62	0.63
1:C:165:VAL:CG1	1:C:173:PHE:CZ	2.83	0.61
1:B:165:VAL:CG1	1:B:173:PHE:CE2	2.83	0.61
1:A:165:VAL:CG1	1:A:173:PHE:CE2	2.83	0.61
1:C:353:GLN:NE2	1:C:355:ARG:HD2	2.15	0.61
1:C:165:VAL:HG13	1:C:173:PHE:CZ	2.37	0.60
2:C:501:HEM:HMB1	2:C:501:HEM:HBB2	1.84	0.60
1:B:165:VAL:HG13	1:B:173:PHE:CZ	2.37	0.60
1:A:170:GLU:HA	1:A:173:PHE:CD2	2.37	0.59
1:C:165:VAL:CG1	1:C:173:PHE:CE2	2.84	0.59
1:C:173:PHE:CE1	1:C:211:TYR:CE2	2.90	0.59
1:B:173:PHE:CE1	1:B:211:TYR:CE2	2.91	0.59
1:A:173:PHE:CE1	1:A:211:TYR:CE2	2.90	0.59
1:A:165:VAL:HG13	1:A:173:PHE:CZ	2.37	0.59
1:C:170:GLU:HA	1:C:173:PHE:CD2	2.37	0.59
1:C:260:THR:HG23	2:C:501:HEM:HAB	1.85	0.58
1:B:170:GLU:HA	1:B:173:PHE:CD2	2.38	0.58
1:C:219:ARG:HD2	1:C:228:MET:HE2	1.86	0.58
1:B:342:GLY:H	4:B:503:EDO:H12	1.69	0.58
1:A:361:LYS:NZ	1:B:193:GLU:OE2	2.38	0.57
1:A:219:ARG:HD2	1:A:228:MET:HE2	1.87	0.57
1:B:219:ARG:HD2	1:B:228:MET:HE2	1.87	0.56
1:A:216:ILE:HG13	1:A:228:MET:CE	2.39	0.53
1:C:256:ALA:HB2	7:C:513:D12:H72	1.92	0.52
1:C:216:ILE:HG13	1:C:228:MET:CE	2.40	0.52
1:B:216:ILE:HG13	1:B:228:MET:CE	2.41	0.51
1:B:154:LEU:HB3	1:B:155:PRO:HD3	1.93	0.50
4:C:505:EDO:H22	4:C:508:EDO:H22	1.94	0.49
1:B:184:LEU:HD11	7:B:509:D12:H52	1.94	0.49
1:C:260:THR:CG2	1:C:261:THR:N	2.76	0.49
1:B:260:THR:HG21	2:B:501:HEM:CHC	2.42	0.49
1:A:181:ALA:HB2	1:A:259:GLU:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ALA:HB2	1:C:259:GLU:HG3	1.95	0.48
1:A:154:LEU:HB3	1:A:155:PRO:HD3	1.96	0.48
1:C:216:ILE:HG13	1:C:228:MET:HE3	1.94	0.48
1:B:260:THR:CG2	1:B:261:THR:N	2.76	0.48
1:B:260:THR:HG22	1:B:261:THR:H	1.78	0.47
1:C:260:THR:HG21	2:C:501:HEM:CHC	2.44	0.47
1:B:181:ALA:HB2	1:B:259:GLU:HG3	1.97	0.47
1:C:113:SER:CB	4:C:508:EDO:H11	2.45	0.47
1:A:156:VAL:HG22	1:A:258:HIS:CD2	2.50	0.46
1:C:154:LEU:HB3	1:C:155:PRO:HD3	1.98	0.46
1:A:216:ILE:HG13	1:A:228:MET:HE1	1.98	0.45
1:C:260:THR:CG2	1:C:261:THR:H	2.29	0.45
1:C:260:THR:HG22	1:C:261:THR:H	1.81	0.45
2:B:501:HEM:HBB2	2:B:501:HEM:HMB1	1.98	0.45
1:A:18:LEU:HD21	1:A:37:ARG:HD3	1.99	0.45
1:B:18:LEU:HD21	1:B:37:ARG:HD3	1.99	0.45
1:C:113:SER:HB2	4:C:508:EDO:H11	1.99	0.44
1:A:102:PRO:HG3	1:B:48:GLU:HG3	1.99	0.44
1:C:156:VAL:HG22	1:C:258:HIS:CD2	2.52	0.44
1:C:18:LEU:HD21	1:C:37:ARG:HD3	1.99	0.44
1:B:368:GLY:HA3	2:B:501:HEM:C3C	2.53	0.44
1:B:73:ARG:O	1:B:76:SER:HB3	2.17	0.44
1:A:179:LEU:HD13	1:A:200[B]:GLU:HG3	2.00	0.44
1:A:368:GLY:HA3	2:A:501:HEM:C3C	2.53	0.44
1:A:73:ARG:O	1:A:76:SER:HB3	2.18	0.43
1:A:112:VAL:HG23	1:A:367:LEU:HD21	2.00	0.43
1:C:109:ARG:HE	4:C:508:EDO:C1	2.31	0.43
1:B:216:ILE:HG13	1:B:228:MET:HE1	1.99	0.43
1:B:303:VAL:HG22	1:B:404:LEU:CD2	2.49	0.43
1:A:222:THR:HG21	1:C:114:LYS:HD2	2.01	0.43
1:B:260:THR:CG2	1:B:261:THR:H	2.32	0.43
1:B:156:VAL:HG22	1:B:258:HIS:CD2	2.54	0.43
1:B:112:VAL:HG23	1:B:367:LEU:HD21	2.01	0.43
1:B:260:THR:CG2	2:B:501:HEM:CHC	2.96	0.42
1:A:216:ILE:HG13	1:A:228:MET:HE3	2.01	0.42
1:A:342:GLY:H	4:A:504:EDO:C1	2.28	0.42
1:C:368:GLY:HA3	2:C:501:HEM:C3C	2.54	0.42
4:C:505:EDO:H22	4:C:508:EDO:C2	2.50	0.42
1:C:260:THR:CG2	2:C:501:HEM:CHC	2.98	0.42
1:C:303:VAL:HG22	1:C:404:LEU:CD2	2.50	0.41
4:C:509:EDO:H11	8:C:727:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:HG23	1:C:367:LEU:HD21	2.03	0.41
1:C:73:ARG:O	1:C:76:SER:HB3	2.20	0.41
1:A:179:LEU:CD1	1:A:200[B]:GLU:HG3	2.51	0.41
1:A:303:VAL:HG22	1:A:404:LEU:CD2	2.52	0.40
1:A:65:ARG:CZ	1:B:191:THR:O	2.69	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	389/418 (93%)	383 (98%)	6 (2%)	0	100	100
1	B	390/418 (93%)	385 (99%)	5 (1%)	0	100	100
1	C	388/418 (93%)	381 (98%)	7 (2%)	0	100	100
All	All	1167/1254 (93%)	1149 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/337 (94%)	315 (99%)	3 (1%)	84	83
1	B	319/337 (95%)	314 (98%)	5 (2%)	70	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	317/337 (94%)	312 (98%)	5 (2%)	70	66
All	All	954/1011 (94%)	941 (99%)	13 (1%)	74	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	119	ARG
1	A	414	VAL
1	B	28	ARG
1	B	140	ASP
1	B	143	GLU
1	B	260	THR
1	B	414	VAL
1	C	28	ARG
1	C	203	LYS
1	C	260	THR
1	C	389	GLU
1	C	414	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	C	353	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 31 ligands modelled in this entry, 5 are monoatomic - leaving 26 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	$\# Z > 2$
2	HEM	A	501	1	30,50,50	2.44	10 (33%)	24,82,82	2.46	11 (45%)
3	PO4	A	502	6	4,4,4	0.59	0	6,6,6	0.27	0
3	PO4	A	503	5	4,4,4	0.41	0	6,6,6	0.28	0
4	EDO	A	504	-	3,3,3	0.39	0	2,2,2	0.73	0
4	EDO	A	505	-	3,3,3	0.40	0	2,2,2	0.29	0
4	EDO	A	508	-	3,3,3	0.62	0	2,2,2	0.11	0
7	D12	A	509	-	11,11,11	0.33	0	10,10,10	0.64	0
2	HEM	B	501	1	30,50,50	2.46	9 (30%)	24,82,82	2.45	11 (45%)
3	PO4	B	502	6	4,4,4	0.55	0	6,6,6	0.26	0
4	EDO	B	503	-	3,3,3	0.31	0	2,2,2	0.97	0
4	EDO	B	504	-	3,3,3	0.48	0	2,2,2	0.47	0
4	EDO	B	505	-	3,3,3	0.49	0	2,2,2	0.17	0
4	EDO	B	506	-	3,3,3	0.46	0	2,2,2	0.50	0
4	EDO	B	507	-	3,3,3	0.47	0	2,2,2	0.51	0
7	D12	B	509	-	11,11,11	0.43	0	10,10,10	0.45	0
2	HEM	C	501	1	30,50,50	2.42	7 (23%)	24,82,82	2.48	13 (54%)
3	PO4	C	502	6	4,4,4	0.35	0	6,6,6	0.29	0
3	PO4	C	503	5	4,4,4	0.46	0	6,6,6	0.28	0
4	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	C	505	-	3,3,3	0.72	0	2,2,2	0.18	0
4	EDO	C	506	-	3,3,3	0.33	0	2,2,2	1.15	0
4	EDO	C	507	-	3,3,3	0.67	0	2,2,2	0.11	0
4	EDO	C	508	-	3,3,3	0.56	0	2,2,2	0.46	0
4	EDO	C	509	-	3,3,3	0.45	0	2,2,2	0.56	0
4	EDO	C	510	-	3,3,3	0.44	0	2,2,2	0.58	0
7	D12	C	513	-	11,11,11	0.25	0	10,10,10	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	0/10/54/54	0/0/8/8
3	PO4	A	502	6	-	0/0/0/0	0/0/0/0
3	PO4	A	503	5	-	0/0/0/0	0/0/0/0
4	EDO	A	504	-	-	0/1/1/1	0/0/0/0
4	EDO	A	505	-	-	0/1/1/1	0/0/0/0
4	EDO	A	508	-	-	0/1/1/1	0/0/0/0
7	D12	A	509	-	-	0/9/9/9	0/0/0/0
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	PO4	B	502	6	-	0/0/0/0	0/0/0/0
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0
4	EDO	B	505	-	-	0/1/1/1	0/0/0/0
4	EDO	B	506	-	-	0/1/1/1	0/0/0/0
4	EDO	B	507	-	-	0/1/1/1	0/0/0/0
7	D12	B	509	-	-	0/9/9/9	0/0/0/0
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8
3	PO4	C	502	6	-	0/0/0/0	0/0/0/0
3	PO4	C	503	5	-	0/0/0/0	0/0/0/0
4	EDO	C	504	-	-	0/1/1/1	0/0/0/0
4	EDO	C	505	-	-	0/1/1/1	0/0/0/0
4	EDO	C	506	-	-	0/1/1/1	0/0/0/0
4	EDO	C	507	-	-	0/1/1/1	0/0/0/0
4	EDO	C	508	-	-	0/1/1/1	0/0/0/0
4	EDO	C	509	-	-	0/1/1/1	0/0/0/0
4	EDO	C	510	-	-	0/1/1/1	0/0/0/0
7	D12	C	513	-	-	0/9/9/9	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-9.10	1.43	1.51
2	B	501	HEM	C3B-C4B	-9.10	1.43	1.51
2	C	501	HEM	C3B-C4B	-8.99	1.43	1.51
2	B	501	HEM	C3D-C4D	-5.86	1.44	1.51
2	C	501	HEM	C3D-C4D	-5.45	1.44	1.51
2	A	501	HEM	C3D-C4D	-5.37	1.44	1.51
2	C	501	HEM	C2C-C1C	-3.55	1.45	1.52
2	B	501	HEM	C2C-C1C	-3.42	1.46	1.52
2	A	501	HEM	C2C-C1C	-3.31	1.46	1.52
2	A	501	HEM	C2B-C1B	-2.36	1.44	1.51
2	C	501	HEM	C2B-C1B	-2.26	1.44	1.51
2	C	501	HEM	C2D-C1D	-2.24	1.44	1.51
2	B	501	HEM	C2B-C1B	-2.23	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C2D-C1D	-2.14	1.44	1.51
2	A	501	HEM	C2D-C1D	-2.05	1.45	1.51
2	B	501	HEM	C4C-NC	2.01	1.38	1.36
2	A	501	HEM	C4C-NC	2.13	1.38	1.36
2	B	501	HEM	CMA-C3A	2.14	1.56	1.51
2	A	501	HEM	C1C-NC	2.20	1.38	1.36
2	A	501	HEM	C3C-CAC	2.24	1.55	1.51
2	C	501	HEM	C1C-NC	2.32	1.38	1.36
2	A	501	HEM	CMA-C3A	2.46	1.56	1.51
2	B	501	HEM	FE-NC	2.67	2.06	1.95
2	A	501	HEM	FE-NC	2.82	2.06	1.95
2	B	501	HEM	C1C-NC	2.82	1.39	1.36
2	C	501	HEM	FE-NC	2.87	2.07	1.95

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3C-CAC-CBC	-3.53	119.03	124.46
2	C	501	HEM	CAA-C2A-C1A	-3.40	123.31	127.01
2	A	501	HEM	C3C-CAC-CBC	-3.19	119.56	124.46
2	C	501	HEM	CMA-C3A-C4A	-2.72	123.87	128.36
2	C	501	HEM	CBD-CAD-C3D	-2.63	105.90	113.55
2	A	501	HEM	CBD-CAD-C3D	-2.53	106.19	113.55
2	B	501	HEM	CMA-C3A-C4A	-2.51	124.21	128.36
2	B	501	HEM	CAA-C2A-C1A	-2.49	124.30	127.01
2	A	501	HEM	CMA-C3A-C4A	-2.49	124.24	128.36
2	A	501	HEM	C3B-CAB-CBB	-2.33	120.88	124.46
2	B	501	HEM	CAA-CBA-CGA	-2.31	108.51	112.75
2	C	501	HEM	C3C-CAC-CBC	-2.29	120.94	124.46
2	A	501	HEM	CAA-CBA-CGA	-2.17	108.77	112.75
2	B	501	HEM	CBD-CAD-C3D	-2.16	107.28	113.55
2	C	501	HEM	C3B-CAB-CBB	-2.09	121.25	124.46
2	C	501	HEM	CAA-CBA-CGA	-2.07	108.96	112.75
2	C	501	HEM	C3B-C4B-NB	-2.03	107.74	111.63
2	A	501	HEM	CMD-C2D-C3D	2.48	125.30	114.35
2	B	501	HEM	CMD-C2D-C3D	2.54	125.56	114.35
2	B	501	HEM	C2D-C3D-C4D	2.59	105.90	101.50
2	C	501	HEM	CMD-C2D-C3D	2.68	126.21	114.35
2	A	501	HEM	C2D-C3D-C4D	2.73	106.13	101.50
2	C	501	HEM	C2D-C3D-C4D	2.92	106.44	101.50
2	B	501	HEM	CAD-C3D-C2D	3.97	124.62	113.22
2	C	501	HEM	CMB-C2B-C3B	4.01	126.53	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CAD-C3D-C2D	4.16	125.19	113.22
2	B	501	HEM	CMB-C2B-C3B	4.28	127.22	116.53
2	C	501	HEM	CAD-C3D-C2D	4.29	125.56	113.22
2	C	501	HEM	CAD-C3D-C4D	4.39	127.96	112.47
2	A	501	HEM	CMB-C2B-C3B	4.47	127.70	116.53
2	B	501	HEM	CMC-C2C-C3C	4.58	127.95	116.53
2	A	501	HEM	CAD-C3D-C4D	4.60	128.68	112.47
2	A	501	HEM	CMC-C2C-C3C	4.67	128.19	116.53
2	C	501	HEM	CMC-C2C-C3C	4.73	128.34	116.53
2	B	501	HEM	CAD-C3D-C4D	4.82	129.47	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	1	0
4	A	504	EDO	2	0
2	B	501	HEM	5	0
4	B	503	EDO	1	0
7	B	509	D12	1	0
2	C	501	HEM	5	0
4	C	505	EDO	2	0
4	C	508	EDO	6	0
4	C	509	EDO	1	0
7	C	513	D12	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	391/418 (93%)	0.07	11 (2%) 56 60	5, 14, 30, 40	16 (4%)
1	B	391/418 (93%)	0.19	12 (3%) 52 56	5, 14, 30, 40	22 (5%)
1	C	391/418 (93%)	0.11	9 (2%) 64 67	5, 14, 30, 40	29 (7%)
All	All	1173/1254 (93%)	0.12	32 (2%) 58 61	5, 14, 30, 40	67 (5%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	PHE	4.2
1	A	140	ASP	4.2
1	B	173	PHE	3.7
1	C	139	VAL	3.5
1	C	414	VAL	3.5
1	B	140	ASP	3.4
1	A	65	ARG	3.3
1	C	140	ASP	3.2
1	C	142	PRO	3.1
1	A	84	ALA	3.1
1	B	414	VAL	3.1
1	C	394	GLY	3.1
1	A	394	GLY	3.0
1	B	394	GLY	3.0
1	A	414	VAL	2.8
1	B	318	THR	2.8
1	B	65	ARG	2.8
1	B	142	PRO	2.7
1	B	139	VAL	2.6
1	A	142	PRO	2.6
1	B	143	GLU	2.5
1	C	65	ARG	2.5
1	A	207	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	139	VAL	2.5
1	C	141	GLY	2.4
1	B	141	GLY	2.4
1	C	411	SER	2.3
1	A	83	LEU	2.3
1	C	44[A]	LEU	2.2
1	B	84	ALA	2.2
1	A	240	GLN	2.1
1	B	15	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

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
7	D12	B	509	12/12	0.86	0.51	20.20	46,48,52,52	0
3	PO4	A	503	5/5	0.92	0.40	16.34	28,29,29,30	5
7	D12	C	513	12/12	0.93	0.37	13.86	40,42,47,48	0
3	PO4	C	503	5/5	0.95	0.34	13.72	26,27,29,29	5
4	EDO	B	506	4/4	0.90	0.22	12.58	50,51,53,53	0
4	EDO	C	508	4/4	0.64	0.42	12.11	32,33,35,36	0
4	EDO	A	508	4/4	0.93	0.29	12.02	34,34,35,35	0
7	D12	A	509	12/12	0.93	0.27	11.61	40,42,48,48	0
4	EDO	C	505	4/4	0.89	0.30	11.01	34,34,35,35	0
4	EDO	C	507	4/4	0.95	0.24	8.94	35,35,35,36	0
2	HEM	B	501	43/43	0.97	0.25	7.59	17,20,23,31	0
2	HEM	C	501	43/43	0.97	0.25	6.85	17,20,23,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	C	504	4/4	0.73	0.24	6.26	44,49,51,54	0
2	HEM	A	501	43/43	0.97	0.21	6.11	17,20,23,32	0
4	EDO	C	506	4/4	0.82	0.26	5.48	34,39,40,41	0
4	EDO	B	504	4/4	0.93	0.34	4.95	39,43,44,45	0
4	EDO	A	504	4/4	0.87	0.25	4.39	35,39,40,47	0
4	EDO	A	505	4/4	0.92	0.32	3.82	42,45,47,49	0
4	EDO	C	510	4/4	0.90	0.18	2.95	50,50,51,51	0
4	EDO	C	509	4/4	0.88	0.19	1.43	42,46,48,52	0
4	EDO	B	503	4/4	0.92	0.20	0.75	35,39,40,47	0
4	EDO	B	507	4/4	0.88	0.16	0.62	49,50,51,52	0
6	K	B	508	1/1	0.97	0.08	-2.02	39,39,39,39	0
5	NA	A	506	1/1	0.94	0.25	-	40,40,40,40	0
3	PO4	C	502	5/5	0.92	0.19	-	44,49,49,49	0
6	K	A	507	1/1	0.97	0.10	-	40,40,40,40	0
3	PO4	A	502	5/5	0.92	0.20	-	23,28,28,29	5
4	EDO	B	505	4/4	0.90	0.23	-	35,42,43,46	0
5	NA	C	511	1/1	0.93	0.29	-	40,40,40,40	0
6	K	C	512	1/1	0.97	0.12	-	39,39,39,39	0
3	PO4	B	502	5/5	0.92	0.18	-	25,29,30,31	5

6.5 Other polymers [i](#)

There are no such residues in this entry.