Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:43 PM GMT

PDB ID	:	4AAL
Title	:	MacA wild-type oxidized
Authors	:	Seidel, J.
Deposited on	:	2011-12-05
Resolution	:	1.84 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

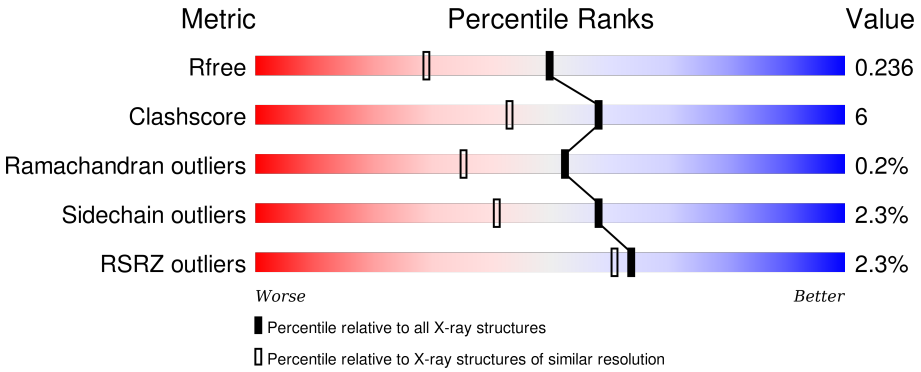
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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 <=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	341	3% 84% 9% • 6%
1	B	341	% 86% 7% • 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5841 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 C551 PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	3	0
			2447	1553	426	455	13			
1	B	319	Total	C	N	O	S	0	4	0
			2449	1553	426	457	13			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	TRP	-	EXPRESSION TAG	UNP Q74FY6
A	7	SER	-	EXPRESSION TAG	UNP Q74FY6
A	8	HIS	-	EXPRESSION TAG	UNP Q74FY6
A	9	PRO	-	EXPRESSION TAG	UNP Q74FY6
A	10	GLN	-	EXPRESSION TAG	UNP Q74FY6
A	11	PHE	-	EXPRESSION TAG	UNP Q74FY6
A	12	GLU	-	EXPRESSION TAG	UNP Q74FY6
A	13	LYS	-	EXPRESSION TAG	UNP Q74FY6
A	14	GLY	-	EXPRESSION TAG	UNP Q74FY6
A	15	ALA	-	EXPRESSION TAG	UNP Q74FY6
A	16	GLU	-	EXPRESSION TAG	UNP Q74FY6
A	17	THR	-	EXPRESSION TAG	UNP Q74FY6
A	18	ALA	-	EXPRESSION TAG	UNP Q74FY6
A	19	VAL	-	EXPRESSION TAG	UNP Q74FY6
A	20	PRO	-	EXPRESSION TAG	UNP Q74FY6
A	21	ASN	-	EXPRESSION TAG	UNP Q74FY6
A	22	SER	-	EXPRESSION TAG	UNP Q74FY6
B	6	TRP	-	EXPRESSION TAG	UNP Q74FY6
B	7	SER	-	EXPRESSION TAG	UNP Q74FY6
B	8	HIS	-	EXPRESSION TAG	UNP Q74FY6
B	9	PRO	-	EXPRESSION TAG	UNP Q74FY6
B	10	GLN	-	EXPRESSION TAG	UNP Q74FY6
B	11	PHE	-	EXPRESSION TAG	UNP Q74FY6
B	12	GLU	-	EXPRESSION TAG	UNP Q74FY6
B	13	LYS	-	EXPRESSION TAG	UNP Q74FY6

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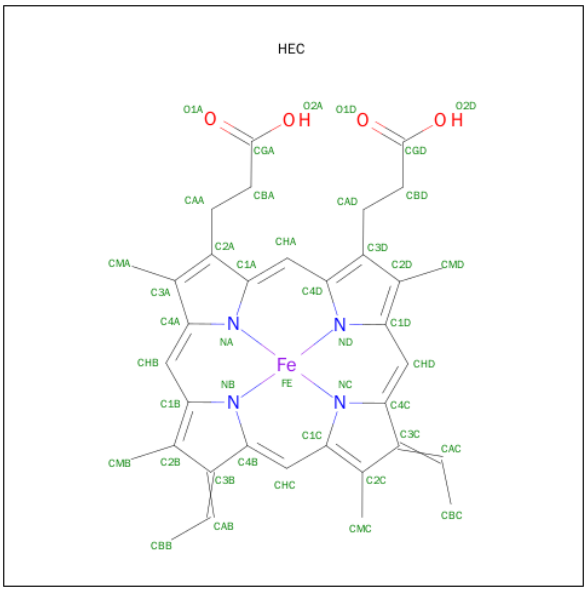
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLY	-	EXPRESSION TAG	UNP Q74FY6
B	15	ALA	-	EXPRESSION TAG	UNP Q74FY6
B	16	GLU	-	EXPRESSION TAG	UNP Q74FY6
B	17	THR	-	EXPRESSION TAG	UNP Q74FY6
B	18	ALA	-	EXPRESSION TAG	UNP Q74FY6
B	19	VAL	-	EXPRESSION TAG	UNP Q74FY6
B	20	PRO	-	EXPRESSION TAG	UNP Q74FY6
B	21	ASN	-	EXPRESSION TAG	UNP Q74FY6
B	22	SER	-	EXPRESSION TAG	UNP Q74FY6

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

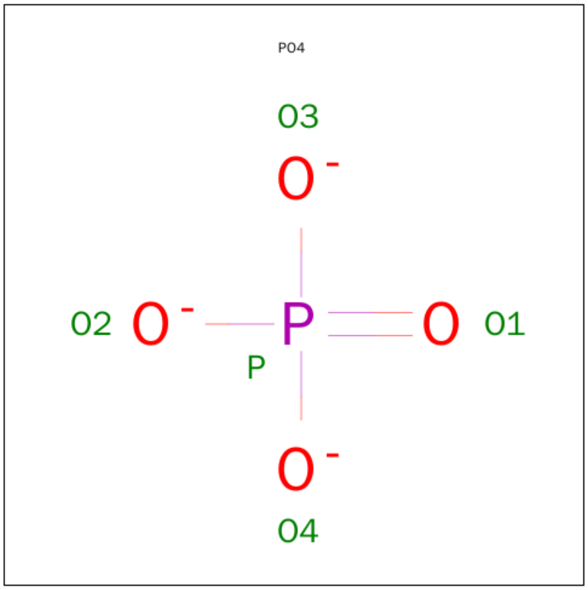


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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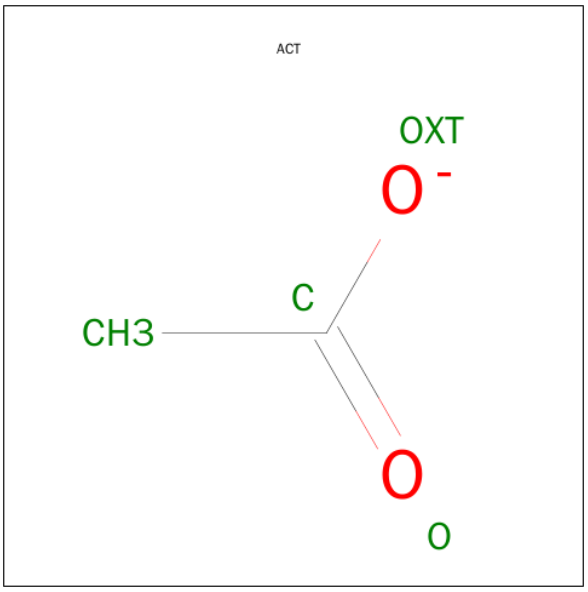
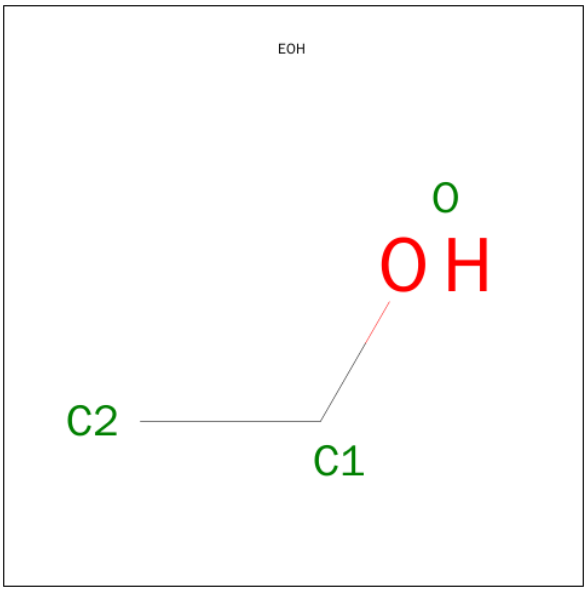
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 2 1	0	0

- Molecule 7 is water.

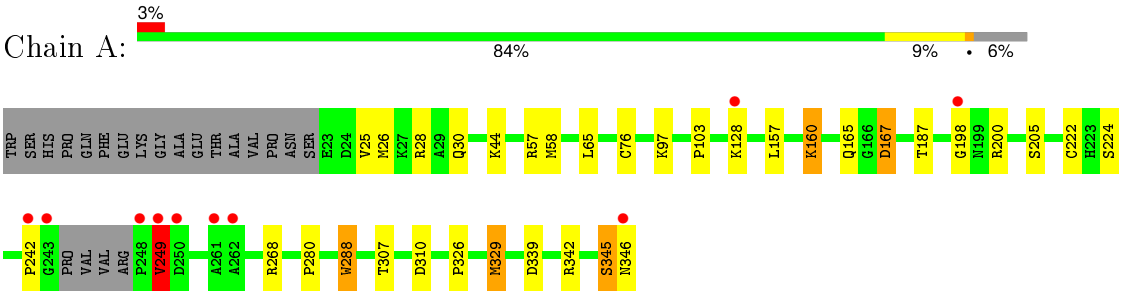
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	344	Total O 344 344	0	0
7	B	285	Total O 285 285	0	0

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.

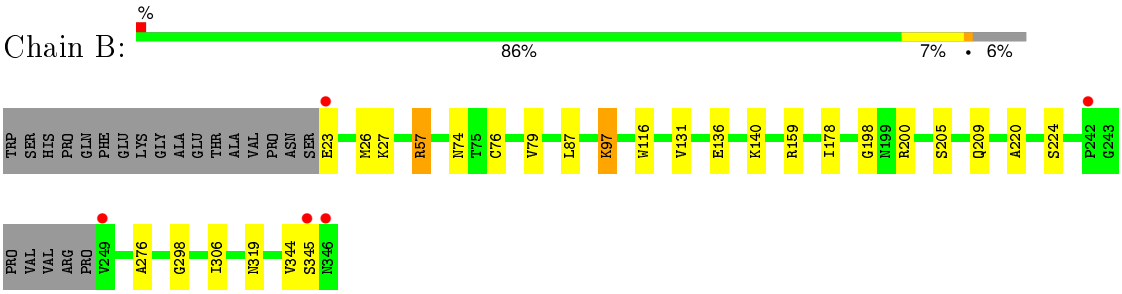
- Molecule 1: CYTOCHROME C551 PEROXIDASE

Chain A:



- Molecule 1: CYTOCHROME C551 PEROXIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.03Å 118.03Å 242.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	102.06 – 1.84 47.08 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.0 (102.06-1.84) 98.1 (47.08-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.6.0113	Depositor
R, R_{free}	0.189 , 0.237 0.189 , 0.236	Depositor DCC
R_{free} test set	4281 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 85453 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5841	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HEC, CA, EOH, PO4, ACT

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	0.96	2/2514 (0.1%)	1.00	13/3413 (0.4%)
1	B	0.94	1/2515 (0.0%)	0.96	2/3414 (0.1%)
All	All	0.95	3/5029 (0.1%)	0.98	15/6827 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	SER	CA-CB	6.21	1.62	1.52
1	A	288	TRP	CD2-CE2	5.81	1.48	1.41
1	B	116	TRP	CD2-CE2	5.08	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	57	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	A	268	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	268	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	342	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	57	ARG	NE-CZ-NH2	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200[A]	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	200[B]	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	200[A]	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	200[B]	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	65	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	249	VAL	N-CA-C	5.14	124.88	111.00
1	A	329[A]	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	329[B]	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	167	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	LYS	Peptide
1	A	249	VAL	Peptide
1	B	344	VAL	Peptide

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	2447	0	2446	24	0
1	B	2449	0	2444	28	0
2	A	86	0	60	7	0
2	B	86	0	61	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	55	0	0	1	0
4	B	60	0	0	1	0
5	A	12	0	9	0	0
5	B	12	0	9	1	0
6	A	3	0	6	0	0
7	A	344	0	0	7	1
7	B	285	0	0	9	1
All	All	5841	0	5035	58	1

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 6.

All (58) 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:B:76:CYS:SG	2:B:423:HEC:CAC	2.07	1.43
1:B:23:GLU:HG3	1:B:200:ARG:NH2	1.64	1.13
5:B:1362:ACT:H3	7:B:2282:HOH:O	1.50	1.10
1:B:76:CYS:SG	2:B:423:HEC:HAC	1.97	1.03
1:B:23:GLU:HB3	7:B:2001:HOH:O	1.64	0.97
1:A:329[B]:MET:SD	7:A:2306:HOH:O	2.24	0.95
1:B:76:CYS:SG	2:B:423:HEC:C3C	2.65	0.84
1:A:222:CYS:SG	2:A:424:HEC:C3C	2.67	0.81
1:B:23:GLU:CB	7:B:2001:HOH:O	2.24	0.79
1:A:76:CYS:SG	2:A:423:HEC:C3C	2.71	0.78
1:B:23:GLU:CG	1:B:200:ARG:NH2	2.45	0.77
1:B:74:ASN:HD21	1:B:79:VAL:H	1.32	0.77
1:B:23:GLU:HG3	1:B:200:ARG:HH21	1.49	0.76
1:B:76:CYS:SG	2:B:423:HEC:CBC	2.74	0.76
1:A:76:CYS:SG	2:A:423:HEC:CBC	2.73	0.75
1:B:57:ARG:NH1	7:B:2041:HOH:O	2.17	0.74
1:A:167:ASP:OD1	7:A:2195:HOH:O	2.05	0.73
1:A:222:CYS:SG	2:A:424:HEC:CBC	2.75	0.73
1:B:136[B]:GLU:HG3	7:B:2124:HOH:O	1.88	0.72
1:B:57:ARG:NH1	7:B:2040:HOH:O	2.15	0.72
1:A:345:SER:HA	7:A:2331:HOH:O	1.91	0.70
1:A:26:MET:HE3	1:A:198:GLY:HA2	1.75	0.69
2:B:423:HEC:HBC3	2:B:423:HEC:HMC1	1.75	0.69
1:B:26:MET:HE1	7:B:2189:HOH:O	1.92	0.68
1:A:165:GLN:OE1	7:A:2191:HOH:O	2.11	0.68
1:B:26:MET:CE	7:B:2007:HOH:O	2.44	0.64
1:B:74:ASN:ND2	1:B:79:VAL:H	1.98	0.61
1:B:26:MET:HE3	1:B:198:GLY:HA2	1.84	0.59
1:A:339:ASP:OD1	7:A:2323:HOH:O	2.17	0.56
1:B:23:GLU:CG	1:B:200:ARG:CZ	2.83	0.56
2:B:424:HEC:HMC1	2:B:424:HEC:HBC3	1.88	0.55
1:B:97:LYS:HD3	7:B:2220:HOH:O	2.08	0.53
1:B:23:GLU:HG2	1:B:200:ARG:CZ	2.39	0.52
4:A:1351:PO4:O4	7:A:2278:HOH:O	2.19	0.52
1:A:25:VAL:HG12	7:A:2006:HOH:O	2.08	0.52
2:B:424:HEC:HBB3	2:B:424:HEC:HMB1	1.92	0.51
1:A:187:THR:HG22	1:A:326:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:HH12	1:A:329[B]:MET:CE	2.25	0.49
1:B:159:ARG:NH2	4:B:1350:PO4:O4	2.39	0.49
2:A:424:HEC:HBB3	2:A:424:HEC:HMB1	1.96	0.47
1:B:26:MET:CE	1:B:198:GLY:HA2	2.44	0.47
1:A:97:LYS:HE2	1:A:97:LYS:HA	1.97	0.47
1:B:220:ALA:O	1:B:224:SER:HB3	2.14	0.47
1:B:76:CYS:CB	2:B:423:HEC:C3C	2.93	0.47
1:A:58:MET:SD	1:A:157:LEU:HD13	2.56	0.46
1:A:26:MET:CE	1:A:30:GLN:HE22	2.29	0.46
1:B:205:SER:O	1:B:209:GLN:HG3	2.16	0.44
1:B:298:GLY:HA3	1:B:306:ILE:HG12	2.00	0.44
1:A:157:LEU:HD23	1:A:160[B]:LYS:HE2	1.99	0.43
1:A:103:PRO:HD3	2:A:423:HEC:CAD	2.48	0.43
1:A:76:CYS:CB	2:A:423:HEC:C3C	2.96	0.43
1:A:26:MET:CE	1:A:198:GLY:HA2	2.48	0.43
1:A:26:MET:HE3	1:A:30:GLN:HE22	1.84	0.43
1:A:280:PRO:HB3	1:A:288:TRP:CD2	2.53	0.43
1:B:276:ALA:HB2	1:B:319:ASN:HD22	1.84	0.42
1:A:307:THR:O	1:A:310:ASP:HB2	2.20	0.41
1:B:178:ILE:HG21	2:B:423:HEC:HMB1	2.03	0.41
1:A:57:ARG:HH12	1:A:329[B]:MET:HE1	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2081:HOH:O	7:B:2264:HOH:O[8_445]	1.93	0.27

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	319/341 (94%)	307 (96%)	11 (3%)	1 (0%)	46 29
1	B	319/341 (94%)	310 (97%)	9 (3%)	0	100 100
All	All	638/682 (94%)	617 (97%)	20 (3%)	1 (0%)	52 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	PRO

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	266/281 (95%)	259 (97%)	7 (3%)	54 35
1	B	266/281 (95%)	260 (98%)	6 (2%)	58 41
All	All	532/562 (95%)	519 (98%)	13 (2%)	58 39

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

Mol	Chain	Res	Type
1	A	44	LYS
1	A	160[A]	LYS
1	A	160[B]	LYS
1	A	205	SER
1	A	249	VAL
1	A	345	SER
1	A	346	ASN
1	B	27	LYS
1	B	87	LEU
1	B	97	LYS
1	B	131	VAL
1	B	140	LYS
1	B	345	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	126	GLN
1	A	139	ASN
1	A	209	GLN
1	A	325	GLN
1	A	346	ASN
1	B	74	ASN
1	B	143	ASN
1	B	209	GLN
1	B	319	ASN

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 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	A	1348	-	4,4,4	0.40	0	6,6,6	0.29	0
4	PO4	A	1349	-	4,4,4	0.54	0	6,6,6	0.27	0
4	PO4	A	1350	-	4,4,4	0.44	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PO4	A	1351	-	4,4,4	0.42	0	6,6,6	0.29	0
4	PO4	A	1352	-	4,4,4	0.36	0	6,6,6	0.29	0
4	PO4	A	1353	-	4,4,4	0.45	0	6,6,6	0.29	0
4	PO4	A	1354	-	4,4,4	0.24	0	6,6,6	0.30	0
4	PO4	A	1355	-	4,4,4	0.43	0	6,6,6	0.29	0
4	PO4	A	1356	-	4,4,4	0.42	0	6,6,6	0.36	0
4	PO4	A	1357	-	4,4,4	0.69	0	6,6,6	0.37	0
5	ACT	A	1358	-	1,3,3	1.63	0	0,3,3	0.00	-
5	ACT	A	1359	-	1,3,3	1.39	0	0,3,3	0.00	-
5	ACT	A	1360	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-
6	EOH	A	1361	-	2,2,2	0.36	0	1,1,1	0.69	0
4	PO4	A	1362	-	4,4,4	0.35	0	6,6,6	0.31	0
2	HEC	A	423	1	24,50,50	1.48	3 (12%)	19,82,82	2.98	9 (47%)
2	HEC	A	424	1	24,50,50	1.30	3 (12%)	19,82,82	2.80	7 (36%)
4	PO4	B	1348	-	4,4,4	0.38	0	6,6,6	0.29	0
4	PO4	B	1349	-	4,4,4	0.46	0	6,6,6	0.27	0
4	PO4	B	1350	-	4,4,4	0.36	0	6,6,6	0.29	0
4	PO4	B	1351	-	4,4,4	0.62	0	6,6,6	0.29	0
4	PO4	B	1352	-	4,4,4	0.54	0	6,6,6	0.36	0
4	PO4	B	1353	-	4,4,4	0.57	0	6,6,6	0.27	0
4	PO4	B	1354	-	4,4,4	0.52	0	6,6,6	0.33	0
4	PO4	B	1355	-	4,4,4	0.34	0	6,6,6	0.31	0
4	PO4	B	1356	-	4,4,4	0.46	0	6,6,6	0.30	0
4	PO4	B	1357	-	4,4,4	0.64	0	6,6,6	0.25	0
4	PO4	B	1358	-	4,4,4	0.29	0	6,6,6	0.33	0
4	PO4	B	1359	-	4,4,4	0.47	0	6,6,6	0.31	0
5	ACT	B	1360	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
5	ACT	B	1361	-	1,3,3	2.18	1 (100%)	0,3,3	0.00	-
5	ACT	B	1362	-	1,3,3	0.89	0	0,3,3	0.00	-
2	HEC	B	423	1	24,50,50	1.37	4 (16%)	19,82,82	3.29	10 (52%)
2	HEC	B	424	1	24,50,50	1.28	3 (12%)	19,82,82	2.62	8 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	1348	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1349	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1350	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	1351	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1352	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1353	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1354	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1355	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1356	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1357	-	-	0/0/0/0	0/0/0/0
5	ACT	A	1358	-	-	0/0/0/0	0/0/0/0
5	ACT	A	1359	-	-	0/0/0/0	0/0/0/0
5	ACT	A	1360	-	-	0/0/0/0	0/0/0/0
6	EOH	A	1361	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1362	-	-	0/0/0/0	0/0/0/0
2	HEC	A	423	1	-	0/6/54/54	0/0/8/8
2	HEC	A	424	1	-	0/6/54/54	0/0/8/8
4	PO4	B	1348	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1349	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1350	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1351	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1352	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1353	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1354	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1355	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1356	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1357	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1358	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1359	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1360	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1361	-	-	0/0/0/0	0/0/0/0
5	ACT	B	1362	-	-	0/0/0/0	0/0/0/0
2	HEC	B	423	1	-	0/6/54/54	0/0/8/8
2	HEC	B	424	1	-	0/6/54/54	0/0/8/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	423	HEC	C4B-NB	-4.67	1.30	1.36
2	A	424	HEC	CBC-CAC	-3.47	1.35	1.49
2	B	423	HEC	C4B-NB	-3.38	1.32	1.36
2	B	424	HEC	CBC-CAC	-3.28	1.36	1.49
2	B	423	HEC	CBC-CAC	-3.12	1.36	1.49
2	B	423	HEC	CBB-CAB	-2.65	1.38	1.49
2	A	423	HEC	CBB-CAB	-2.36	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	424	HEC	C4B-NB	-2.27	1.33	1.36
2	A	424	HEC	CBB-CAB	-2.23	1.40	1.49
2	B	424	HEC	CBB-CAB	-2.21	1.40	1.49
2	A	423	HEC	CBC-CAC	-2.06	1.41	1.49
5	B	1361	ACT	CH3-C	2.18	1.51	1.48
2	B	423	HEC	C4A-NA	2.26	1.39	1.36
2	B	424	HEC	C3B-C4B	2.37	1.48	1.42
5	A	1360	ACT	CH3-C	2.68	1.52	1.48
5	B	1360	ACT	CH3-C	2.93	1.52	1.48

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	424	HEC	CBB-CAB-C3B	-8.04	109.49	127.35
2	B	423	HEC	CBD-CAD-C3D	-7.68	98.77	112.53
2	A	423	HEC	CBB-CAB-C3B	-7.61	110.44	127.35
2	B	423	HEC	CBB-CAB-C3B	-7.17	111.41	127.35
2	B	424	HEC	CBB-CAB-C3B	-6.90	112.03	127.35
2	A	423	HEC	CBD-CAD-C3D	-4.89	103.77	112.53
2	B	423	HEC	C3B-C4B-NB	-4.59	102.28	110.94
2	A	424	HEC	CBD-CAD-C3D	-4.29	104.84	112.53
2	B	423	HEC	CAA-CBA-CGA	-4.17	105.10	112.75
2	A	423	HEC	C3B-C4B-NB	-4.07	103.26	110.94
2	A	423	HEC	CAA-CBA-CGA	-3.94	105.53	112.75
2	B	424	HEC	C3B-C4B-NB	-3.94	103.51	110.94
2	B	424	HEC	CBD-CAD-C3D	-3.79	105.73	112.53
2	A	424	HEC	C3B-C4B-NB	-3.52	104.29	110.94
2	A	424	HEC	CMB-C2B-C1B	-3.51	122.56	128.36
2	B	424	HEC	CBC-CAC-C3C	-3.44	119.71	127.35
2	A	423	HEC	CMB-C2B-C1B	-3.40	122.73	128.36
2	A	424	HEC	CBA-CAA-C2A	-3.39	106.45	112.53
2	A	423	HEC	CBA-CAA-C2A	-3.37	106.49	112.53
2	B	423	HEC	CBC-CAC-C3C	-3.35	119.90	127.35
2	B	423	HEC	CMB-C2B-C1B	-3.15	123.15	128.36
2	B	424	HEC	CBA-CAA-C2A	-3.06	107.05	112.53
2	B	424	HEC	CAD-C3D-C4D	-2.96	123.80	127.01
2	A	423	HEC	CMC-C2C-C1C	-2.86	123.63	128.36
2	A	424	HEC	CMD-C2D-C1D	-2.70	123.90	128.36
2	B	423	HEC	CMC-C2C-C1C	-2.59	124.07	128.36
2	B	424	HEC	C3C-C4C-NC	-2.54	106.14	110.94
2	A	424	HEC	CMC-C2C-C1C	-2.30	124.57	128.36
2	B	423	HEC	C3C-C4C-NC	-2.26	106.67	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	423	HEC	CAA-C2A-C3A	-2.13	122.93	129.00
2	B	423	HEC	CAA-C2A-C3A	-2.09	123.03	129.00
2	B	424	HEC	CMC-C2C-C1C	-2.06	124.96	128.36
2	A	423	HEC	CAA-C2A-C1A	2.44	129.66	127.01
2	B	423	HEC	CMA-C3A-C2A	2.59	130.66	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1351	PO4	1	0
2	A	423	HEC	4	0
2	A	424	HEC	3	0
4	B	1350	PO4	1	0
5	B	1362	ACT	1	0
2	B	423	HEC	7	0
2	B	424	HEC	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, 95^{th} 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	320/341 (93%)	-0.12	10 (3%) 52 48	21, 31, 56, 98	0
1	B	319/341 (93%)	-0.21	5 (1%) 74 73	22, 32, 54, 124	0
All	All	639/682 (93%)	-0.17	15 (2%) 64 61	21, 32, 55, 124	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	346	ASN	11.3
1	B	345	SER	6.1
1	B	23	GLU	5.2
1	A	249	VAL	5.0
1	A	242	PRO	3.7
1	A	248	PRO	3.4
1	A	243	GLY	3.1
1	A	346	ASN	3.0
1	A	261	ALA	2.8
1	B	249	VAL	2.4
1	B	242	PRO	2.3
1	A	262	ALA	2.3
1	A	250	ASP	2.2
1	A	128	LYS	2.1
1	A	198	GLY	2.1

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, 95^{th} 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
4	PO4	A	1353	5/5	0.96	0.21	1.33	42,56,63,68	0
4	PO4	B	1356	5/5	0.89	0.14	1.32	68,91,97,97	0
3	CA	B	425	1/1	1.00	0.10	1.26	25,25,25,25	0
4	PO4	B	1352	5/5	0.97	0.15	1.05	62,63,67,71	0
4	PO4	A	1357	5/5	0.96	0.13	0.87	43,53,60,65	0
4	PO4	B	1355	5/5	0.96	0.13	0.83	66,68,75,81	0
2	HEC	A	423	43/43	0.99	0.13	0.61	19,22,29,31	0
2	HEC	B	423	43/43	0.99	0.08	0.34	21,23,31,40	0
2	HEC	A	424	43/43	0.98	0.10	0.31	23,27,31,32	0
4	PO4	B	1349	5/5	0.94	0.15	0.24	67,70,79,80	0
2	HEC	B	424	43/43	0.98	0.08	-0.13	23,29,33,35	0
3	CA	A	425	1/1	1.00	0.09	-0.27	25,25,25,25	0
4	PO4	B	1358	5/5	0.90	0.26	-	55,61,74,77	0
4	PO4	B	1348	5/5	0.88	0.22	-	81,89,105,107	0
5	ACT	B	1360	4/4	0.93	0.18	-	50,59,61,66	0
5	ACT	A	1358	4/4	0.87	0.10	-	58,58,66,69	0
4	PO4	A	1352	5/5	0.96	0.24	-	66,73,81,82	0
4	PO4	A	1350	5/5	0.82	0.12	-	61,71,86,87	0
4	PO4	A	1348	5/5	0.87	0.19	-	58,60,77,90	0
4	PO4	A	1362	5/5	0.87	0.21	-	68,78,83,97	0
4	PO4	A	1351	5/5	0.85	0.29	-	67,74,96,99	0
4	PO4	B	1354	5/5	0.95	0.11	-	51,59,60,62	0
4	PO4	A	1356	5/5	0.94	0.10	-	63,63,66,73	0
5	ACT	B	1361	4/4	0.79	0.26	-	78,82,83,89	0
6	EOH	A	1361	3/3	0.94	0.07	-	50,50,54,55	0
4	PO4	B	1359	5/5	0.94	0.14	-	53,60,68,80	0
4	PO4	A	1355	5/5	0.90	0.20	-	60,67,81,84	0
4	PO4	A	1354	5/5	0.95	0.12	-	70,70,81,93	0
4	PO4	B	1351	5/5	0.97	0.16	-	53,64,66,69	0
5	ACT	A	1360	4/4	0.84	0.19	-	54,61,67,72	0
4	PO4	A	1349	5/5	0.83	0.25	-	65,71,89,102	0
5	ACT	B	1362	4/4	0.88	0.16	-	43,45,51,68	0
5	ACT	A	1359	4/4	0.93	0.08	-	56,58,59,61	0
4	PO4	B	1353	5/5	0.95	0.13	-	69,74,84,86	0
4	PO4	B	1350	5/5	0.90	0.26	-	74,79,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PO4	B	1357	5/5	0.70	0.21	-	60,81,98,103	0

6.5 Other polymers (i)

There are no such residues in this entry.