Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:35 PM GMT

PDB ID	:	4M25
Title	:	Crystal structure of non-heme iron oxygenase OrfP in complex with Fe and alpha-ketoglutaric acid
Authors	:	Chang, C.Y.; Liu, Y.C.; Lyu, S.Y.; Wu, C.C.; Li, T.L.
Deposited on	:	2013-08-05
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:

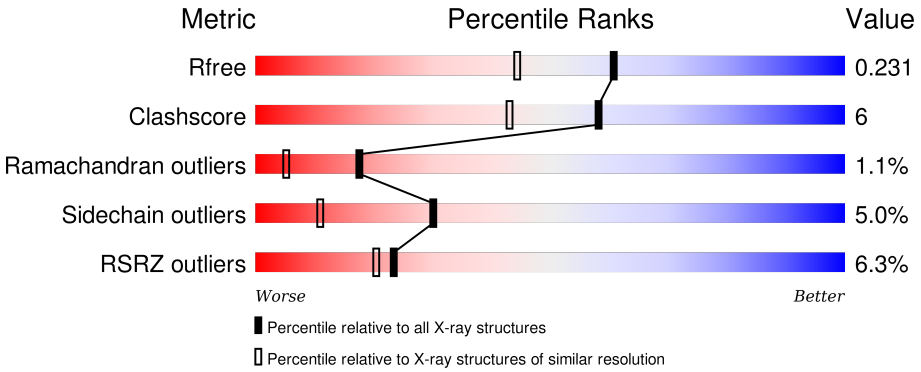
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	364	4% 79% 12% • 8%
1	B	364	7% 70% 14% • • 13%
1	C	364	5% 75% 9% • 13%
1	D	364	6% 74% 11% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11546 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 L-arginine beta-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2697	1697	488	505	7			
1	B	317	Total	C	N	O	S	0	0	0
			2541	1600	461	473	7			
1	C	317	Total	C	N	O	S	0	0	0
			2541	1600	461	473	7			
1	D	314	Total	C	N	O	S	0	1	0
			2525	1593	456	469	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
A	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
A	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
A	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
A	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
A	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
A	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
A	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
A	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
A	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
A	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
A	0	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-19	MET	-	EXPRESSION TAG	UNP G9MBV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
B	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
B	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
B	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
B	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
B	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
B	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
B	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
B	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
B	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
B	0	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
C	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
C	-17	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
C	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
C	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
C	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
C	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
C	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
C	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
C	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
C	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
C	0	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-19	MET	-	EXPRESSION TAG	UNP G9MBV2
D	-18	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-17	SER	-	EXPRESSION TAG	UNP G9MBV2

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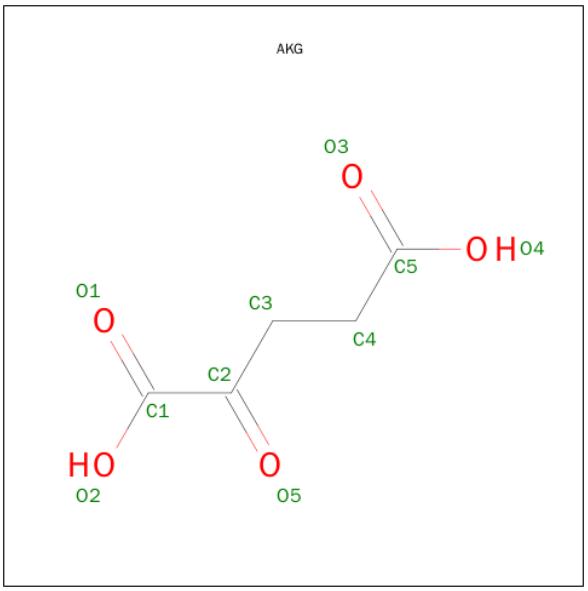
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-15	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-14	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-13	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-12	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-11	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-10	HIS	-	EXPRESSION TAG	UNP G9MBV2
D	-9	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-8	SER	-	EXPRESSION TAG	UNP G9MBV2
D	-7	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-6	LEU	-	EXPRESSION TAG	UNP G9MBV2
D	-5	VAL	-	EXPRESSION TAG	UNP G9MBV2
D	-4	PRO	-	EXPRESSION TAG	UNP G9MBV2
D	-3	ARG	-	EXPRESSION TAG	UNP G9MBV2
D	-2	GLY	-	EXPRESSION TAG	UNP G9MBV2
D	-1	SER	-	EXPRESSION TAG	UNP G9MBV2
D	0	HIS	-	EXPRESSION TAG	UNP G9MBV2

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0

- Molecule 4 is water.

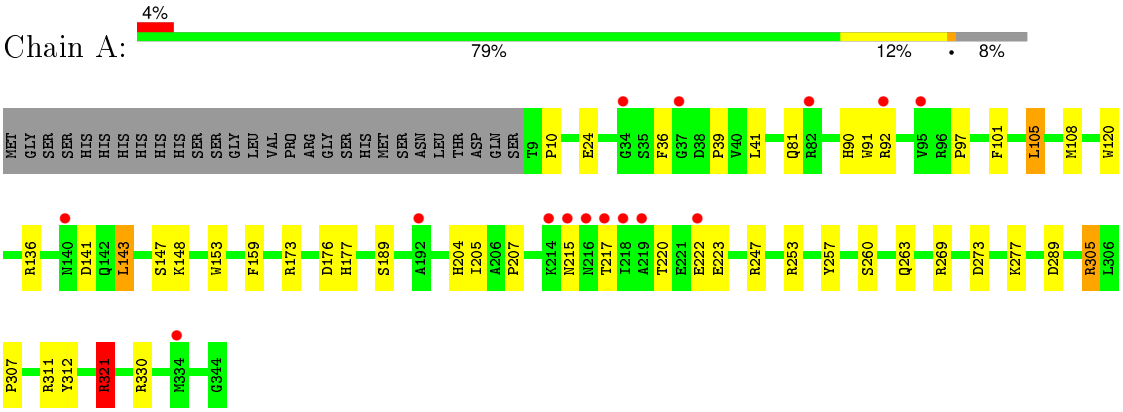
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	404	Total O 404 404	0	0
4	B	263	Total O 263 263	0	0
4	C	291	Total O 291 291	0	0
4	D	236	Total O 236 236	0	0

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.

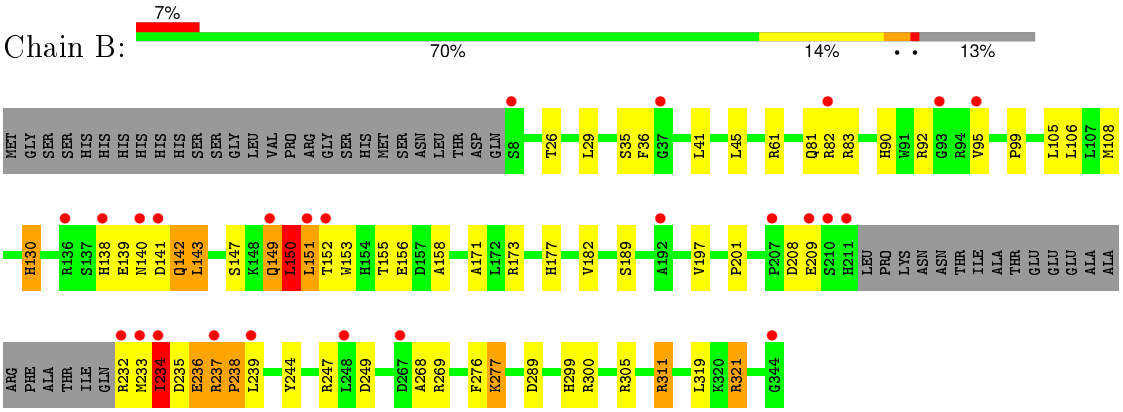
- Molecule 1: L-arginine beta-hydroxylase

Chain A:



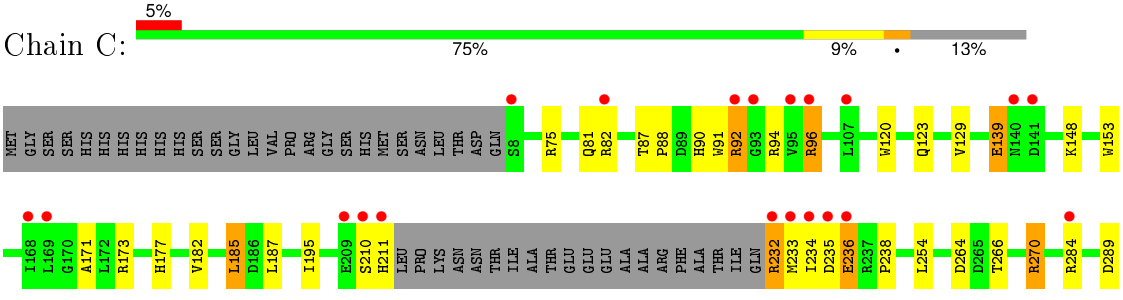
- Molecule 1: L-arginine beta-hydroxylase

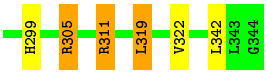
Chain B:



- Molecule 1: L-arginine beta-hydroxylase

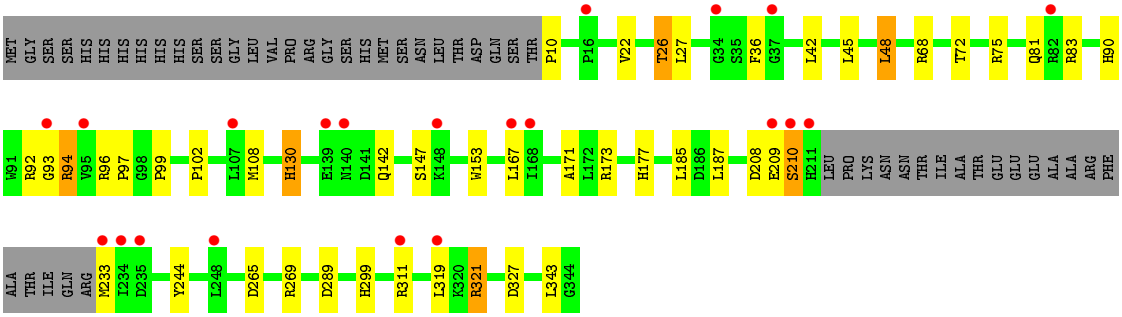
Chain C:





• Molecule 1: L-arginine beta-hydroxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.20Å 117.26Å 96.56Å 90.00° 91.86° 90.00°	Depositor
Resolution (Å)	30.00 – 1.84 26.70 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.84) 99.4 (26.70-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.194 , 0.232 0.195 , 0.231	Depositor DCC
R_{free} test set	6597 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.5	EDS
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 130687 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: AKG, FE

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	0.69	3/2767 (0.1%)	0.80	2/3764 (0.1%)
1	B	0.68	1/2608 (0.0%)	0.79	3/3545 (0.1%)
1	C	0.70	1/2608 (0.0%)	0.84	3/3545 (0.1%)
1	D	0.65	1/2592 (0.0%)	0.77	1/3523 (0.0%)
All	All	0.68	6/10575 (0.1%)	0.80	9/14377 (0.1%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	TRP	CD2-CE2	5.86	1.48	1.41
1	A	91	TRP	CD2-CE2	5.56	1.48	1.41
1	D	153	TRP	CD2-CE2	5.46	1.47	1.41
1	C	153	TRP	CD2-CE2	5.26	1.47	1.41
1	B	153	TRP	CD2-CE2	5.15	1.47	1.41
1	A	120	TRP	CD2-CE2	5.03	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	305	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	321	ARG	NE-CZ-NH2	-5.96	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	319	LEU	CA-CB-CG	5.80	128.64	115.30
1	B	150	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	61	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	185	LEU	CB-CG-CD2	5.20	119.84	111.00
1	D	48	LEU	CB-CG-CD1	5.17	119.78	111.00
1	B	236	GLU	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2697	0	2612	29	1
1	B	2541	0	2456	40	0
1	C	2541	0	2456	24	1
1	D	2525	0	2442	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	404	0	0	10	0
4	B	263	0	0	9	0
4	C	291	0	0	4	0
4	D	236	0	0	7	0
All	All	11546	0	9982	120	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 (120) 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:75:ARG:HD2	4:C:754:HOH:O	1.53	1.06
1:B:239:LEU:HB2	4:B:665:HOH:O	1.60	1.00
1:D:26:THR:HG23	1:D:102:PRO:HB3	1.51	0.93
1:D:244:TYR:OH	1:D:299:HIS:ND1	2.02	0.92
1:B:90:HIS:HD2	1:B:92:ARG:H	1.20	0.88
1:B:150:LEU:O	1:B:151:LEU:HB2	1.71	0.88
1:C:232:ARG:HH11	1:C:232:ARG:HG2	1.40	0.86
1:C:90:HIS:HD2	1:C:92:ARG:H	1.24	0.82
1:B:150:LEU:HD12	1:B:305:ARG:H	1.48	0.78
1:D:26:THR:HG21	4:D:566:HOH:O	1.84	0.77
1:B:150:LEU:HD13	1:B:152:THR:H	1.55	0.72
1:A:177:HIS:HD2	1:A:289:ASP:OD1	1.72	0.71
1:D:26:THR:HG23	1:D:102:PRO:CB	2.19	0.71
1:A:90:HIS:HD2	1:A:92:ARG:H	1.39	0.70
1:B:244:TYR:OH	1:B:299:HIS:ND1	2.21	0.70
1:D:26:THR:CG2	1:D:102:PRO:HB3	2.22	0.68
1:D:90:HIS:HD2	1:D:92:ARG:H	1.42	0.68
1:A:269:ARG:HD3	4:A:762:HOH:O	1.93	0.68
1:A:36:PHE:CE1	1:A:108:MET:HG3	2.29	0.68
1:B:90:HIS:CD2	1:B:92:ARG:H	2.07	0.67
1:A:141:ASP:HB2	1:A:143:LEU:HD22	1.76	0.66
1:B:201:PRO:O	4:B:665:HOH:O	2.14	0.65
1:C:177:HIS:HD2	1:C:289:ASP:OD1	1.80	0.64
1:A:90:HIS:CD2	1:A:92:ARG:H	2.15	0.63
1:D:177:HIS:HD2	1:D:289:ASP:OD1	1.82	0.63
1:B:269:ARG:HD3	4:B:756:HOH:O	1.99	0.63
1:A:177:HIS:HE1	4:A:726:HOH:O	1.81	0.62
1:A:222:GLU:HG2	1:A:223:GLU:N	2.15	0.62
1:B:237:ARG:CG	1:B:238:PRO:HD3	2.29	0.62
1:A:277:LYS:HG3	4:A:902:HOH:O	2.01	0.61
1:B:141:ASP:HB2	1:B:143:LEU:HD22	1.83	0.61
1:B:36:PHE:CE1	1:B:108:MET:HG3	2.36	0.60
1:D:321:ARG:HD3	4:D:621:HOH:O	2.02	0.60
1:B:305:ARG:HD3	4:B:685:HOH:O	2.02	0.59
1:D:265:ASP:O	1:D:269:ARG:HG3	2.03	0.58
1:C:236:GLU:O	1:C:238:PRO:HD3	2.03	0.58
1:C:91:TRP:CZ3	1:C:92:ARG:HD3	2.39	0.57
1:A:305:ARG:HD3	4:A:708:HOH:O	2.05	0.57
1:B:142:GLN:HG3	1:B:142:GLN:O	2.05	0.57
1:B:247:ARG:NH1	4:B:601:HOH:O	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLN:HG3	1:A:269:ARG:NH2	2.20	0.57
1:D:93:GLY:O	1:D:94:ARG:O	2.22	0.56
1:A:176:ASP:OD2	1:A:311:ARG:NH2	2.39	0.56
1:C:75:ARG:CD	4:C:754:HOH:O	2.30	0.55
1:D:10:PRO:O	1:D:72:THR:HG22	2.07	0.55
1:B:130:HIS:HD2	4:B:700:HOH:O	1.89	0.54
1:D:327:ASP:OD1	4:D:584:HOH:O	2.18	0.54
1:D:167[B]:LEU:HD22	1:D:167[B]:LEU:N	2.22	0.54
1:B:35:SER:HB2	4:B:626:HOH:O	2.07	0.54
1:B:150:LEU:HD13	1:B:152:THR:N	2.22	0.54
1:B:130:HIS:HE1	4:B:640:HOH:O	1.90	0.54
1:D:10:PRO:N	4:D:699:HOH:O	2.41	0.53
1:A:222:GLU:HG2	1:A:223:GLU:H	1.73	0.53
1:C:139:GLU:OE2	1:C:148:LYS:HE2	2.08	0.53
1:C:171:ALA:HA	1:C:319:LEU:HD22	1.90	0.53
1:D:130:HIS:HE1	4:D:599:HOH:O	1.91	0.53
1:A:204:HIS:HB3	1:A:260:SER:HB2	1.91	0.53
1:B:234:ILE:HA	1:B:235:ASP:HB2	1.91	0.52
1:A:273:ASP:OD1	4:A:763:HOH:O	2.19	0.52
1:C:91:TRP:CH2	1:C:92:ARG:HD3	2.44	0.51
1:B:150:LEU:HB3	1:B:305:ARG:O	2.11	0.51
1:A:148:LYS:O	1:A:307:PRO:HB3	2.10	0.51
1:C:90:HIS:CD2	1:C:92:ARG:H	2.15	0.51
1:C:311:ARG:HB2	1:C:311:ARG:HH11	1.76	0.51
1:B:237:ARG:HG3	1:B:238:PRO:HD3	1.92	0.51
1:D:97:PRO:HD2	4:D:617:HOH:O	2.11	0.50
1:B:171:ALA:HA	1:B:319:LEU:HD22	1.92	0.50
1:B:239:LEU:CB	4:B:665:HOH:O	2.33	0.49
1:C:232:ARG:NH1	1:C:232:ARG:HG2	2.15	0.49
1:B:249:ASP:CG	1:B:300:ARG:HH22	2.15	0.49
1:D:244:TYR:HH	1:D:299:HIS:CE1	2.23	0.48
1:A:39:PRO:HD2	4:A:814:HOH:O	2.14	0.48
1:C:96:ARG:HA	1:C:96:ARG:HD2	1.68	0.47
1:A:41:LEU:HD21	1:A:105:LEU:HD11	1.96	0.47
1:B:83:ARG:O	1:B:99:PRO:HB2	2.16	0.46
1:D:244:TYR:OH	1:D:299:HIS:CE1	2.66	0.46
1:D:81:GLN:NE2	1:D:173:ARG:HE	2.13	0.46
1:C:305:ARG:HD3	4:C:668:HOH:O	2.15	0.45
1:A:215:ASN:HB3	1:A:217:THR:HG23	1.97	0.45
1:A:321:ARG:HD3	4:A:590:HOH:O	2.16	0.45
1:D:83:ARG:O	1:D:99:PRO:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:NE2	1:B:173:ARG:HE	2.15	0.44
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.53	0.44
1:A:205:ILE:HD12	1:A:253:ARG:CZ	2.47	0.44
1:B:235:ASP:N	1:B:236:GLU:HB3	2.32	0.44
1:C:87:THR:HA	1:C:88:PRO:HD3	1.89	0.44
1:B:208:ASP:OD1	1:B:209:GLU:N	2.50	0.44
1:B:150:LEU:HD12	1:B:305:ARG:N	2.26	0.44
1:A:24:GLU:HG2	4:A:803:HOH:O	2.18	0.43
1:B:26:THR:HG21	1:B:106:LEU:HB2	2.00	0.43
1:D:94:ARG:N	4:D:615:HOH:O	2.40	0.43
1:B:276:PHE:HD1	1:B:277:LYS:HD3	1.83	0.43
1:A:330:ARG:HD2	4:A:722:HOH:O	2.18	0.43
1:B:156:GLU:OE2	1:B:321:ARG:NH2	2.52	0.43
1:C:81:GLN:HE22	1:C:173:ARG:HE	1.67	0.43
1:C:129:VAL:HG22	1:C:322:VAL:HG22	2.01	0.43
1:D:171:ALA:HA	1:D:319:LEU:HD22	2.01	0.42
1:B:233:MET:O	1:B:233:MET:HG3	2.19	0.42
1:A:136:ARG:HA	1:A:312:TYR:CZ	2.54	0.42
1:C:264:ASP:HB2	4:C:617:HOH:O	2.20	0.42
1:C:120:TRP:HB2	1:C:123:GLN:HB2	2.01	0.42
1:D:22:VAL:O	1:D:26:THR:HB	2.19	0.42
1:B:41:LEU:HD21	1:B:105:LEU:HD21	2.01	0.42
1:B:177:HIS:HD2	1:B:289:ASP:OD1	2.02	0.42
1:A:159:PHE:CG	1:A:207:PRO:HA	2.55	0.42
1:D:208:ASP:HB3	1:D:210:SER:HB2	2.01	0.42
1:C:187:LEU:HD22	1:C:195:ILE:HD11	2.01	0.42
1:B:138:HIS:HB3	1:B:143:LEU:HD21	2.00	0.42
1:C:266:THR:HG22	1:C:270:ARG:NH2	2.34	0.42
1:D:343:LEU:N	1:D:343:LEU:HD12	2.35	0.42
1:A:263:GLN:HG3	1:A:269:ARG:HH21	1.84	0.41
1:C:232:ARG:N	1:C:232:ARG:HD3	2.36	0.41
1:B:197:VAL:HG11	1:B:268:ALA:HA	2.02	0.41
1:A:97:PRO:HB2	1:A:101:PHE:HB2	2.03	0.41
1:B:311:ARG:HB2	1:B:311:ARG:HH11	1.84	0.41
1:A:81:GLN:NE2	1:A:173:ARG:HH11	2.17	0.41
1:A:10:PRO:HA	4:A:649:HOH:O	2.20	0.40
1:B:155:THR:HB	1:B:158:ALA:HB2	2.03	0.40
1:C:82:ARG:HH11	1:C:82:ARG:HG2	1.86	0.40
1:D:177:HIS:CD2	1:D:289:ASP:OD1	2.70	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)
1:A:257:TYR:OH	1:C:270:ARG:NH2[2_546]	2.03	0.17

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	335/364 (92%)	326 (97%)	7 (2%)	2 (1%)	30 14
1	B	313/364 (86%)	293 (94%)	14 (4%)	6 (2%)	10 1
1	C	313/364 (86%)	300 (96%)	10 (3%)	3 (1%)	19 6
1	D	311/364 (85%)	303 (97%)	5 (2%)	3 (1%)	19 6
All	All	1272/1456 (87%)	1222 (96%)	36 (3%)	14 (1%)	17 5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LEU
1	B	237	ARG
1	C	235	ASP
1	D	94	ARG
1	B	150	LEU
1	C	210	SER
1	D	147	SER
1	A	147	SER
1	A	220	THR
1	B	139	GLU
1	D	210	SER
1	B	234	ILE
1	C	234	ILE
1	B	238	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	287/311 (92%)	282 (98%)	5 (2%)	68 54
1	B	271/311 (87%)	253 (93%)	18 (7%)	21 5
1	C	271/311 (87%)	255 (94%)	16 (6%)	24 7
1	D	269/311 (86%)	253 (94%)	16 (6%)	24 7
All	All	1098/1244 (88%)	1043 (95%)	55 (5%)	30 11

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	143	LEU
1	A	189	SER
1	A	247	ARG
1	A	321	ARG
1	B	29	LEU
1	B	45	LEU
1	B	82	ARG
1	B	95	VAL
1	B	130	HIS
1	B	140	ASN
1	B	142	GLN
1	B	143	LEU
1	B	147	SER
1	B	149	GLN
1	B	150	LEU
1	B	182	VAL
1	B	189	SER
1	B	232	ARG
1	B	234	ILE
1	B	277	LYS
1	B	311	ARG
1	B	321	ARG
1	C	92	ARG

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Mol	Chain	Res	Type
1	C	94	ARG
1	C	96	ARG
1	C	139	GLU
1	C	182	VAL
1	C	185	LEU
1	C	211	HIS
1	C	232	ARG
1	C	233	MET
1	C	236	GLU
1	C	254	LEU
1	C	270	ARG
1	C	284	ARG
1	C	299	HIS
1	C	311	ARG
1	C	342	LEU
1	D	26	THR
1	D	27	LEU
1	D	42	LEU
1	D	45	LEU
1	D	48	LEU
1	D	68	ARG
1	D	75	ARG
1	D	96	ARG
1	D	130	HIS
1	D	142	GLN
1	D	185	LEU
1	D	187	LEU
1	D	209	GLU
1	D	233	MET
1	D	311	ARG
1	D	321	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	138	HIS
1	A	177	HIS
1	A	263	GLN
1	B	57	GLN

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Mol	Chain	Res	Type
1	B	81	GLN
1	B	90	HIS
1	B	130	HIS
1	B	177	HIS
1	B	211	HIS
1	C	57	GLN
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	142	GLN
1	C	177	HIS
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	130	HIS
1	D	177	HIS
1	D	263	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\|>2$
3	AKG	A	403	2	3,9,9	0.50	0	4,11,11	0.56	0
3	AKG	B	403	2	3,9,9	0.76	0	4,11,11	0.51	0
3	AKG	C	403	2	3,9,9	0.45	0	4,11,11	0.43	0
3	AKG	D	403	2	3,9,9	0.58	0	4,11,11	0.86	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
3	AKG	A	403	2	-	0/3/9/9	0/0/0/0
3	AKG	B	403	2	-	0/3/9/9	0/0/0/0
3	AKG	C	403	2	-	0/3/9/9	0/0/0/0
3	AKG	D	403	2	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	336/364 (92%)	0.05	15 (4%)	37	33	16, 27, 53, 116	6 (1%)
1	B	317/364 (87%)	0.25	25 (7%)	15	14	19, 32, 72, 97	3 (0%)
1	C	317/364 (87%)	0.08	20 (6%)	23	20	16, 27, 57, 92	4 (1%)
1	D	314/364 (86%)	0.19	21 (6%)	21	18	17, 32, 61, 80	3 (0%)
All	All	1284/1456 (88%)	0.14	81 (6%)	23	20	16, 30, 61, 116	16 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	16.2
1	A	216	ASN	10.0
1	C	234	ILE	6.8
1	C	236	GLU	5.8
1	B	151	LEU	5.7
1	A	214	LYS	5.7
1	C	233	MET	5.2
1	A	219	ALA	5.1
1	B	37	GLY	4.7
1	B	237	ARG	4.7
1	B	209	GLU	4.6
1	C	211	HIS	4.6
1	D	234	ILE	4.3
1	D	209	GLU	4.3
1	C	210	SER	4.2
1	A	92	ARG	4.0
1	B	211	HIS	3.9
1	A	217	THR	3.9
1	A	215	ASN	3.8
1	B	234	ILE	3.7
1	A	334	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	95	VAL	3.4
1	C	82	ARG	3.4
1	B	93	GLY	3.3
1	D	319	LEU	3.3
1	D	210	SER	3.2
1	D	34	GLY	3.2
1	C	140	ASN	3.1
1	C	235	ASP	3.0
1	B	136	ARG	3.0
1	B	239	LEU	3.0
1	C	93	GLY	3.0
1	A	192	ALA	2.9
1	C	209	GLU	2.9
1	D	233	MET	2.9
1	A	95	VAL	2.8
1	D	235	ASP	2.8
1	D	148	LYS	2.8
1	B	248	LEU	2.7
1	D	37	GLY	2.7
1	D	107	LEU	2.6
1	C	92	ARG	2.6
1	B	344	GLY	2.6
1	B	140	ASN	2.6
1	A	37	GLY	2.6
1	D	95	VAL	2.6
1	C	168	ILE	2.5
1	D	82	ARG	2.5
1	D	93	GLY	2.5
1	D	16	PRO	2.5
1	D	168	ILE	2.5
1	B	192	ALA	2.5
1	B	152	THR	2.5
1	C	169	LEU	2.5
1	D	167[A]	LEU	2.5
1	D	248	LEU	2.4
1	A	140	ASN	2.4
1	C	8	SER	2.4
1	C	232	ARG	2.4
1	B	233	MET	2.4
1	B	82	ARG	2.3
1	D	211	HIS	2.2
1	B	141	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	GLN	2.2
1	A	222	GLU	2.2
1	D	311	ARG	2.2
1	D	140	ASN	2.2
1	C	96	ARG	2.2
1	B	232	ARG	2.2
1	B	267	ASP	2.1
1	C	107	LEU	2.1
1	B	207	PRO	2.1
1	C	95	VAL	2.1
1	B	8	SER	2.1
1	B	210	SER	2.1
1	A	82	ARG	2.1
1	B	138	HIS	2.1
1	C	141	ASP	2.0
1	D	139	GLU	2.0
1	C	284	ARG	2.0
1	A	34	GLY	2.0

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, 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
3	AKG	C	403	10/10	0.98	0.16	0.40	26,26,27,28	0
3	AKG	A	403	10/10	0.96	0.09	-0.47	24,25,26,27	0
2	FE	D	402	1/1	0.98	0.12	-0.54	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AKG	D	403	10/10	0.95	0.10	-0.62	27,29,32,32	0
2	FE	B	402	1/1	0.98	0.07	-1.09	48,48,48,48	0
3	AKG	B	403	10/10	0.96	0.08	-1.21	29,30,34,36	0
2	FE	C	401	1/1	1.00	0.09	-1.81	22,22,22,22	0
2	FE	A	401	1/1	1.00	0.07	-	24,24,24,24	0
2	FE	D	401	1/1	1.00	0.08	-	23,23,23,23	0
2	FE	C	402	1/1	0.99	0.08	-	48,48,48,48	0
2	FE	A	402	1/1	0.99	0.02	-	26,26,26,26	0
2	FE	B	401	1/1	0.98	0.06	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.