



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:10 PM UTC

PDB ID : 4M25 / pdb_00004m25
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

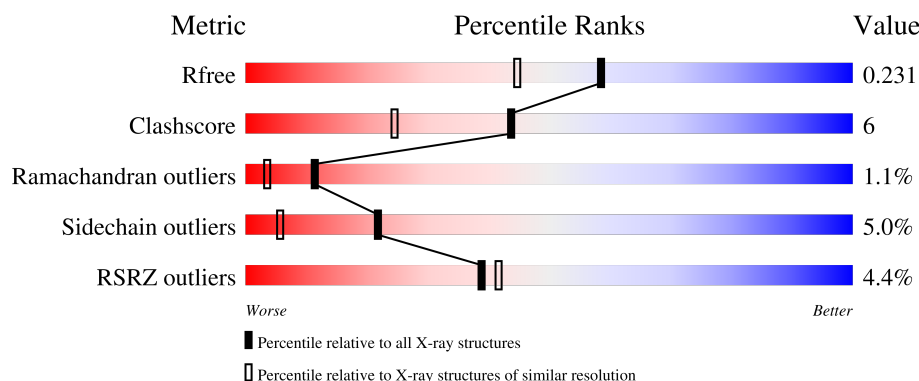
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	364	4% 79% 12% 8%
1	B	364	6% 69% 15% 13%
1	C	364	3% 74% 11% 13%
1	D	364	2% 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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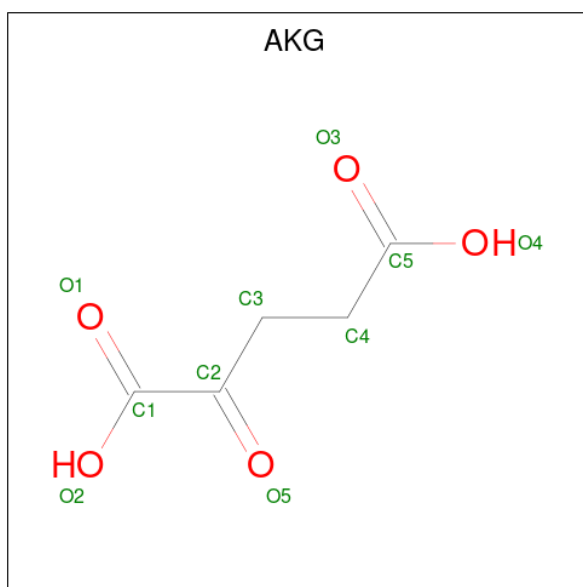
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9MBV2
D	-15	HIS	-	expression tag	UNP G9MBV2
D	-14	HIS	-	expression tag	UNP G9MBV2
D	-13	HIS	-	expression tag	UNP G9MBV2
D	-12	HIS	-	expression tag	UNP G9MBV2
D	-11	HIS	-	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 (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



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

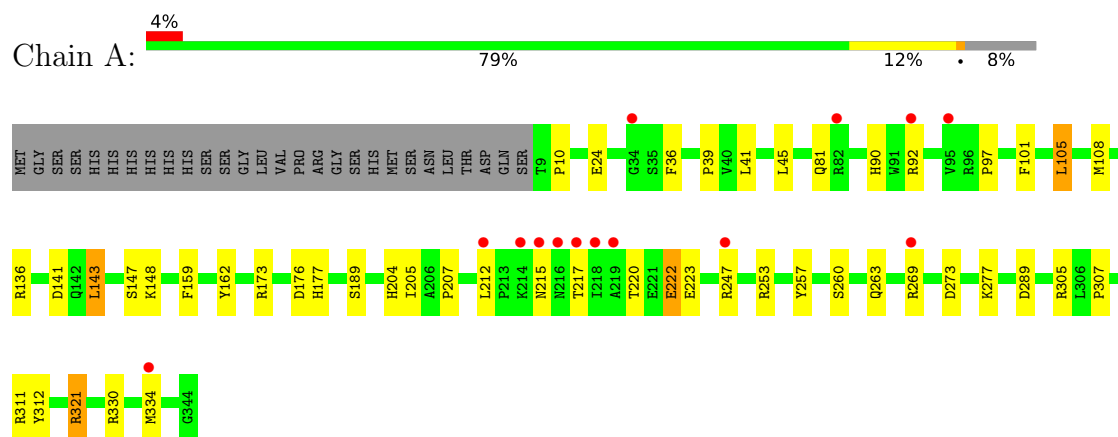
- Molecule 4 is water.

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

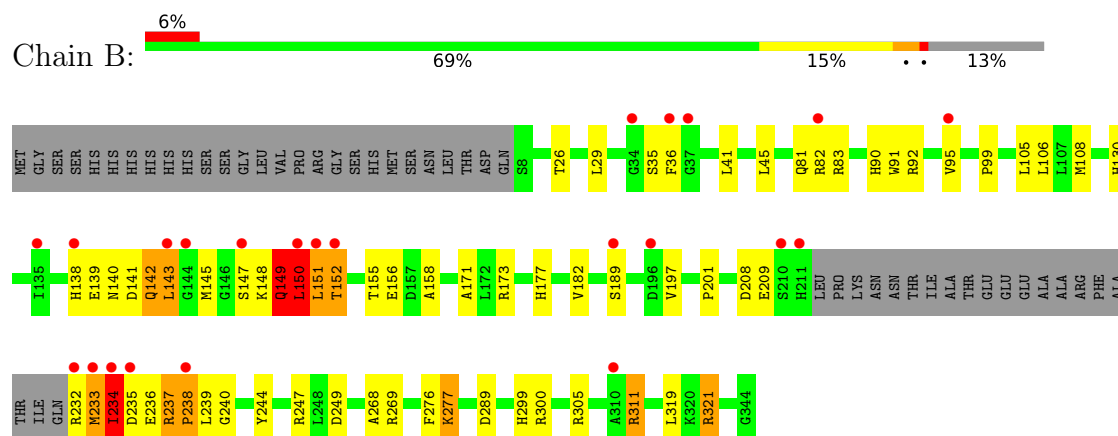
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

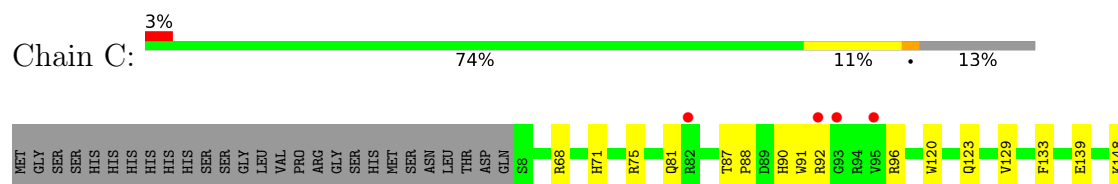
- Molecule 1: L-arginine beta-hydroxylase

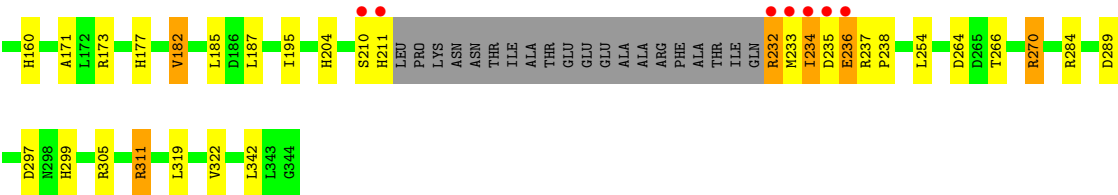


- Molecule 1: L-arginine beta-hydroxylase

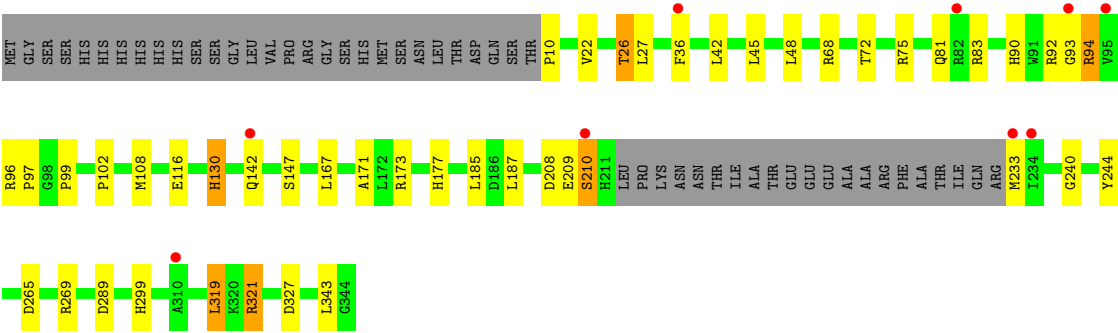


- Molecule 1: L-arginine beta-hydroxylase





● Molecule 1: L-arginine beta-hydroxylase



4 Data and refinement statistics

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 30.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.84) 99.5 (30.00-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	6600 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: FE, AKG

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	0.93	0/2767	0.95	2/3764 (0.1%)
1	B	0.94	0/2608	0.94	2/3545 (0.1%)
1	C	0.96	4/2608 (0.2%)	0.98	5/3545 (0.1%)
1	D	0.88	0/2592	0.91	4/3523 (0.1%)
All	All	0.93	4/10575 (0.0%)	0.95	13/14377 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	HIS	CG-CD2	5.72	1.42	1.35
1	C	71	HIS	CG-CD2	5.62	1.42	1.35
1	C	299	HIS	CE1-NE2	5.19	1.37	1.32
1	C	160	HIS	CG-CD2	5.18	1.41	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLN	N-CA-C	6.72	119.94	109.52
1	D	240	GLY	CA-C-N	6.41	126.59	120.31
1	D	240	GLY	C-N-CA	6.41	126.59	120.31
1	C	133	PHE	CA-C-N	-6.38	113.10	119.99
1	C	133	PHE	C-N-CA	-6.38	113.10	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ARG	CA-C-N	-5.95	114.14	120.03
1	C	237	ARG	C-N-CA	-5.95	114.14	120.03
1	D	116	GLU	CA-C-N	-5.31	114.45	119.76
1	D	116	GLU	C-N-CA	-5.31	114.45	119.76
1	C	182	VAL	CB-CA-C	5.29	118.65	110.28
1	B	233	MET	N-CA-C	5.10	117.08	109.59
1	A	45	LEU	CA-C-N	-5.01	113.88	119.19
1	A	45	LEU	C-N-CA	-5.01	113.88	119.19

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

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	30	1
1	B	2541	0	2456	42	0
1	C	2541	0	2456	24	1
1	D	2525	0	2442	28	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	8	0
All	All	11546	0	9982	124	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 (124) 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:HG2	1:C:232:ARG:HH11	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:36:PHE:CE1	1:A:108:MET:HG3	2.29	0.68
1:A:269:ARG:HD3	4:A:762:HOH:O	1.93	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:B:269:ARG:HD3	4:B:756:HOH:O	1.99	0.63
1:D:177:HIS:HD2	1:D:289:ASP:OD1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HD3	4:A:708:HOH:O	2.05	0.57
1:B:142:GLN:O	1:B:142:GLN:HG3	2.05	0.57
1:B:247:ARG:NH1	4:B:601:HOH:O	1.99	0.57
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:249:ASP:CG	1:B:300:ARG:HH22	2.15	0.54
1:B:130:HIS:HD2	4:B:700:HOH:O	1.89	0.54
1:D:167[B]:LEU:N	1:D:167[B]:LEU:HD22	2.22	0.54
1:D:327:ASP:OD1	4:D:584:HOH:O	2.18	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:A:162:TYR:CE2	1:A:334:MET:HE3	2.44	0.52
1:A:273:ASP:OD1	4:A:763:HOH:O	2.19	0.52
1:B:234:ILE:HA	1:B:235:ASP:HB2	1.91	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:HH11	1:C:311:ARG:HB2	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:HG2	1:C:232:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASN:HB3	1:A:217:THR:HG23	1.97	0.45
1:C:305:ARG:HD3	4:C:668:HOH:O	2.15	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
1:B:81:GLN:NE2	1:B:173:ARG:HE	2.15	0.44
1:A:205:ILE:HD12	1:A:253:ARG:CZ	2.47	0.44
1:D:36:PHE:CE1	1:D:108:MET:HG3	2.53	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:D:208:ASP:CG	4:D:657:HOH:O	2.61	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:B:233:MET:O	1:B:233:MET:HG3	2.19	0.42
1:D:171:ALA:HA	1:D:319:LEU:HD22	2.01	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:B:41:LEU:HD21	1:B:105:LEU:HD21	2.01	0.42
1:D:22:VAL:O	1:D:26:THR:HB	2.19	0.42
1:B:177:HIS:HD2	1:B:289:ASP:OD1	2.02	0.42
1:C:297:ASP:C	1:C:297:ASP:OD1	2.63	0.42
1:A:159:PHE:CG	1:A:207:PRO:HA	2.55	0.42
1:C:187:LEU:HD22	1:C:195:ILE:HD11	2.01	0.42
1:D:208:ASP:HB3	1:D:210:SER:HB2	2.01	0.42
1:B:138:HIS:HB3	1:B:143:LEU:HD21	2.00	0.42
1:B:91:TRP:HD1	1:B:145:MET:HE2	1.85	0.42
1:C:266:THR:HG22	1:C:270:ARG:NH2	2.34	0.42
1:D:343:LEU:HD12	1:D:343:LEU:N	2.35	0.42
1:A:263:GLN:HG3	1:A:269:ARG:HH21	1.84	0.41
1:B:197:VAL:HG11	1:B:268:ALA:HA	2.02	0.41
1:C:232:ARG:N	1:C:232:ARG:HD3	2.36	0.41
1:A:97:PRO:HB2	1:A:101:PHE:HB2	2.03	0.41
1:B:311:ARG:HH11	1:B:311:ARG:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:NE2	1:A:173:ARG:HH11	2.17	0.41
1:B:201:PRO:HA	1:B:240:GLY:C	2.46	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: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%)	21	9
1	B	313/364 (86%)	293 (94%)	14 (4%)	6 (2%)	6	0
1	C	313/364 (86%)	300 (96%)	10 (3%)	3 (1%)	12	4
1	D	311/364 (85%)	303 (97%)	5 (2%)	3 (1%)	12	4
All	All	1272/1456 (87%)	1222 (96%)	36 (3%)	14 (1%)	11	3

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	280 (98%)	7 (2%)	43	25
1	B	271/311 (87%)	252 (93%)	19 (7%)	14	2
1	C	271/311 (87%)	258 (95%)	13 (5%)	23	6
1	D	269/311 (86%)	253 (94%)	16 (6%)	18	4
All	All	1098/1244 (88%)	1043 (95%)	55 (5%)	22	6

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	212	LEU
1	A	222	GLU
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	140	ASN

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Mol	Chain	Res	Type
1	B	142	GLN
1	B	143	LEU
1	B	147	SER
1	B	148	LYS
1	B	149	GLN
1	B	150	LEU
1	B	152	THR
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	68	ARG
1	C	182	VAL
1	C	185	LEU
1	C	211	HIS
1	C	232	ARG
1	C	233	MET
1	C	234	ILE
1	C	236	GLU
1	C	254	LEU
1	C	270	ARG
1	C	284	ARG
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	319	LEU

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Mol	Chain	Res	Type
1	D	321	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	A	90	HIS
1	A	123	GLN
1	A	138	HIS
1	A	177	HIS
1	B	81	GLN
1	B	90	HIS
1	B	130	HIS
1	B	138	HIS
1	B	149	GLN
1	B	177	HIS
1	B	211	HIS
1	C	81	GLN
1	C	90	HIS
1	C	123	GLN
1	C	138	HIS
1	C	142	GLN
1	C	177	HIS
1	C	290	GLN
1	D	57	GLN
1	D	81	GLN
1	D	90	HIS
1	D	130	HIS
1	D	177	HIS
1	D	204	HIS
1	D	263	GLN
1	D	290	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	403	2	9,9,9	2.19	2 (22%)	11,11,11	1.39	2 (18%)
3	AKG	D	403	2	9,9,9	1.70	1 (11%)	11,11,11	2.37	4 (36%)
3	AKG	C	403	2	9,9,9	1.84	1 (11%)	11,11,11	1.72	3 (27%)
3	AKG	A	403	2	9,9,9	1.59	1 (11%)	11,11,11	1.53	2 (18%)

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	B	403	2	-	1/9/9/9	-
3	AKG	D	403	2	-	3/9/9/9	-
3	AKG	C	403	2	-	1/9/9/9	-
3	AKG	A	403	2	-	1/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	AKG	C2-C1	-4.92	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	AKG	C2-C1	-4.41	1.46	1.53
3	D	403	AKG	C2-C1	-4.28	1.47	1.53
3	A	403	AKG	C2-C1	-3.53	1.48	1.53
3	B	403	AKG	O1-C1	2.74	1.29	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	AKG	O1-C1-C2	-5.67	114.75	121.81
3	B	403	AKG	C3-C2-C1	3.17	121.25	115.86
3	C	403	AKG	C3-C2-C1	3.15	121.21	115.86
3	D	403	AKG	O2-C1-C2	3.00	121.91	113.59
3	A	403	AKG	C3-C2-C1	2.92	120.82	115.86
3	C	403	AKG	O2-C1-C2	2.83	121.43	113.59
3	D	403	AKG	O4-C5-C4	2.56	122.08	114.00
3	A	403	AKG	O1-C1-C2	-2.37	118.87	121.81
3	D	403	AKG	C3-C2-C1	2.35	119.86	115.86
3	B	403	AKG	O1-C1-C2	-2.30	118.95	121.81
3	C	403	AKG	O1-C1-C2	-2.03	119.29	121.81

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	AKG	C1-C2-C3-C4
3	D	403	AKG	C1-C2-C3-C4
3	A	403	AKG	C1-C2-C3-C4
3	C	403	AKG	C1-C2-C3-C4
3	D	403	AKG	C3-C4-C5-O4
3	D	403	AKG	C3-C4-C5-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	336/364 (92%)	-0.02	14 (4%)	40 43	8, 26, 53, 116	7 (2%)
1	B	317/364 (87%)	0.35	23 (7%)	21 22	18, 32, 72, 97	3 (0%)
1	C	317/364 (87%)	0.03	11 (3%)	47 51	16, 26, 57, 92	4 (1%)
1	D	314/364 (86%)	0.20	9 (2%)	53 58	11, 32, 61, 80	4 (1%)
All	All	1284/1456 (88%)	0.14	57 (4%)	39 42	8, 29, 61, 116	18 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	ARG	6.2
1	A	218	ILE	6.1
1	B	234	ILE	5.4
1	C	234	ILE	5.4
1	B	151	LEU	5.4
1	A	269	ARG	4.9
1	A	334	MET	4.8
1	D	233	MET	4.8
1	A	92	ARG	4.7
1	B	82	ARG	4.7
1	C	82	ARG	4.6
1	D	234	ILE	4.6
1	A	82	ARG	4.4
1	A	219	ALA	4.3
1	D	82	ARG	4.1
1	C	93	GLY	3.7
1	B	152	THR	3.4
1	C	95	VAL	3.4
1	B	150	LEU	3.4
1	B	36	PHE	3.2
1	B	143	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	93	GLY	3.2
1	A	214	LYS	3.1
1	A	217	THR	3.1
1	C	210	SER	3.1
1	B	95	VAL	3.0
1	C	233	MET	3.0
1	B	211	HIS	2.9
1	C	235	ASP	2.8
1	A	215	ASN	2.8
1	A	216	ASN	2.8
1	B	138	HIS	2.8
1	D	95	VAL	2.8
1	C	236	GLU	2.8
1	B	235	ASP	2.7
1	C	211	HIS	2.7
1	B	189	SER	2.6
1	B	238	PRO	2.6
1	B	233	MET	2.5
1	B	232	ARG	2.5
1	B	144	GLY	2.4
1	B	196	ASP	2.3
1	A	247	ARG	2.3
1	A	212	LEU	2.3
1	B	37	GLY	2.2
1	B	210	SER	2.2
1	B	147	SER	2.2
1	D	310	ALA	2.1
1	A	95	VAL	2.1
1	B	34	GLY	2.1
1	C	232	ARG	2.1
1	B	135	ILE	2.1
1	D	210	SER	2.1
1	D	142	GLN	2.1
1	D	36	PHE	2.0
1	B	310	ALA	2.0
1	A	34	GLY	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 [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	AKG	B	403	10/10	0.94	0.07	29,30,34,36	0
3	AKG	D	403	10/10	0.94	0.07	27,29,32,32	0
3	AKG	C	403	10/10	0.97	0.06	26,26,27,28	0
3	AKG	A	403	10/10	0.97	0.05	24,25,26,27	0
2	FE	B	401	1/1	0.98	0.03	30,30,30,30	0
2	FE	B	402	1/1	0.98	0.11	48,48,48,48	0
2	FE	C	402	1/1	0.98	0.12	48,48,48,48	0
2	FE	D	402	1/1	0.98	0.13	47,47,47,47	0
2	FE	D	401	1/1	0.99	0.02	23,23,23,23	0
2	FE	A	402	1/1	0.99	0.04	26,26,26,26	0
2	FE	C	401	1/1	1.00	0.01	22,22,22,22	0
2	FE	A	401	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.