Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 12:53 am GMT

PDB ID	:	1OII
Title	:	Crystal structure of the alkylsulfatase AtsK, a non-heme Fe(II) alphaketoglutarate dependent Dioxygenase in complex with iron and alphaketoglutarate
Authors	:	Mueller, I.; Kahnert, A.; Pape, T.; Dierks, T.; Meyer-Klauke, W.; Kertesz, M.A.; Uson, I.
Deposited on	:	2003-06-18
Resolution	:	2.19 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 (i) 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 (i)) were used in the production of this report:

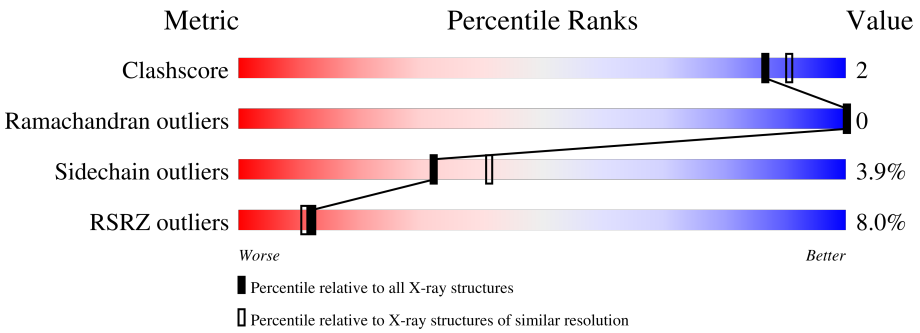
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.19 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	301	7% 75% 8% • 16%
1	B	301	7% 76% 7% • 16%
1	C	301	6% 73% 5% • 21%
1	D	301	7% 75% • • 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8211 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.

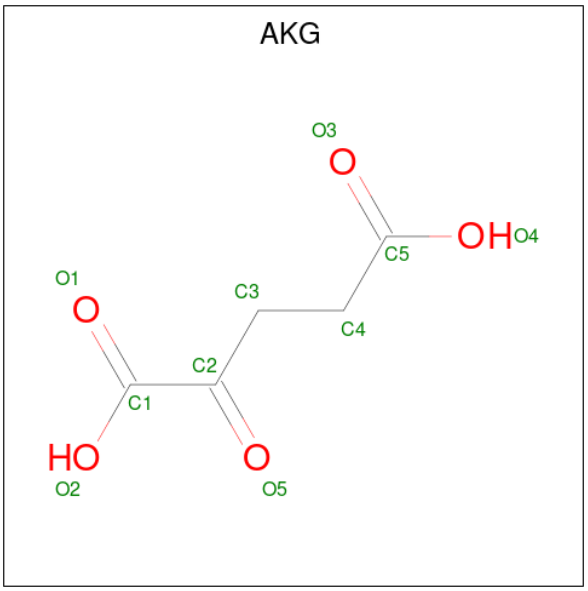
- Molecule 1 is a protein called PUTATIVE ALKYLSULFATASE ATSK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	253	1948	1232	358	358	0	0	0
1	B	253	1965	1243	363	359	0	0	0
1	C	237	1811	1148	330	333	0	0	0
1	D	245	1870	1185	347	338	0	0	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

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



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

- Molecule 4 is water.

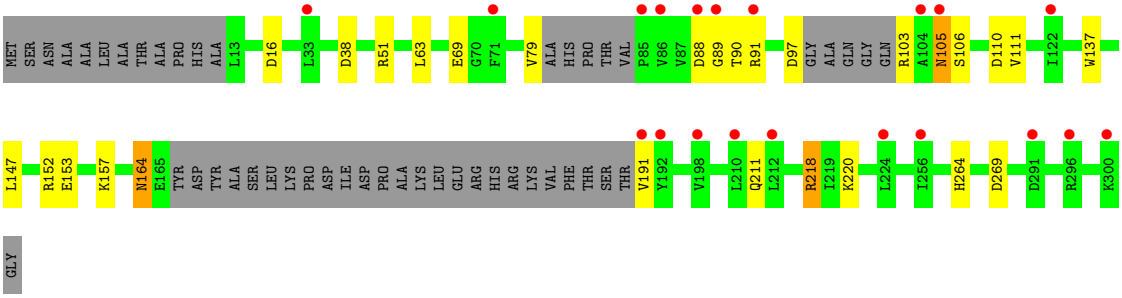
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	150	150	150	0	0
4	B	155	155	155	0	0
4	C	151	151	151	0	0
4	D	117	117	117	0	0

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.

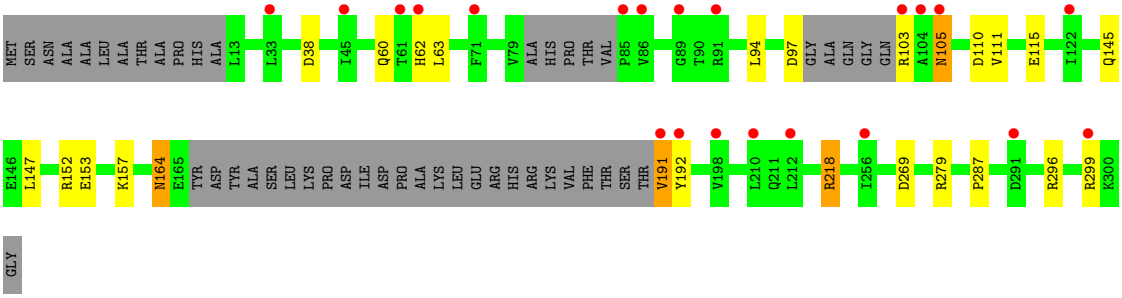
• Molecule 1: PUTATIVE ALKYLSULFATASE ATSK

Chain A:



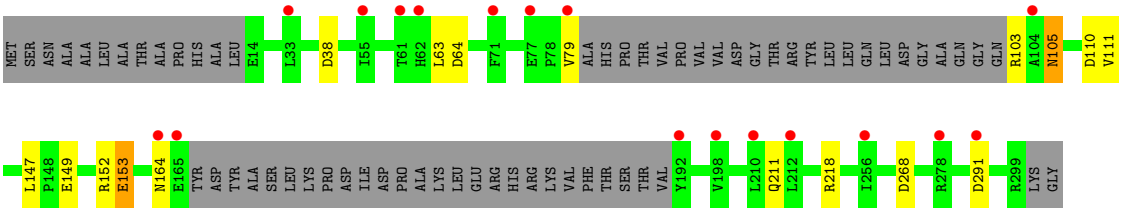
• Molecule 1: PUTATIVE ALKYLSULFATASE ATSK

Chain B:



• Molecule 1: PUTATIVE ALKYLSULFATASE ATSK

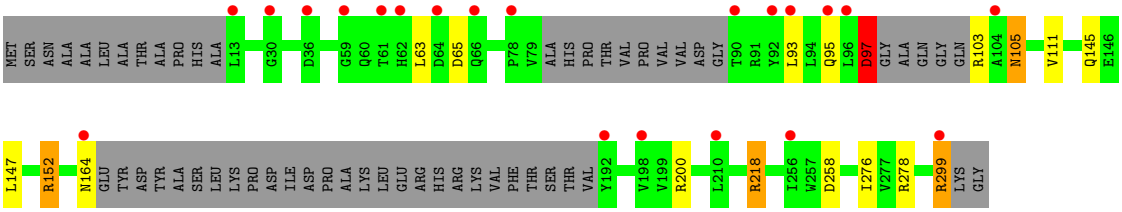
Chain C:



• Molecule 1: PUTATIVE ALKYLSULFATASE ATSK

Chain D:

7%
75%
19%


MET SER ASN ALA ALA LEU ALA THR ALA PRO HIS ALA L13 G30 D36 G59 Q60 T61 H62 L63 D64 D65 Q66 P78 V79 ALA HIS PRO THR VAL PRO VAL VAL ASP GLY T90 R91 Y92 L93 L94 Q95 L96 D97 GLY ALA GLN GLY GLN R103 A104 N105 V111 Q145 E146
L147 R152 N164 GLU TYR ASP TYR ALA SER LEU LYS PRO ASP ILE ASP PRO ALA LYS LEU GLU ARG HIS ARG LYS VAL PHE THR SER THR VAL Y192 V198 V199 R200 L210 R218 I256 W257 D258 I276 V277 R278 R299 LYS GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.42Å 147.33Å 158.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.19 20.34 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.19) 97.6 (20.34-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.195 , 0.220 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8211	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3198e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: FE2, 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	0.88	0/1991	1.00	11/2715 (0.4%)
1	B	0.89	0/2009	1.03	8/2740 (0.3%)
1	C	0.89	2/1854 (0.1%)	1.06	11/2534 (0.4%)
1	D	0.88	1/1913 (0.1%)	0.99	8/2614 (0.3%)
All	All	0.89	3/7767 (0.0%)	1.02	38/10603 (0.4%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	GLU	CG-CD	6.09	1.61	1.51
1	D	145	GLN	CG-CD	5.36	1.63	1.51
1	C	153	GLU	CD-OE1	5.17	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	218	ARG	NE-CZ-NH1	-16.16	112.22	120.30
1	C	218	ARG	NE-CZ-NH2	15.78	128.19	120.30
1	B	103	ARG	NE-CZ-NH2	12.70	126.65	120.30
1	B	103	ARG	NE-CZ-NH1	-12.62	113.99	120.30
1	D	103	ARG	NE-CZ-NH1	-12.10	114.25	120.30
1	D	103	ARG	NE-CZ-NH2	11.19	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	C	103	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	A	103	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	B	38	ASP	CB-CG-OD2	10.13	127.42	118.30
1	C	103	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	B	269	ASP	CB-CG-OD2	8.87	126.29	118.30
1	A	38	ASP	CB-CG-OD2	8.12	125.60	118.30
1	C	218	ARG	CD-NE-CZ	7.50	134.10	123.60
1	A	269	ASP	CB-CG-OD2	7.35	124.91	118.30
1	D	97	ASP	CB-CG-OD2	7.03	124.63	118.30
1	A	110	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	218	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	200	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	218	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	B	218	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	110	ASP	CB-CG-OD2	6.59	124.23	118.30
1	D	218	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	97	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	218	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	218	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	97	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	64	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	103	ARG	CD-NE-CZ	5.65	131.51	123.60
1	C	110	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	38	ASP	CB-CG-OD2	5.53	123.27	118.30
1	C	291	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	152	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	89	GLY	N-CA-C	-5.32	99.81	113.10
1	A	103	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	16	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	268	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	258	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	ASP	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	1948	0	1892	7	0
1	B	1965	0	1920	9	0
1	C	1811	0	1738	6	0
1	D	1870	0	1783	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	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	1	0
4	A	150	0	0	1	0
4	B	155	0	0	1	0
4	C	151	0	0	1	0
4	D	117	0	0	1	0
All	All	8211	0	7349	32	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 2.

All (32) 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:211:GLN:HG2	4:C:2055:HOH:O	1.73	0.88
1:A:211:GLN:HG2	4:A:2058:HOH:O	1.76	0.85
1:A:164:ASN:HD21	1:A:191:VAL:HA	1.45	0.80
1:D:95:GLN:OE1	1:D:278:ARG:NH2	2.21	0.71
3:D:1301:AKG:C2	4:D:2116:HOH:O	2.42	0.66
1:B:153:GLU:O	1:B:157:LYS:HD2	1.99	0.63
1:B:164:ASN:HD21	1:B:191:VAL:HA	1.62	0.63
1:A:153:GLU:O	1:A:157:LYS:HD2	2.00	0.61
1:D:97:ASP:HB3	1:D:276:ILE:HG12	1.83	0.59
1:A:69:GLU:OE2	1:A:90:THR:HB	2.03	0.59
1:C:79:VAL:O	1:C:79:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LEU:HB2	1:D:152:ARG:HG2	1.89	0.53
1:C:105:ASN:HD22	1:C:105:ASN:H	1.57	0.53
1:A:105:ASN:H	1:A:105:ASN:HD22	1.57	0.53
1:B:105:ASN:H	1:B:105:ASN:HD22	1.57	0.51
1:D:105:ASN:HD22	1:D:105:ASN:H	1.58	0.51
1:D:93:LEU:HD21	1:D:278:ARG:HD3	1.91	0.51
1:C:79:VAL:O	1:C:79:VAL:CG2	2.62	0.48
1:D:95:GLN:OE1	1:D:278:ARG:NE	2.46	0.47
1:D:65:ASP:CB	1:D:93:LEU:HD22	2.46	0.46
1:B:147:LEU:HB2	1:B:152:ARG:HG2	1.97	0.46
1:D:299:ARG:HD3	1:D:299:ARG:C	2.36	0.45
1:A:147:LEU:HB2	1:A:152:ARG:HG2	2.00	0.44
1:B:60:GLN:HA	1:B:62:HIS:CE1	2.53	0.43
1:B:164:ASN:ND2	1:B:192:TYR:H	2.16	0.43
1:C:147:LEU:HB2	1:C:152:ARG:HG2	2.00	0.43
1:B:191:VAL:HG13	4:B:2154:HOH:O	2.19	0.42
1:B:115:GLU:O	1:B:287:PRO:HD3	2.20	0.42
1:D:95:GLN:OE1	1:D:278:ARG:CZ	2.68	0.42
1:C:149:GLU:O	1:C:153:GLU:HG3	2.20	0.42
1:A:137:TRP:CD1	1:A:264:HIS:HB3	2.55	0.40
1:B:94:LEU:HD23	1:B:279:ARG:NH1	2.36	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	245/301 (81%)	239 (98%)	6 (2%)	0	100	100
1	B	245/301 (81%)	237 (97%)	8 (3%)	0	100	100
1	C	231/301 (77%)	223 (96%)	8 (4%)	0	100	100
1	D	237/301 (79%)	230 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	958/1204 (80%)	929 (97%)	29 (3%)	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	197/244 (81%)	187 (95%)	10 (5%)	24	29
1	B	201/244 (82%)	192 (96%)	9 (4%)	27	34
1	C	180/244 (74%)	176 (98%)	4 (2%)	52	65
1	D	182/244 (75%)	175 (96%)	7 (4%)	33	42
All	All	760/976 (78%)	730 (96%)	30 (4%)	32	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	63	LEU
1	A	79	VAL
1	A	91	ARG
1	A	105	ASN
1	A	106	SER
1	A	111	VAL
1	A	164	ASN
1	A	218	ARG
1	A	220	LYS
1	B	63	LEU
1	B	105	ASN
1	B	111	VAL
1	B	145	GLN
1	B	164	ASN
1	B	191	VAL
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	296	ARG
1	B	299	ARG
1	C	63	LEU
1	C	105	ASN
1	C	111	VAL
1	C	164	ASN
1	D	63	LEU
1	D	97	ASP
1	D	105	ASN
1	D	111	VAL
1	D	164	ASN
1	D	218	ARG
1	D	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	164	ASN
1	B	105	ASN
1	B	164	ASN
1	C	105	ASN
1	C	164	ASN
1	D	105	ASN
1	D	164	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	1302	2	9,9,9	0.75	1 (11%)	11,11,11	2.56	2 (18%)
3	AKG	C	1301	2	9,9,9	0.56	0	11,11,11	2.16	4 (36%)
3	AKG	A	1302	2	9,9,9	0.50	0	11,11,11	2.04	4 (36%)
3	AKG	D	1301	2	9,9,9	0.52	0	11,11,11	2.19	3 (27%)

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	1302	2	-	1/9/9/9	-
3	AKG	C	1301	2	-	1/9/9/9	-
3	AKG	A	1302	2	-	3/9/9/9	-
3	AKG	D	1301	2	-	1/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	AKG	C3-C2	-2.03	1.48	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1302	AKG	C4-C3-C2	-6.70	100.40	113.03
3	C	1301	AKG	C4-C3-C2	-5.04	103.54	113.03
3	B	1302	AKG	C3-C4-C5	-4.50	103.93	113.60
3	D	1301	AKG	C4-C3-C2	-4.13	105.26	113.03
3	A	1302	AKG	C3-C4-C5	-4.11	104.76	113.60
3	D	1301	AKG	C3-C4-C5	-3.86	105.30	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1302	AKG	C4-C3-C2	-3.51	106.41	113.03
3	D	1301	AKG	C3-C2-C1	3.46	122.39	115.97
3	C	1301	AKG	C3-C2-C1	2.42	120.47	115.97
3	C	1301	AKG	C3-C4-C5	-2.27	108.72	113.60
3	C	1301	AKG	O4-C5-C4	2.11	120.80	114.03
3	A	1302	AKG	O2-C1-C2	2.05	119.58	113.97
3	A	1302	AKG	C3-C2-C1	2.03	119.74	115.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	AKG	C1-C2-C3-C4
3	B	1302	AKG	C1-C2-C3-C4
3	C	1301	AKG	C1-C2-C3-C4
3	D	1301	AKG	C1-C2-C3-C4
3	A	1302	AKG	C3-C4-C5-O4
3	A	1302	AKG	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1301	AKG	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	253/301 (84%)	0.22	20 (7%)	12	11	20, 32, 57, 78	0
1	B	253/301 (84%)	0.17	21 (8%)	11	10	20, 32, 55, 84	0
1	C	237/301 (78%)	0.14	17 (7%)	15	14	20, 31, 52, 75	0
1	D	245/301 (81%)	0.28	21 (8%)	10	9	20, 32, 58, 81	0
All	All	988/1204 (82%)	0.20	79 (7%)	12	11	20, 32, 55, 84	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	HIS	5.5
1	A	86	VAL	5.3
1	D	61	THR	5.0
1	D	92	TYR	4.7
1	B	191	VAL	4.4
1	B	299	ARG	4.2
1	D	299	ARG	4.1
1	C	79	VAL	4.0
1	C	61	THR	3.7
1	B	122	ILE	3.7
1	A	122	ILE	3.4
1	A	104	ALA	3.4
1	A	33	LEU	3.4
1	A	212	LEU	3.3
1	C	210	LEU	3.3
1	B	61	THR	3.3
1	B	210	LEU	3.3
1	A	88	ASP	3.2
1	B	104	ALA	3.2
1	D	192	TYR	3.2
1	D	59	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	198	VAL	3.1
1	A	198	VAL	3.0
1	B	85	PRO	3.0
1	A	224	LEU	3.0
1	D	90	THR	2.9
1	C	165	GLU	2.9
1	D	164	ASN	2.9
1	A	191	VAL	2.9
1	A	210	LEU	2.9
1	D	13	LEU	2.9
1	D	198	VAL	2.8
1	B	105	ASN	2.8
1	C	256	ILE	2.8
1	C	192	TYR	2.8
1	B	291	ASP	2.8
1	A	85	PRO	2.8
1	D	93	LEU	2.8
1	D	78	PRO	2.7
1	C	104	ALA	2.6
1	B	86	VAL	2.6
1	D	210	LEU	2.6
1	C	62	HIS	2.6
1	B	62	HIS	2.6
1	A	71	PHE	2.5
1	D	104	ALA	2.5
1	A	192	TYR	2.5
1	B	192	TYR	2.5
1	C	164	ASN	2.5
1	C	291	ASP	2.5
1	A	89	GLY	2.5
1	D	30	GLY	2.5
1	A	291	ASP	2.4
1	C	77	GLU	2.4
1	D	64	ASP	2.4
1	D	256	ILE	2.4
1	A	256	ILE	2.4
1	B	256	ILE	2.4
1	B	71	PHE	2.4
1	D	95	GLN	2.3
1	D	36	ASP	2.3
1	A	300	LYS	2.3
1	B	91	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	55	ILE	2.3
1	B	33	LEU	2.2
1	C	278	ARG	2.2
1	B	212	LEU	2.2
1	C	33	LEU	2.2
1	D	96	LEU	2.2
1	B	103	ARG	2.2
1	A	105	ASN	2.2
1	B	45	ILE	2.1
1	A	91	ARG	2.1
1	C	212	LEU	2.1
1	B	89	GLY	2.1
1	A	296	ARG	2.0
1	D	66	GLN	2.0
1	B	198	VAL	2.0
1	C	71	PHE	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 monosaccharides 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(Å^2)	Q<0.9
3	AKG	A	1302	10/10	0.88	0.22	26,32,34,35	10
3	AKG	B	1302	10/10	0.92	0.21	25,28,30,30	10
3	AKG	D	1301	10/10	0.92	0.20	24,29,32,32	10
3	AKG	C	1301	10/10	0.94	0.15	23,26,30,33	10
2	FE2	A	1301	1/1	1.00	0.06	21,21,21,21	1
2	FE2	B	1301	1/1	1.00	0.07	21,21,21,21	1
2	FE2	C	1300	1/1	1.00	0.07	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	D	1300	1/1	1.00	0.06	22,22,22,22	1

6.5 Other polymers (i)

There are no such residues in this entry.