Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:05 PM GMT

PDB ID	:	3W21
Title	:	Crystal Structure of a Novel N-Substituted L-Amino Acid Dioxygenase in complex with alpha-KG from Burkholderia ambifaria AMMD
Authors	:	Qin, H.M.; Miyakawa, T.; Jia, M.Z.; Nakamura, A.; Ohtsuka, J.; Xue, Y.L.; Kawashima, T.; Kasahara, T.; Hibi, M.; Ogawa, J.; Tanokura, M.
Deposited on	:	2012-11-26
Resolution	:	1.98 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:

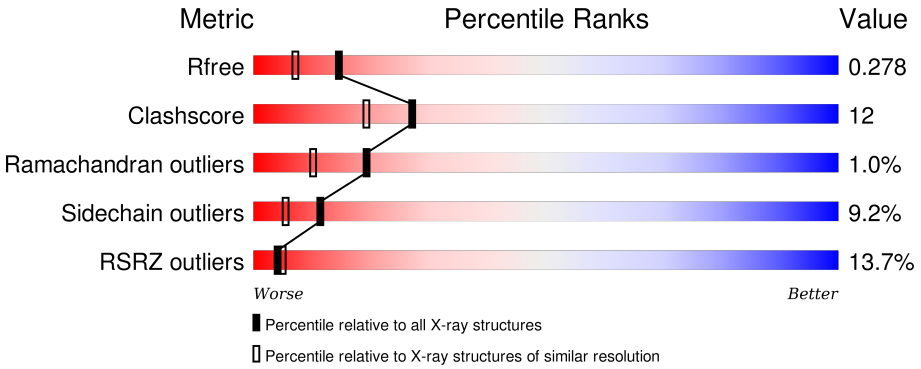
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	273	12% 66% 21% 5% • 7%
1	B	273	12% 67% 19% • • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4103 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.

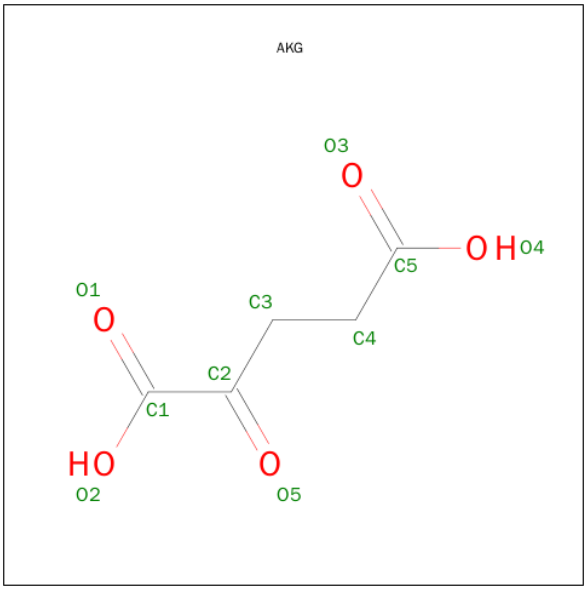
- Molecule 1 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	Se	0	2	0
			2001	1255	351	381	3	11			
1	B	250	Total	C	N	O	S	Se	0	0	0
			1952	1224	342	373	3	10			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- 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

- Molecule 4 is water.

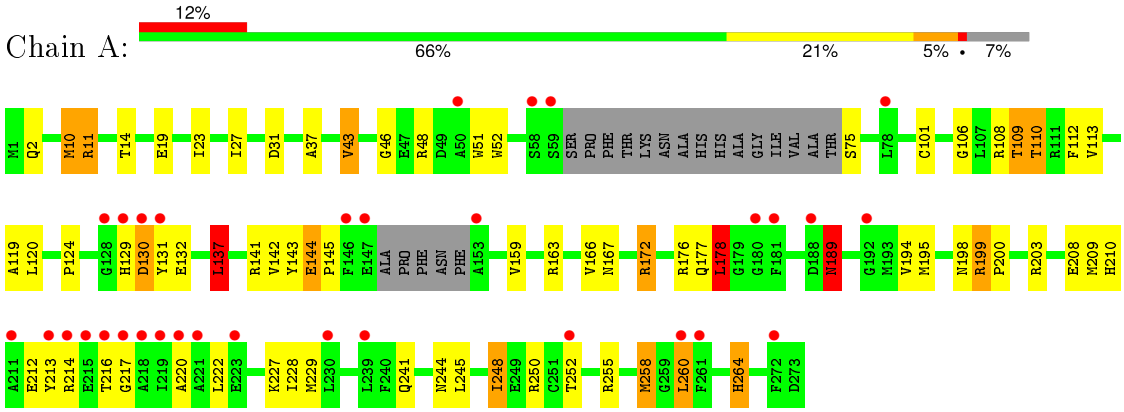
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	63	Total O 63 63	0	0

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.

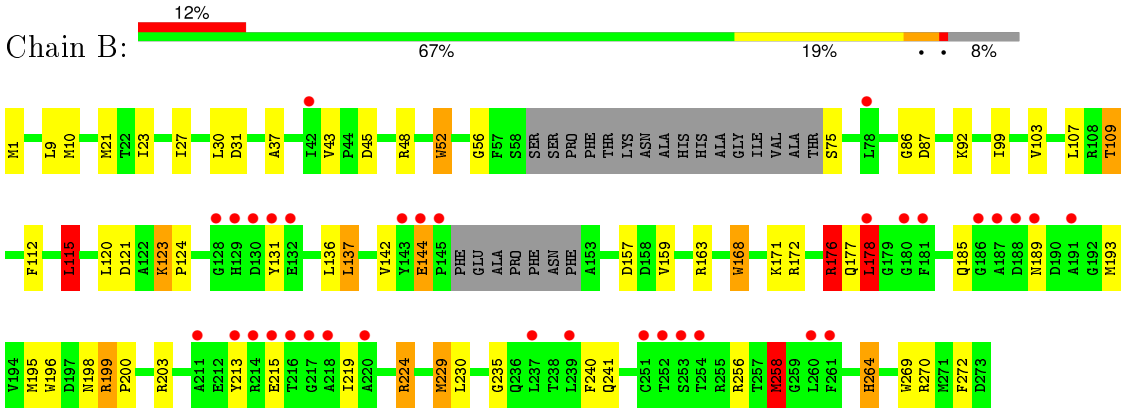
- Molecule 1: Putative uncharacterized protein

Chain A:



- Molecule 1: Putative uncharacterized protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.59Å 71.14Å 147.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.80 – 1.98 32.80 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.1 (32.80-1.98) 98.1 (32.80-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	8.10 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.212 , 0.278 0.211 , 0.278	Depositor DCC
R_{free} test set	1858 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 36601 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4103	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: ZN, 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	0.91	2/2039 (0.1%)	1.18	13/2740 (0.5%)
1	B	0.92	5/1984 (0.3%)	1.05	11/2671 (0.4%)
All	All	0.92	7/4023 (0.2%)	1.12	24/5411 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	MSE	SE-CE	-5.96	1.60	1.95
1	B	196	TRP	CD2-CE2	5.62	1.48	1.41
1	A	51	TRP	CD2-CE2	5.42	1.47	1.41
1	B	52	TRP	CD2-CE2	5.17	1.47	1.41
1	B	269	TRP	CD2-CE2	5.13	1.47	1.41
1	B	168	TRP	CD2-CE2	5.10	1.47	1.41
1	A	52	TRP	CD2-CE2	5.04	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	ARG	NE-CZ-NH2	-17.37	111.62	120.30
1	B	199	ARG	NE-CZ-NH2	-13.49	113.56	120.30
1	A	199	ARG	NE-CZ-NH1	12.83	126.72	120.30
1	A	141	ARG	NE-CZ-NH1	10.15	125.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	141	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	178	LEU	CB-CG-CD1	8.07	124.72	111.00
1	A	172	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	199	ARG	CD-NE-CZ	7.08	133.51	123.60
1	B	176	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	A	172	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	87	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	178	LEU	CB-CG-CD1	6.33	121.76	111.00
1	B	115	LEU	CA-CB-CG	5.95	128.97	115.30
1	A	11	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	B	176	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	260	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	260	LEU	CB-CG-CD2	5.44	120.25	111.00
1	B	199	ARG	CG-CD-NE	-5.44	100.37	111.80
1	B	157	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	A	258	MSE	N-CA-CB	-5.33	101.00	110.60
1	B	115	LEU	CB-CG-CD1	5.16	119.78	111.00
1	A	137	LEU	CB-CG-CD1	5.16	119.76	111.00
1	B	123	LYS	CD-CE-NZ	-5.14	99.87	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	GLY	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	2001	0	1919	47	0
1	B	1952	0	1862	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	4	2	0
4	A	75	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	63	0	0	3	0
All	All	4103	0	3785	93	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 12.

All (93) 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:43:VAL:HG12	1:B:235:GLY:HA2	1.42	1.01
1:B:43:VAL:CG1	1:B:235:GLY:HA2	1.96	0.94
1:B:185:GLN:HE21	1:B:256:ARG:HE	1.16	0.93
1:B:9:LEU:HB2	4:B:419:HOH:O	1.68	0.93
1:B:159:VAL:H	1:B:177:GLN:HE22	1.26	0.82
1:B:112:PHE:HB2	1:B:258:MSE:HE1	1.63	0.81
1:A:159:VAL:H	1:A:177:GLN:HE22	1.29	0.77
1:A:194:VAL:HG22	1:A:229[A]:MSE:HG2	1.68	0.75
1:A:176:ARG:O	1:A:178:LEU:HD13	1.88	0.73
1:A:176:ARG:HH21	1:A:241:GLN:HE22	1.36	0.72
1:A:217:GLY:HA2	4:A:433:HOH:O	1.89	0.71
1:A:209:MSE:HE1	4:A:401:HOH:O	1.89	0.71
1:B:176:ARG:O	1:B:178:LEU:HD13	1.91	0.70
1:B:9:LEU:HD12	4:B:419:HOH:O	1.91	0.69
1:B:185:GLN:NE2	1:B:256:ARG:HE	1.88	0.69
1:A:110:THR:CG2	1:A:113:VAL:H	2.06	0.68
1:A:27:ILE:HD13	1:A:120:LEU:HD11	1.78	0.66
1:B:27:ILE:HD13	1:B:120:LEU:HD11	1.76	0.65
1:A:43:VAL:HG22	1:A:48:ARG:HG3	1.76	0.65
1:A:212:GLU:O	1:A:216:THR:HB	1.97	0.64
1:B:43:VAL:HG12	1:B:235:GLY:CA	2.22	0.64
1:B:213:TYR:HB2	1:B:219:ILE:HD11	1.80	0.63
1:B:193:MSE:HE2	1:B:195:MSE:HE2	1.80	0.63
1:B:168:TRP:O	1:B:171:LYS:HE3	2.00	0.62
1:B:176:ARG:HD3	1:B:241:GLN:NE2	2.14	0.62
1:B:31:ASP:OD2	1:B:264:HIS:HD2	1.83	0.61
1:A:199:ARG:HH22	1:A:241:GLN:HE21	1.49	0.61
1:A:10:MSE:HE2	1:A:37:ALA:O	2.02	0.60
1:B:112:PHE:HB2	1:B:258:MSE:CE	2.31	0.60
1:A:75:SER:N	1:B:131:TYR:HH	1.98	0.60
1:B:45:ASP:HA	1:B:48:ARG:CZ	2.32	0.60
1:A:131:TYR:HH	1:B:75:SER:N	1.99	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:THR:HG23	1:A:113:VAL:H	1.68	0.59
1:A:222:LEU:HD21	1:A:245:LEU:HD23	1.85	0.58
1:B:163:ARG:HA	1:B:203:ARG:HG2	1.86	0.58
1:A:37:ALA:HB2	1:A:195:MSE:HE1	1.84	0.58
1:B:56:GLY:HA3	1:B:109:THR:HG22	1.86	0.58
1:A:132:GLU:O	1:A:132:GLU:HG3	2.04	0.57
1:A:195:MSE:HE3	1:A:228:ILE:HD12	1.87	0.56
1:B:159:VAL:N	1:B:177:GLN:HE22	2.02	0.55
1:B:193:MSE:HE1	1:B:240:PHE:CD2	2.42	0.55
1:B:198:ASN:HD22	1:B:200:PRO:HD3	1.72	0.55
1:A:31:ASP:OD2	1:A:264:HIS:HD2	1.90	0.54
1:A:144:GLU:CG	1:A:145:PRO:HD2	2.37	0.54
1:B:9:LEU:CB	4:B:419:HOH:O	2.38	0.54
1:B:195:MSE:CE	1:B:230:LEU:HD11	2.38	0.53
1:A:189:ASN:OD1	1:A:250:ARG:O	2.28	0.52
1:A:130:ASP:N	1:A:130:ASP:OD2	2.43	0.52
1:A:199:ARG:HH22	1:A:241:GLN:NE2	2.08	0.51
1:B:37:ALA:HB2	1:B:195:MSE:HE1	1.92	0.51
1:A:131:TYR:HB3	1:B:99:ILE:HD11	1.93	0.51
1:A:124:PRO:HB3	1:A:137:LEU:HD13	1.93	0.49
1:A:199:ARG:HH21	1:A:244:ASN:HD21	1.60	0.49
1:A:248:ILE:HD11	3:A:302:AKG:H42	1.95	0.49
1:A:255:ARG:NH2	3:A:302:AKG:O3	2.44	0.49
1:A:106:GLY:O	1:A:109:THR:HG22	2.13	0.49
1:A:144:GLU:HG2	1:A:145:PRO:HD2	1.95	0.48
1:A:189:ASN:HB2	1:A:252:THR:OG1	2.14	0.48
1:B:30:LEU:HB3	1:B:178:LEU:HD11	1.95	0.48
1:A:23:ILE:HG22	1:A:27:ILE:HD12	1.96	0.48
1:B:120:LEU:O	1:B:121:ASP:HB3	2.14	0.48
1:B:23:ILE:CD1	1:B:115:LEU:HG	2.43	0.48
1:A:199:ARG:HH21	1:A:244:ASN:ND2	2.12	0.47
1:A:2:GLN:HE22	1:A:119:ALA:HA	1.78	0.47
1:B:43:VAL:CG1	1:B:235:GLY:CA	2.83	0.47
1:A:2:GLN:NE2	4:A:414:HOH:O	2.46	0.47
1:B:103:VAL:HG12	1:B:107:LEU:HG	1.96	0.47
1:B:229:MSE:HB2	1:B:229:MSE:HE2	1.95	0.47
1:A:163:ARG:HA	1:A:203:ARG:HG2	1.96	0.46
1:B:199:ARG:HH22	1:B:241:GLN:NE2	2.13	0.46
1:A:210:HIS:O	1:A:214:ARG:HG2	2.16	0.46
1:A:166:VAL:HG13	1:A:167:ASN:N	2.32	0.45
1:A:198:ASN:HD22	1:A:200:PRO:HD3	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LYS:O	1:B:270:ARG:HA	2.17	0.45
1:B:112:PHE:CB	1:B:258:MSE:CE	2.95	0.44
1:B:176:ARG:CD	1:B:241:GLN:NE2	2.79	0.43
1:B:176:ARG:HD3	1:B:241:GLN:HE22	1.80	0.43
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.18	0.43
1:A:172:ARG:HD3	4:A:410:HOH:O	2.17	0.42
1:A:176:ARG:HH21	1:A:241:GLN:NE2	2.10	0.42
1:A:167:ASN:OD1	1:B:86:GLY:HA2	2.20	0.42
1:B:258:MSE:HB3	1:B:258:MSE:HE3	1.85	0.42
1:B:213:TYR:HB2	1:B:219:ILE:CD1	2.48	0.42
1:B:124:PRO:HB3	1:B:137:LEU:HD13	2.00	0.42
1:B:52:TRP:CZ3	1:B:256:ARG:HB3	2.54	0.41
1:A:132:GLU:HB3	4:A:417:HOH:O	2.20	0.41
1:B:112:PHE:CB	1:B:258:MSE:HE1	2.40	0.41
1:B:136:LEU:O	1:B:272:PHE:HA	2.20	0.41
1:A:176:ARG:HD3	1:A:176:ARG:HA	1.95	0.41
1:B:176:ARG:HH21	1:B:241:GLN:HE22	1.69	0.41
1:B:224:ARG:HD2	1:B:224:ARG:HA	1.86	0.41
1:A:143:TYR:CE2	1:A:255:ARG:NH2	2.90	0.40
1:A:112:PHE:HB2	1:A:258:MSE:SE	2.71	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	249/273 (91%)	240 (96%)	5 (2%)	4 (2%)	12 4
1	B	244/273 (89%)	241 (99%)	2 (1%)	1 (0%)	39 31
All	All	493/546 (90%)	481 (98%)	7 (1%)	5 (1%)	19 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	108	ARG
1	A	129	HIS
1	A	220	ALA
1	B	215	GLU

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	205/211 (97%)	184 (90%)	21 (10%)	9 4
1	B	198/211 (94%)	181 (91%)	17 (9%)	13 6
All	All	403/422 (96%)	365 (91%)	38 (9%)	11 5

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MSE
1	A	11	ARG
1	A	14	THR
1	A	19	GLU
1	A	43	VAL
1	A	101	CYS
1	A	109	THR
1	A	110	THR
1	A	130	ASP
1	A	137	LEU
1	A	142	VAL
1	A	144	GLU
1	A	178	LEU
1	A	189	ASN
1	A	208[A]	GLU
1	A	208[B]	GLU
1	A	213	TYR
1	A	227	LYS
1	A	248	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	LEU
1	A	264	HIS
1	B	1	MSE
1	B	10	MSE
1	B	21	MSE
1	B	92	LYS
1	B	109	THR
1	B	115	LEU
1	B	137	LEU
1	B	142	VAL
1	B	144	GLU
1	B	172	ARG
1	B	176	ARG
1	B	178	LEU
1	B	189	ASN
1	B	224	ARG
1	B	229	MSE
1	B	258	MSE
1	B	264	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	177	GLN
1	A	185	GLN
1	A	198	ASN
1	A	233	GLN
1	A	241	GLN
1	A	244	ASN
1	A	264	HIS
1	B	28	HIS
1	B	177	GLN
1	B	185	GLN
1	B	198	ASN
1	B	233	GLN
1	B	241	GLN
1	B	244	ASN
1	B	264	HIS

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	302	2	3,9,9	0.34	0	4,11,11	1.55	1 (25%)

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	302	2	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	AKG	C3-C4-C5	-2.81	107.59	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	AKG	2	0

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, 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	243/273 (89%)	0.70	32 (13%)	4	5	23, 37, 71, 95	0
1	B	240/273 (87%)	0.71	34 (14%)	4	4	26, 38, 73, 90	0
All	All	483/546 (88%)	0.71	66 (13%)	4	5	23, 37, 72, 95	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ALA	8.6
1	A	213	TYR	7.6
1	A	146	PHE	6.2
1	B	131	TYR	5.4
1	B	145	PRO	5.2
1	B	213	TYR	5.1
1	B	218	ALA	4.9
1	A	220	ALA	4.9
1	B	254	THR	4.9
1	B	252	THR	4.7
1	A	129	HIS	4.5
1	B	251	CYS	4.5
1	A	128	GLY	4.4
1	B	187	ALA	4.1
1	A	153	ALA	3.9
1	A	216	THR	3.8
1	A	260	LEU	3.8
1	B	143	TYR	3.7
1	B	188	ASP	3.7
1	A	214	ARG	3.7
1	B	211	ALA	3.7
1	B	129	HIS	3.7
1	B	130	ASP	3.6
1	A	217	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	58	SER	3.5
1	B	186	GLY	3.5
1	B	216	THR	3.4
1	B	261	PHE	3.3
1	B	215	GLU	3.3
1	A	130	ASP	3.1
1	B	189	ASN	3.0
1	A	215	GLU	3.0
1	A	147	GLU	3.0
1	A	261	PHE	3.0
1	B	253	SER	3.0
1	A	59	SER	2.9
1	A	223	GLU	2.9
1	B	220	ALA	2.9
1	A	131	TYR	2.8
1	B	78	LEU	2.7
1	B	237	LEU	2.7
1	A	188	ASP	2.6
1	B	128	GLY	2.6
1	B	217	GLY	2.6
1	A	252	THR	2.6
1	B	144	GLU	2.6
1	B	214	ARG	2.6
1	B	260	LEU	2.5
1	A	221	ALA	2.5
1	A	181	PHE	2.4
1	A	78	LEU	2.4
1	B	42	ILE	2.3
1	A	239	LEU	2.3
1	A	50	ALA	2.3
1	A	180	GLY	2.2
1	B	181	PHE	2.2
1	A	219	ILE	2.2
1	B	191	ALA	2.2
1	B	239	LEU	2.2
1	A	192	GLY	2.2
1	B	180	GLY	2.2
1	A	272	PHE	2.1
1	A	211	ALA	2.1
1	B	132	GLU	2.1
1	A	230	LEU	2.1
1	B	178	LEU	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	A	302	10/10	0.91	0.17	0.15	47,61,65,68	0
2	ZN	A	301	1/1	0.99	0.06	-	33,33,33,33	1
2	ZN	B	301	1/1	0.90	0.24	-	53,53,53,53	1

6.5 Other polymers (i)

There are no such residues in this entry.