Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2016 – 11:51 PM EDT

PDB ID	:	5DAB
Title	:	Crystal structure of FTO-IN115
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Deposited on	:	2015-08-19
Resolution	:	2.10 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:

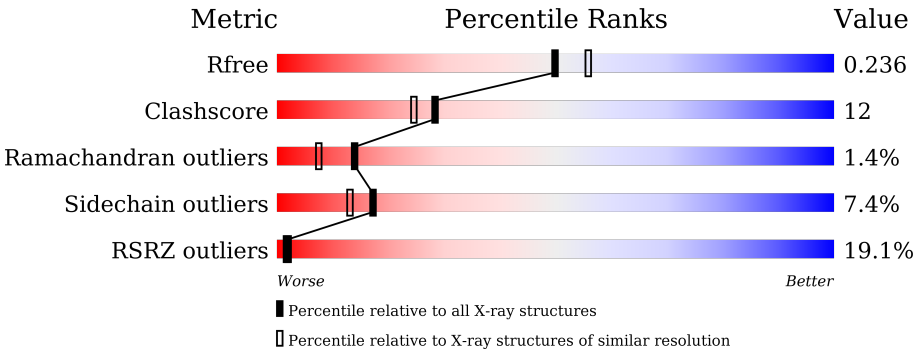
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	479	17% 69% 17% · 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	603	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3673 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 Alpha-ketoglutarate-dependent dioxygenase FTO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3513	2229	607	655	22			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	LEU	-	expression tag	UNP Q9C0B1
A	28	GLU	-	expression tag	UNP Q9C0B1
A	29	SER	-	expression tag	UNP Q9C0B1
A	30	HIS	-	expression tag	UNP Q9C0B1
A	31	MET	-	expression tag	UNP Q9C0B1
A	188	ASP	GLN	conflict	UNP Q9C0B1
A	189	VAL	ASP	conflict	UNP Q9C0B1

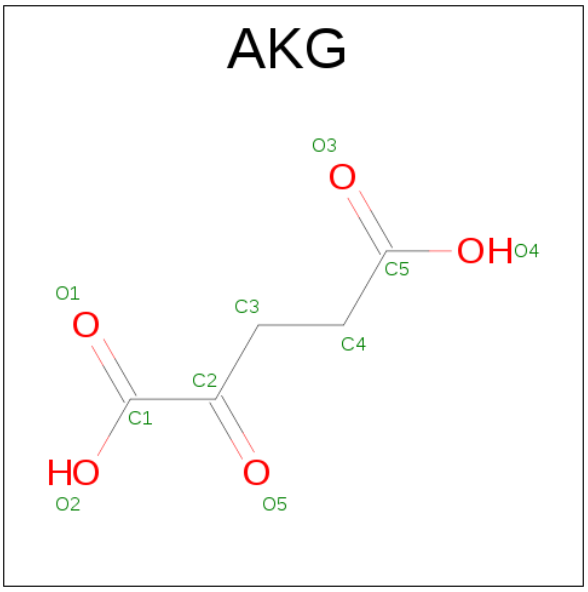
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Cl	0	0
			9	9		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

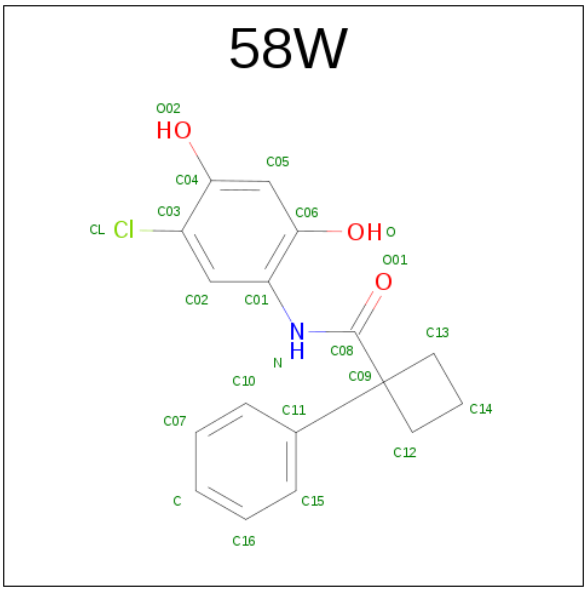
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	5	5	0	0

- Molecule 5 is N-(5-chloro-2,4-dihydroxyphenyl)-1-phenylcyclobutanecarboxamide (three-letter code: 58W) (formula: $C_{17}H_{16}ClNO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	A	1	22	17	1	1	3	0	0

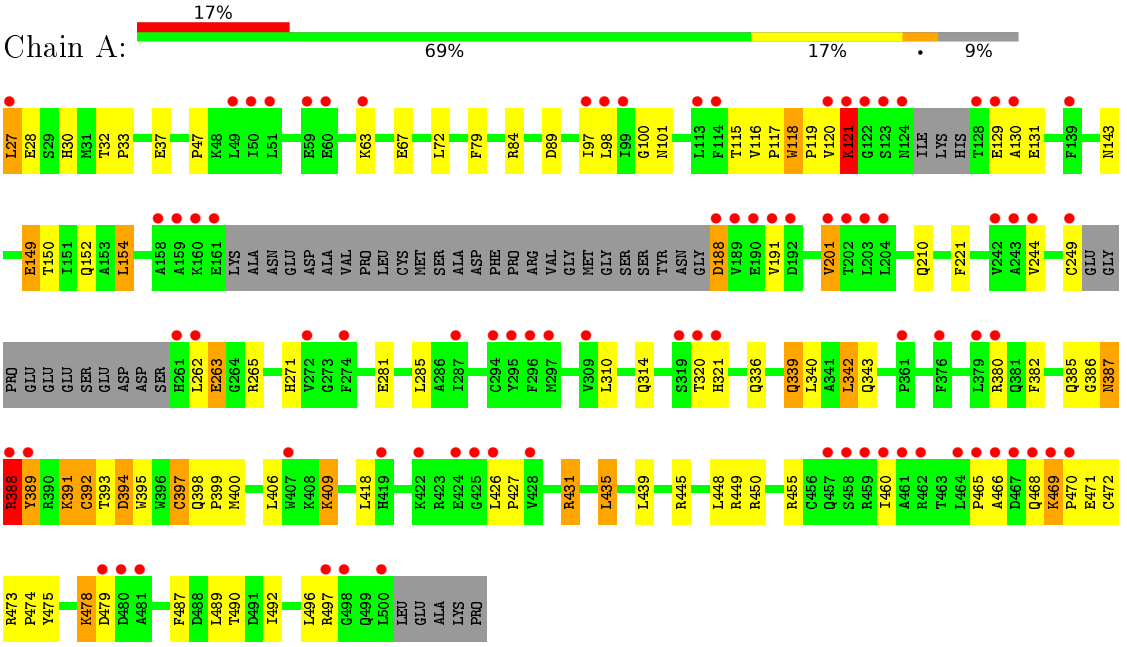
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	118	Total O 118 118	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: Alpha-ketoglutarate-dependent dioxygenase FTO



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	142.68Å 142.68Å 82.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.91 – 2.10 28.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (28.91-2.10) 96.6 (28.91-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.210 , 0.241 0.204 , 0.236	Depositor DCC
R_{free} test set	1746 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3673	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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, 0.333 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: 58W, FE2, AKG, CL

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	0.38	0/3597	0.48	1/4879 (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})
1	A	388	ARG	N-CA-C	6.28	127.97	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3513	0	3404	80	0
2	A	9	0	0	1	0
3	A	1	0	0	0	0
4	A	10	0	4	2	0
5	A	22	0	0	0	0
6	A	118	0	0	4	0
All	All	3673	0	3408	81	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 (81) 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:A:391:LYS:O	1:A:391:LYS:HG3	1.46	1.06
1:A:387:ASN:O	1:A:388:ARG:HG3	1.76	0.85
1:A:393:THR:O	1:A:394:ASP:HB3	1.80	0.81
1:A:387:ASN:O	1:A:388:ARG:CG	2.30	0.79
1:A:393:THR:O	1:A:394:ASP:CB	2.30	0.79
1:A:387:ASN:O	1:A:388:ARG:CB	2.29	0.77
1:A:450:ARG:HH22	1:A:490:THR:HG21	1.50	0.75
1:A:79:PHE:HZ	1:A:391:LYS:HE2	1.52	0.74
1:A:389:TYR:C	1:A:391:LYS:N	2.38	0.72
1:A:389:TYR:C	1:A:391:LYS:H	1.90	0.71
1:A:478:LYS:NZ	1:A:478:LYS:HB2	2.06	0.70
1:A:450:ARG:NH2	1:A:490:THR:HG21	2.08	0.69
1:A:439:LEU:HD21	1:A:497:ARG:HD3	1.77	0.65
1:A:30:HIS:HE1	1:A:265:ARG:H	1.44	0.65
4:A:611:AKG:H32	6:A:762:HOH:O	1.96	0.64
1:A:143:ASN:OD1	1:A:321:HIS:HD2	1.80	0.64
1:A:119:PRO:HG3	6:A:729:HOH:O	2.00	0.61
1:A:394:ASP:OD1	1:A:394:ASP:C	2.40	0.60
1:A:98:LEU:HD11	1:A:201:VAL:CG1	2.33	0.59
1:A:380:ARG:HH22	1:A:487:PHE:HE2	1.51	0.58
1:A:389:TYR:N	1:A:389:TYR:CD1	2.71	0.57
1:A:79:PHE:CZ	1:A:391:LYS:HE2	2.37	0.57
1:A:380:ARG:NH2	1:A:487:PHE:HE2	2.02	0.57
1:A:387:ASN:O	1:A:388:ARG:HB2	2.04	0.57
1:A:262:LEU:O	1:A:263:GLU:CB	2.52	0.57
1:A:492:ILE:O	1:A:496:LEU:HD13	2.05	0.57
1:A:394:ASP:O	1:A:394:ASP:CG	2.41	0.56
1:A:121:LYS:NZ	1:A:121:LYS:HB2	2.20	0.56
1:A:380:ARG:NH2	1:A:487:PHE:CE2	2.74	0.56
1:A:97:ILE:HD11	1:A:116:VAL:HG21	1.89	0.55
1:A:30:HIS:CE1	1:A:265:ARG:H	2.23	0.55
1:A:244:VAL:HG22	1:A:320:THR:HG22	1.88	0.54
1:A:398:GLN:HB3	1:A:399:PRO:HD3	1.89	0.54
1:A:387:ASN:ND2	1:A:387:ASN:O	2.29	0.54
1:A:63:LYS:O	1:A:67:GLU:HG2	2.09	0.52
1:A:478:LYS:HB2	1:A:478:LYS:HZ3	1.75	0.52
1:A:409:LYS:HA	1:A:409:LYS:HE3	1.90	0.52
1:A:101:ASN:O	1:A:115:THR:HG21	2.09	0.51
1:A:389:TYR:O	1:A:393:THR:N	2.30	0.51
1:A:445:ARG:O	1:A:449:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:HA2	1:A:118:TRP:CE2	2.45	0.51
1:A:394:ASP:OD1	1:A:394:ASP:O	2.30	0.50
1:A:468:GLN:O	1:A:469:LYS:O	2.30	0.50
1:A:98:LEU:HD11	1:A:201:VAL:HG11	1.94	0.49
1:A:98:LEU:HD11	1:A:201:VAL:HG13	1.94	0.49
1:A:385:GLN:O	1:A:386:GLY:C	2.49	0.48
1:A:472:CYS:O	1:A:475:TYR:HB2	2.14	0.48
1:A:388:ARG:O	1:A:392:CYS:SG	2.70	0.47
1:A:489:LEU:HD21	6:A:702:HOH:O	2.14	0.47
1:A:380:ARG:NH1	1:A:474:PRO:HD2	2.28	0.47
1:A:47:PRO:HD2	2:A:601:CL:CL	2.52	0.46
1:A:382:PHE:CD2	1:A:400:MET:HG2	2.50	0.46
1:A:27:LEU:HD23	1:A:28:GLU:H	1.80	0.46
1:A:188:ASP:O	1:A:191:VAL:HB	2.16	0.46
1:A:339:GLN:HG3	1:A:340:LEU:N	2.29	0.46
1:A:129:GLU:O	1:A:131:GLU:N	2.50	0.45
1:A:465:PRO:O	1:A:469:LYS:HE3	2.16	0.45
1:A:249:CYS:SG	1:A:314:GLN:HB3	2.56	0.45
1:A:150:THR:HG22	1:A:154:LEU:HD22	1.98	0.45
1:A:320:THR:HG21	4:A:611:AKG:H31	1.99	0.45
1:A:339:GLN:O	1:A:343:GLN:HG3	2.17	0.45
1:A:121:LYS:HZ1	1:A:121:LYS:HB2	1.81	0.45
1:A:30:HIS:HD2	1:A:221:PHE:O	2.02	0.43
1:A:431:ARG:O	1:A:435:LEU:HD13	2.19	0.43
1:A:79:PHE:CD1	1:A:387:ASN:HB2	2.53	0.43
1:A:32:THR:HB	1:A:33:PRO:HD2	1.99	0.43
1:A:89:ASP:HB2	1:A:460:ILE:HD12	2.01	0.43
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.81	0.42
1:A:478:LYS:HZ2	1:A:478:LYS:HB2	1.84	0.42
1:A:393:THR:HG23	1:A:394:ASP:N	2.34	0.42
1:A:84:ARG:HH11	1:A:455:ARG:CG	2.33	0.42
1:A:389:TYR:O	1:A:391:LYS:N	2.52	0.42
1:A:471:GLU:HG2	1:A:473:ARG:HG3	2.01	0.42
1:A:117:PRO:HG3	1:A:395:TRP:CD1	2.55	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD12	1.81	0.41
1:A:394:ASP:HB2	1:A:397:CYS:SG	2.61	0.41
1:A:271:HIS:HB2	1:A:310:LEU:HD12	2.02	0.41
1:A:466:ALA:HA	1:A:469:LYS:CE	2.50	0.41
1:A:149:GLU:O	1:A:152:GLN:HB3	2.20	0.41
1:A:336:GLN:HG3	6:A:775:HOH:O	2.21	0.41
1:A:426:LEU:HA	1:A:427:PRO:HD2	1.91	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	426/479 (89%)	404 (95%)	16 (4%)	6 (1%)	14 7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	LYS
1	A	263	GLU
1	A	388	ARG
1	A	397	CYS
1	A	121	LYS
1	A	130	ALA

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	380/423 (90%)	352 (93%)	28 (7%)	17 13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	GLU

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	118	TRP
1	A	120	VAL
1	A	121	LYS
1	A	149	GLU
1	A	154	LEU
1	A	188	ASP
1	A	201	VAL
1	A	210	GLN
1	A	281	GLU
1	A	285	LEU
1	A	339	GLN
1	A	342	LEU
1	A	387	ASN
1	A	389	TYR
1	A	391	LYS
1	A	392	CYS
1	A	394	ASP
1	A	406	LEU
1	A	409	LYS
1	A	418	LEU
1	A	431	ARG
1	A	435	LEU
1	A	448	LEU
1	A	478	LYS
1	A	479	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	321	HIS
1	A	336	GLN
1	A	339	GLN
1	A	430	GLN
1	A	446	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AKG	A	611	3	3,9,9	0.69	0	4,11,11	1.13	0
5	58W	A	612	-	24,24,24	1.40	5 (20%)	30,35,35	1.00	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	A	611	3	-	0/3/9/9	0/0/0/0
5	58W	A	612	-	-	0/16/24/24	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	612	58W	C09-C11	-3.41	1.47	1.53
5	A	612	58W	C13-C09	-2.32	1.49	1.55
5	A	612	58W	C12-C09	-2.29	1.49	1.55
5	A	612	58W	C09-C08	-2.05	1.49	1.53
5	A	612	58W	C08-N	3.18	1.43	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	612	58W	C01-N-C08	-2.45	120.38	127.71
5	A	612	58W	C05-C04-C03	2.72	119.71	118.29

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
4	A	611	AKG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	434/479 (90%)	0.82	83 (19%) 2 2	46, 71, 128, 160	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	THR	12.4
1	A	262	LEU	6.4
1	A	465	PRO	6.0
1	A	466	ALA	5.9
1	A	122	GLY	5.9
1	A	129	GLU	5.5
1	A	479	ASP	5.3
1	A	27	LEU	5.3
1	A	189	VAL	5.1
1	A	462	ARG	5.0
1	A	457	GLN	4.9
1	A	459	ARG	4.9
1	A	467	ASP	4.8
1	A	261	HIS	4.8
1	A	295	TYR	4.7
1	A	203	LEU	4.7
1	A	123	SER	4.7
1	A	428	VAL	4.3
1	A	158	ALA	4.3
1	A	424	GLU	4.1
1	A	124	ASN	3.9
1	A	244	VAL	3.9
1	A	497	ARG	3.9
1	A	190	GLU	3.8
1	A	204	LEU	3.8
1	A	458	SER	3.8
1	A	188	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	389	TYR	3.6
1	A	243	ALA	3.6
1	A	191	VAL	3.5
1	A	159	ALA	3.4
1	A	160	LYS	3.4
1	A	481	ALA	3.3
1	A	296	PHE	3.3
1	A	422	LYS	3.3
1	A	49	LEU	3.2
1	A	272	VAL	3.2
1	A	464	LEU	3.2
1	A	500	LEU	3.2
1	A	201	VAL	3.2
1	A	161	GLU	3.2
1	A	469	LYS	3.2
1	A	59	GLU	3.1
1	A	461	ALA	3.1
1	A	470	PRO	3.0
1	A	99	ILE	3.0
1	A	202	THR	2.9
1	A	274	PHE	2.9
1	A	97	ILE	2.9
1	A	425	GLY	2.9
1	A	379	LEU	2.9
1	A	249	CYS	2.9
1	A	460	ILE	2.8
1	A	63	LYS	2.8
1	A	51	LEU	2.8
1	A	121	LYS	2.8
1	A	407	TRP	2.8
1	A	60	GLU	2.7
1	A	480	ASP	2.7
1	A	120	VAL	2.6
1	A	320	THR	2.6
1	A	319	SER	2.6
1	A	498	GLY	2.5
1	A	113	LEU	2.5
1	A	426	LEU	2.5
1	A	388	ARG	2.4
1	A	50	ILE	2.4
1	A	287	ILE	2.4
1	A	98	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	242	VAL	2.4
1	A	380	ARG	2.4
1	A	297	MET	2.4
1	A	468	GLN	2.4
1	A	192	ASP	2.4
1	A	376	PHE	2.3
1	A	294	CYS	2.3
1	A	114	PHE	2.3
1	A	419	HIS	2.2
1	A	130	ALA	2.1
1	A	361	PRO	2.1
1	A	309	VAL	2.1
1	A	321	HIS	2.0
1	A	139	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 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
2	CL	A	603	1/1	0.87	0.38	7.18	112,112,112,112	0
4	AKG	A	611	10/10	0.83	0.26	0.39	61,69,79,82	0
5	58W	A	612	22/22	0.90	0.12	-0.37	65,72,80,85	0
2	CL	A	601	1/1	0.91	0.11	-0.77	83,83,83,83	0
2	CL	A	608	1/1	0.94	0.05	-3.12	98,98,98,98	0
3	FE2	A	610	1/1	0.90	0.16	-	106,106,106,106	0
2	CL	A	606	1/1	0.88	0.29	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	A	604	1/1	0.94	0.39	-	96,96,96,96	0
2	CL	A	609	1/1	0.91	0.07	-	116,116,116,116	0
2	CL	A	602	1/1	0.69	0.24	-	101,101,101,101	0
2	CL	A	605	1/1	0.88	0.08	-	92,92,92,92	0
2	CL	A	607	1/1	0.70	0.15	-	120,120,120,120	0

6.5 Other polymers

There are no such residues in this entry.