Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 09:17 am GMT

PDB ID	:	6GEM
Title	:	FeII-Dependent Halogenase Wi-WelO15
Authors	:	Srinivasan, V.
Deposited on	:	2018-04-26
Resolution	:	3.46 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:

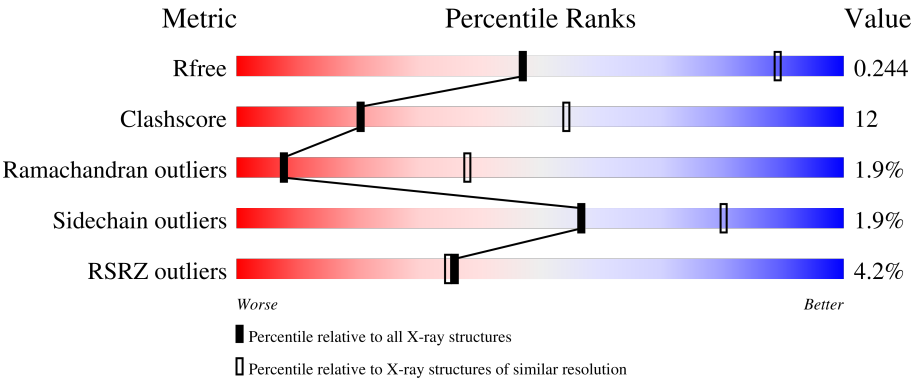
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.46 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	308	69% 20% 9%
1	B	308	3% 65% 24% 9%
1	C	308	9% 65% 21% 9%
1	D	308	3% 68% 22% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8836 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2198	1398	371	419	10			
1	B	280	Total	C	N	O	S	0	0	0
			2198	1398	371	419	10			
1	C	280	Total	C	N	O	S	0	0	0
			2198	1398	371	419	10			
1	D	280	Total	C	N	O	S	0	0	0
			2198	1398	371	419	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A075X7F9
A	-16	GLY	-	expression tag	UNP A0A075X7F9
A	-15	SER	-	expression tag	UNP A0A075X7F9
A	-14	SER	-	expression tag	UNP A0A075X7F9
A	-13	HIS	-	expression tag	UNP A0A075X7F9
A	-12	HIS	-	expression tag	UNP A0A075X7F9
A	-11	HIS	-	expression tag	UNP A0A075X7F9
A	-10	HIS	-	expression tag	UNP A0A075X7F9
A	-9	HIS	-	expression tag	UNP A0A075X7F9
A	-8	HIS	-	expression tag	UNP A0A075X7F9
A	-7	SER	-	expression tag	UNP A0A075X7F9
A	-6	GLN	-	expression tag	UNP A0A075X7F9
A	-5	ASP	-	expression tag	UNP A0A075X7F9
A	-4	PRO	-	expression tag	UNP A0A075X7F9
A	-3	ASN	-	expression tag	UNP A0A075X7F9
A	-2	SER	-	expression tag	UNP A0A075X7F9
A	-1	SER	-	expression tag	UNP A0A075X7F9
A	0	SER	-	expression tag	UNP A0A075X7F9
A	6	ILE	VAL	conflict	UNP A0A075X7F9
A	284	ASN	ASP	conflict	UNP A0A075X7F9
B	-17	MET	-	initiating methionine	UNP A0A075X7F9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	GLY	-	expression tag	UNP A0A075X7F9
B	-15	SER	-	expression tag	UNP A0A075X7F9
B	-14	SER	-	expression tag	UNP A0A075X7F9
B	-13	HIS	-	expression tag	UNP A0A075X7F9
B	-12	HIS	-	expression tag	UNP A0A075X7F9
B	-11	HIS	-	expression tag	UNP A0A075X7F9
B	-10	HIS	-	expression tag	UNP A0A075X7F9
B	-9	HIS	-	expression tag	UNP A0A075X7F9
B	-8	HIS	-	expression tag	UNP A0A075X7F9
B	-7	SER	-	expression tag	UNP A0A075X7F9
B	-6	GLN	-	expression tag	UNP A0A075X7F9
B	-5	ASP	-	expression tag	UNP A0A075X7F9
B	-4	PRO	-	expression tag	UNP A0A075X7F9
B	-3	ASN	-	expression tag	UNP A0A075X7F9
B	-2	SER	-	expression tag	UNP A0A075X7F9
B	-1	SER	-	expression tag	UNP A0A075X7F9
B	0	SER	-	expression tag	UNP A0A075X7F9
B	6	ILE	VAL	conflict	UNP A0A075X7F9
B	284	ASN	ASP	conflict	UNP A0A075X7F9
C	-17	MET	-	initiating methionine	UNP A0A075X7F9
C	-16	GLY	-	expression tag	UNP A0A075X7F9
C	-15	SER	-	expression tag	UNP A0A075X7F9
C	-14	SER	-	expression tag	UNP A0A075X7F9
C	-13	HIS	-	expression tag	UNP A0A075X7F9
C	-12	HIS	-	expression tag	UNP A0A075X7F9
C	-11	HIS	-	expression tag	UNP A0A075X7F9
C	-10	HIS	-	expression tag	UNP A0A075X7F9
C	-9	HIS	-	expression tag	UNP A0A075X7F9
C	-8	HIS	-	expression tag	UNP A0A075X7F9
C	-7	SER	-	expression tag	UNP A0A075X7F9
C	-6	GLN	-	expression tag	UNP A0A075X7F9
C	-5	ASP	-	expression tag	UNP A0A075X7F9
C	-4	PRO	-	expression tag	UNP A0A075X7F9
C	-3	ASN	-	expression tag	UNP A0A075X7F9
C	-2	SER	-	expression tag	UNP A0A075X7F9
C	-1	SER	-	expression tag	UNP A0A075X7F9
C	0	SER	-	expression tag	UNP A0A075X7F9
C	6	ILE	VAL	conflict	UNP A0A075X7F9
C	284	ASN	ASP	conflict	UNP A0A075X7F9
D	-17	MET	-	initiating methionine	UNP A0A075X7F9
D	-16	GLY	-	expression tag	UNP A0A075X7F9
D	-15	SER	-	expression tag	UNP A0A075X7F9

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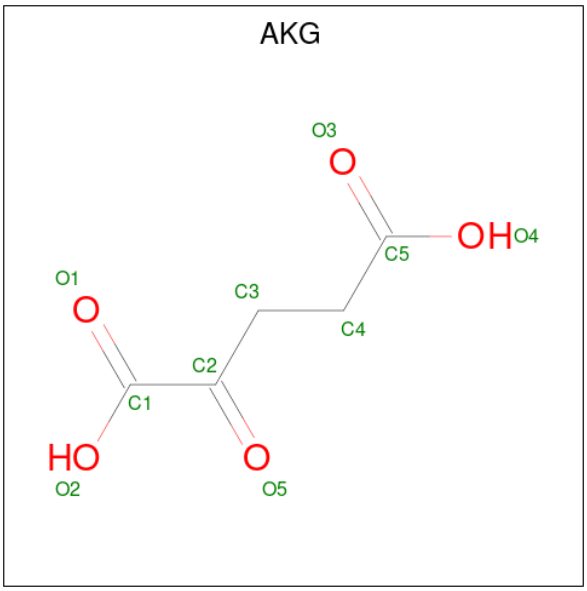
Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	SER	-	expression tag	UNP A0A075X7F9
D	-13	HIS	-	expression tag	UNP A0A075X7F9
D	-12	HIS	-	expression tag	UNP A0A075X7F9
D	-11	HIS	-	expression tag	UNP A0A075X7F9
D	-10	HIS	-	expression tag	UNP A0A075X7F9
D	-9	HIS	-	expression tag	UNP A0A075X7F9
D	-8	HIS	-	expression tag	UNP A0A075X7F9
D	-7	SER	-	expression tag	UNP A0A075X7F9
D	-6	GLN	-	expression tag	UNP A0A075X7F9
D	-5	ASP	-	expression tag	UNP A0A075X7F9
D	-4	PRO	-	expression tag	UNP A0A075X7F9
D	-3	ASN	-	expression tag	UNP A0A075X7F9
D	-2	SER	-	expression tag	UNP A0A075X7F9
D	-1	SER	-	expression tag	UNP A0A075X7F9
D	0	SER	-	expression tag	UNP A0A075X7F9
D	6	ILE	VAL	conflict	UNP A0A075X7F9
D	284	ASN	ASP	conflict	UNP A0A075X7F9

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

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

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



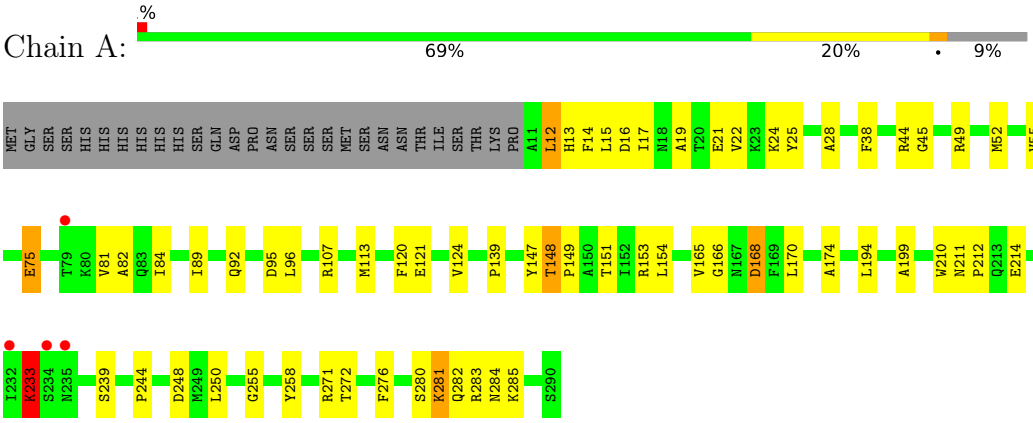
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0

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.

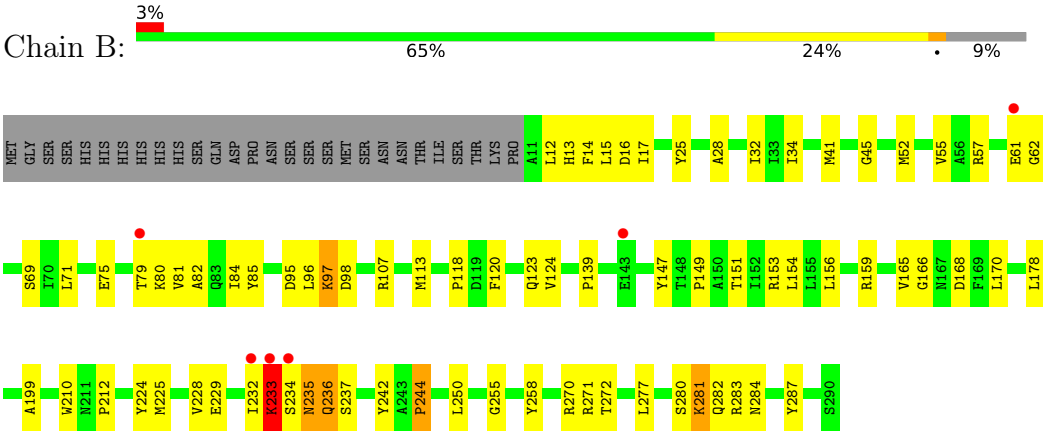
• Molecule 1: Oxidoreductase

Chain A:



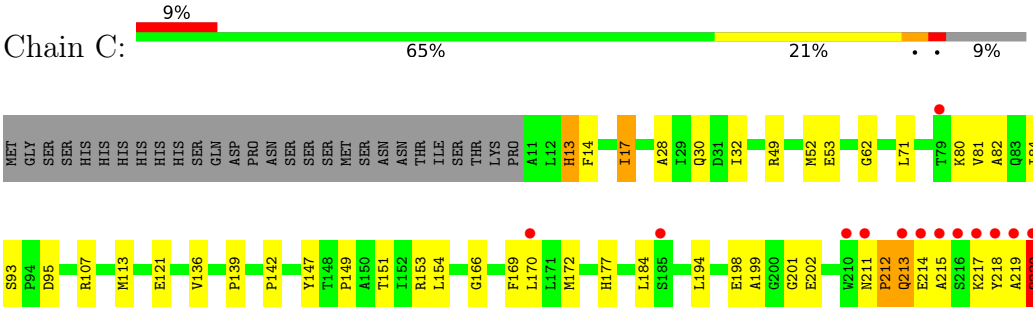
• Molecule 1: Oxidoreductase

Chain B:

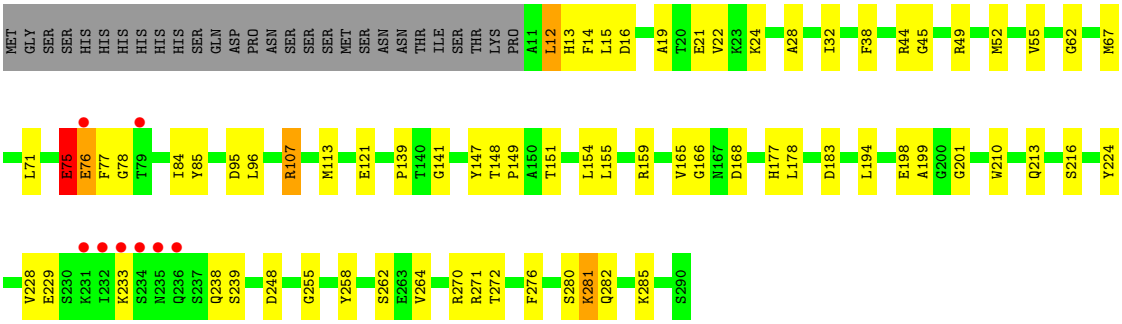


• Molecule 1: Oxidoreductase

Chain C:



• Molecule 1: Oxidoreductase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.83Å 155.45Å 133.23Å 90.00° 126.91° 90.00°	Depositor
Resolution (Å)	49.19 – 3.46 49.19 – 3.46	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.19-3.46) 98.7 (49.19-3.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.191 , 0.242 0.199 , 0.244	Depositor DCC
R_{free} test set	2064 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: 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	0.60	0/2249	0.78	2/3046 (0.1%)
1	B	0.56	0/2249	0.77	3/3046 (0.1%)
1	C	0.57	1/2249 (0.0%)	0.84	3/3046 (0.1%)
1	D	0.63	0/2249	0.85	6/3046 (0.2%)
All	All	0.59	1/8996 (0.0%)	0.81	14/12184 (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	A	0	1
1	B	0	2
1	C	0	5
1	D	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	224	TYR	CD1-CE1	-5.71	1.30	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	12	LEU	CB-CG-CD2	6.77	122.50	111.00
1	A	12	LEU	CA-CB-CG	6.53	130.32	115.30
1	D	12	LEU	CA-CB-CG	6.32	129.84	115.30
1	C	236	GLN	CA-CB-CG	6.28	127.22	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	226	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	12	LEU	CB-CG-CD2	5.49	120.33	111.00
1	B	12	LEU	CA-CB-CG	5.43	127.80	115.30
1	D	107	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	75	GLU	CA-CB-CG	5.41	125.31	113.40
1	A	12	LEU	CB-CG-CD2	5.37	120.12	111.00
1	C	221	MET	N-CA-C	5.29	125.28	111.00
1	D	285	LYS	N-CA-CB	-5.21	101.22	110.60
1	B	277	LEU	CA-CB-CG	5.16	127.17	115.30
1	D	285	LYS	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	LYS	Peptide
1	B	233	LYS	Peptide
1	B	235	ASN	Peptide
1	C	219	ALA	Peptide
1	C	220	GLN	Peptide
1	C	226	ASP	Peptide
1	C	232	ILE	Peptide
1	C	233	LYS	Peptide
1	D	233	LYS	Peptide
1	D	75	GLU	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	2198	0	2133	45	0
1	B	2198	0	2133	58	0
1	C	2198	0	2133	70	0
1	D	2198	0	2133	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
3	D	10	0	4	0	0
All	All	8836	0	8548	215	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 (215) 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:13:HIS:O	1:B:13:HIS:ND1	2.07	0.87
1:C:213:GLN:HG2	1:C:214:GLU:H	1.41	0.86
1:A:13:HIS:ND1	1:A:13:HIS:O	2.13	0.81
1:D:76:GLU:HG3	1:D:77:PHE:CE1	2.17	0.80
1:C:225:MET:HA	1:C:228:VAL:HB	1.65	0.78
1:C:13:HIS:O	1:C:13:HIS:ND1	2.14	0.78
1:D:166:GLY:HA3	1:D:255:GLY:HA2	1.66	0.77
1:D:76:GLU:HG3	1:D:77:PHE:CD1	2.20	0.77
1:A:107:ARG:HD3	1:A:149:PRO:HD3	1.66	0.76
1:C:215:ALA:HA	1:C:224:TYR:CE2	2.23	0.74
1:D:13:HIS:O	1:D:13:HIS:ND1	2.23	0.72
1:C:218:TYR:HB2	1:C:224:TYR:OH	1.90	0.71
1:C:215:ALA:HA	1:C:224:TYR:HE2	1.57	0.69
1:B:15:LEU:HB3	1:B:17:ILE:HG12	1.75	0.69
1:C:214:GLU:HA	1:C:217:LYS:HG2	1.75	0.69
1:D:154:LEU:HD13	1:D:271:ARG:HG2	1.75	0.68
1:D:107:ARG:HD3	1:D:149:PRO:HD3	1.74	0.68
1:C:226:ASP:OD1	1:C:227:ASP:HB3	1.94	0.68
1:D:75:GLU:HG3	1:D:78:GLY:C	2.17	0.65
1:D:52:MET:HE3	1:D:194:LEU:HA	1.79	0.64
1:B:151:THR:HB	1:B:153:ARG:HH12	1.61	0.64
1:D:201:GLY:H	1:D:262:SER:HB2	1.63	0.64
1:A:95:ASP:OD1	1:A:96:LEU:N	2.31	0.64
1:D:95:ASP:OD1	1:D:96:LEU:N	2.31	0.64
1:C:139:PRO:HB2	1:C:147:TYR:CD1	2.33	0.64
1:C:154:LEU:HD13	1:C:271:ARG:HG2	1.79	0.64
1:C:244:PRO:HG3	1:C:250:LEU:HD12	1.80	0.64
1:D:75:GLU:CA	1:D:77:PHE:H	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLU:HA	1:D:77:PHE:H	1.63	0.63
1:D:28:ALA:O	1:D:32:ILE:HG13	1.99	0.63
1:C:107:ARG:HD3	1:C:149:PRO:HD3	1.79	0.62
1:B:236:GLN:HG2	1:B:237:SER:H	1.63	0.62
1:B:244:PRO:HG3	1:B:250:LEU:HD12	1.81	0.61
1:C:52:MET:HE3	1:C:194:LEU:HA	1.83	0.61
1:A:151:THR:HB	1:A:153:ARG:HH12	1.66	0.61
1:B:166:GLY:HA3	1:B:255:GLY:HA2	1.83	0.61
1:C:211:ASN:CG	1:C:212:PRO:HD3	2.21	0.60
1:C:211:ASN:OD1	1:C:212:PRO:HD3	2.01	0.60
1:A:84:ILE:HD11	1:A:151:THR:HG21	1.82	0.60
1:A:15:LEU:HB3	1:A:17:ILE:HG12	1.84	0.60
1:B:236:GLN:HG2	1:B:237:SER:N	2.17	0.59
1:B:95:ASP:OD1	1:B:96:LEU:N	2.36	0.59
1:D:201:GLY:N	1:D:262:SER:HB2	2.18	0.59
1:B:232:ILE:O	1:B:234:SER:N	2.33	0.58
1:A:14:PHE:HB3	1:D:199:ALA:HB2	1.86	0.58
1:B:224:TYR:O	1:B:228:VAL:HG23	2.03	0.58
1:C:215:ALA:O	1:C:224:TYR:OH	2.06	0.57
1:C:218:TYR:HB2	1:C:224:TYR:CE1	2.39	0.57
1:B:199:ALA:HB2	1:C:14:PHE:HB3	1.86	0.57
1:A:166:GLY:HA3	1:A:255:GLY:HA2	1.87	0.57
1:B:280:SER:O	1:B:282:GLN:N	2.38	0.57
1:D:75:GLU:O	1:D:75:GLU:HG2	2.05	0.56
1:C:153:ARG:HD2	3:C:302:AKG:O3	2.06	0.56
1:D:229:GLU:OE2	1:D:238:GLN:HB2	2.05	0.56
1:A:139:PRO:HB2	1:A:147:TYR:CD1	2.41	0.55
1:A:151:THR:HB	1:A:153:ARG:NH1	2.22	0.55
1:C:202:GLU:H	1:C:262:SER:HB2	1.70	0.55
1:C:229:GLU:O	1:C:233:LYS:HG3	2.07	0.55
1:D:224:TYR:O	1:D:228:VAL:HG23	2.06	0.55
1:B:280:SER:HB3	1:B:287:TYR:CD2	2.43	0.54
1:B:28:ALA:O	1:B:32:ILE:HG13	2.06	0.54
1:B:79:THR:C	1:B:80:LYS:HD3	2.27	0.54
1:A:244:PRO:HG3	1:A:250:LEU:HD12	1.89	0.54
1:C:142:PRO:HG3	1:C:177:HIS:CD2	2.43	0.54
1:A:210:TRP:CH2	1:A:212:PRO:HB3	2.43	0.54
1:C:199:ALA:HB3	1:C:265:ILE:HB	1.91	0.53
1:B:14:PHE:HB3	1:C:199:ALA:HB2	1.90	0.53
1:D:139:PRO:HB2	1:D:147:TYR:CD1	2.43	0.53
1:C:220:GLN:OE1	1:C:221:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ARG:NH1	1:B:272:THR:HG21	2.23	0.53
1:B:15:LEU:HD12	1:B:41:MET:HG2	1.90	0.52
1:C:232:ILE:HD11	1:C:238:GLN:HB3	1.91	0.52
1:A:19:ALA:O	1:A:22:VAL:HB	2.09	0.52
1:C:84:ILE:HD11	1:C:151:THR:HG21	1.91	0.52
1:A:67:MET:O	1:A:67:MET:HG3	2.08	0.52
1:A:224:TYR:O	1:A:228:VAL:HG23	2.09	0.51
1:A:280:SER:O	1:A:282:GLN:N	2.43	0.51
1:C:270:ARG:NH1	1:C:272:THR:HG21	2.25	0.51
1:B:139:PRO:HB2	1:B:147:TYR:CD1	2.45	0.51
1:A:81:VAL:HG22	1:A:82:ALA:H	1.75	0.51
1:C:49:ARG:O	1:C:53:GLU:HG2	2.10	0.51
1:D:44:ARG:HA	1:D:248:ASP:OD1	2.11	0.51
1:D:280:SER:O	1:D:282:GLN:N	2.43	0.51
1:B:107:ARG:HD3	1:B:149:PRO:HD3	1.92	0.51
1:B:233:LYS:HG3	1:B:235:ASN:ND2	2.26	0.51
1:B:168:ASP:OD1	1:B:210:TRP:CZ3	2.64	0.51
1:B:210:TRP:CH2	1:B:212:PRO:HB3	2.45	0.51
1:C:28:ALA:O	1:C:32:ILE:HG13	2.11	0.51
1:C:201:GLY:N	1:C:262:SER:HB2	2.25	0.51
1:B:55:VAL:HG13	1:B:113:MET:HE3	1.93	0.51
1:B:165:VAL:HG23	1:B:258:TYR:CD2	2.46	0.50
1:D:14:PHE:O	1:D:15:LEU:HG	2.11	0.50
1:D:168:ASP:OD1	1:D:210:TRP:CZ3	2.63	0.50
1:A:199:ALA:HB2	1:D:14:PHE:HB3	1.92	0.50
1:C:107:ARG:HD2	1:C:121:GLU:OE2	2.11	0.50
1:C:229:GLU:HG2	1:C:233:LYS:CE	2.42	0.50
1:C:215:ALA:CA	1:C:224:TYR:HE2	2.22	0.50
1:D:52:MET:CE	1:D:194:LEU:HD23	2.42	0.49
1:D:52:MET:HE3	1:D:194:LEU:HD23	1.94	0.49
1:A:12:LEU:HD22	1:A:38:PHE:HB2	1.93	0.49
1:D:12:LEU:HD22	1:D:38:PHE:HB2	1.94	0.49
1:C:218:TYR:HB2	1:C:224:TYR:CZ	2.47	0.49
1:C:232:ILE:CD1	1:C:238:GLN:HB3	2.42	0.49
1:D:21:GLU:HB2	1:D:24:LYS:HD2	1.94	0.49
1:C:80:LYS:HB3	1:C:80:LYS:HE3	1.55	0.48
1:B:45:GLY:HA2	1:C:49:ARG:NH1	2.28	0.48
1:B:233:LYS:HE3	1:B:235:ASN:HD21	1.77	0.48
1:C:166:GLY:HA3	1:C:255:GLY:HA2	1.96	0.48
1:C:227:ASP:OD2	1:C:228:VAL:N	2.45	0.48
1:C:280:SER:O	1:C:282:GLN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:HB	1:B:153:ARG:NH1	2.28	0.48
1:A:55:VAL:HG13	1:A:113:MET:HE3	1.96	0.48
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.52	0.48
1:D:165:VAL:HG23	1:D:258:TYR:CD2	2.49	0.48
1:B:84:ILE:HD11	1:B:151:THR:HG21	1.96	0.48
1:B:97:LYS:HB2	1:B:98:ASP:OD1	2.13	0.47
1:B:97:LYS:H	1:B:97:LYS:HG3	1.45	0.47
1:C:30:GLN:HG3	1:C:279:PHE:HZ	1.79	0.47
1:B:52:MET:HE3	1:B:194:LEU:HA	1.96	0.47
1:B:34:ILE:HD13	1:B:283:ARG:HE	1.79	0.47
1:D:270:ARG:NH1	1:D:272:THR:HG21	2.29	0.47
1:A:280:SER:O	1:A:283:ARG:N	2.48	0.47
1:A:281:LYS:HD2	1:A:281:LYS:HA	1.65	0.47
1:D:12:LEU:HD22	1:D:38:PHE:CB	2.45	0.47
1:C:93:SER:HB2	1:C:95:ASP:OD1	2.15	0.46
1:C:90:VAL:HG13	1:C:172:MET:SD	2.55	0.46
1:C:71:LEU:HB2	1:C:85:TYR:CE1	2.51	0.46
1:A:165:VAL:HG23	1:A:258:TYR:CD2	2.50	0.46
1:A:75:GLU:H	1:A:75:GLU:HG2	1.52	0.46
1:C:236:GLN:NE2	1:C:237:SER:H	2.14	0.46
1:D:107:ARG:NH1	1:D:121:GLU:OE1	2.50	0.45
1:D:281:LYS:HD2	1:D:281:LYS:HA	1.75	0.45
1:A:153:ARG:HB2	1:A:272:THR:HG23	1.98	0.45
1:B:280:SER:HB3	1:B:287:TYR:HD2	1.82	0.45
1:B:281:LYS:HD2	1:B:281:LYS:HA	1.79	0.45
1:B:118:PRO:HG2	1:B:123:GLN:HG3	1.98	0.45
1:B:234:SER:O	1:B:235:ASN:ND2	2.50	0.45
1:C:81:VAL:HG22	1:C:82:ALA:H	1.81	0.45
1:D:159:ARG:HH11	1:D:159:ARG:HG3	1.81	0.45
1:A:49:ARG:NH1	1:D:45:GLY:HA2	2.31	0.45
1:A:92:GLN:O	1:A:174:ALA:HB2	2.17	0.45
1:C:201:GLY:H	1:C:262:SER:HB2	1.82	0.45
1:D:165:VAL:HG13	1:D:255:GLY:O	2.17	0.45
1:A:52:MET:HE3	1:A:194:LEU:HD23	1.99	0.45
1:B:52:MET:HE3	1:B:194:LEU:HD23	1.99	0.45
1:B:57:ARG:O	1:B:61:GLU:HG3	2.17	0.45
1:C:71:LEU:HD13	1:C:85:TYR:CE1	2.52	0.45
1:B:66:GLY:O	1:B:69:SER:OG	2.35	0.44
1:D:15:LEU:O	1:D:16:ASP:C	2.55	0.44
1:D:84:ILE:HD11	1:D:151:THR:HG21	1.98	0.44
1:B:25:TYR:HB3	1:B:28:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:VAL:HG13	1:D:113:MET:HE3	1.98	0.44
1:B:13:HIS:HB3	1:B:242:TYR:OH	2.16	0.44
1:C:220:GLN:HB3	1:C:221:MET:H	1.75	0.44
1:C:220:GLN:OE1	1:C:220:GLN:HA	2.17	0.44
1:B:52:MET:CE	1:B:194:LEU:HD23	2.47	0.44
1:B:79:THR:O	1:B:80:LYS:HD3	2.18	0.44
1:D:19:ALA:O	1:D:22:VAL:HB	2.17	0.44
1:A:233:LYS:HB2	1:A:233:LYS:HE3	1.65	0.44
1:C:280:SER:O	1:C:283:ARG:N	2.51	0.44
1:A:44:ARG:HA	1:A:248:ASP:OD1	2.18	0.44
1:C:170:LEU:HD21	1:C:184:LEU:HD22	2.00	0.43
1:A:25:TYR:HB3	1:A:28:ALA:HB2	1.99	0.43
1:D:148:THR:HG22	1:D:149:PRO:HD2	1.99	0.43
1:A:284:ASN:HB2	1:A:285:LYS:H	1.56	0.43
1:C:153:ARG:HB2	1:C:272:THR:HG23	1.99	0.43
1:D:155:LEU:HB3	1:D:264:VAL:HG21	2.00	0.43
1:A:49:ARG:CZ	1:D:45:GLY:HA2	2.49	0.43
1:C:281:LYS:HD2	1:C:281:LYS:HA	1.67	0.43
1:D:15:LEU:HD23	1:D:15:LEU:HA	1.68	0.43
1:C:229:GLU:O	1:C:233:LYS:HE3	2.18	0.43
1:C:211:ASN:HB3	1:C:213:GLN:HE22	1.83	0.43
1:C:218:TYR:CB	1:C:224:TYR:HE1	2.31	0.43
1:B:120:PHE:O	1:B:124:VAL:HG23	2.19	0.43
1:C:213:GLN:O	1:C:217:LYS:HE2	2.18	0.43
1:C:227:ASP:O	1:C:229:GLU:N	2.52	0.43
1:B:178:LEU:H	1:B:178:LEU:HD12	1.83	0.43
1:C:239:SER:OG	1:C:240:VAL:N	2.50	0.43
1:A:148:THR:HG22	1:A:149:PRO:HD2	2.01	0.42
1:A:168:ASP:OD1	1:A:210:TRP:CZ3	2.72	0.42
1:B:81:VAL:HG22	1:B:82:ALA:H	1.84	0.42
1:C:17:ILE:HD13	1:C:17:ILE:HA	1.76	0.42
1:D:75:GLU:HA	1:D:76:GLU:HG2	2.01	0.42
1:B:156:LEU:O	1:B:159:ARG:HB2	2.19	0.42
1:C:218:TYR:CZ	1:C:226:ASP:OD2	2.73	0.42
1:A:89:ILE:HD12	1:A:147:TYR:HE2	1.85	0.42
1:B:97:LYS:HE3	1:B:98:ASP:OD1	2.20	0.42
1:B:170:LEU:HD21	1:B:184:LEU:HD22	2.02	0.42
1:B:45:GLY:HA2	1:C:49:ARG:CZ	2.50	0.42
1:B:225:MET:O	1:B:229:GLU:HG3	2.19	0.42
1:A:154:LEU:HD13	1:A:271:ARG:HG2	2.02	0.41
1:B:15:LEU:O	1:C:198:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:TYR:CD2	1:C:223:GLU:HG3	2.55	0.41
1:A:107:ARG:NH1	1:A:121:GLU:OE1	2.53	0.41
1:A:15:LEU:O	1:A:16:ASP:C	2.58	0.41
1:A:211:ASN:ND2	1:A:214:GLU:HB3	2.34	0.41
1:B:153:ARG:HB2	1:B:272:THR:HG23	2.02	0.41
1:D:183:ASP:N	1:D:281:LYS:N	2.69	0.41
1:C:169:PHE:HA	1:C:172:MET:SD	2.60	0.41
1:C:218:TYR:CG	1:C:224:TYR:CE1	3.09	0.41
1:D:213:GLN:O	1:D:216:SER:OG	2.39	0.41
1:A:45:GLY:HA2	1:D:49:ARG:CZ	2.51	0.41
1:C:136:VAL:HG22	1:C:286:ILE:HB	2.01	0.41
1:D:178:LEU:HD12	1:D:178:LEU:H	1.85	0.41
1:A:15:LEU:O	1:D:198:GLU:HA	2.21	0.41
1:B:71:LEU:HD13	1:B:85:TYR:CZ	2.55	0.41
1:C:218:TYR:OH	1:C:226:ASP:OD2	2.27	0.40
1:D:71:LEU:HD13	1:D:85:TYR:CE1	2.56	0.40
1:D:141:GLY:HA2	1:D:177:HIS:HE1	1.85	0.40
1:B:154:LEU:HD13	1:B:271:ARG:HG2	2.02	0.40
1:B:233:LYS:HG3	1:B:235:ASN:HD21	1.85	0.40
1:A:120:PHE:O	1:A:124:VAL:HG23	2.21	0.40
1:A:21:GLU:HB2	1:A:24:LYS:HD2	2.03	0.40
1:B:15:LEU:O	1:B:16:ASP:C	2.60	0.40
1:D:183:ASP:N	1:D:281:LYS:H	2.20	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	278/308 (90%)	250 (90%)	25 (9%)	3 (1%)	14 50
1	B	278/308 (90%)	245 (88%)	28 (10%)	5 (2%)	8 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	278/308 (90%)	239 (86%)	29 (10%)	10 (4%)	3 25
1	D	278/308 (90%)	250 (90%)	25 (9%)	3 (1%)	14 50
All	All	1112/1232 (90%)	984 (88%)	107 (10%)	21 (2%)	8 38

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	LYS
1	A	281	LYS
1	B	75	GLU
1	B	233	LYS
1	B	281	LYS
1	C	213	GLN
1	C	227	ASP
1	C	234	SER
1	C	281	LYS
1	D	76	GLU
1	D	281	LYS
1	C	228	VAL
1	B	236	GLN
1	C	220	GLN
1	C	236	GLN
1	C	13	HIS
1	B	62	GLY
1	A	62	GLY
1	C	62	GLY
1	D	62	GLY
1	C	212	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	235/266 (88%)	229 (97%)	6 (3%)	46 74
1	B	235/266 (88%)	232 (99%)	3 (1%)	69 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	235/266 (88%)	229 (97%)	6 (3%)	46 74
1	D	235/266 (88%)	232 (99%)	3 (1%)	69 86
All	All	940/1064 (88%)	922 (98%)	18 (2%)	57 80

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	MET
1	A	75	GLU
1	A	148	THR
1	A	168	ASP
1	A	239	SER
1	A	276	PHE
1	B	97	LYS
1	B	244	PRO
1	B	284	ASN
1	C	17	ILE
1	C	113	MET
1	C	227	ASP
1	C	232	ILE
1	C	237	SER
1	C	284	ASN
1	D	67	MET
1	D	239	SER
1	D	276	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	B	235	ASN
1	C	177	HIS
1	C	220	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 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	C	302	2	9,9,9	1.16	0	11,11,11	1.40	2 (18%)
3	AKG	D	302	2	9,9,9	1.22	1 (11%)	11,11,11	1.46	2 (18%)
3	AKG	A	302	2	9,9,9	1.00	0	11,11,11	1.87	3 (27%)
3	AKG	B	302	2	9,9,9	0.99	0	11,11,11	2.05	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	C	302	2	-	5/9/9/9	-
3	AKG	D	302	2	-	8/9/9/9	-
3	AKG	A	302	2	-	4/9/9/9	-
3	AKG	B	302	2	-	4/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	AKG	O3-C5	2.04	1.28	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	AKG	O1-C1-C2	-3.76	116.69	121.72
3	B	302	AKG	C4-C3-C2	-3.63	106.19	113.03
3	A	302	AKG	C4-C3-C2	-3.21	106.98	113.03
3	A	302	AKG	O1-C1-C2	-3.05	117.64	121.72
3	B	302	AKG	O2-C1-C2	2.95	122.05	113.97
3	D	302	AKG	C4-C3-C2	-2.94	107.50	113.03
3	A	302	AKG	O2-C1-C2	2.75	121.48	113.97
3	C	302	AKG	C3-C2-C1	2.26	120.16	115.97
3	D	302	AKG	C3-C2-C1	2.15	119.96	115.97
3	C	302	AKG	O2-C1-O1	-2.10	118.79	123.61

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	AKG	O1-C1-C2-O5
3	A	302	AKG	O1-C1-C2-C3
3	A	302	AKG	O2-C1-C2-C3
3	B	302	AKG	O1-C1-C2-O5
3	B	302	AKG	O1-C1-C2-C3
3	B	302	AKG	O2-C1-C2-C3
3	C	302	AKG	C1-C2-C3-C4
3	D	302	AKG	O1-C1-C2-C3
3	D	302	AKG	O2-C1-C2-O5
3	D	302	AKG	O2-C1-C2-C3
3	D	302	AKG	C2-C3-C4-C5
3	C	302	AKG	C2-C3-C4-C5
3	A	302	AKG	C1-C2-C3-C4
3	D	302	AKG	C1-C2-C3-C4
3	D	302	AKG	O1-C1-C2-O5
3	C	302	AKG	O2-C1-C2-O5
3	D	302	AKG	C3-C4-C5-O3
3	D	302	AKG	C3-C4-C5-O4
3	C	302	AKG	C3-C4-C5-O3
3	B	302	AKG	C1-C2-C3-C4
3	C	302	AKG	C3-C4-C5-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	AKG	1	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	280/308 (90%)	-0.47	4 (1%) 75 72	3, 14, 51, 104	0
1	B	280/308 (90%)	-0.23	8 (2%) 51 49	12, 30, 68, 100	0
1	C	280/308 (90%)	0.26	27 (9%) 8 10	12, 36, 129, 155	0
1	D	280/308 (90%)	-0.46	8 (2%) 51 49	2, 14, 59, 96	0
All	All	1120/1232 (90%)	-0.23	47 (4%) 36 35	2, 23, 80, 155	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	SER	8.7
1	C	222	GLN	8.6
1	C	216	SER	7.0
1	C	234	SER	6.5
1	C	236	GLN	6.5
1	C	235	ASN	6.0
1	C	215	ALA	5.8
1	C	221	MET	5.7
1	C	223	GLU	5.5
1	C	214	GLU	5.4
1	C	231	LYS	5.0
1	C	219	ALA	4.8
1	C	225	MET	4.5
1	C	227	ASP	4.3
1	C	213	GLN	4.1
1	B	79	THR	3.8
1	C	233	LYS	3.8
1	C	218	TYR	3.7
1	C	217	LYS	3.6
1	C	237	SER	3.6
1	D	234	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	231	LYS	3.4
1	C	232	ILE	3.2
1	D	232	ILE	3.1
1	A	79	THR	3.1
1	B	232	ILE	3.1
1	D	233	LYS	3.0
1	C	79	THR	3.0
1	D	79	THR	2.9
1	C	220	GLN	2.9
1	A	235	ASN	2.8
1	A	234	SER	2.8
1	B	65	GLY	2.7
1	D	235	ASN	2.7
1	B	233	LYS	2.7
1	C	210	TRP	2.7
1	C	211	ASN	2.6
1	B	234	SER	2.6
1	C	185	SER	2.4
1	B	63	ASN	2.3
1	C	226	ASP	2.3
1	B	61	GLU	2.2
1	A	232	ILE	2.2
1	D	236	GLN	2.1
1	D	76	GLU	2.1
1	C	170	LEU	2.0
1	B	143	GLU	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, 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	B-factors(Å^2)	Q<0.9
3	AKG	D	302	10/10	0.91	0.22	22,35,46,47	0
3	AKG	A	302	10/10	0.94	0.17	18,30,40,42	0
3	AKG	B	302	10/10	0.95	0.17	21,37,48,49	0
2	FE	B	301	1/1	0.96	0.07	52,52,52,52	0
3	AKG	C	302	10/10	0.97	0.17	37,45,54,55	0
2	FE	A	301	1/1	0.97	0.06	44,44,44,44	0
2	FE	C	301	1/1	0.98	0.05	49,49,49,49	0
2	FE	D	301	1/1	0.98	0.04	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.