Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2026 – 01:29 PM UTC

PDB ID	:	4BXF / pdb_00004bxf
Title	:	60S ribosomal protein L27A histidine hydroxylase (MINA53 Y209C) in complex with MN(II), 2-oxoglutarate (2OG) and 60S ribosomal protein L27A (RPL27A G37C) peptide fragment
Authors	:	Chowdhury, R.; Schofield, C.J.
Deposited on	:	2013-07-10
Resolution	:	2.05 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 (1)) were used in the production of this report:

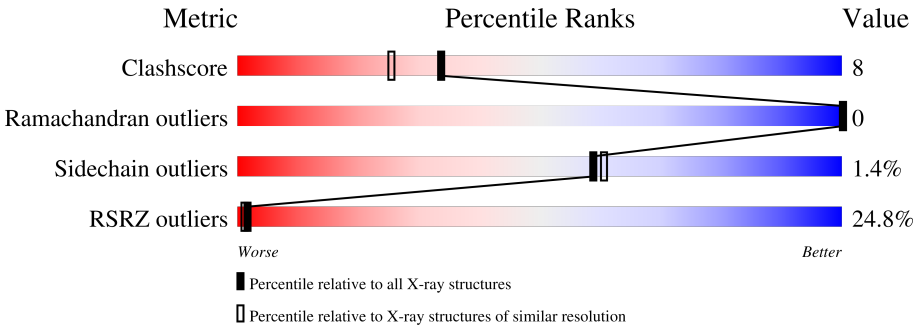
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	442	17%, 80%, 16%, ·
1	B	442	29%, 74%, 21%, · 5%
2	C	19	16%, 37%, 11%, 53%
2	D	19	26%, 37%, 5%, 58%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7077 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 BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE MINA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3331	2137	570	611	13			
1	B	422	Total	C	N	O	S	0	0	0
			3256	2086	558	599	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP Q8IUF8
A	25	MET	-	expression tag	UNP Q8IUF8
A	209	CYS	TYR	engineered mutation	UNP Q8IUF8
B	24	SER	-	expression tag	UNP Q8IUF8
B	25	MET	-	expression tag	UNP Q8IUF8
B	209	CYS	TYR	engineered mutation	UNP Q8IUF8

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	S	0	0	0
			72	44	18	9	1			
2	D	8	Total	C	N	O	S	0	0	0
			64	38	17	8	1			

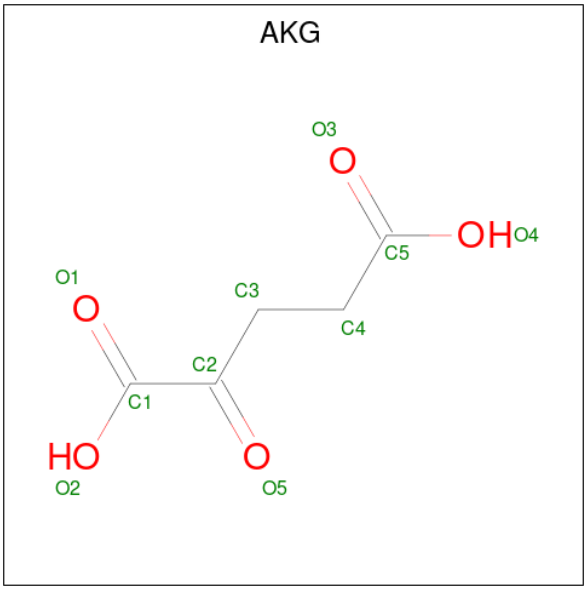
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	CYS	GLY	engineered mutation	UNP P46776
D	37	CYS	GLY	engineered mutation	UNP P46776

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



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

- Molecule 5 is water.

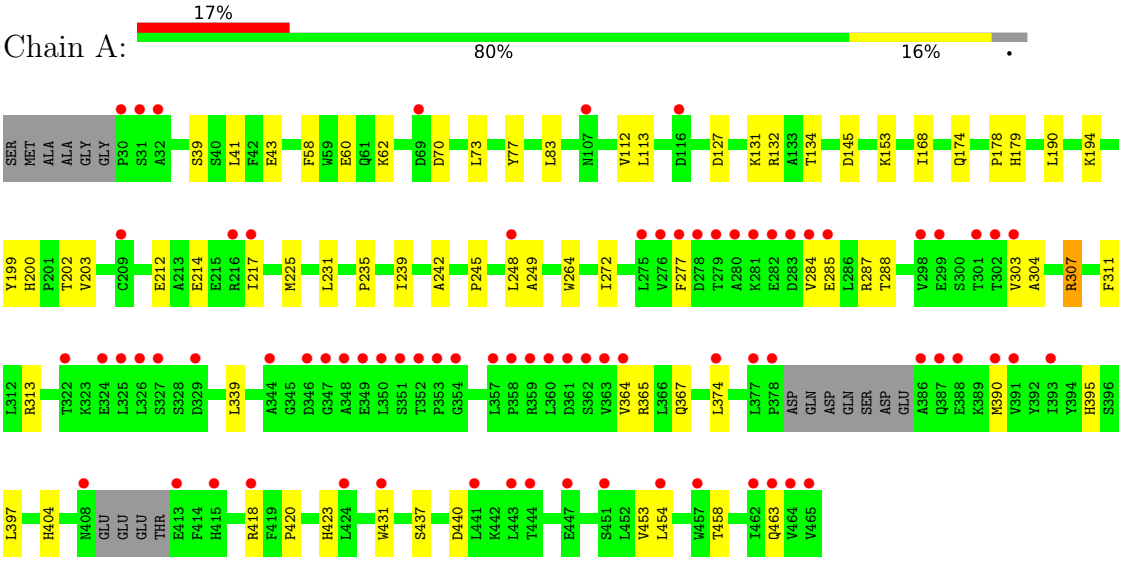
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	229	Total O 229 229	0	0
5	B	101	Total O 101 101	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

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.

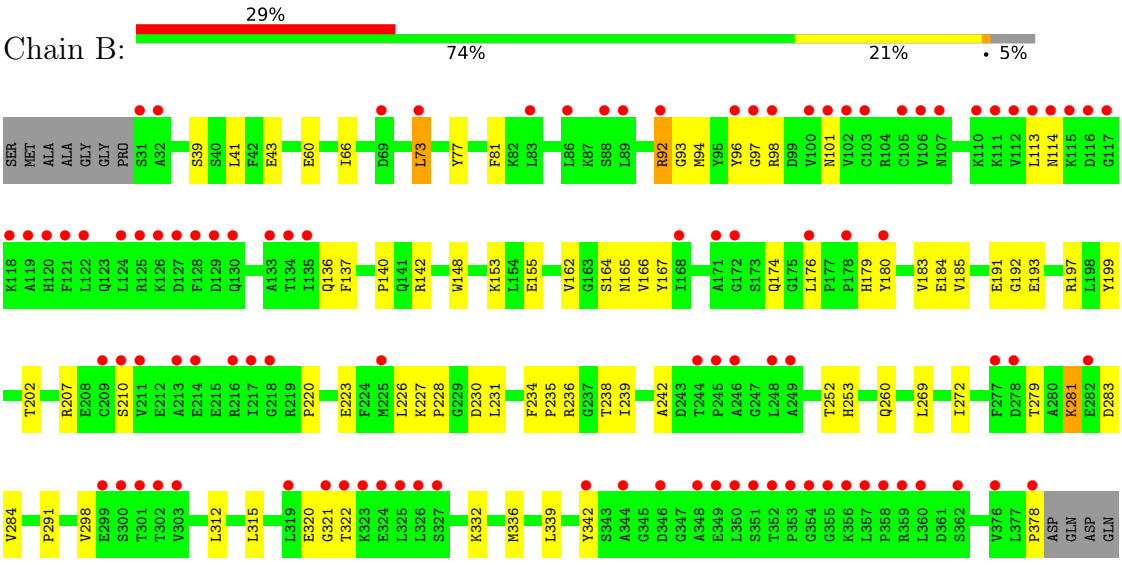
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE MINA

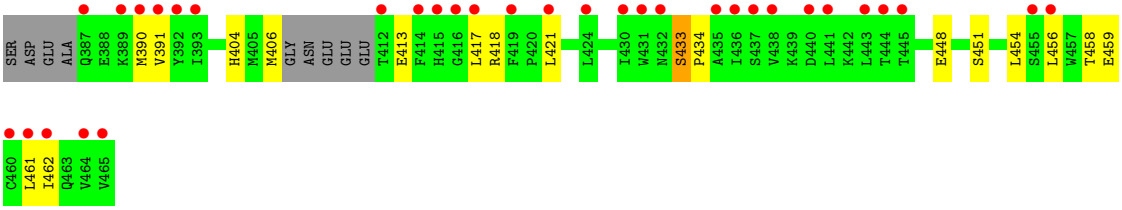
Chain A:



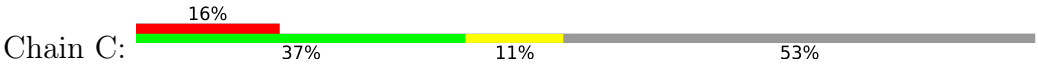
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE MINA

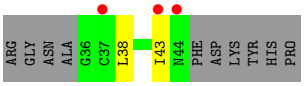
Chain B:



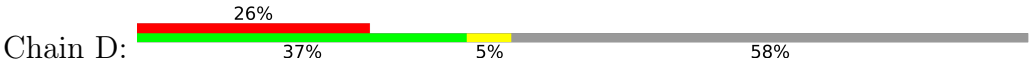


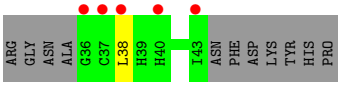
• Molecule 2: 60S RIBOSOMAL PROTEIN L27A





• Molecule 2: 60S RIBOSOMAL PROTEIN L27A





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.34Å 88.39Å 167.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.83 – 2.05 64.83 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (64.83-2.05) 92.4 (64.83-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.05Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.220 , 0.221 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7077	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: MN, 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	0.52	0/3411	0.83	2/4630 (0.0%)
1	B	0.40	0/3335	0.83	5/4535 (0.1%)
2	C	0.59	0/74	0.85	0/98
2	D	0.44	0/66	0.83	0/87
All	All	0.46	0/6886	0.83	7/9350 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	VAL	N-CA-C	7.43	120.97	113.47
1	A	202	THR	N-CA-C	-7.16	103.52	112.90
1	B	378	PRO	N-CA-CB	6.25	109.87	103.00
1	B	321	GLY	N-CA-C	6.01	127.42	113.18
1	B	185	VAL	N-CA-C	5.94	118.00	108.85
1	A	145	ASP	N-CA-C	5.75	117.55	111.28
1	B	433	SER	N-CA-C	5.04	116.42	110.07

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	3331	0	3246	51	0
1	B	3256	0	3091	57	0
2	C	72	0	64	2	0
2	D	64	0	53	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	4	1	0
5	A	229	0	0	2	0
5	B	101	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	7077	0	6462	101	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 8.

All (101) 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:92:ARG:HH11	1:B:92:ARG:HG2	1.39	0.86
1:A:374:LEU:HD13	1:B:298:VAL:HG12	1.65	0.79
1:B:92:ARG:HG2	1:B:92:ARG:NH1	1.97	0.78
1:A:285:GLU:OE2	1:A:307:ARG:NH1	2.20	0.74
1:A:272:ILE:HD13	1:B:272:ILE:HD13	1.72	0.70
1:A:390:MET:HG3	1:A:418:ARG:HD3	1.73	0.70
1:B:332:LYS:HG3	1:B:336:MET:HE2	1.73	0.70
1:B:97:GLY:HA2	1:B:101:ASN:HD21	1.58	0.69
1:A:203:VAL:HG22	1:B:281:LYS:HD2	1.74	0.68
1:B:456:LEU:HB3	1:B:462:ILE:HD13	1.78	0.66
1:B:41:LEU:HD22	1:B:153:LYS:HB2	1.79	0.65
1:B:93:GLY:O	1:B:94:MET:HE2	1.96	0.65
1:B:390:MET:HE3	1:B:418:ARG:HG2	1.79	0.64
1:A:41:LEU:HD22	1:A:153:LYS:HB2	1.79	0.64
1:A:390:MET:HE3	1:A:418:ARG:HG2	1.82	0.60
1:B:142:ARG:NH1	1:B:406:MET:HE2	2.18	0.58
1:A:41:LEU:HD22	1:A:153:LYS:CB	2.35	0.57
1:B:448:GLU:HA	1:B:451:SER:HB3	1.86	0.57
1:B:41:LEU:HD22	1:B:153:LYS:CB	2.35	0.57
1:B:179:HIS:CG	2:D:38:LEU:HD12	2.40	0.57
1:A:214:GLU:HG3	1:A:217:ILE:HD11	1.88	0.56
1:B:191:GLU:HB2	1:B:252:THR:HB	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG12	1:A:287:ARG:NH2	2.22	0.55
1:A:272:ILE:HD11	1:B:312:LEU:HD21	1.88	0.55
1:A:199:TYR:HB2	1:A:239:ILE:HB	1.88	0.54
1:A:225:MET:HE1	1:A:245:PRO:HG2	1.89	0.54
1:A:454:LEU:O	1:A:458:THR:HG23	2.07	0.54
1:A:284:VAL:O	1:A:288:THR:HG23	2.08	0.53
1:A:225:MET:HE1	1:A:245:PRO:CG	2.38	0.52
1:A:194:LYS:N	1:A:225:MET:HE3	2.25	0.52
1:B:92:ARG:HH11	1:B:92:ARG:CG	2.14	0.52
1:B:461:LEU:O	1:B:462:ILE:HD12	2.10	0.51
1:A:374:LEU:HD11	1:A:431:TRP:CZ2	2.45	0.51
1:B:417:LEU:HD11	1:B:459:GLU:HG3	1.93	0.50
1:B:202:THR:HG23	1:B:239:ILE:HD11	1.93	0.50
1:B:391:VAL:HG23	1:B:421:LEU:HA	1.94	0.49
1:B:96:TYR:HB3	1:B:114:ASN:HD22	1.78	0.49
1:B:456:LEU:CB	1:B:462:ILE:HD13	2.43	0.49
1:A:437:SER:HB2	1:A:440:ASP:OD2	2.12	0.49
1:B:39:SER:O	1:B:43:GLU:HG3	2.13	0.48
1:A:420:PRO:HG2	1:A:423:HIS:ND1	2.28	0.48
2:C:43:ILE:HD12	2:C:43:ILE:N	2.29	0.48
1:B:199:TYR:CE2	1:B:220:PRO:HG3	2.48	0.48
1:A:178:PRO:HG2	1:A:212:GLU:O	2.15	0.47
1:B:137:PHE:HE2	1:B:140:PRO:HA	1.79	0.47
1:B:73:LEU:HD22	1:B:77:TYR:CE1	2.49	0.47
1:A:339:LEU:HG	1:A:404:HIS:CE1	2.49	0.47
1:B:454:LEU:O	1:B:458:THR:HG23	2.15	0.47
1:A:367:GLN:CD	1:A:463:GLN:HB2	2.40	0.46
1:A:231:LEU:C	1:A:231:LEU:HD23	2.41	0.46
1:B:81:PHE:CD1	1:B:166:VAL:HG11	2.51	0.46
1:A:364:VAL:HG11	1:A:453:VAL:HG11	1.98	0.46
1:B:179:HIS:CD2	2:D:38:LEU:HD12	2.50	0.46
1:B:167:TYR:HB2	1:B:253:HIS:CE1	2.51	0.46
1:B:433:SER:HA	1:B:434:PRO:HD3	1.81	0.45
1:A:365:ARG:NH1	1:A:367:GLN:HG2	2.32	0.45
1:B:155:GLU:HG2	1:B:162:VAL:HG23	1.97	0.45
1:A:313:ARG:HH22	1:B:320:GLU:CD	2.24	0.45
1:B:279:THR:CG2	1:B:283:ASP:HB3	2.46	0.45
1:A:70:ASP:HB3	1:A:73:LEU:HB2	1.99	0.45
1:B:66:ILE:HD12	1:B:231:LEU:HD22	1.98	0.45
1:B:180:TYR:CZ	1:B:210:SER:HB3	2.52	0.44
1:B:164:SER:C	1:B:165:ASN:HD22	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HG	1:B:404:HIS:CD2	2.52	0.44
1:B:192:GLY:O	1:B:228:PRO:HD3	2.18	0.43
1:A:285:GLU:HG2	1:A:311:PHE:HE1	1.83	0.43
1:A:248:LEU:C	1:A:248:LEU:HD12	2.44	0.43
1:B:60:GLU:HA	1:B:235:PRO:HB3	2.01	0.43
1:A:127:ASP:OD1	1:A:131:LYS:HD2	2.18	0.43
1:A:395:HIS:ND1	1:A:397:LEU:HB2	2.34	0.43
1:B:174:GLN:HG3	1:B:242:ALA:O	2.18	0.43
1:A:307:ARG:CG	1:A:307:ARG:HH11	2.32	0.43
1:A:174:GLN:HG3	1:A:242:ALA:O	2.19	0.43
1:B:176:LEU:HD12	4:B:901:AKG:H42	2.00	0.43
1:B:136:GLN:HA	1:B:166:VAL:O	2.19	0.42
1:A:58:PHE:CE1	1:A:62:LYS:HE3	2.55	0.42
1:A:132:ARG:HD3	5:A:2101:HOH:O	2.19	0.42
1:B:148:TRP:CZ2	1:B:342:TYR:HA	2.54	0.42
1:A:77:TYR:O	1:A:190:LEU:HD22	2.19	0.42
1:A:200:HIS:HE1	5:A:2124:HOH:O	2.01	0.42
1:B:227:LYS:HG2	1:B:230:ASP:OD2	2.20	0.42
1:B:183:VAL:HG12	1:B:260:GLN:HB2	2.02	0.42
1:B:231:LEU:C	1:B:231:LEU:HD23	2.45	0.42
1:A:179:HIS:CG	2:C:38:LEU:HD12	2.55	0.42
1:A:83:LEU:HD13	1:A:168:ILE:HG21	2.01	0.41
1:A:339:LEU:HG	1:A:404:HIS:CD2	2.54	0.41
1:A:39:SER:O	1:A:43:GLU:HG3	2.20	0.41
1:B:234:PHE:CD1	1:B:238:THR:HB	2.55	0.41
1:A:272:ILE:CD1	1:B:272:ILE:HD13	2.45	0.41
1:A:277:PHE:CE2	1:B:269:LEU:HD12	2.56	0.41
1:B:197:ARG:HG2	1:B:223:GLU:HG3	2.02	0.41
1:A:112:VAL:C	1:A:113:LEU:HD12	2.46	0.41
1:A:248:LEU:HD12	1:A:249:ALA:N	2.36	0.41
1:B:184:GLU:OE2	1:B:236:ARG:HG2	2.21	0.41
1:A:60:GLU:HA	1:A:235:PRO:HB3	2.03	0.41
1:A:367:GLN:NE2	1:A:463:GLN:HB2	2.35	0.41
1:B:193:GLU:HA	1:B:226:LEU:O	2.20	0.41
1:B:113:LEU:N	1:B:113:LEU:HD12	2.36	0.41
1:A:194:LYS:C	1:A:225:MET:HE3	2.46	0.40
1:A:264:TRP:CZ2	1:B:291:PRO:HD3	2.56	0.40
1:A:303:VAL:HG13	1:A:304:ALA:N	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	419/442 (95%)	405 (97%)	14 (3%)	0	100	100
1	B	416/442 (94%)	407 (98%)	9 (2%)	0	100	100
2	C	7/19 (37%)	7 (100%)	0	0	100	100
2	D	6/19 (32%)	6 (100%)	0	0	100	100
All	All	848/922 (92%)	825 (97%)	23 (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	356/394 (90%)	354 (99%)	2 (1%)	78	83
1	B	336/394 (85%)	328 (98%)	8 (2%)	43	40
2	C	7/16 (44%)	7 (100%)	0	100	100
2	D	6/16 (38%)	6 (100%)	0	100	100
All	All	705/820 (86%)	695 (99%)	10 (1%)	59	60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	THR
1	A	307	ARG

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Mol	Chain	Res	Type
1	B	73	LEU
1	B	92	ARG
1	B	98	ARG
1	B	207	ARG
1	B	281	LYS
1	B	315	LEU
1	B	322	THR
1	B	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	HIS
1	A	408	ASN
1	B	101	ASN
1	B	136	GLN
1	B	200	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	B	901	3	9,9,9	1.27	0	11,11,11	1.62	2 (18%)
4	AKG	A	901	3	9,9,9	1.24	0	11,11,11	1.61	2 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	B	901	3	-	1/9/9/9	-
4	AKG	A	901	3	-	0/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	AKG	O1-C1-C2	-3.29	117.72	121.81
4	A	901	AKG	O1-C1-C2	-3.02	118.06	121.81
4	A	901	AKG	C3-C2-C1	2.60	120.28	115.86
4	B	901	AKG	C3-C2-C1	2.53	120.16	115.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	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
4	B	901	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

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	425/442 (96%)	0.92	76 (17%) 3 3	20, 37, 92, 100	6 (1%)
1	B	422/442 (95%)	1.49	130 (30%) 1 0	21, 53, 100, 100	6 (1%)
2	C	9/19 (47%)	1.71	3 (33%) 1 0	27, 38, 61, 63	0
2	D	8/19 (42%)	2.47	5 (62%) 0 0	48, 62, 87, 87	0
All	All	864/922 (93%)	1.22	214 (24%) 2 1	20, 46, 98, 100	12 (1%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	LYS	6.2
1	A	325	LEU	5.4
1	A	350	LEU	5.4
1	A	277	PHE	5.3
1	A	278	ASP	5.3
1	B	412	THR	5.1
1	A	284	VAL	5.1
1	A	276	VAL	5.0
1	B	116	ASP	5.0
1	B	414	PHE	5.0
1	A	30	PRO	4.9
1	B	462	ILE	4.8
1	B	119	ALA	4.6
1	B	211	VAL	4.5
1	B	444	THR	4.5
1	B	106	VAL	4.4
1	A	303	VAL	4.3
1	A	348	ALA	4.3
1	A	465	VAL	4.2
1	A	386	ALA	4.2
1	B	378	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	43	ILE	4.1
2	C	44	ASN	4.0
1	B	415	HIS	4.0
1	B	319	LEU	4.0
2	D	37	CYS	4.0
1	B	350	LEU	3.9
1	B	417	LEU	3.9
2	D	43	ILE	3.9
1	B	121	PHE	3.9
1	B	124	LEU	3.7
1	B	249	ALA	3.7
1	B	213	ALA	3.7
1	B	246	ALA	3.7
1	B	117	GLY	3.6
1	B	128	PHE	3.6
1	B	217	ILE	3.6
1	B	105	CYS	3.6
1	A	357	LEU	3.6
1	B	118	LYS	3.5
1	B	31	SER	3.5
1	A	349	GLU	3.5
1	B	216	ARG	3.5
1	A	280	ALA	3.4
1	A	324	GLU	3.4
1	B	110	LYS	3.4
1	B	349	GLU	3.4
2	C	37	CYS	3.4
1	A	279	THR	3.4
2	D	38	LEU	3.3
1	B	209	CYS	3.3
1	B	357	LEU	3.3
1	B	461	LEU	3.3
1	B	129	ASP	3.3
1	A	354	GLY	3.3
1	B	355	GLY	3.3
1	A	31	SER	3.2
1	B	89	LEU	3.2
1	B	352	THR	3.2
1	B	113	LEU	3.1
1	B	214	GLU	3.1
1	B	464	VAL	3.1
1	B	302	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	115	LYS	3.1
1	A	344	ALA	3.0
1	B	100	VAL	3.0
1	B	441	LEU	3.0
1	A	322	THR	3.0
1	B	301	THR	3.0
1	B	322	THR	3.0
1	A	415	HIS	3.0
1	B	300	SER	3.0
1	B	325	LEU	3.0
1	B	443	LEU	3.0
1	B	387	GLN	3.0
1	B	133	ALA	3.0
1	B	348	ALA	3.0
1	A	248	LEU	3.0
1	A	326	LEU	3.0
1	B	465	VAL	3.0
1	A	285	GLU	3.0
1	A	116	ASP	3.0
1	A	361	ASP	3.0
1	B	391	VAL	2.9
1	B	354	GLY	2.9
1	B	393	ILE	2.9
1	B	421	LEU	2.9
1	A	299	GLU	2.9
1	A	388	GLU	2.9
1	A	408	ASN	2.9
1	A	32	ALA	2.9
1	A	346	ASP	2.9
1	B	358	PRO	2.9
1	B	125	ARG	2.8
1	B	103	CYS	2.8
1	B	438	VAL	2.8
1	B	419	PHE	2.8
1	A	301	THR	2.8
1	B	299	GLU	2.8
1	B	218	GLY	2.8
1	A	107	ASN	2.7
1	B	135	ILE	2.7
1	B	430	ILE	2.7
1	A	413	GLU	2.7
1	B	277	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	392	TYR	2.7
1	A	351	SER	2.7
1	B	327	SER	2.7
1	A	359	ARG	2.7
1	B	360	LEU	2.7
1	B	107	ASN	2.7
1	B	321	GLY	2.7
1	A	387	GLN	2.6
1	A	275	LEU	2.6
1	A	360	LEU	2.6
2	D	36	GLY	2.6
1	B	83	LEU	2.6
1	B	346	ASP	2.6
1	B	342	TYR	2.6
1	B	112	VAL	2.6
1	A	282	GLU	2.6
1	B	122	LEU	2.6
1	B	431	TRP	2.6
1	B	111	LYS	2.5
1	A	283	ASP	2.5
1	B	282	GLU	2.5
1	A	364	VAL	2.5
1	B	120	HIS	2.5
1	B	356	LYS	2.5
1	B	351	SER	2.5
1	B	455	SER	2.5
1	B	326	LEU	2.5
1	A	457	TRP	2.5
1	A	347	GLY	2.5
1	B	416	GLY	2.5
1	B	92	ARG	2.5
1	B	69	ASP	2.5
1	A	352	THR	2.5
1	A	464	VAL	2.4
1	B	437	SER	2.4
1	A	378	PRO	2.4
1	A	374	LEU	2.4
1	B	432	ASN	2.4
1	B	324	GLU	2.4
1	A	302	THR	2.4
1	B	245	PRO	2.4
1	B	390	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	130	GLN	2.4
1	B	88	SER	2.4
1	A	216	ARG	2.4
1	B	96	TYR	2.4
1	B	73	LEU	2.4
1	B	101	ASN	2.4
1	B	303	VAL	2.4
1	A	447	GLU	2.3
1	B	32	ALA	2.3
1	B	86	LEU	2.3
1	B	176	LEU	2.3
1	B	126	LYS	2.3
1	B	323	LYS	2.3
1	B	244	THR	2.3
1	A	463	GLN	2.3
1	B	248	LEU	2.3
1	A	298	VAL	2.3
1	A	363	VAL	2.3
1	B	102	VAL	2.3
1	A	377	LEU	2.3
1	B	210	SER	2.3
2	D	40	HIS	2.3
1	A	393	ILE	2.3
1	A	443	LEU	2.3
1	A	329	ASP	2.2
1	A	390	MET	2.2
1	B	171	ALA	2.2
1	A	327	SER	2.2
1	B	98	ARG	2.2
1	A	358	PRO	2.2
1	A	217	ILE	2.2
1	A	462	ILE	2.2
1	B	278	ASP	2.2
1	B	436	ILE	2.2
1	B	440	ASP	2.2
1	B	114	ASN	2.2
1	B	225	MET	2.2
1	A	353	PRO	2.1
1	B	353	PRO	2.1
1	B	445	THR	2.2
1	A	391	VAL	2.1
1	A	441	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	454	LEU	2.1
1	B	178	PRO	2.1
1	B	97	GLY	2.1
1	B	172	GLY	2.1
1	B	376	VAL	2.1
1	A	418	ARG	2.1
1	A	424	LEU	2.1
1	B	424	LEU	2.1
1	B	460	CYS	2.1
1	B	127	ASP	2.1
1	B	180	TYR	2.1
1	A	431	TRP	2.1
1	B	344	ALA	2.1
1	B	435	ALA	2.1
1	A	451	SER	2.1
1	B	362	SER	2.1
1	A	69	ASP	2.1
1	B	134	THR	2.1
1	B	359	ARG	2.1
1	B	456	LEU	2.0
1	A	209	CYS	2.0
1	B	389	LYS	2.0
1	B	168	ILE	2.0
1	A	362	SER	2.0
1	A	444	THR	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	AKG	B	901	10/10	0.90	0.13	48,52,58,58	0
4	AKG	A	901	10/10	0.96	0.07	27,32,38,40	0
3	MN	B	601	1/1	0.98	0.04	45,45,45,45	0
3	MN	A	601	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.