



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:19 PM GMT

PDB ID : 3THT  
Title : Crystal structure and RNA binding properties of the RRM/AlkB domains in human ABH8, an enzyme catalyzing tRNA hypermodification, Northeast Structural Genomics Consortium Target HR5601B  
Authors : Pastore, C.; Topalidou, I.; Forouhar, F.; Yan, A.C.; Levy, M.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2011-08-19  
Resolution : 3.01 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

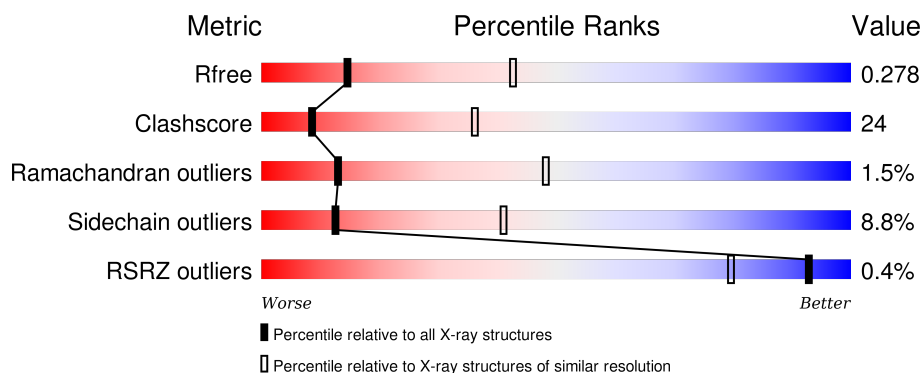
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	345	<div> <div> <div></div> <div>48%</div> <div>35%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	345	<div> <div> <div></div> <div>48%</div> <div>38%</div> <div>• •</div> <div>10%</div> </div> </div>
1	C	345	<div> <div> <div></div> <div>46%</div> <div>34%</div> <div>6%</div> <div>14%</div> </div> </div>
1	D	345	<div> <div> <div></div> <div>48%</div> <div>36%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9758 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 Alkylated DNA repair protein alkB homolog 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2393	1517	413	450	13			
1	B	312	Total	C	N	O	S	0	0	0
			2462	1565	426	458	13			
1	C	295	Total	C	N	O	S	0	0	0
			2344	1486	406	439	13			
1	D	302	Total	C	N	O	S	0	0	0
			2411	1532	416	450	13			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ASN	-	EXPRESSION TAG	UNP Q96BT7
A	357	LEU	-	EXPRESSION TAG	UNP Q96BT7
A	358	TYR	-	EXPRESSION TAG	UNP Q96BT7
A	359	PHE	-	EXPRESSION TAG	UNP Q96BT7
A	360	GLN	-	EXPRESSION TAG	UNP Q96BT7
A	361	GLY	-	EXPRESSION TAG	UNP Q96BT7
A	362	LEU	-	EXPRESSION TAG	UNP Q96BT7
A	363	GLU	-	EXPRESSION TAG	UNP Q96BT7
A	364	HIS	-	EXPRESSION TAG	UNP Q96BT7
A	365	HIS	-	EXPRESSION TAG	UNP Q96BT7
A	366	HIS	-	EXPRESSION TAG	UNP Q96BT7
A	367	HIS	-	EXPRESSION TAG	UNP Q96BT7
A	368	HIS	-	EXPRESSION TAG	UNP Q96BT7
A	369	HIS	-	EXPRESSION TAG	UNP Q96BT7
B	356	ASN	-	EXPRESSION TAG	UNP Q96BT7
B	357	LEU	-	EXPRESSION TAG	UNP Q96BT7
B	358	TYR	-	EXPRESSION TAG	UNP Q96BT7
B	359	PHE	-	EXPRESSION TAG	UNP Q96BT7
B	360	GLN	-	EXPRESSION TAG	UNP Q96BT7
B	361	GLY	-	EXPRESSION TAG	UNP Q96BT7
B	362	LEU	-	EXPRESSION TAG	UNP Q96BT7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	363	GLU	-	EXPRESSION TAG	UNP Q96BT7
B	364	HIS	-	EXPRESSION TAG	UNP Q96BT7
B	365	HIS	-	EXPRESSION TAG	UNP Q96BT7
B	366	HIS	-	EXPRESSION TAG	UNP Q96BT7
B	367	HIS	-	EXPRESSION TAG	UNP Q96BT7
B	368	HIS	-	EXPRESSION TAG	UNP Q96BT7
B	369	HIS	-	EXPRESSION TAG	UNP Q96BT7
C	356	ASN	-	EXPRESSION TAG	UNP Q96BT7
C	357	LEU	-	EXPRESSION TAG	UNP Q96BT7
C	358	TYR	-	EXPRESSION TAG	UNP Q96BT7
C	359	PHE	-	EXPRESSION TAG	UNP Q96BT7
C	360	GLN	-	EXPRESSION TAG	UNP Q96BT7
C	361	GLY	-	EXPRESSION TAG	UNP Q96BT7
C	362	LEU	-	EXPRESSION TAG	UNP Q96BT7
C	363	GLU	-	EXPRESSION TAG	UNP Q96BT7
C	364	HIS	-	EXPRESSION TAG	UNP Q96BT7
C	365	HIS	-	EXPRESSION TAG	UNP Q96BT7
C	366	HIS	-	EXPRESSION TAG	UNP Q96BT7
C	367	HIS	-	EXPRESSION TAG	UNP Q96BT7
C	368	HIS	-	EXPRESSION TAG	UNP Q96BT7
C	369	HIS	-	EXPRESSION TAG	UNP Q96BT7
D	356	ASN	-	EXPRESSION TAG	UNP Q96BT7
D	357	LEU	-	EXPRESSION TAG	UNP Q96BT7
D	358	TYR	-	EXPRESSION TAG	UNP Q96BT7
D	359	PHE	-	EXPRESSION TAG	UNP Q96BT7
D	360	GLN	-	EXPRESSION TAG	UNP Q96BT7
D	361	GLY	-	EXPRESSION TAG	UNP Q96BT7
D	362	LEU	-	EXPRESSION TAG	UNP Q96BT7
D	363	GLU	-	EXPRESSION TAG	UNP Q96BT7
D	364	HIS	-	EXPRESSION TAG	UNP Q96BT7
D	365	HIS	-	EXPRESSION TAG	UNP Q96BT7
D	366	HIS	-	EXPRESSION TAG	UNP Q96BT7
D	367	HIS	-	EXPRESSION TAG	UNP Q96BT7
D	368	HIS	-	EXPRESSION TAG	UNP Q96BT7
D	369	HIS	-	EXPRESSION TAG	UNP Q96BT7

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

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

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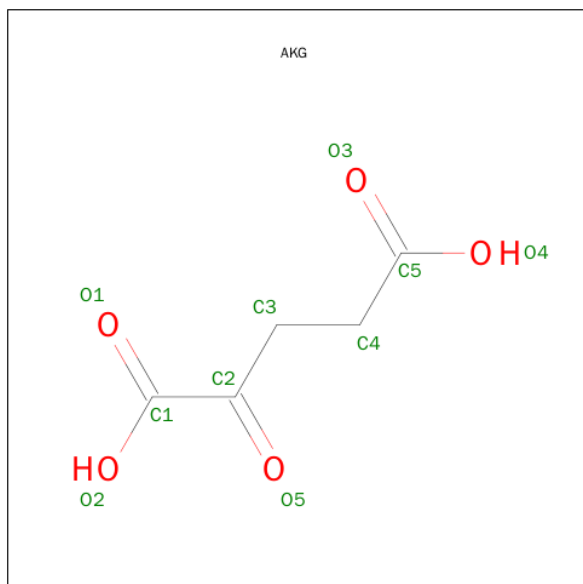
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



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

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

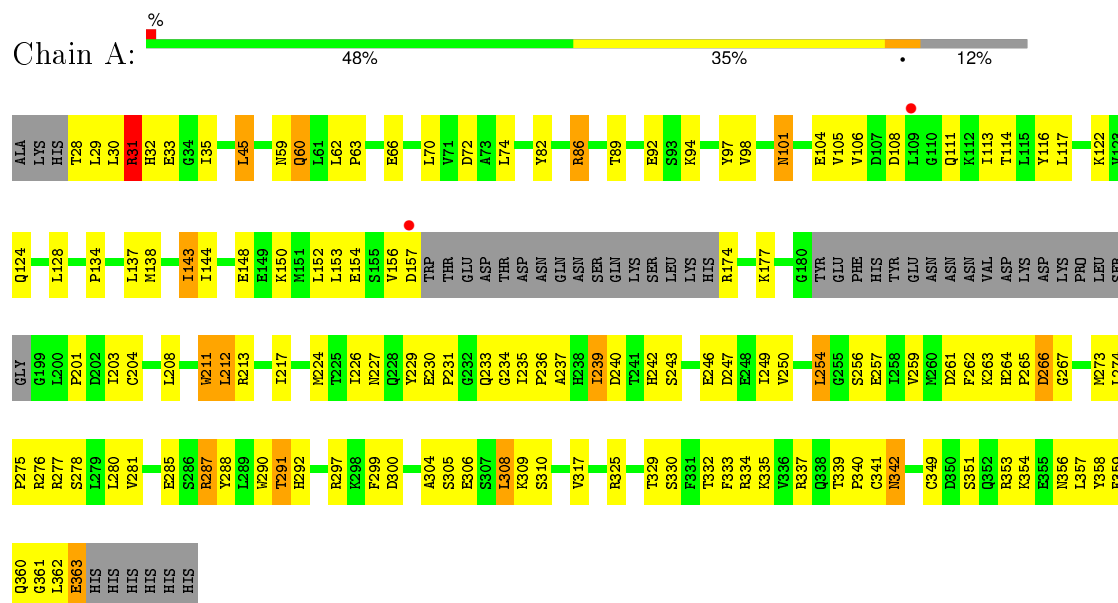
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	31	Total	O	0	0
			31	31		
5	C	18	Total	O	0	0
			18	18		
5	D	31	Total	O	0	0
			31	31		

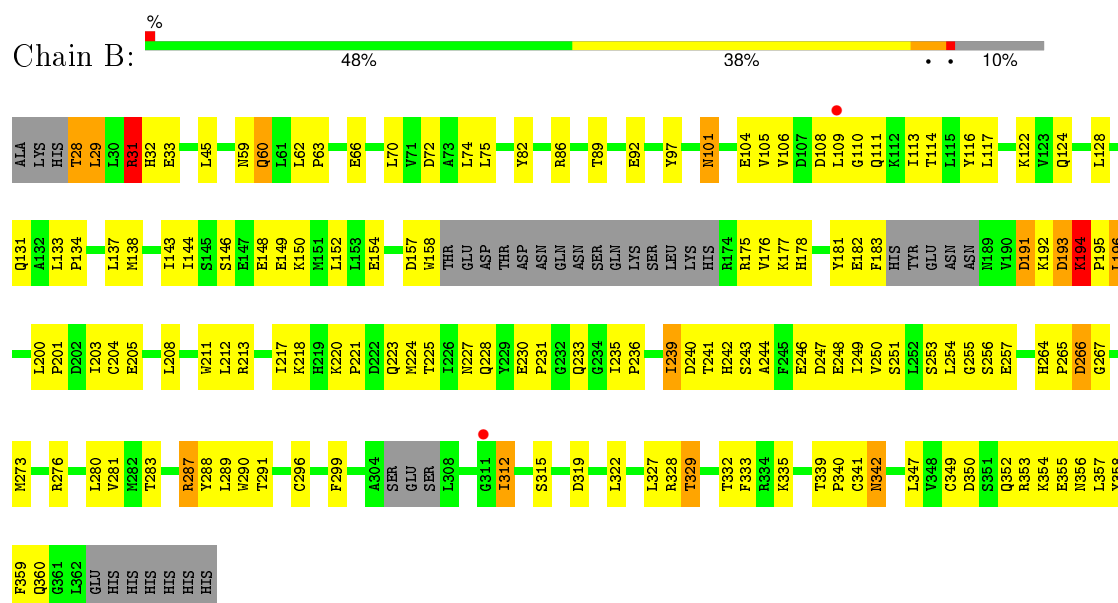
### 3 Residue-property plots

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.

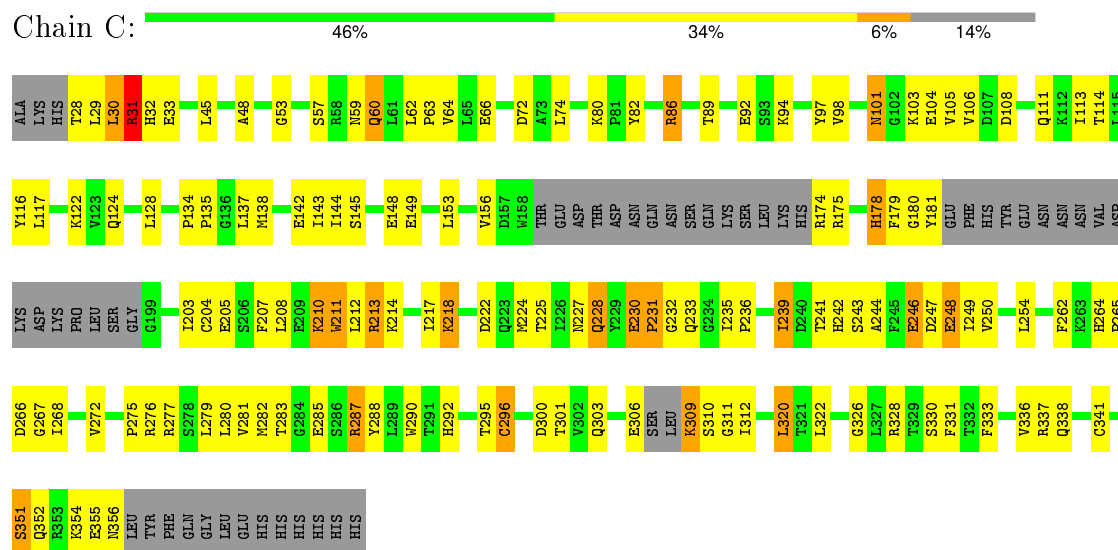
- Molecule 1: Alkylated DNA repair protein alkB homolog 8



- Molecule 1: Alkylated DNA repair protein alkB homolog 8



• Molecule 1: Alkylated DNA repair protein alkB homolog 8





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.17Å 73.28Å 149.81Å 90.00° 112.73° 90.00°	Depositor
Resolution (Å)	39.06 – 3.01 40.08 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.06-3.01) 96.3 (40.08-3.01)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.220 , 0.277 0.220 , 0.278	Depositor DCC
$R_{free}$ test set	2898 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 29876 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, 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	0.45	0/2439	0.82	6/3295 (0.2%)
1	B	0.46	0/2511	0.68	5/3393 (0.1%)
1	C	0.44	0/2390	0.84	6/3229 (0.2%)
1	D	0.46	0/2461	0.66	5/3328 (0.2%)
All	All	0.45	0/9801	0.76	22/13245 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ARG	NE-CZ-NH2	21.04	130.82	120.30
1	C	86	ARG	NE-CZ-NH1	-20.84	109.88	120.30
1	A	31	ARG	NE-CZ-NH1	-20.53	110.04	120.30
1	A	31	ARG	NE-CZ-NH2	20.23	130.41	120.30
1	C	86	ARG	CD-NE-CZ	10.97	138.96	123.60
1	A	31	ARG	CD-NE-CZ	10.31	138.04	123.60
1	C	31	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	D	31	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	C	31	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	31	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	31	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	86	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	31	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	86	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	D	86	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	D	86	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	86	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	86	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	363	GLU	CB-CA-C	5.31	121.02	110.40
1	B	31	ARG	CD-NE-CZ	5.12	130.77	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	ARG	CD-NE-CZ	5.06	130.69	123.60
1	C	31	ARG	CD-NE-CZ	5.01	130.61	123.60

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	2393	0	2412	113	0
1	B	2462	0	2465	132	0
1	C	2344	0	2357	121	0
1	D	2411	0	2422	99	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	4	1	0
4	C	10	0	4	1	0
4	D	10	0	4	0	0
5	A	20	0	0	3	0
5	B	31	0	0	8	0
5	C	18	0	0	5	0
5	D	31	0	0	3	0
All	All	9758	0	9672	459	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 24.

All (459) 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:149:GLU:HG3	1:B:254:LEU:HD22	1.34	1.08
1:B:28:THR:HG23	1:B:29:LEU:HD22	1.31	1.05
1:D:306:GLU:HB3	1:D:309:LYS:HB3	1.37	1.03
1:B:230:GLU:H	1:B:233:GLN:HE21	1.09	0.93
1:C:203:ILE:HD12	1:C:203:ILE:H	1.38	0.88
1:B:196:LEU:HD13	1:B:196:LEU:H	1.37	0.86
1:B:194:LYS:HE3	1:B:194:LYS:HA	1.58	0.86
1:B:230:GLU:HG2	1:B:327:LEU:HD13	1.59	0.84
1:C:210:LYS:NZ	1:C:213:ARG:HH11	1.77	0.83
1:B:356:ASN:ND2	1:B:358:TYR:HB3	1.95	0.81
1:A:156:VAL:HG13	1:A:157:ASP:H	1.45	0.81
1:C:210:LYS:HZ2	1:C:213:ARG:HH11	1.26	0.81
1:B:196:LEU:HD13	1:B:196:LEU:N	1.95	0.80
1:D:239:ILE:HG23	1:D:291:THR:HG22	1.64	0.79
1:C:268:ILE:HD12	1:C:268:ILE:H	1.48	0.79
1:B:265:PRO:HG3	1:B:289:LEU:HD11	1.64	0.78
1:C:320:LEU:HD23	1:C:320:LEU:H	1.48	0.77
1:D:264:HIS:HD2	1:D:266:ASP:H	1.33	0.76
1:C:178:HIS:HA	1:C:225:THR:HG22	1.66	0.75
1:D:309:LYS:HD3	1:D:310:SER:O	1.86	0.75
1:A:259:VAL:HG12	1:A:273:MET:HG2	1.67	0.75
1:B:192:LYS:HD2	1:B:195:PRO:HG3	1.67	0.75
1:A:308:LEU:HD12	1:A:308:LEU:H	1.50	0.74
1:C:134:PRO:HB3	1:C:290:TRP:CE2	2.22	0.73
1:B:239:ILE:HD11	1:B:288:TYR:O	1.88	0.73
1:A:124:GLN:HB3	1:B:128:LEU:HD12	1.69	0.73
1:C:104:GLU:HG2	1:C:114:THR:HG22	1.70	0.73
1:B:264:HIS:HD2	1:B:266:ASP:HB2	1.52	0.73
1:A:250:VAL:HG12	1:A:281:VAL:HG13	1.68	0.73
1:B:230:GLU:N	1:B:233:GLN:HE21	1.87	0.72
1:B:104:GLU:HG2	1:B:114:THR:HG22	1.70	0.72
1:D:104:GLU:HG2	1:D:114:THR:HG22	1.72	0.72
1:B:109:LEU:HD22	1:B:296:CYS:O	1.90	0.72
1:D:339:THR:HB	1:D:340:PRO:HD2	1.71	0.71
1:B:29:LEU:HD22	1:B:29:LEU:H	1.54	0.71
1:A:104:GLU:HG2	1:A:114:THR:HG22	1.71	0.71
1:D:258:ILE:HD11	1:D:294:ILE:HG21	1.73	0.71
1:B:143:ILE:HG23	1:B:144:ILE:HG23	1.72	0.70
1:C:28:THR:HG23	1:C:29:LEU:H	1.55	0.70
1:B:352:GLN:O	1:B:355:GLU:HG2	1.91	0.70
1:C:204:CYS:O	1:C:208:LEU:HD22	1.92	0.69
1:A:254:LEU:HD23	1:A:254:LEU:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:VAL:HG12	1:D:281:VAL:HA	1.75	0.69
1:C:204:CYS:HA	1:C:207:PHE:HD2	1.59	0.68
1:A:342:ASN:HD22	1:A:342:ASN:H	1.42	0.68
1:C:248:GLU:HA	1:C:283:THR:HG22	1.75	0.67
1:A:201:PRO:HB2	1:A:203:ILE:HG12	1.76	0.67
1:C:231:PRO:HG3	1:C:326:GLY:C	2.14	0.67
1:C:217:ILE:HD12	1:C:248:GLU:CD	2.14	0.67
1:B:194:LYS:O	1:B:196:LEU:HD13	1.93	0.67
1:B:342:ASN:H	1:B:342:ASN:HD22	1.42	0.67
1:C:218:LYS:HB3	5:C:379:HOH:O	1.95	0.67
1:B:192:LYS:HG2	1:B:195:PRO:CD	2.25	0.67
1:C:205:GLU:HA	1:C:208:LEU:HD23	1.77	0.67
1:C:122:LYS:HD3	1:C:124:GLN:HE21	1.60	0.67
1:D:303:GLN:HA	1:D:320:LEU:HD23	1.77	0.67
1:D:28:THR:HG23	1:D:29:LEU:H	1.58	0.67
1:C:235:ILE:HG13	1:C:236:PRO:HD2	1.77	0.66
1:B:230:GLU:H	1:B:233:GLN:NE2	1.87	0.66
1:D:150:LYS:HE3	1:D:154:GLU:OE2	1.95	0.66
1:C:312:ILE:N	1:C:312:ILE:HD12	2.10	0.66
1:B:256:SER:O	1:B:328:ARG:HG3	1.96	0.65
1:D:235:ILE:HG13	1:D:236:PRO:HD2	1.79	0.65
1:A:342:ASN:N	1:A:342:ASN:HD22	1.94	0.65
1:D:356:ASN:OD1	1:D:358:TYR:HB3	1.97	0.65
1:B:134:PRO:HB3	1:B:290:TRP:CE2	2.32	0.65
1:D:122:LYS:HD3	1:D:124:GLN:HE21	1.62	0.65
1:C:239:ILE:HD11	1:C:287:ARG:O	1.97	0.64
1:A:177:LYS:HB3	1:A:226:ILE:HB	1.79	0.64
1:C:117:LEU:N	1:C:117:LEU:HD12	2.13	0.64
1:A:246:GLU:HG3	1:A:335:LYS:CE	2.28	0.64
1:B:28:THR:HG23	1:B:29:LEU:CD2	2.18	0.64
1:D:228:GLN:HG2	1:D:327:LEU:HD11	1.79	0.64
1:A:213:ARG:HG2	1:A:213:ARG:HH21	1.61	0.64
1:C:143:ILE:HG23	1:C:144:ILE:HG23	1.80	0.64
1:B:201:PRO:HG2	1:B:204:CYS:SG	2.37	0.63
1:A:128:LEU:HD12	1:B:124:GLN:HB3	1.80	0.63
1:B:192:LYS:O	1:B:195:PRO:HD2	1.99	0.63
1:C:233:GLN:HA	1:C:296:CYS:SG	2.37	0.63
1:A:249:ILE:HG23	1:A:334:ARG:HG2	1.81	0.63
1:A:262:PHE:O	1:A:263:LYS:HD3	1.97	0.63
1:A:306:GLU:HG2	1:A:309:LYS:HD2	1.79	0.63
1:C:264:HIS:HD2	1:C:266:ASP:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ASP:O	1:D:287:ARG:HD2	1.99	0.62
1:C:145:SER:OG	1:C:148:GLU:HG3	2.00	0.62
1:B:134:PRO:HB3	1:B:290:TRP:CD2	2.35	0.61
1:C:246:GLU:O	1:C:287:ARG:NH1	2.33	0.61
1:A:275:PRO:CD	1:A:310:SER:HB3	2.30	0.61
1:B:122:LYS:HD3	1:B:124:GLN:HE21	1.64	0.61
1:C:312:ILE:H	1:C:312:ILE:HD12	1.65	0.61
1:C:174:ARG:HE	1:C:227:ASN:ND2	1.98	0.61
1:B:117:LEU:HD12	1:B:117:LEU:N	2.15	0.61
1:D:33:GLU:HG2	1:D:82:TYR:CE2	2.36	0.61
1:D:28:THR:HG23	1:D:29:LEU:HD12	1.81	0.61
1:D:29:LEU:HD13	1:D:30:LEU:N	2.15	0.61
1:A:339:THR:HB	1:A:340:PRO:HD2	1.83	0.61
1:C:33:GLU:HG2	1:C:82:TYR:CE2	2.37	0.60
1:C:175:ARG:HB2	1:C:228:GLN:HB3	1.83	0.60
1:A:353:ARG:HB2	1:A:359:PHE:HD1	1.65	0.60
1:A:122:LYS:HD3	1:A:124:GLN:HE21	1.66	0.60
1:A:117:LEU:HD12	1:A:117:LEU:N	2.17	0.60
1:A:274:LEU:HD21	1:A:280:LEU:HD22	1.83	0.59
1:B:33:GLU:HG2	1:B:82:TYR:CE2	2.37	0.59
1:C:134:PRO:HB3	1:C:290:TRP:CZ2	2.37	0.59
1:C:137:LEU:HD11	1:C:280:LEU:HD11	1.84	0.59
1:B:230:GLU:HG2	1:B:327:LEU:CD1	2.31	0.59
1:C:241:THR:HB	1:C:244:ALA:HB3	1.84	0.59
1:A:246:GLU:HG3	1:A:335:LYS:HE3	1.82	0.59
1:B:264:HIS:CG	1:B:265:PRO:HD2	2.37	0.59
1:D:202:ASP:C	1:D:204:CYS:H	2.06	0.59
1:C:174:ARG:HE	1:C:227:ASN:HD22	1.50	0.59
1:A:264:HIS:HD2	1:A:266:ASP:H	1.48	0.59
1:B:194:LYS:H	1:B:195:PRO:HD2	1.67	0.58
1:C:246:GLU:OE2	1:C:337:ARG:HA	2.03	0.58
1:A:212:LEU:HD22	1:A:217:ILE:HG23	1.86	0.58
1:A:353:ARG:HB2	1:A:359:PHE:CD1	2.38	0.58
1:B:194:LYS:O	1:B:196:LEU:CD1	2.51	0.58
1:D:29:LEU:CD1	1:D:29:LEU:H	2.16	0.58
1:B:31:ARG:NH2	1:B:32:HIS:HB2	2.19	0.58
1:D:356:ASN:O	1:D:357:LEU:HB3	2.02	0.58
1:D:226:ILE:HA	1:D:330:SER:O	2.03	0.58
1:C:28:THR:HG23	1:C:29:LEU:N	2.19	0.57
1:A:33:GLU:HG2	1:A:82:TYR:CE2	2.39	0.57
1:D:117:LEU:HD12	1:D:117:LEU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:HIS:CD2	1:D:266:ASP:H	2.20	0.57
1:C:213:ARG:HG3	1:C:213:ARG:HH21	1.68	0.57
1:A:134:PRO:HB3	1:A:290:TRP:CE2	2.39	0.57
1:C:268:ILE:HD12	1:C:268:ILE:N	2.17	0.57
1:D:276:ARG:O	1:D:277:ARG:HB2	2.03	0.57
1:D:263:LYS:HB2	1:D:263:LYS:NZ	2.20	0.57
1:C:211:TRP:HB3	1:C:217:ILE:HG22	1.86	0.57
1:C:301:THR:HG22	1:C:322:LEU:HD23	1.87	0.56
1:D:315:SER:O	1:D:316:ASP:HB2	2.05	0.56
1:B:257:GLU:H	1:B:257:GLU:CD	2.08	0.56
1:A:137:LEU:HD23	1:A:138:MET:N	2.21	0.56
1:A:297:ARG:HD2	1:A:300:ASP:OD2	2.06	0.56
1:D:200:LEU:HD23	1:D:201:PRO:HD2	1.87	0.56
1:A:148:GLU:O	1:A:152:LEU:HD13	2.05	0.56
1:B:220:LYS:O	1:B:335:LYS:HE3	2.06	0.56
1:B:212:LEU:HD23	1:B:217:ILE:HG23	1.87	0.55
1:B:241:THR:HG22	1:B:244:ALA:H	1.70	0.55
1:B:183:PHE:CB	1:B:191:ASP:HA	2.36	0.55
1:C:337:ARG:HH11	1:C:341:CYS:HA	1.72	0.55
1:B:264:HIS:CD2	1:B:266:ASP:H	2.24	0.55
1:D:31:ARG:NH1	5:D:374:HOH:O	2.39	0.55
1:B:253:SER:HB3	5:B:6:HOH:O	2.06	0.55
1:B:242:HIS:HB3	1:B:341:CYS:SG	2.47	0.55
1:A:267:GLY:HA2	5:A:384:HOH:O	2.06	0.55
1:B:255:GLY:O	1:B:276:ARG:NE	2.40	0.55
1:C:264:HIS:CD2	1:C:266:ASP:H	2.23	0.55
1:A:263:LYS:O	1:A:291:THR:HG22	2.08	0.54
1:A:239:ILE:HD13	1:A:240:ASP:O	2.07	0.54
1:A:273:MET:O	1:A:275:PRO:HD3	2.07	0.54
1:A:358:TYR:CZ	1:A:362:LEU:HD11	2.42	0.54
1:C:124:GLN:HB3	1:D:128:LEU:HD12	1.90	0.54
1:B:144:ILE:CD1	1:B:254:LEU:HD21	2.38	0.54
1:C:203:ILE:H	1:C:203:ILE:CD1	2.14	0.54
1:B:264:HIS:CD2	1:B:266:ASP:HB2	2.38	0.54
1:D:130:PRO:HA	5:D:9:HOH:O	2.07	0.54
1:D:297:ARG:HD2	1:D:299:PHE:O	2.08	0.54
1:D:177:LYS:HD2	1:D:179:PHE:CE2	2.42	0.54
1:A:349:CYS:O	1:A:353:ARG:HG2	2.09	0.53
1:C:31:ARG:NH2	1:C:32:HIS:HB2	2.23	0.53
1:B:218:LYS:H	1:B:248:GLU:CD	2.11	0.53
1:D:337:ARG:HG2	1:D:339:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:HIS:HD2	1:C:266:ASP:HB2	1.74	0.53
1:C:175:ARG:HG3	1:C:228:GLN:NE2	2.24	0.53
1:D:213:ARG:HG2	1:D:213:ARG:HH21	1.73	0.53
1:C:320:LEU:HD23	1:C:320:LEU:N	2.22	0.53
1:B:111:GLN:HE22	1:B:296:CYS:HB2	1.74	0.53
1:B:196:LEU:HD22	1:B:196:LEU:H	1.74	0.53
1:B:62:LEU:HB3	1:B:63:PRO:HD3	1.91	0.53
1:B:217:ILE:HD13	1:B:250:VAL:HG11	1.91	0.53
1:A:237:ALA:HB1	1:A:291:THR:OG1	2.08	0.53
1:D:264:HIS:CD2	1:D:265:PRO:HD2	2.45	0.52
1:B:217:ILE:HD13	1:B:250:VAL:CG1	2.39	0.52
1:C:143:ILE:HD13	1:C:279:LEU:HB2	1.91	0.52
1:A:62:LEU:HB3	1:A:63:PRO:HD3	1.91	0.52
1:A:242:HIS:HB3	1:A:341:CYS:SG	2.50	0.52
1:D:31:ARG:NH2	1:D:32:HIS:HB2	2.24	0.52
1:C:241:THR:HB	1:C:244:ALA:CB	2.40	0.52
1:C:32:HIS:CG	1:C:267:GLY:HA3	2.45	0.52
1:C:276:ARG:O	1:C:277:ARG:HB2	2.09	0.52
1:D:62:LEU:HB3	1:D:63:PRO:HD3	1.90	0.52
1:C:178:HIS:CA	1:C:225:THR:HG22	2.39	0.52
1:B:224:MET:HG3	1:B:333:PHE:CE2	2.45	0.52
1:C:247:ASP:O	1:C:249:ILE:HG13	2.09	0.52
1:A:261:ASP:HB3	1:A:263:LYS:HE3	1.92	0.52
1:A:254:LEU:HD23	1:A:254:LEU:H	1.75	0.52
1:B:342:ASN:HD22	1:B:342:ASN:N	2.03	0.52
1:B:221:PRO:HG3	1:B:333:PHE:HB3	1.92	0.52
1:B:192:LYS:HG2	1:B:195:PRO:HD2	1.92	0.52
1:D:143:ILE:HG12	1:D:211:TRP:CH2	2.45	0.52
1:C:135:PRO:HG2	1:C:285:GLU:HB3	1.92	0.52
1:B:196:LEU:N	1:B:196:LEU:CD1	2.67	0.51
1:A:259:VAL:HG23	1:A:259:VAL:O	2.10	0.51
1:B:133:LEU:HB3	1:B:137:LEU:HD23	1.91	0.51
1:C:137:LEU:HD12	1:C:282:MET:HG2	1.93	0.51
1:C:62:LEU:HB3	1:C:63:PRO:HD3	1.92	0.51
1:B:246:GLU:O	1:B:287:ARG:NH1	2.43	0.51
1:D:28:THR:HG23	1:D:29:LEU:N	2.25	0.51
1:A:31:ARG:NH2	1:A:32:HIS:HB2	2.25	0.51
1:C:285:GLU:HB2	5:C:378:HOH:O	2.10	0.51
1:C:149:GLU:HG3	1:C:254:LEU:HD22	1.93	0.51
1:A:213:ARG:NH2	1:A:213:ARG:HG2	2.24	0.51
1:D:203:ILE:HG22	1:D:203:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HD3	1:A:310:SER:HB3	1.92	0.51
1:D:143:ILE:HG23	1:D:144:ILE:HG23	1.92	0.51
1:A:243:SER:HB3	1:A:351:SER:OG	2.11	0.51
1:C:210:LYS:NZ	1:C:213:ARG:NH1	2.54	0.51
1:B:256:SER:HA	1:B:276:ARG:HD2	1.91	0.51
1:B:356:ASN:C	1:B:358:TYR:H	2.14	0.50
1:D:101:ASN:ND2	1:D:116:TYR:HA	2.26	0.50
1:B:213:ARG:HD3	5:B:372:HOH:O	2.11	0.50
1:B:192:LYS:HG2	1:B:195:PRO:HD3	1.94	0.50
1:C:175:ARG:HB2	1:C:228:GLN:CB	2.42	0.50
1:A:86:ARG:HD3	1:B:131:GLN:OE1	2.11	0.50
1:B:138:MET:HG2	1:B:281:VAL:HB	1.94	0.50
1:B:32:HIS:CD2	1:B:267:GLY:HA3	2.47	0.50
1:D:223:GLN:NE2	1:D:224:MET:O	2.44	0.50
1:C:272:VAL:HA	1:C:311:GLY:O	2.12	0.50
1:A:156:VAL:HG13	1:A:157:ASP:N	2.21	0.50
1:B:111:GLN:NE2	1:B:296:CYS:HB2	2.26	0.50
1:C:337:ARG:NH1	1:C:341:CYS:HA	2.27	0.50
1:C:137:LEU:CD1	1:C:282:MET:HG2	2.42	0.50
1:C:301:THR:HG22	1:C:322:LEU:CD2	2.42	0.50
1:B:144:ILE:HD11	1:B:254:LEU:HD21	1.93	0.50
1:B:29:LEU:HD13	1:B:29:LEU:N	2.27	0.50
1:C:268:ILE:H	1:C:268:ILE:CD1	2.20	0.49
1:B:144:ILE:HD11	1:B:254:LEU:CD2	2.43	0.49
1:A:174:ARG:HH21	1:A:227:ASN:ND2	2.09	0.49
1:D:64:VAL:HG13	1:D:103:LYS:NZ	2.27	0.49
1:B:196:LEU:N	1:B:196:LEU:HD22	2.28	0.49
1:B:256:SER:OG	1:B:328:ARG:HB2	2.13	0.49
1:B:176:VAL:HG12	1:B:177:LYS:N	2.26	0.49
1:A:211:TRP:HB3	1:A:217:ILE:HG22	1.95	0.49
1:B:354:LYS:HA	1:B:360:GLN:NE2	2.26	0.49
1:C:53:GLY:HA2	5:C:24:HOH:O	2.11	0.49
1:C:174:ARG:NE	1:C:227:ASN:HD22	2.11	0.49
1:D:257:GLU:CD	1:D:257:GLU:H	2.16	0.49
1:A:297:ARG:HD3	1:A:299:PHE:O	2.12	0.49
1:C:250:VAL:HA	1:C:280:LEU:O	2.12	0.49
1:D:250:VAL:HA	1:D:280:LEU:O	2.13	0.48
1:A:262:PHE:CE1	1:A:292:HIS:HB3	2.48	0.48
1:A:342:ASN:N	1:A:342:ASN:ND2	2.61	0.48
1:C:264:HIS:CD2	1:C:266:ASP:HB2	2.48	0.48
1:C:247:ASP:O	1:C:248:GLU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ASP:O	1:C:249:ILE:N	2.46	0.48
1:C:210:LYS:HZ2	1:C:213:ARG:NH1	2.04	0.48
1:B:224:MET:HA	1:B:332:THR:O	2.13	0.48
1:A:204:CYS:O	1:A:208:LEU:HD13	2.13	0.48
1:B:137:LEU:HD11	1:B:280:LEU:HD11	1.96	0.48
1:A:208:LEU:HD11	1:A:333:PHE:CE2	2.49	0.48
1:D:274:LEU:HD21	1:D:280:LEU:HD13	1.96	0.48
1:D:29:LEU:C	1:D:29:LEU:HD22	2.34	0.48
1:A:264:HIS:CD2	1:A:266:ASP:H	2.28	0.48
1:B:181:TYR:C	1:B:183:PHE:H	2.17	0.48
1:C:264:HIS:CG	1:C:265:PRO:HD2	2.49	0.48
1:A:230:GLU:H	1:A:233:GLN:CG	2.25	0.48
1:D:177:LYS:HD2	1:D:179:PHE:CZ	2.49	0.48
1:B:150:LYS:O	1:B:154:GLU:HG3	2.14	0.48
1:A:342:ASN:HB3	5:A:379:HOH:O	2.13	0.48
1:A:230:GLU:O	1:A:233:GLN:HG2	2.14	0.48
1:D:278:SER:HB3	5:D:4:HOH:O	2.14	0.47
1:B:175:ARG:HH11	1:B:175:ARG:HG2	1.79	0.47
1:B:105:VAL:HG23	1:B:113:ILE:HG13	1.96	0.47
1:C:222:ASP:OD2	1:C:336:VAL:HG23	2.14	0.47
1:C:203:ILE:N	1:C:203:ILE:HD12	2.18	0.47
1:D:29:LEU:HD12	1:D:29:LEU:H	1.78	0.47
1:A:254:LEU:N	1:A:254:LEU:CD2	2.77	0.47
1:B:178:HIS:ND1	1:B:225:THR:HG23	2.30	0.47
1:D:106:VAL:HA	1:D:111:GLN:O	2.14	0.47
1:B:101:ASN:ND2	1:B:116:TYR:HA	2.30	0.47
1:B:28:THR:HG23	1:B:29:LEU:H	1.79	0.47
1:C:101:ASN:ND2	1:C:116:TYR:HA	2.30	0.47
1:B:289:LEU:HD12	1:B:289:LEU:O	2.14	0.47
1:A:105:VAL:HG23	1:A:113:ILE:HG13	1.97	0.47
1:B:148:GLU:O	1:B:152:LEU:HG	2.15	0.47
1:C:128:LEU:HD12	1:D:124:GLN:HB3	1.97	0.47
1:D:224:MET:HG3	1:D:333:PHE:CE2	2.50	0.47
1:C:213:ARG:HG3	1:C:213:ARG:NH2	2.30	0.47
1:C:208:LEU:H	1:C:208:LEU:HD22	1.79	0.47
1:C:106:VAL:HA	1:C:111:GLN:O	2.14	0.47
1:D:232:GLY:HA2	1:D:297:ARG:O	2.16	0.46
1:D:253:SER:O	1:D:254:LEU:HD23	2.16	0.46
1:D:264:HIS:CD2	1:D:265:PRO:CD	2.99	0.46
1:A:246:GLU:OE2	1:A:337:ARG:HG3	2.14	0.46
1:B:60:GLN:O	1:B:63:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ILE:HD13	1:B:312:ILE:H	1.80	0.46
1:A:101:ASN:ND2	1:A:116:TYR:HA	2.30	0.46
1:A:60:GLN:O	1:A:63:PRO:HD2	2.15	0.46
1:D:270:VAL:HG13	1:D:312:ILE:HG23	1.97	0.46
1:A:227:ASN:HB2	1:A:330:SER:OG	2.16	0.46
1:A:143:ILE:HG22	1:A:277:ARG:O	2.15	0.46
1:A:354:LYS:HE3	1:A:354:LYS:HA	1.98	0.46
1:D:152:LEU:HD21	1:D:207:PHE:CE2	2.51	0.46
1:B:349:CYS:SG	1:B:352:GLN:HG3	2.56	0.46
1:D:235:ILE:HG22	1:D:294:ILE:HD12	1.97	0.46
1:C:64:VAL:HG13	1:C:103:LYS:NZ	2.31	0.46
1:C:105:VAL:HG23	1:C:113:ILE:HG13	1.96	0.46
1:D:285:GLU:HG2	1:D:290:TRP:CD1	2.50	0.46
1:D:205:GLU:OE2	1:D:209:GLU:OE1	2.34	0.46
1:B:106:VAL:HA	1:B:111:GLN:O	2.16	0.45
1:D:132:ALA:C	1:D:312:ILE:HD11	2.35	0.45
1:C:262:PHE:CE1	1:C:292:HIS:HB3	2.51	0.45
1:A:106:VAL:HA	1:A:111:GLN:O	2.15	0.45
1:B:235:ILE:HG13	1:B:236:PRO:HD2	1.97	0.45
1:B:240:ASP:O	1:B:287:ARG:NH2	2.49	0.45
1:B:291:THR:HG23	5:B:377:HOH:O	2.16	0.45
1:C:138:MET:HB3	1:C:281:VAL:HB	1.98	0.45
1:A:259:VAL:CG1	1:A:273:MET:HG2	2.42	0.45
1:A:246:GLU:HG3	1:A:335:LYS:HE2	1.95	0.45
1:C:338:GLN:OE1	1:C:338:GLN:HA	2.16	0.45
1:A:134:PRO:HB3	1:A:290:TRP:CD2	2.52	0.45
1:C:309:LYS:HE3	1:C:309:LYS:HA	1.96	0.45
1:A:235:ILE:O	1:A:235:ILE:HG23	2.16	0.45
1:B:339:THR:HB	1:B:340:PRO:HD2	1.98	0.45
1:A:153:LEU:HG	1:A:254:LEU:HD12	1.99	0.45
1:B:196:LEU:CD1	1:B:196:LEU:H	2.07	0.45
1:A:264:HIS:CG	1:A:265:PRO:HD2	2.52	0.45
1:D:347:LEU:O	1:D:353:ARG:HD2	2.17	0.45
1:B:241:THR:HG22	1:B:243:SER:H	1.82	0.45
1:A:357:LEU:HD22	1:A:357:LEU:H	1.81	0.45
1:A:357:LEU:O	1:A:360:GLN:HB3	2.16	0.45
1:A:254:LEU:HD23	1:A:329:THR:O	2.17	0.45
1:A:285:GLU:HG2	1:A:290:TRP:CD1	2.52	0.45
1:A:70:LEU:HA	5:A:381:HOH:O	2.16	0.45
1:C:94:LYS:O	1:C:98:VAL:HG22	2.17	0.45
1:A:247:ASP:HB2	1:A:288:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASN:O	1:B:358:TYR:N	2.51	0.44
1:C:337:ARG:HH21	1:C:337:ARG:HG3	1.82	0.44
1:C:231:PRO:HG3	1:C:326:GLY:CA	2.48	0.44
1:B:158:TRP:CZ2	1:B:228:GLN:HB2	2.52	0.44
1:A:235:ILE:HG13	1:A:236:PRO:HD2	1.99	0.44
1:A:224:MET:HG2	1:A:332:THR:O	2.18	0.44
1:D:258:ILE:HG12	1:D:259:VAL:H	1.82	0.44
1:D:60:GLN:O	1:D:63:PRO:HD2	2.18	0.44
1:D:62:LEU:O	1:D:66:GLU:HG3	2.18	0.44
1:C:210:LYS:O	1:C:214:LYS:HD3	2.17	0.44
1:B:347:LEU:O	1:B:353:ARG:HD2	2.18	0.44
1:A:263:LYS:HB2	1:A:291:THR:HG23	1.98	0.44
1:B:235:ILE:O	1:B:235:ILE:HG23	2.16	0.44
1:C:354:LYS:C	1:C:356:ASN:H	2.21	0.44
1:B:89:THR:OG1	1:B:92:GLU:HG3	2.17	0.44
1:A:257:GLU:HB3	1:A:275:PRO:HA	1.99	0.44
1:A:174:ARG:NH2	1:A:227:ASN:ND2	2.66	0.44
1:C:97:TYR:O	1:C:101:ASN:HB2	2.18	0.44
1:B:247:ASP:OD2	1:B:283:THR:HA	2.17	0.44
1:C:337:ARG:NH2	5:C:17:HOH:O	2.46	0.44
1:C:330:SER:C	1:C:331:PHE:HD1	2.21	0.44
1:A:229:TYR:CD2	1:A:234:GLY:HA2	2.53	0.44
1:C:242:HIS:NE2	1:C:288:TYR:HD1	2.16	0.43
1:D:248:GLU:HA	1:D:283:THR:HG22	2.00	0.43
1:A:59:ASN:N	1:A:59:ASN:HD22	2.15	0.43
1:B:70:LEU:HA	5:B:373:HOH:O	2.18	0.43
1:C:250:VAL:HB	1:C:279:LEU:HD11	2.00	0.43
1:D:202:ASP:C	1:D:204:CYS:N	2.72	0.43
1:A:356:ASN:OD1	1:A:358:TYR:HB3	2.18	0.43
1:C:60:GLN:O	1:C:63:PRO:HD2	2.18	0.43
1:C:178:HIS:N	1:C:178:HIS:ND1	2.67	0.43
1:A:208:LEU:O	1:A:211:TRP:HB2	2.19	0.43
1:D:97:TYR:O	1:D:101:ASN:HB2	2.19	0.43
1:D:94:LYS:O	1:D:98:VAL:HG22	2.18	0.43
1:B:110:GLY:N	5:B:7:HOH:O	2.50	0.43
1:D:282:MET:HG2	1:D:287:ARG:HB3	2.00	0.43
1:B:59:ASN:N	1:B:59:ASN:HD22	2.16	0.43
1:C:275:PRO:CD	1:C:310:SER:HB3	2.48	0.43
1:C:303:GLN:HA	1:C:320:LEU:HA	2.00	0.43
1:B:200:LEU:HG	1:B:201:PRO:HD2	2.00	0.43
1:C:62:LEU:O	1:C:66:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:MET:HA	1:D:332:THR:O	2.19	0.43
1:D:31:ARG:NH2	1:D:266:ASP:O	2.51	0.43
1:C:230:GLU:O	1:C:232:GLY:N	2.51	0.43
1:D:264:HIS:CG	1:D:265:PRO:HD2	2.54	0.43
1:C:29:LEU:HD12	1:C:30:LEU:N	2.34	0.43
1:D:246:GLU:O	1:D:287:ARG:NH1	2.50	0.43
1:D:173:HIS:CD2	1:D:233:GLN:HE21	2.37	0.43
1:D:29:LEU:N	1:D:29:LEU:CD1	2.80	0.43
1:B:157:ASP:O	1:B:158:TRP:HB2	2.18	0.43
1:B:248:GLU:HB3	5:B:13:HOH:O	2.18	0.43
1:D:262:PHE:HA	1:D:291:THR:O	2.19	0.42
1:D:143:ILE:HG22	1:D:277:ARG:O	2.18	0.42
1:C:243:SER:HB3	1:C:351:SER:HB3	1.99	0.42
1:B:328:ARG:NH2	4:B:403:AKG:O4	2.50	0.42
1:D:247:ASP:O	1:D:287:ARG:CD	2.66	0.42
1:B:221:PRO:CG	1:B:333:PHE:HB3	2.50	0.42
1:A:229:TYR:HD2	1:A:234:GLY:HA2	1.84	0.42
1:B:350:ASP:HB3	5:B:374:HOH:O	2.17	0.42
1:B:194:LYS:HB2	1:B:195:PRO:HD3	2.00	0.42
1:C:204:CYS:O	1:C:207:PHE:HB2	2.19	0.42
1:A:261:ASP:O	1:A:292:HIS:HA	2.18	0.42
1:B:175:ARG:HG2	1:B:175:ARG:NH1	2.33	0.42
1:B:97:TYR:O	1:B:101:ASN:HB2	2.20	0.42
1:D:242:HIS:ND1	1:D:349:CYS:HA	2.34	0.42
1:A:45:LEU:HD12	1:A:45:LEU:O	2.20	0.42
1:B:212:LEU:CD2	1:B:217:ILE:HG23	2.49	0.42
1:C:89:THR:OG1	1:C:92:GLU:HG3	2.20	0.42
1:A:361:GLY:C	1:A:363:GLU:H	2.23	0.42
1:A:250:VAL:HG22	1:A:333:PHE:HB2	2.01	0.42
1:D:145:SER:OG	1:D:147:GLU:HG2	2.19	0.42
1:D:105:VAL:HG23	1:D:113:ILE:HG13	2.00	0.42
1:B:250:VAL:HA	1:B:280:LEU:O	2.20	0.42
1:A:32:HIS:CG	1:A:267:GLY:HA3	2.54	0.42
1:A:239:ILE:HD13	1:A:239:ILE:C	2.40	0.42
1:B:62:LEU:O	1:B:66:GLU:HG3	2.20	0.42
1:A:62:LEU:O	1:A:66:GLU:HG3	2.19	0.42
1:D:334:ARG:HH11	1:D:334:ARG:HG3	1.85	0.42
1:A:247:ASP:HA	1:A:287:ARG:HD3	2.01	0.42
1:D:230:GLU:O	1:D:231:PRO:C	2.57	0.42
1:D:235:ILE:HG23	1:D:235:ILE:O	2.20	0.42
1:D:143:ILE:HG12	1:D:211:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:NH2	1:B:359:PHE:HB3	2.34	0.42
1:C:153:LEU:O	1:C:156:VAL:HG22	2.20	0.42
1:D:201:PRO:HG2	1:D:204:CYS:SG	2.60	0.41
1:A:97:TYR:O	1:A:101:ASN:HB2	2.20	0.41
1:A:143:ILE:HG23	1:A:144:ILE:N	2.35	0.41
1:A:94:LYS:O	1:A:98:VAL:HG22	2.19	0.41
1:C:204:CYS:O	1:C:207:PHE:N	2.52	0.41
1:D:101:ASN:ND2	1:D:117:LEU:H	2.19	0.41
1:A:275:PRO:HG2	1:A:278:SER:HB3	2.02	0.41
1:A:227:ASN:O	1:A:329:THR:HA	2.19	0.41
1:C:228:GLN:HE21	1:C:228:GLN:HB3	1.59	0.41
1:A:256:SER:HA	1:A:276:ARG:HD2	2.02	0.41
1:B:227:ASN:O	1:B:329:THR:HA	2.20	0.41
1:A:89:THR:OG1	1:A:92:GLU:HG3	2.19	0.41
1:B:196:LEU:HD22	1:B:196:LEU:O	2.20	0.41
1:A:30:LEU:HB3	1:A:35:ILE:HB	2.03	0.41
1:B:264:HIS:HD2	1:B:266:ASP:H	1.68	0.41
1:C:48:ALA:HB3	1:C:116:TYR:HB2	2.02	0.41
1:A:317:VAL:HG13	1:B:75:LEU:HG	2.01	0.41
1:B:312:ILE:HD13	1:B:312:ILE:N	2.36	0.41
1:C:328:ARG:HH12	4:C:403:AKG:C5	2.34	0.41
1:C:179:PHE:HB2	1:C:224:MET:O	2.21	0.41
1:B:356:ASN:C	1:B:358:TYR:N	2.73	0.41
1:D:339:THR:HB	1:D:340:PRO:CD	2.47	0.41
1:D:128:LEU:HD21	1:D:268:ILE:HG12	2.02	0.41
1:C:337:ARG:HD2	5:C:370:HOH:O	2.20	0.41
1:B:204:CYS:O	1:B:205:GLU:C	2.57	0.41
1:C:59:ASN:HD22	1:C:59:ASN:N	2.18	0.41
1:A:300:ASP:CG	1:A:325:ARG:HE	2.23	0.41
1:D:213:ARG:HG2	1:D:213:ARG:NH2	2.36	0.41
1:D:89:THR:OG1	1:D:92:GLU:HG3	2.20	0.41
1:D:237:ALA:HA	1:D:292:HIS:O	2.21	0.41
1:A:150:LYS:O	1:A:154:GLU:HG2	2.21	0.41
1:A:275:PRO:HG3	1:A:310:SER:HB3	2.02	0.40
1:B:134:PRO:HG2	1:B:137:LEU:HD22	2.02	0.40
1:C:33:GLU:OE2	1:C:80:LYS:NZ	2.46	0.40
1:C:180:GLY:C	1:C:181:TYR:CD1	2.94	0.40
1:B:249:ILE:HG12	5:B:378:HOH:O	2.21	0.40
1:C:57:SER:OG	1:C:60:GLN:HB2	2.21	0.40
1:C:224:MET:HG3	1:C:333:PHE:CE2	2.57	0.40
1:D:240:ASP:O	1:D:241:THR:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.88	0.40
1:A:276:ARG:O	1:A:277:ARG:HB2	2.22	0.40
1:D:314:THR:O	1:D:317:VAL:HG22	2.22	0.40
1:B:299:PHE:HB3	1:B:322:LEU:HG	2.04	0.40
1:B:322:LEU:HA	1:B:322:LEU:HD12	1.95	0.40
1:C:212:LEU:HD23	1:C:217:ILE:O	2.21	0.40
1:C:143:ILE:CD1	1:C:279:LEU:HD22	2.52	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	296/345 (86%)	267 (90%)	26 (9%)	3 (1%)	19	59
1	B	304/345 (88%)	269 (88%)	29 (10%)	6 (2%)	9	39
1	C	287/345 (83%)	258 (90%)	24 (8%)	5 (2%)	11	44
1	D	296/345 (86%)	270 (91%)	22 (7%)	4 (1%)	14	50
All	All	1183/1380 (86%)	1064 (90%)	101 (8%)	18 (2%)	13	48

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	191	ASP
1	C	246	GLU
1	C	248	GLU
1	A	305	SER
1	B	182	GLU
1	B	239	ILE
1	C	355	GLU
1	D	203	ILE

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Mol	Chain	Res	Type
1	C	231	PRO
1	C	30	LEU
1	D	310	SER
1	D	343	CYS
1	A	231	PRO
1	A	304	ALA
1	B	193	ASP
1	B	231	PRO
1	B	194	LYS
1	D	284	GLY

### 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	270/311 (87%)	251 (93%)	19 (7%)	19	53
1	B	273/311 (88%)	246 (90%)	27 (10%)	10	34
1	C	264/311 (85%)	238 (90%)	26 (10%)	10	35
1	D	272/311 (88%)	249 (92%)	23 (8%)	13	43
All	All	1079/1244 (87%)	984 (91%)	95 (9%)	12	41

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	29	LEU
1	A	31	ARG
1	A	45	LEU
1	A	60	GLN
1	A	72	ASP
1	A	74	LEU
1	A	101	ASN
1	A	108	ASP
1	A	143	ILE
1	A	211	TRP

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	239	ILE
1	A	254	LEU
1	A	266	ASP
1	A	287	ARG
1	A	291	THR
1	A	308	LEU
1	A	342	ASN
1	B	28	THR
1	B	29	LEU
1	B	31	ARG
1	B	45	LEU
1	B	60	GLN
1	B	72	ASP
1	B	74	LEU
1	B	101	ASN
1	B	108	ASP
1	B	146	SER
1	B	193	ASP
1	B	194	LYS
1	B	196	LEU
1	B	203	ILE
1	B	208	LEU
1	B	211	TRP
1	B	223	GLN
1	B	251	SER
1	B	266	ASP
1	B	273	MET
1	B	287	ARG
1	B	312	ILE
1	B	315	SER
1	B	319	ASP
1	B	329	THR
1	B	342	ASN
1	B	357	LEU
1	C	31	ARG
1	C	45	LEU
1	C	60	GLN
1	C	72	ASP
1	C	74	LEU
1	C	86	ARG
1	C	101	ASN

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Mol	Chain	Res	Type
1	C	108	ASP
1	C	142	GLU
1	C	178	HIS
1	C	210	LYS
1	C	211	TRP
1	C	213	ARG
1	C	218	LYS
1	C	228	GLN
1	C	230	GLU
1	C	239	ILE
1	C	287	ARG
1	C	295	THR
1	C	296	CYS
1	C	300	ASP
1	C	306	GLU
1	C	309	LYS
1	C	320	LEU
1	C	351	SER
1	C	352	GLN
1	D	29	LEU
1	D	31	ARG
1	D	45	LEU
1	D	60	GLN
1	D	72	ASP
1	D	74	LEU
1	D	101	ASN
1	D	108	ASP
1	D	118	ASN
1	D	138	MET
1	D	146	SER
1	D	147	GLU
1	D	178	HIS
1	D	200	LEU
1	D	206	SER
1	D	208	LEU
1	D	211	TRP
1	D	251	SER
1	D	273	MET
1	D	287	ARG
1	D	337	ARG
1	D	357	LEU
1	D	358	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	101	ASN
1	A	111	GLN
1	A	124	GLN
1	A	227	ASN
1	A	264	HIS
1	A	303	GLN
1	A	342	ASN
1	B	32	HIS
1	B	49	ASN
1	B	59	ASN
1	B	101	ASN
1	B	111	GLN
1	B	124	GLN
1	B	233	GLN
1	B	264	HIS
1	B	303	GLN
1	B	338	GLN
1	B	342	ASN
1	B	356	ASN
1	C	49	ASN
1	C	59	ASN
1	C	101	ASN
1	C	111	GLN
1	C	124	GLN
1	C	131	GLN
1	C	227	ASN
1	C	228	GLN
1	C	264	HIS
1	C	352	GLN
1	D	32	HIS
1	D	49	ASN
1	D	59	ASN
1	D	101	ASN
1	D	111	GLN
1	D	124	GLN
1	D	173	HIS
1	D	228	GLN
1	D	264	HIS
1	D	303	GLN

### 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 12 ligands modelled in this entry, 8 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	$\# Z  > 2$
4	AKG	A	403	3	3,9,9	1.35	1 (33%)	4,11,11	0.41	0
4	AKG	B	403	3	3,9,9	0.75	0	4,11,11	0.51	0
4	AKG	C	403	3	3,9,9	0.94	0	4,11,11	0.35	0
4	AKG	D	403	3	3,9,9	0.92	0	4,11,11	0.25	0

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	403	3	-	0/3/9/9	0/0/0/0
4	AKG	B	403	3	-	0/3/9/9	0/0/0/0
4	AKG	C	403	3	-	0/3/9/9	0/0/0/0
4	AKG	D	403	3	-	0/3/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	AKG	C3-C2	2.30	1.54	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	AKG	1	0
4	C	403	AKG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/345 (87%)	-0.26	2 (0%) 89 70	21, 48, 77, 93	0
1	B	312/345 (90%)	-0.35	2 (0%) 90 73	21, 40, 70, 88	0
1	C	295/345 (85%)	-0.17	0 100 100	31, 49, 75, 90	0
1	D	302/345 (87%)	-0.25	1 (0%) 94 84	23, 42, 80, 96	0
All	All	1211/1380 (87%)	-0.26	5 (0%) 93 79	21, 44, 76, 96	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	4.2
1	B	109	LEU	3.2
1	D	306	GLU	2.4
1	A	157	ASP	2.1
1	B	311	GLY	2.1

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	AKG	C	403	10/10	0.93	0.24	1.75	62,64,66,67	0
4	AKG	B	403	10/10	0.96	0.23	1.55	43,44,45,46	0
4	AKG	A	403	10/10	0.93	0.22	1.11	46,47,51,52	0
4	AKG	D	403	10/10	0.96	0.16	-0.61	39,42,43,44	0
2	ZN	B	401	1/1	1.00	0.11	-1.68	30,30,30,30	0
2	ZN	A	401	1/1	0.98	0.12	-2.10	37,37,37,37	0
2	ZN	D	401	1/1	0.99	0.07	-2.54	40,40,40,40	0
2	ZN	C	401	1/1	0.99	0.09	-3.04	51,51,51,51	0
3	MN	D	402	1/1	0.98	0.14	-	33,33,33,33	0
3	MN	B	402	1/1	0.99	0.08	-	28,28,28,28	0
3	MN	A	402	1/1	0.91	0.12	-	40,40,40,40	0
3	MN	C	402	1/1	0.97	0.14	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.