



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:36 PM UTC

PDB ID : 3THT / pdb_00003tht
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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

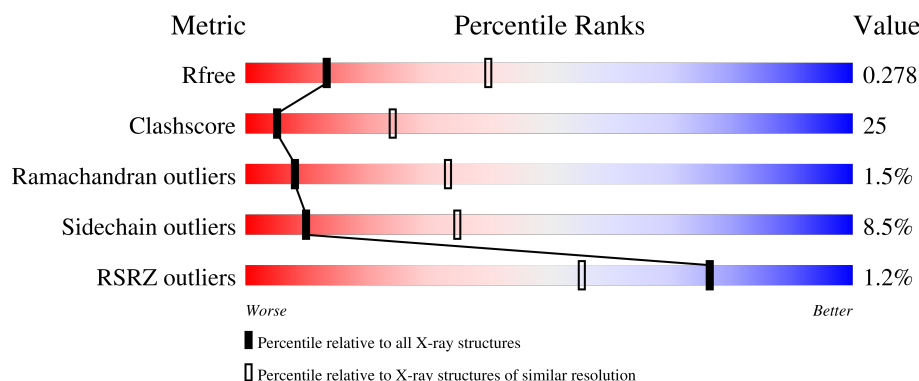
1 Overall quality at a glance

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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 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 $\leq 5\%$. 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	% 48% 34% 5% 12%
1	B	345	% 48% 37% 5% 10%
1	C	345	45% 34% 6% 14%
1	D	345	% 47% 36% • 12%

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 (CCD ID: ZN) (formula: Zn).

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

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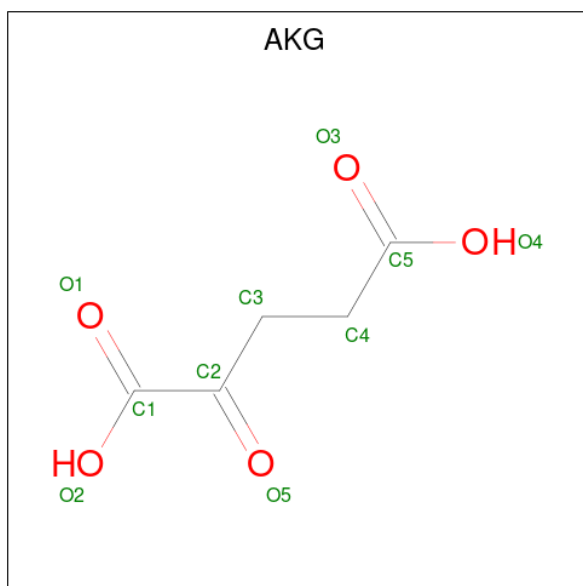
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

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

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

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



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		

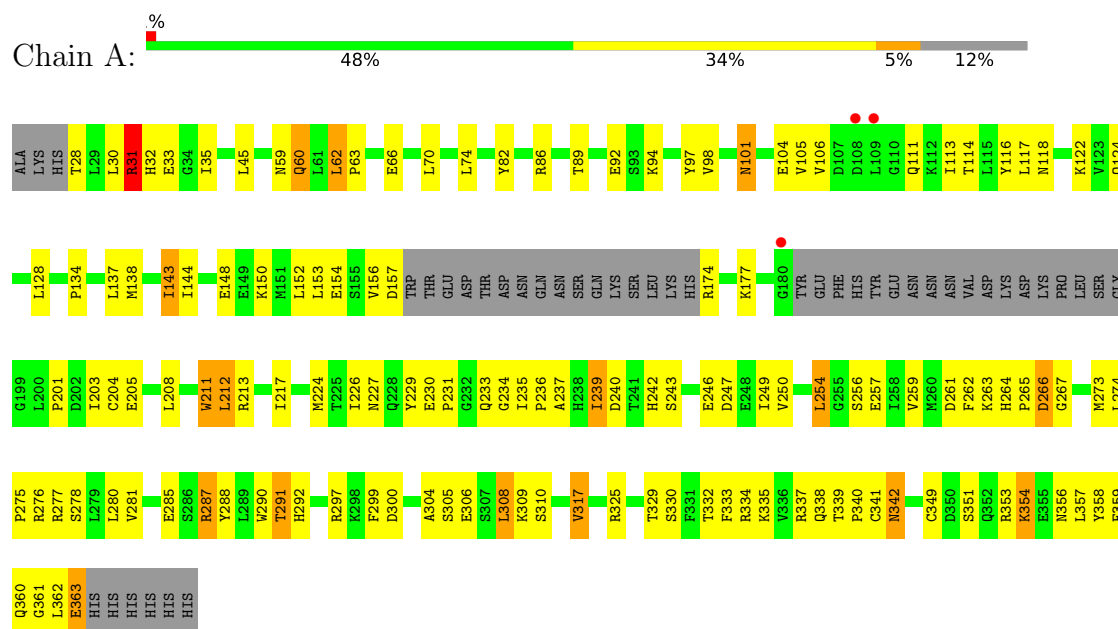
- Molecule 5 is water.

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, 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.

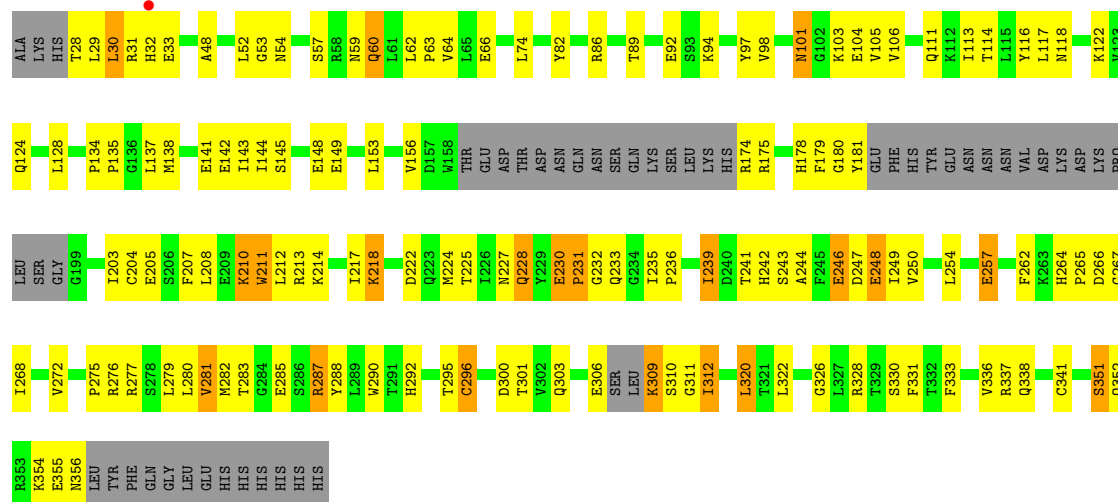
- Molecule 1: Alkylated DNA repair protein alkB homolog 8



GLU
HIS
HIS
HIS
HIS
HIS

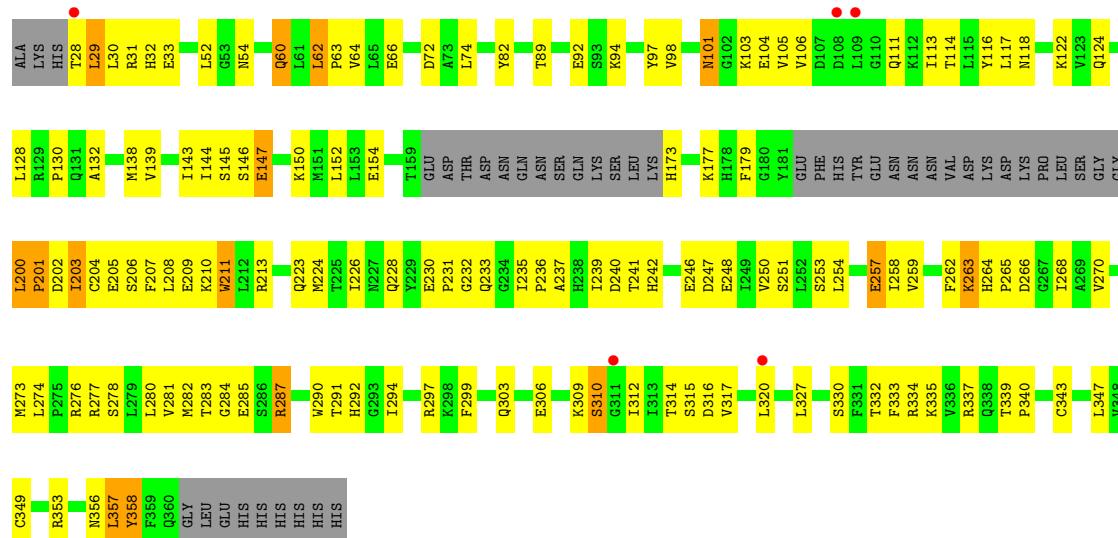
• Molecule 1: Alkylated DNA repair protein alkB homolog 8

Chain C:  45% 34% 6% 14%



• Molecule 1: Alkylated DNA repair protein alkB homolog 8

Chain D:  47% 36% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.17Å 73.28Å 149.81Å 90.00° 112.73° 90.00°	Depositor
Resolution (Å)	39.06 – 3.01 39.06 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.06-3.01) 96.4 (39.06-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2 & Xtalview	Depositor
R, R_{free}	0.220 , 0.277 0.220 , 0.278	Depositor DCC
R_{free} test set	2990 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9758	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: AKG, MN, ZN

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	0.54	0/2439	0.95	6/3295 (0.2%)
1	B	0.56	1/2511 (0.0%)	0.88	0/3393
1	C	0.51	0/2390	0.94	4/3229 (0.1%)
1	D	0.54	0/2461	0.89	1/3328 (0.0%)
All	All	0.54	1/9801 (0.0%)	0.91	11/13245 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	MET	SD-CE	5.01	1.92	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ARG	NE-CZ-NH2	12.91	130.82	119.20
1	A	31	ARG	NE-CZ-NH2	12.46	130.41	119.20
1	C	86	ARG	NE-CZ-NH1	-11.62	109.88	121.50
1	A	31	ARG	NE-CZ-NH1	-11.46	110.04	121.50
1	C	86	ARG	CD-NE-CZ	10.40	138.96	124.40
1	A	31	ARG	CD-NE-CZ	9.74	138.04	124.40
1	A	317	VAL	N-CA-C	-5.76	107.67	113.20
1	A	363	GLU	CB-CA-C	5.75	121.02	110.10
1	A	205	GLU	N-CA-C	-5.73	105.12	111.71
1	C	281	VAL	CB-CA-C	-5.45	104.73	111.32
1	D	201	PRO	N-CA-C	5.26	119.47	111.11

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	115	0
1	B	2462	0	2465	138	0
1	C	2344	0	2357	125	0
1	D	2411	0	2422	102	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	474	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 25.

All (474) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLU:HG2	1:B:327:LEU:HD13	1.59	0.84
1:C:210:LYS:HZ2	1:C:213:ARG:HH11	1.24	0.83
1:C:210:LYS:NZ	1:C:213:ARG:HH11	1.77	0.83
1:A:156:VAL:HG13	1:A:157:ASP:H	1.45	0.81
1:B:356:ASN:ND2	1:B:358:TYR:HB3	1.95	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:H	1:C:320:LEU:HD23	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:A:250:VAL:HG12	1:A:281:VAL:HG13	1.68	0.73
1:B:264:HIS:HD2	1:B:266:ASP:HB2	1.52	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:C:231:PRO:HG3	1:C:326:GLY:C	2.14	0.72
1:B:109:LEU:HD22	1:B:296:CYS:O	1.90	0.72
1:C:217:ILE:HD12	1:C:248:GLU:CD	2.14	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:A:254:LEU:N	1:A:254:LEU:HD23	2.08	0.69
1:C:204:CYS:O	1:C:208:LEU:HD22	1.92	0.69
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:A:201:PRO:HB2	1:A:203:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:HA	1:C:283:THR:HG22	1.75	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:28:THR:HG23	1:D:29:LEU:H	1.58	0.67
1:D:303:GLN:HA	1:D:320:LEU:HD23	1.77	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:HD22	1:A:342:ASN:N	1.94	0.65
1:B:257:GLU:HB2	1:B:273:MET:HE1	1.77	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:A:246:GLU:HG3	1:A:335:LYS:CE	2.28	0.64
1:C:117:LEU:HD12	1:C:117:LEU:N	2.13	0.64
1:A:213:ARG:HG2	1:A:213:ARG:HH21	1.61	0.64
1:B:28:THR:HG23	1:B:29:LEU:CD2	2.18	0.64
1:D:202:ASP:C	1:D:204:CYS:H	2.06	0.64
1:D:228:GLN:HG2	1:D:327:LEU:HD11	1.79	0.64
1:C:143:ILE:HG23	1:C:144:ILE:HG23	1.80	0.64
1:A:128:LEU:HD12	1:B:124:GLN:HB3	1.80	0.63
1:B:201:PRO:HG2	1:B:204:CYS:SG	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:C:312:ILE:H	1.65	0.61
1:B:117:LEU:N	1:B:117:LEU:HD12	2.15	0.61
1:C:174:ARG:HE	1:C:227:ASN:ND2	1.98	0.61
1:D:33:GLU:HG2	1:D:82:TYR:CE2	2.36	0.61
1:B:257:GLU:H	1:B:257:GLU:CD	2.08	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:117:LEU:HD12	1:A:117:LEU:N	2.17	0.60
1:A:122:LYS:HD3	1:A:124:GLN:HE21	1.66	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:A:264:HIS:HD2	1:A:266:ASP:H	1.48	0.59
1:C:174:ARG:HE	1:C:227:ASN:HD22	1.50	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:B:218:LYS:H	1:B:248:GLU:CD	2.11	0.58
1:A:353:ARG:HB2	1:A:359:PHE:CD1	2.38	0.58
1:B:31:ARG:NH2	1:B:32:HIS:HB2	2.19	0.58
1:B:194:LYS:O	1:B:196:LEU:CD1	2.51	0.58
1:D:29:LEU:H	1:D:29:LEU:CD1	2.16	0.58
1:D:226:ILE:HA	1:D:330:SER:O	2.03	0.58
1:D:356:ASN:O	1:D:357:LEU:HB3	2.02	0.58
1:A:33:GLU:HG2	1:A:82:TYR:CE2	2.39	0.57
1:C:28:THR:HG23	1:C:29:LEU:N	2.19	0.57
1:D:117:LEU:N	1:D:117:LEU:HD12	2.19	0.57
1:D:264:HIS:CD2	1:D:266:ASP:H	2.20	0.57
1:A:134:PRO:HB3	1:A:290:TRP:CE2	2.39	0.57
1:C:213:ARG:HH21	1:C:213:ARG:HG3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:315:SER:O	1:D:316:ASP:HB2	2.05	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:253:SER:HB3	5:B:6:HOH:O	2.06	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:356:ASN:C	1:B:358:TYR:H	2.14	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:239:ILE:HD13	1:A:240:ASP:O	2.07	0.54
1:A:263:LYS:O	1:A:291:THR:HG22	2.08	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:B:264:HIS:CD2	1:B:266:ASP:HB2	2.38	0.54
1:C:203:ILE:H	1:C:203:ILE:CD1	2.14	0.54
1:D:130:PRO:HA	5:D:9:HOH:O	2.07	0.54
1:D:177:LYS:HD2	1:D:179:PHE:CE2	2.42	0.54
1:D:297:ARG:HD2	1:D:299:PHE:O	2.08	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:C:282:MET:HE1	1:C:292:HIS:CE1	2.43	0.53
1:C:175:ARG:HG3	1:C:228:GLN:NE2	2.24	0.53
1:C:264:HIS:HD2	1:C:266:ASP:HB2	1.74	0.53
1:D:337:ARG:HG2	1:D:339:THR:O	2.08	0.53
1:C:247:ASP:O	1:C:248:GLU:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLU:CD	1:D:257:GLU:H	2.16	0.53
1:D:213:ARG:HG2	1:D:213:ARG:HH21	1.73	0.53
1:B:111:GLN:HE22	1:B:296:CYS:HB2	1.74	0.53
1:C:320:LEU:HD23	1:C:320:LEU:N	2.22	0.53
1:B:181:TYR:C	1:B:183:PHE:H	2.17	0.53
1:B:196:LEU:H	1:B:196:LEU:HD22	1.74	0.53
1:D:29:LEU:C	1:D:29:LEU:HD22	2.34	0.53
1:B:62:LEU:HB3	1:B:63:PRO:HD3	1.91	0.53
1:A:237:ALA:HB1	1:A:291:THR:OG1	2.08	0.53
1:B:217:ILE:HD13	1:B:250:VAL:HG11	1.91	0.53
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:D:264:HIS:CD2	1:D:265:PRO:HD2	2.45	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:C:32:HIS:CG	1:C:267:GLY:HA3	2.45	0.52
1:C:241:THR:HB	1:C:244:ALA:CB	2.40	0.52
1:C:276:ARG:O	1:C:277:ARG:HB2	2.09	0.52
1:D:31:ARG:NH2	1:D:32:HIS:HB2	2.24	0.52
1:D:62:LEU:HB3	1:D:63:PRO:HD3	1.90	0.52
1:B:224:MET:HG3	1:B:333:PHE:CE2	2.45	0.52
1:C:178:HIS:CA	1:C:225:THR:HG22	2.39	0.52
1:A:261:ASP:HB3	1:A:263:LYS:HE3	1.92	0.52
1:C:247:ASP:O	1:C:249:ILE:HG13	2.09	0.52
1:A:254:LEU:HD23	1:A:254:LEU:H	1.75	0.52
1:B:221:PRO:HG3	1:B:333:PHE:HB3	1.92	0.52
1:B:342:ASN:HD22	1:B:342:ASN:N	2.03	0.52
1:B:192:LYS:HG2	1:B:195:PRO:HD2	1.92	0.52
1:C:135:PRO:HG2	1:C:285:GLU:HB3	1.92	0.52
1:D:143:ILE:HG12	1:D:211:TRP:CH2	2.45	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:B:246:GLU:O	1:B:287:ARG:NH1	2.43	0.51
1:C:62:LEU:HB3	1:C:63:PRO:HD3	1.92	0.51
1:C:137:LEU:HD12	1:C:282:MET:HG2	1.93	0.51
1:A:31:ARG:NH2	1:A:32:HIS:HB2	2.25	0.51
1:D:28:THR:HG23	1:D:29:LEU:N	2.25	0.51
1:C:149:GLU:HG3	1:C:254:LEU:HD22	1.93	0.51
1:C:285:GLU:HB2	5:C:378:HOH:O	2.10	0.51
1:A:213:ARG:HG2	1:A:213:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LYS:HZ2	1:C:213:ARG:NH1	2.02	0.51
1:D:203:ILE:HG22	1:D:203:ILE:O	2.11	0.51
1:A:243:SER:HB3	1:A:351:SER:OG	2.11	0.51
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:B:256:SER:HA	1:B:276:ARG:HD2	1.91	0.51
1:C:210:LYS:NZ	1:C:213:ARG:NH1	2.54	0.51
1:B:213:ARG:HD3	5:B:372:HOH:O	2.11	0.50
1:D:101:ASN:ND2	1:D:116:TYR:HA	2.26	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: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:B:32:HIS:CD2	1:B:267:GLY:HA3	2.47	0.50
1:C:272:VAL:HA	1:C:311:GLY:O	2.12	0.50
1:D:132:ALA:C	1:D:312:ILE:HD11	2.35	0.50
1:D:223:GLN:NE2	1:D:224:MET:O	2.44	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:29:LEU:N	1:B:29:LEU:HD13	2.27	0.50
1:B:144:ILE:HD11	1:B:254:LEU:HD21	1.93	0.50
1:C:268:ILE:H	1:C:268:ILE:CD1	2.20	0.49
1:A:174:ARG:HH21	1:A:227:ASN:ND2	2.09	0.49
1:B:144:ILE:HD11	1:B:254:LEU:CD2	2.43	0.49
1:D:64:VAL:HG13	1:D:103:LYS:NZ	2.27	0.49
1:B:176:VAL:HG12	1:B:177:LYS:N	2.26	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: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: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:A:262:PHE:CE1	1:A:292:HIS:HB3	2.48	0.48
1:C:354:LYS:C	1:C:356:ASN:H	2.21	0.48
1:D:250:VAL:HA	1:D:280:LEU:O	2.13	0.48
1:C:264:HIS:CD2	1:C:266:ASP:HB2	2.48	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: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:A:264:HIS:CD2	1:A:266:ASP:H	2.28	0.48
1:D:202:ASP:C	1:D:204:CYS:N	2.72	0.48
1:D:274:LEU:HD21	1:D:280:LEU:HD13	1.96	0.48
1:A:230:GLU:H	1:A:233:GLN:CG	2.25	0.48
1:C:264:HIS:CG	1:C:265:PRO:HD2	2.49	0.48
1:C:330:SER:C	1:C:331:PHE:HD1	2.21	0.48
1:B:150:LYS:O	1:B:154:GLU:HG3	2.14	0.48
1:D:177:LYS:HD2	1:D:179:PHE:CZ	2.49	0.48
1:A:230:GLU:O	1:A:233:GLN:HG2	2.14	0.48
1:A:342:ASN:HB3	5:A:379:HOH:O	2.13	0.48
1:B:105:VAL:HG23	1:B:113:ILE:HG13	1.96	0.47
1:B:175:ARG:HG2	1:B:175:ARG:HH11	1.79	0.47
1:D:278:SER:HB3	5:D:4:HOH:O	2.14	0.47
1:C:222:ASP:OD2	1:C:336:VAL:HG23	2.14	0.47
1:C:203:ILE:HD12	1:C:203:ILE:N	2.18	0.47
1:D:29:LEU:H	1:D:29:LEU:HD12	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: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:B:289:LEU:O	1:B:289:LEU:HD12	2.14	0.47
1:A:239:ILE:HD13	1:A:239:ILE:C	2.40	0.47
1:A:361:GLY:C	1:A:363:GLU:H	2.23	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:106:VAL:HA	1:C:111:GLN:O	2.14	0.47
1:C:208:LEU:HD22	1:C:208:LEU:H	1.79	0.47
1:C:213:ARG:HG3	1:C:213:ARG:NH2	2.30	0.47
1:A:342:ASN:N	1:A:342:ASN:ND2	2.61	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:ND2	1:A:116:TYR:HA	2.30	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
1:B:312:ILE:HD13	1:B:312:ILE:H	1.80	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:143:ILE:HG22	1:A:277:ARG:O	2.15	0.46
1:A:227:ASN:HB2	1:A:330:SER:OG	2.16	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:230:GLU:O	1:D:231:PRO:C	2.57	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:205:GLU:OE2	1:D:209:GLU:OE1	2.34	0.46
1:D:235:ILE:HG22	1:D:294:ILE:HD12	1.97	0.46
1:D:285:GLU:HG2	1:D:290:TRP:CD1	2.50	0.46
1:A:106:VAL:HA	1:A:111:GLN:O	2.15	0.45
1:B:106:VAL:HA	1:B:111:GLN:O	2.16	0.45
1:B:204:CYS:O	1:B:205:GLU:C	2.57	0.45
1:B:235:ILE:HG13	1:B:236:PRO:HD2	1.97	0.45
1:C:262:PHE:CE1	1:C:292:HIS:HB3	2.51	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:B:356:ASN:C	1:B:358:TYR:N	2.73	0.45
1:C:138:MET:HB3	1:C:281:VAL:HB	1.98	0.45
1:A:246:GLU:HG3	1:A:335:LYS:HE2	1.95	0.45
1:A:259:VAL:CG1	1:A:273:MET:HG2	2.42	0.45
1:A:300:ASP:CG	1:A:325:ARG:HE	2.23	0.45
1:C:338:GLN:HA	1:C:338:GLN:OE1	2.16	0.45
1:A:134:PRO:HB3	1:A:290:TRP:CD2	2.52	0.45
1:B:339:THR:HB	1:B:340:PRO:HD2	1.98	0.45
1:C:180:GLY:C	1:C:181:TYR:CD1	2.94	0.45
1:C:309:LYS:HE3	1:C:309:LYS:HA	1.96	0.45
1:A:153:LEU:HG	1:A:254:LEU:HD12	1.99	0.45
1:A:235:ILE:O	1:A:235:ILE:HG23	2.16	0.45
1:A:264:HIS:CG	1:A:265:PRO:HD2	2.52	0.45
1:B:196:LEU:H	1:B:196:LEU:CD1	2.07	0.45
1:D:240:ASP:O	1:D:241:THR:C	2.59	0.45
1:D:347:LEU:O	1:D:353:ARG:HD2	2.17	0.45
1:A:357:LEU:O	1:A:360:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HD22	1:A:357:LEU:H	1.81	0.45
1:B:241:THR:HG22	1:B:243:SER:H	1.82	0.45
1:A:70:LEU:HA	5:A:381:HOH:O	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:247:ASP:HB2	1:A:288:TYR:OH	2.17	0.45
1:C:94:LYS:O	1:C:98:VAL:HG22	2.17	0.45
1:B:356:ASN:O	1:B:358:TYR:N	2.51	0.44
1:C:337:ARG:HG3	1:C:337:ARG:HH21	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:B:239:ILE:O	1:B:240:ASP:C	2.60	0.44
1:A:224:MET:HG2	1:A:332:THR:O	2.18	0.44
1:A:235:ILE:HG13	1:A:236:PRO:HD2	1.99	0.44
1:D:89:THR:HG1	1:D:92:GLU:HG3	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:D:258:ILE:HG12	1:D:259:VAL:H	1.82	0.44
1:B:347:LEU:O	1:B:353:ARG:HD2	2.18	0.44
1:C:210:LYS:O	1:C:214:LYS:HD3	2.17	0.44
1:A:263:LYS:HB2	1:A:291:THR:HG23	1.98	0.44
1:B:89:THR:OG1	1:B:92:GLU:HG3	2.17	0.44
1:B:235:ILE:HG23	1:B:235:ILE:O	2.16	0.44
1:A:174:ARG:NH2	1:A:227:ASN:ND2	2.66	0.44
1:A:257:GLU:HB3	1:A:275:PRO:HA	1.99	0.44
1:B:247:ASP:OD2	1:B:283:THR:HA	2.17	0.44
1:C:97:TYR:O	1:C:101:ASN:HB2	2.18	0.44
1:A:229:TYR:CD2	1:A:234:GLY:HA2	2.53	0.44
1:C:337:ARG:NH2	5:C:17:HOH:O	2.46	0.44
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: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: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:250:VAL:HB	1:C:279:LEU:HD11	2.00	0.43
1:A:208:LEU:O	1:A:211:TRP:HB2	2.19	0.43
1:B:110:GLY:N	5:B:7:HOH:O	2.50	0.43
1:C:178:HIS:ND1	1:C:178:HIS:N	2.67	0.43
1:D:94:LYS:O	1:D:98:VAL:HG22	2.18	0.43
1:D:97:TYR:O	1:D:101:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:282:MET:HG2	1:D:287:ARG:HB3	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
1:C:303:GLN:HA	1:C:320:LEU:HA	2.00	0.43
1:D:224:MET:HA	1:D:332:THR:O	2.19	0.43
1:C:230:GLU:O	1:C:232:GLY:N	2.51	0.43
1:D:31:ARG:NH2	1:D:266:ASP:O	2.51	0.43
1:C:29:LEU:HD12	1:C:30:LEU:N	2.34	0.43
1:D:173:HIS:CD2	1:D:233:GLN:HE21	2.37	0.43
1:D:246:GLU:O	1:D:287:ARG:NH1	2.50	0.43
1:D:264:HIS:CG	1:D:265:PRO:HD2	2.54	0.43
1:B:157:ASP:O	1:B:158:TRP:HB2	2.18	0.43
1:B:218:LYS:C	1:B:219:HIS:ND1	2.77	0.43
1:D:29:LEU:CD1	1:D:29:LEU:N	2.80	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:C:243:SER:HB3	1:C:351:SER:HB3	1.99	0.42
1:D:143:ILE:HG22	1:D:277:ARG:O	2.18	0.42
1:A:229:TYR:HD2	1:A:234:GLY:HA2	1.84	0.42
1:A:247:ASP:CG	1:A:247:ASP:O	2.62	0.42
1:B:221:PRO:CG	1:B:333:PHE:HB3	2.50	0.42
1:B:328:ARG:NH2	4:B:403:AKG:O4	2.50	0.42
1:B:350:ASP:HB3	5:B:374:HOH:O	2.17	0.42
1:D:247:ASP:O	1:D:287:ARG:CD	2.66	0.42
1:A:45:LEU:O	1:A:45:LEU:HD12	2.20	0.42
1:A:261:ASP:O	1:A:292:HIS:HA	2.18	0.42
1:B:97:TYR:O	1:B:101:ASN:HB2	2.20	0.42
1:B:175:ARG:HG2	1:B:175:ARG:NH1	2.33	0.42
1:B:194:LYS:HB2	1:B:195:PRO:HD3	2.00	0.42
1:B:224:MET:HE1	1:B:226:ILE:HD11	2.02	0.42
1:C:52:LEU:C	1:C:54:ASN:H	2.27	0.42
1:C:204:CYS:O	1:C:207:PHE:HB2	2.19	0.42
1:D:242:HIS:ND1	1:D:349:CYS:HA	2.34	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:250:VAL:HG22	1:A:333:PHE:HB2	2.01	0.42
1:C:29:LEU:C	1:C:31:ARG:N	2.76	0.42
1:D:105:VAL:HG23	1:D:113:ILE:HG13	2.00	0.42
1:D:145:SER:OG	1:D:147:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:CYS:O	1:D:205:GLU:C	2.63	0.42
1:A:32:HIS:CG	1:A:267:GLY:HA3	2.54	0.42
1:A:62:LEU:O	1:A:66:GLU:HG3	2.19	0.42
1:B:62:LEU:O	1:B:66:GLU:HG3	2.20	0.42
1:B:250:VAL:HA	1:B:280:LEU:O	2.20	0.42
1:D:334:ARG:HG3	1:D:334:ARG:HH11	1.85	0.42
1:A:247:ASP:HA	1:A:287:ARG:HD3	2.01	0.42
1:B:52:LEU:C	1:B:54:ASN:H	2.28	0.42
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:143:ILE:HG12	1:D:211:TRP:CZ3	2.55	0.42
1:D:235:ILE:O	1:D:235:ILE:HG23	2.20	0.42
1:A:94:LYS:O	1:A:98:VAL:HG22	2.19	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:356:ASN:O	1:A:357:LEU:C	2.61	0.41
1:D:201:PRO:HG2	1:D:204:CYS:SG	2.60	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:227:ASN:O	1:A:329:THR:HA	2.19	0.41
1:A:256:SER:HA	1:A:276:ARG:HD2	2.02	0.41
1:A:275:PRO:HG2	1:A:278:SER:HB3	2.02	0.41
1:C:228:GLN:HB3	1:C:228:GLN:HE21	1.59	0.41
1:B:227:ASN:O	1:B:329:THR:HA	2.20	0.41
1:C:257:GLU:CD	1:C:257:GLU:H	2.26	0.41
1:A:89:THR:OG1	1:A:92:GLU:HG3	2.19	0.41
1:D:52:LEU:C	1:D:54:ASN:H	2.28	0.41
1:A:30:LEU:HB3	1:A:35:ILE:HB	2.03	0.41
1:B:196:LEU:HD22	1:B:196:LEU:O	2.20	0.41
1:A:317:VAL:HG13	1:B:75:LEU:HG	2.01	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:B:312:ILE:HD13	1:B:312:ILE:N	2.36	0.41
1:C:179:PHE:HB2	1:C:224:MET:O	2.21	0.41
1:C:328:ARG:HH12	4:C:403:AKG:C5	2.34	0.41
1:C:59:ASN:N	1:C:59:ASN:HD22	2.18	0.41
1:C:337:ARG:HD2	5:C:370:HOH:O	2.20	0.41
1:D:128:LEU:HD21	1:D:268:ILE:HG12	2.02	0.41
1:D:339:THR:HB	1:D:340:PRO:CD	2.47	0.41
1:A:150:LYS:O	1:A:154:GLU:HG2	2.21	0.41
1:D:213:ARG:HG2	1:D:213:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ALA:HA	1:D:292:HIS:O	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:B:217:ILE:HD12	1:B:248:GLU:CD	2.45	0.40
1:B:249:ILE:HG12	5:B:378:HOH:O	2.21	0.40
1:D:89:THR:OG1	1:D:92:GLU:HG3	2.20	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:A:276:ARG:O	1:A:277:ARG:HB2	2.22	0.40
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.88	0.40
1:B:299:PHE:HB3	1:B:322:LEU:HG	2.04	0.40
1:B:322:LEU:HD12	1:B:322:LEU:HA	1.95	0.40
1:C:141:GLU:CD	1:C:310:SER:OG	2.65	0.40
1:D:314:THR:O	1:D:317:VAL:HG22	2.22	0.40
1:C:143:ILE:CD1	1:C:279:LEU:HD22	2.52	0.40
1:C:212:LEU:HD23	1:C:217:ILE:O	2.21	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%)	12	43
1	B	304/345 (88%)	269 (88%)	29 (10%)	6 (2%)	6	26
1	C	287/345 (83%)	258 (90%)	24 (8%)	5 (2%)	7	30
1	D	296/345 (86%)	270 (91%)	22 (7%)	4 (1%)	9	34
All	All	1183/1380 (86%)	1064 (90%)	101 (8%)	18 (2%)	8	33

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
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 ⓘ

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%)	14	42
1	B	273/311 (88%)	246 (90%)	27 (10%)	7	28
1	C	264/311 (85%)	242 (92%)	22 (8%)	10	35
1	D	272/311 (88%)	248 (91%)	24 (9%)	9	33
All	All	1079/1244 (87%)	987 (92%)	92 (8%)	10	35

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	31	ARG
1	A	60	GLN
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	74	LEU
1	A	101	ASN
1	A	118	ASN
1	A	143	ILE
1	A	211	TRP
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	338	GLN
1	A	342	ASN
1	A	354	LYS
1	B	28	THR
1	B	29	LEU
1	B	31	ARG
1	B	60	GLN
1	B	62	LEU
1	B	74	LEU
1	B	101	ASN
1	B	118	ASN
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	220	LYS
1	B	248	GLU
1	B	251	SER
1	B	257	GLU
1	B	273	MET
1	B	287	ARG
1	B	312	ILE
1	B	315	SER
1	B	320	LEU
1	B	329	THR
1	B	342	ASN
1	B	357	LEU

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Mol	Chain	Res	Type
1	C	60	GLN
1	C	74	LEU
1	C	101	ASN
1	C	118	ASN
1	C	142	GLU
1	C	210	LYS
1	C	211	TRP
1	C	218	LYS
1	C	228	GLN
1	C	230	GLU
1	C	239	ILE
1	C	257	GLU
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	312	ILE
1	C	320	LEU
1	C	351	SER
1	C	352	GLN
1	D	29	LEU
1	D	60	GLN
1	D	62	LEU
1	D	72	ASP
1	D	74	LEU
1	D	101	ASN
1	D	118	ASN
1	D	138	MET
1	D	139	VAL
1	D	146	SER
1	D	147	GLU
1	D	200	LEU
1	D	206	SER
1	D	208	LEU
1	D	210	LYS
1	D	211	TRP
1	D	251	SER
1	D	257	GLU
1	D	263	LYS
1	D	273	MET

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Mol	Chain	Res	Type
1	D	287	ARG
1	D	335	LYS
1	D	357	LEU
1	D	358	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
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	A	352	GLN
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	C	43	GLN
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	C	356	ASN
1	D	32	HIS

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Mol	Chain	Res	Type
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 [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	403	3	9,9,9	1.13	0	11,11,11	1.66	3 (27%)
4	AKG	A	403	3	9,9,9	1.39	1 (11%)	11,11,11	1.62	4 (36%)
4	AKG	D	403	3	9,9,9	1.18	0	11,11,11	1.65	3 (27%)
4	AKG	B	403	3	9,9,9	1.26	1 (11%)	11,11,11	1.52	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	C	403	3	-	7/9/9/9	-
4	AKG	A	403	3	-	6/9/9/9	-
4	AKG	D	403	3	-	8/9/9/9	-
4	AKG	B	403	3	-	3/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	AKG	C3-C2	3.16	1.54	1.51
4	B	403	AKG	C2-C1	-2.66	1.49	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	AKG	C3-C2-C1	3.32	121.50	115.86
4	D	403	AKG	C3-C2-C1	3.18	121.25	115.86
4	B	403	AKG	C3-C2-C1	2.99	120.95	115.86
4	A	403	AKG	C3-C2-C1	2.81	120.62	115.86
4	A	403	AKG	O2-C1-C2	2.46	120.41	113.59
4	D	403	AKG	O2-C1-C2	2.33	120.06	113.59
4	C	403	AKG	O2-C1-C2	2.32	120.03	113.59
4	A	403	AKG	O2-C1-O1	-2.20	118.67	123.90
4	B	403	AKG	O2-C1-C2	2.19	119.67	113.59
4	D	403	AKG	O4-C5-C4	2.16	120.81	114.00
4	C	403	AKG	O4-C5-C4	2.02	120.37	114.00
4	A	403	AKG	O4-C5-O3	-2.00	118.19	123.33

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	AKG	O1-C1-C2-O5
4	A	403	AKG	O1-C1-C2-C3
4	A	403	AKG	O2-C1-C2-C3
4	A	403	AKG	C2-C3-C4-C5
4	B	403	AKG	C1-C2-C3-C4
4	C	403	AKG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	403	AKG	O2-C1-C2-C3
4	C	403	AKG	C2-C3-C4-C5
4	D	403	AKG	O1-C1-C2-O5
4	D	403	AKG	O1-C1-C2-C3
4	D	403	AKG	O2-C1-C2-O5
4	D	403	AKG	O2-C1-C2-C3
4	D	403	AKG	C2-C3-C4-C5
4	B	403	AKG	C2-C3-C4-C5
4	C	403	AKG	O1-C1-C2-O5
4	C	403	AKG	C1-C2-C3-C4
4	D	403	AKG	C1-C2-C3-C4
4	C	403	AKG	C3-C4-C5-O4
4	A	403	AKG	C3-C4-C5-O3
4	C	403	AKG	C3-C4-C5-O3
4	A	403	AKG	C3-C4-C5-O4
4	D	403	AKG	C3-C4-C5-O3
4	B	403	AKG	O5-C2-C3-C4
4	D	403	AKG	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	AKG	1	0
4	B	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, 95th 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	302/345 (87%)	-0.08	3 (0%) 79 59	21, 48, 77, 93	0
1	B	312/345 (90%)	-0.21	5 (1%) 70 47	21, 40, 70, 88	0
1	C	295/345 (85%)	-0.07	1 (0%) 90 79	31, 49, 75, 90	0
1	D	302/345 (87%)	-0.17	5 (1%) 69 46	23, 42, 80, 96	0
All	All	1211/1380 (87%)	-0.13	14 (1%) 76 55	21, 44, 76, 96	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	3.4
1	B	191	ASP	3.2
1	D	311	GLY	3.0
1	D	320	LEU	3.0
1	B	32	HIS	2.5
1	A	108	ASP	2.5
1	C	32	HIS	2.4
1	B	308	LEU	2.4
1	D	109	LEU	2.3
1	B	189	ASN	2.3
1	B	109	LEU	2.2
1	D	108	ASP	2.2
1	D	28	THR	2.1
1	A	180	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 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, 95th 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($\text{\AA}^2$)	Q<0.9
4	AKG	A	403	10/10	0.91	0.11	46,47,51,52	0
4	AKG	B	403	10/10	0.92	0.10	43,44,45,46	0
4	AKG	C	403	10/10	0.93	0.16	62,64,66,67	0
4	AKG	D	403	10/10	0.95	0.10	39,42,43,44	0
3	MN	A	402	1/1	0.97	0.04	40,40,40,40	0
3	MN	D	402	1/1	0.97	0.05	33,33,33,33	0
3	MN	C	402	1/1	0.98	0.05	44,44,44,44	0
2	ZN	A	401	1/1	0.98	0.04	37,37,37,37	0
2	ZN	C	401	1/1	0.99	0.04	51,51,51,51	0
3	MN	B	402	1/1	0.99	0.02	28,28,28,28	0
2	ZN	B	401	1/1	1.00	0.02	30,30,30,30	0
2	ZN	D	401	1/1	1.00	0.01	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.