



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:35 PM UTC

PDB ID : 6IE2 / pdb_00006ie2
Title : Crystal structure of methyladenine demethylase
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Deposited on : 2018-09-13
Resolution : 2.80 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

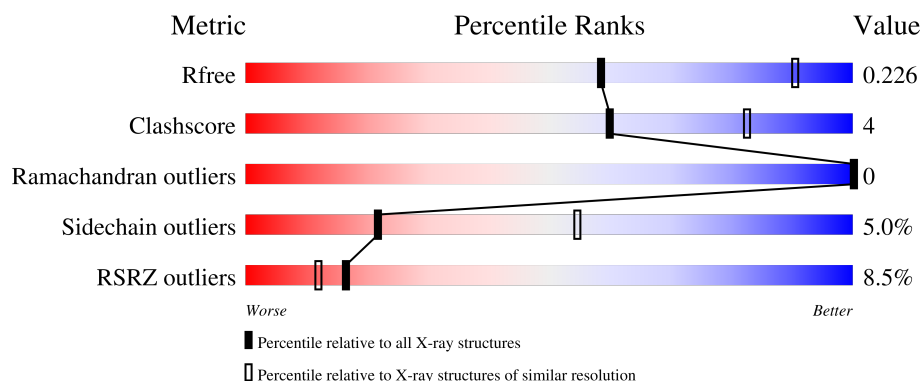
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



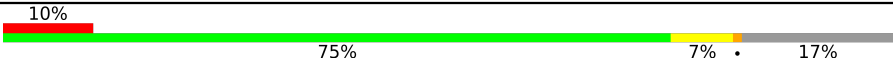
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	389	2% 69% 11% .. 17%
1	B	389	6% 73% 8% .. 17%
1	C	389	5% 72% 10% . 17%
1	D	389	8% 74% 6% .. 17%
1	E	389	6% 68% 12% . 19%

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Mol	Chain	Length	Quality of chain
1	F	389	
1	G	389	
1	H	389	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20660 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 Nucleic acid dioxygenase ALKBH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2505	1609	427	455	14			
1	B	323	Total	C	N	O	S	0	0	0
			2515	1615	430	456	14			
1	C	323	Total	C	N	O	S	0	0	0
			2521	1619	433	455	14			
1	D	323	Total	C	N	O	S	0	0	0
			2506	1611	426	455	14			
1	E	317	Total	C	N	O	S	0	0	0
			2474	1590	425	445	14			
1	F	324	Total	C	N	O	S	0	0	0
			2533	1627	434	458	14			
1	G	323	Total	C	N	O	S	0	0	0
			2519	1617	435	453	14			
1	H	324	Total	C	N	O	S	0	0	0
			2513	1615	431	453	14			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

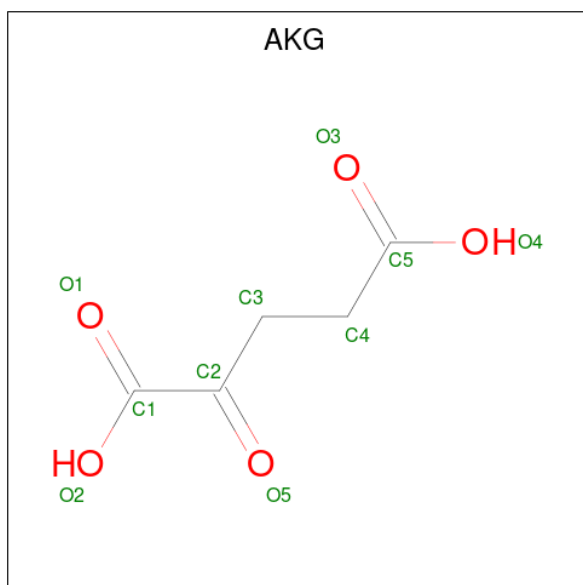
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



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

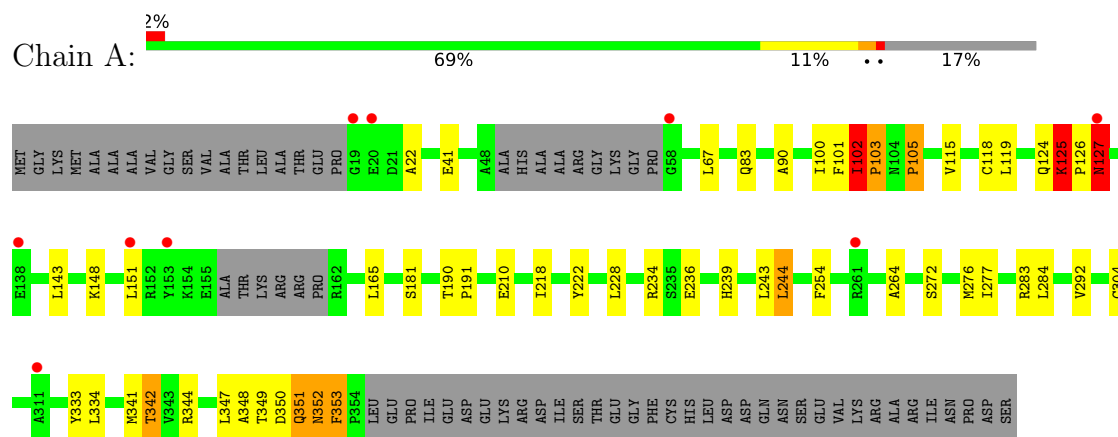
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	68	Total 68	O 68	0	0
4	C	76	Total 76	O 76	0	0
4	D	51	Total 51	O 51	0	0
4	E	60	Total 60	O 60	0	0
4	F	47	Total 47	O 47	0	0
4	G	46	Total 46	O 46	0	0
4	H	53	Total 53	O 53	0	0

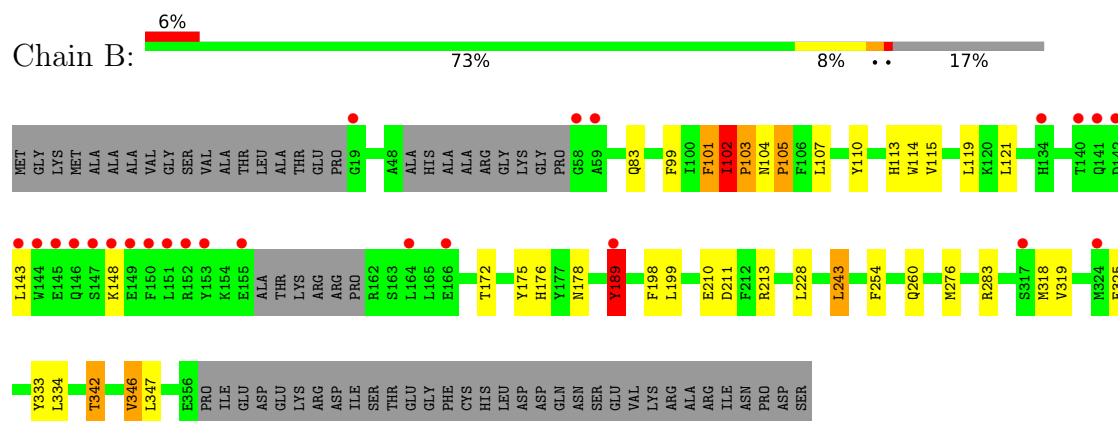
3 Residue-property plots [i](#)

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.

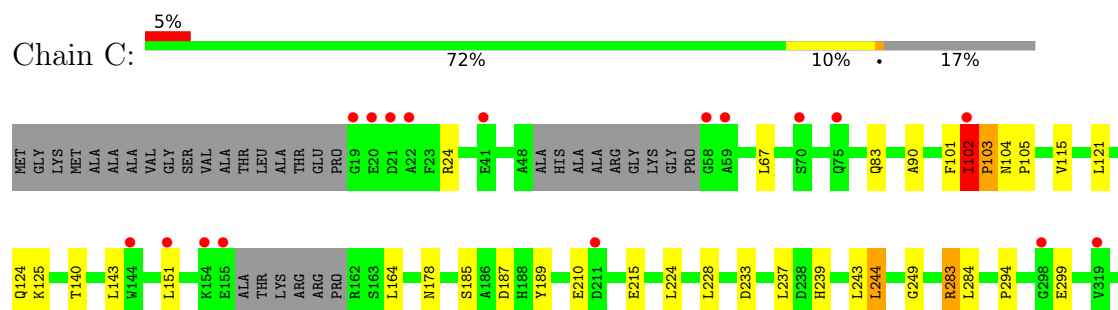
• Molecule 1: Nucleic acid dioxygenase ALKBH1

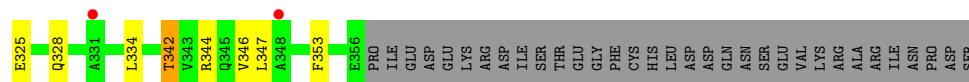


• Molecule 1: Nucleic acid dioxygenase ALKBH1

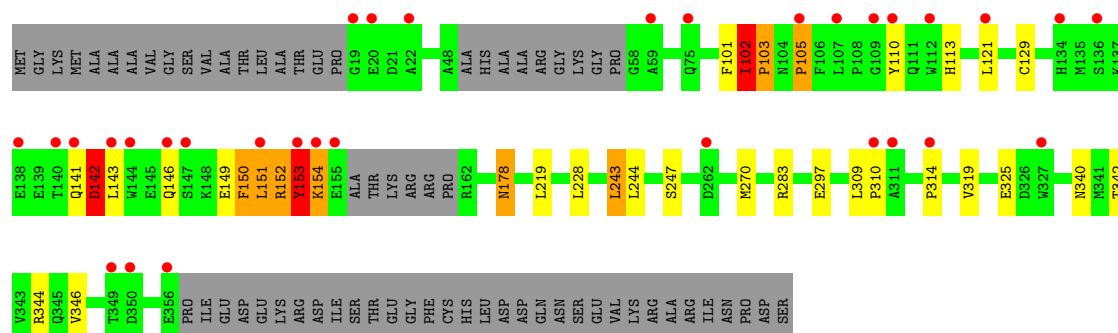
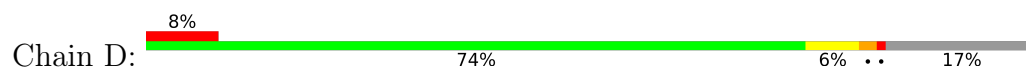


• Molecule 1: Nucleic acid dioxygenase ALKBH1

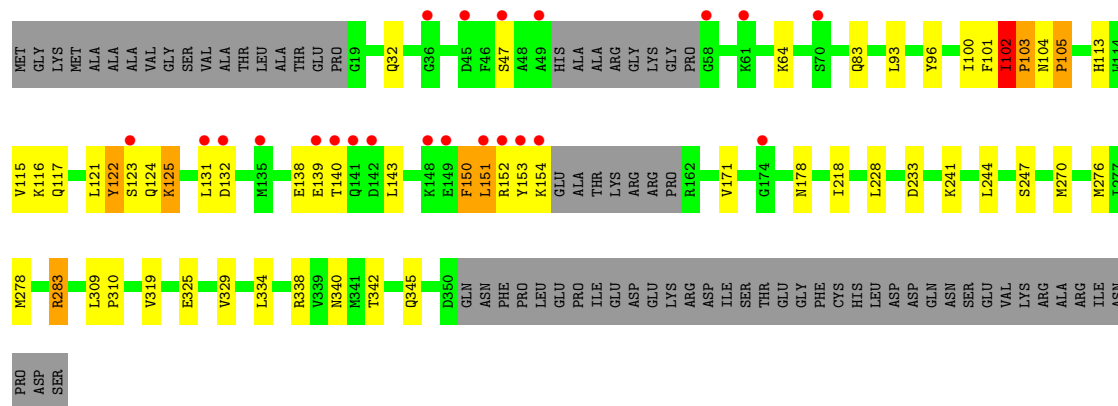




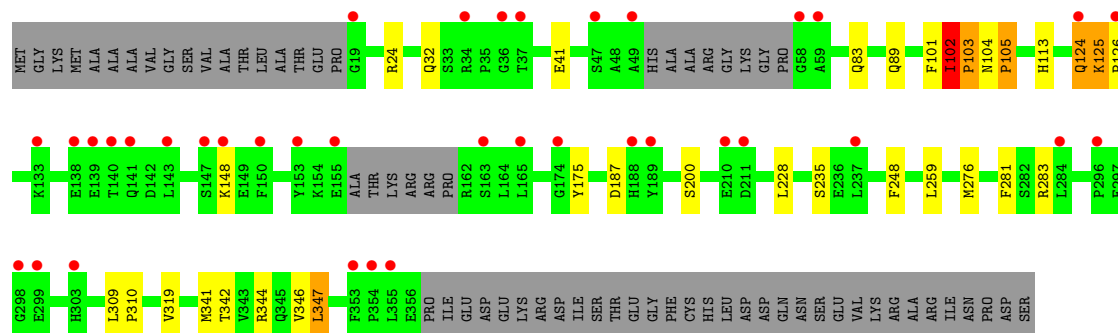
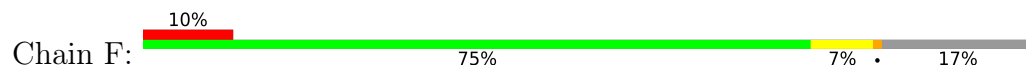
• Molecule 1: Nucleic acid dioxygenase ALKBH1



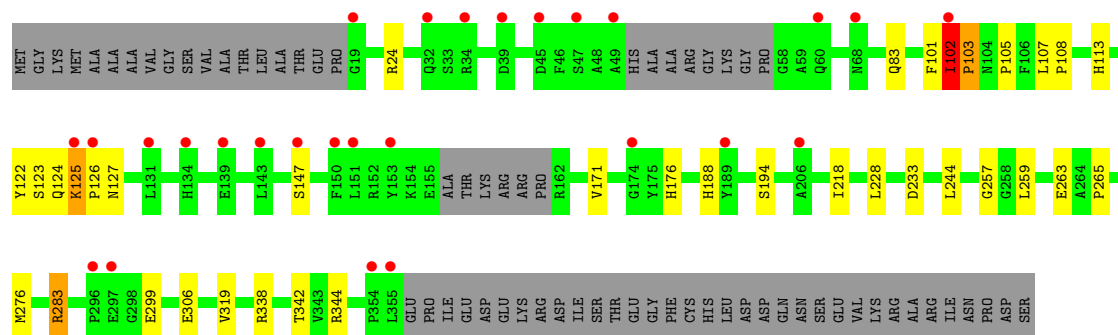
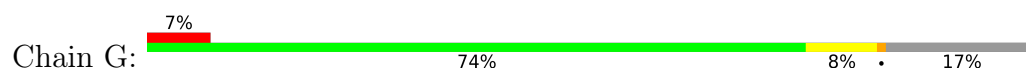
• Molecule 1: Nucleic acid dioxygenase ALKBH1



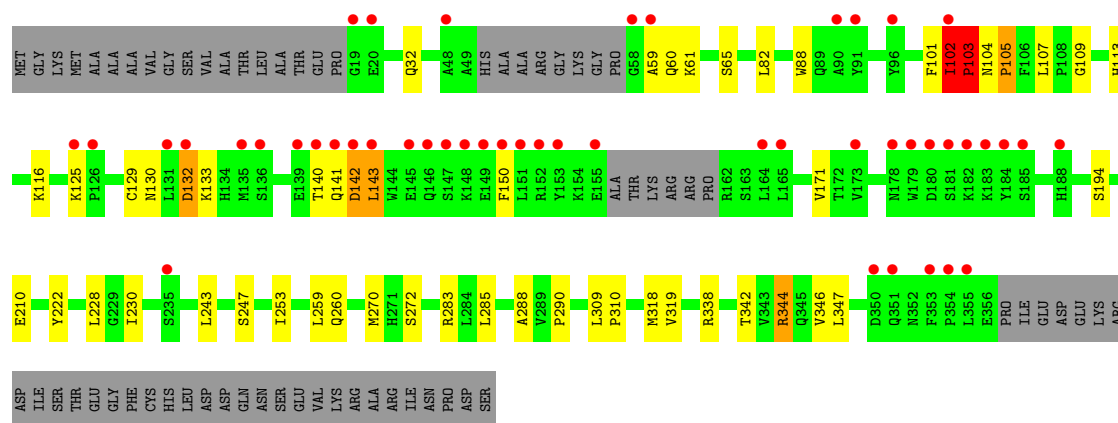
• Molecule 1: Nucleic acid dioxygenase ALKBH1



• Molecule 1: Nucleic acid dioxygenase ALKBH1



• Molecule 1: Nucleic acid dioxygenase ALKBH1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.02Å 99.17Å 126.79Å 106.60° 90.42° 93.14°	Depositor
Resolution (Å)	50.01 – 2.80 50.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.2 (50.01-2.80) 71.2 (50.01-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.216 , 0.254 0.223 , 0.226	Depositor DCC
R_{free} test set	3670 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20660	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: 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	0.61	0/2576	1.37	19/3499 (0.5%)
1	B	0.60	0/2586	1.07	12/3513 (0.3%)
1	C	0.60	0/2592	1.04	12/3519 (0.3%)
1	D	0.61	1/2577 (0.0%)	1.41	24/3502 (0.7%)
1	E	0.59	1/2543 (0.0%)	1.25	31/3452 (0.9%)
1	F	0.56	0/2604	1.06	16/3534 (0.5%)
1	G	0.57	0/2590	1.01	11/3517 (0.3%)
1	H	0.65	1/2584 (0.0%)	1.25	26/3512 (0.7%)
All	All	0.60	3/20652 (0.0%)	1.19	151/28048 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	3
1	D	0	3
1	E	0	2
1	F	0	1
1	G	0	1
1	H	0	3
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	130	ASN	CA-C	9.08	1.64	1.52
1	E	152	ARG	CA-C	5.84	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	PRO	CA-C	5.55	1.60	1.52

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASN	N-CA-C	27.17	150.41	111.56
1	A	127	ASN	CB-CA-C	-27.03	77.22	111.82
1	D	154	LYS	N-CA-C	25.45	145.60	114.04
1	B	102	ILE	CB-CA-C	21.77	150.98	111.36
1	H	102	ILE	CB-CA-C	21.21	149.96	111.36
1	D	153	TYR	N-CA-C	21.02	155.58	110.80
1	A	102	ILE	CB-CA-C	20.15	148.03	111.36
1	H	103	PRO	CB-CA-C	19.27	143.36	111.56
1	D	153	TYR	CB-CA-C	-18.92	72.76	110.42
1	H	102	ILE	CA-C-N	18.90	143.47	119.84
1	H	102	ILE	C-N-CA	18.90	143.47	119.84
1	C	102	ILE	CB-CA-C	18.64	145.28	111.36
1	D	150	PHE	N-CA-C	-18.44	82.48	109.59
1	D	102	ILE	CB-CA-C	17.59	143.37	111.36
1	G	102	ILE	CB-CA-C	16.96	142.23	111.36
1	E	102	ILE	CB-CA-C	16.34	141.10	111.36
1	F	102	ILE	CB-CA-C	16.17	140.79	111.36
1	B	102	ILE	CA-C-N	15.95	139.77	119.84
1	B	102	ILE	C-N-CA	15.95	139.77	119.84
1	A	127	ASN	CA-C-N	15.77	150.35	121.97
1	A	127	ASN	C-N-CA	15.77	150.35	121.97
1	E	154	LYS	CB-CA-C	-15.74	80.20	110.10
1	F	103	PRO	CB-CA-C	15.51	137.16	111.56
1	E	103	PRO	CB-CA-C	15.44	137.03	111.56
1	G	103	PRO	CB-CA-C	15.19	136.63	111.56
1	C	103	PRO	CB-CA-C	15.18	136.61	111.56
1	B	103	PRO	CB-CA-C	15.17	136.59	111.56
1	D	153	TYR	CA-C-N	14.96	148.89	122.42
1	D	153	TYR	C-N-CA	14.96	148.89	122.42
1	A	102	ILE	CA-C-N	14.82	138.37	119.84
1	A	102	ILE	C-N-CA	14.82	138.37	119.84
1	D	154	LYS	CB-CA-C	-14.14	83.98	109.15
1	A	103	PRO	CB-CA-C	14.05	134.75	111.56
1	E	123	SER	CB-CA-C	-13.65	89.04	111.02
1	H	142	ASP	CB-CA-C	-13.62	89.20	111.13
1	E	131	LEU	CB-CA-C	-13.57	88.55	110.94
1	E	152	ARG	N-CA-C	13.29	131.47	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	PRO	CB-CA-C	-13.18	92.41	110.60
1	A	352	ASN	CB-CA-C	12.79	132.28	109.64
1	D	142	ASP	CB-CA-C	-12.71	87.75	110.37
1	A	102	ILE	N-CA-C	-12.68	81.50	108.88
1	A	351	GLN	N-CA-C	-12.64	81.88	107.41
1	D	150	PHE	CB-CA-C	12.55	129.09	110.26
1	G	102	ILE	CA-C-N	12.52	135.49	119.84
1	G	102	ILE	C-N-CA	12.52	135.49	119.84
1	D	102	ILE	CA-C-N	12.46	135.41	119.84
1	D	102	ILE	C-N-CA	12.46	135.41	119.84
1	D	103	PRO	CB-CA-C	12.42	132.06	111.56
1	H	142	ASP	CA-C-N	12.31	137.16	120.54
1	H	142	ASP	C-N-CA	12.31	137.16	120.54
1	E	132	ASP	CB-CA-C	12.09	132.83	110.70
1	F	102	ILE	CA-C-N	12.01	134.86	119.84
1	F	102	ILE	C-N-CA	12.01	134.86	119.84
1	F	125	LYS	CA-C-N	-11.98	107.34	119.56
1	F	125	LYS	C-N-CA	-11.98	107.34	119.56
1	A	125	LYS	CB-CA-C	-11.94	96.91	110.17
1	B	102	ILE	N-CA-C	-11.71	83.59	108.88
1	E	102	ILE	N-CA-C	-11.29	84.48	108.88
1	C	102	ILE	N-CA-C	-11.25	84.59	108.88
1	C	102	ILE	CA-C-N	11.14	133.77	119.84
1	C	102	ILE	C-N-CA	11.14	133.77	119.84
1	A	350	ASP	N-CA-C	11.07	126.66	111.39
1	H	143	LEU	N-CA-C	10.91	124.20	111.11
1	E	47	SER	N-CA-C	10.90	122.74	111.07
1	E	152	ARG	CB-CA-C	-10.90	88.11	109.68
1	F	102	ILE	N-CA-C	-10.68	85.82	108.88
1	C	104	ASN	CB-CA-C	10.63	125.77	109.50
1	C	104	ASN	N-CA-C	-10.52	96.64	109.57
1	F	105	PRO	CB-CA-C	10.33	128.60	111.56
1	A	352	ASN	N-CA-C	-10.29	96.87	110.24
1	D	102	ILE	N-CA-C	-10.26	86.71	108.88
1	D	143	LEU	N-CA-C	9.58	122.61	111.11
1	G	125	LYS	CA-C-N	-9.39	108.10	119.84
1	G	125	LYS	C-N-CA	-9.39	108.10	119.84
1	G	102	ILE	N-CA-C	-9.38	88.62	108.88
1	H	102	ILE	N-CA-C	-9.20	89.00	108.88
1	E	105	PRO	CB-CA-C	8.88	126.21	111.56
1	E	131	LEU	N-CA-C	8.69	122.62	112.72
1	E	151	LEU	N-CA-C	8.64	126.85	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	141	GLN	CB-CA-C	-8.39	96.37	110.56
1	A	105	PRO	CB-CA-C	8.34	125.32	111.56
1	B	105	PRO	CB-CA-C	8.23	125.14	111.56
1	E	102	ILE	CA-C-N	8.23	130.13	119.84
1	E	102	ILE	C-N-CA	8.23	130.13	119.84
1	G	123	SER	CB-CA-C	-8.19	97.95	111.13
1	C	104	ASN	CA-C-N	8.14	130.02	119.84
1	C	104	ASN	C-N-CA	8.14	130.02	119.84
1	H	103	PRO	CA-C-N	8.12	141.62	121.80
1	H	103	PRO	C-N-CA	8.12	141.62	121.80
1	D	154	LYS	CA-C-N	8.10	136.29	121.70
1	D	154	LYS	C-N-CA	8.10	136.29	121.70
1	D	105	PRO	CB-CA-C	7.59	124.09	111.56
1	E	138	GLU	N-CA-C	-7.56	98.69	109.96
1	H	132	ASP	CB-CA-C	7.42	125.19	110.42
1	E	104	ASN	CB-CA-C	7.39	120.75	109.60
1	D	152	ARG	CB-CA-C	7.36	125.06	110.42
1	B	102	ILE	C-N-CD	-7.34	94.89	125.00
1	E	122	TYR	CB-CA-C	-7.24	96.35	110.11
1	H	104	ASN	CA-C-N	6.96	128.54	119.84
1	H	104	ASN	C-N-CA	6.96	128.54	119.84
1	A	102	ILE	C-N-CD	-6.82	97.06	125.00
1	E	47	SER	CB-CA-C	-6.77	100.25	110.88
1	F	102	ILE	C-N-CD	-6.70	97.55	125.00
1	G	125	LYS	CB-CA-C	6.69	123.36	110.17
1	H	102	ILE	C-N-CD	-6.68	97.60	125.00
1	H	59	ALA	CB-CA-C	-6.54	96.93	109.95
1	F	125	LYS	N-CA-C	6.47	124.12	109.81
1	A	353	PHE	CB-CA-C	6.47	119.40	109.50
1	A	125	LYS	N-CA-C	6.46	121.45	109.10
1	E	138	GLU	CB-CA-C	6.44	119.43	110.16
1	H	133	LYS	N-CA-C	6.38	121.20	113.41
1	A	236	GLU	N-CA-C	-6.36	101.96	110.55
1	E	125	LYS	CA-C-N	-6.33	111.93	119.84
1	E	125	LYS	C-N-CA	-6.33	111.93	119.84
1	B	104	ASN	CB-CA-C	6.30	119.11	109.60
1	G	102	ILE	C-N-CD	-6.21	99.52	125.00
1	E	124	GLN	CB-CA-C	6.19	125.10	111.30
1	G	124	GLN	CB-CA-C	6.16	123.62	110.19
1	F	124	GLN	CB-CA-C	6.06	122.95	110.40
1	F	104	ASN	CB-CA-C	6.03	122.05	110.17
1	F	126	PRO	CB-CA-C	-5.93	103.43	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ASP	CA-C-N	5.92	128.54	120.54
1	D	142	ASP	C-N-CA	5.92	128.54	120.54
1	E	131	LEU	CA-C-N	5.88	130.64	120.58
1	E	131	LEU	C-N-CA	5.88	130.64	120.58
1	E	104	ASN	CA-C-N	5.83	127.13	119.84
1	E	104	ASN	C-N-CA	5.83	127.13	119.84
1	E	153	TYR	CB-CA-C	-5.80	99.44	113.19
1	H	143	LEU	CB-CA-C	-5.71	101.67	110.81
1	D	102	ILE	C-N-CD	-5.66	101.79	125.00
1	B	101	PHE	CB-CA-C	5.64	119.53	109.38
1	H	132	ASP	N-CA-C	5.63	122.79	110.80
1	D	141	GLN	CB-CA-C	-5.62	98.77	109.95
1	C	103	PRO	CA-C-N	5.46	128.64	120.83
1	C	103	PRO	C-N-CA	5.46	128.64	120.83
1	H	60	GLN	N-CA-C	5.45	117.93	111.33
1	C	102	ILE	C-N-CD	-5.44	102.70	125.00
1	B	189	TYR	N-CA-C	5.42	117.33	108.55
1	H	107	LEU	CB-CA-C	5.41	119.25	109.61
1	F	103	PRO	N-CA-C	-5.31	101.52	112.47
1	H	125	LYS	CA-C-N	-5.29	113.33	119.47
1	H	125	LYS	C-N-CA	-5.29	113.33	119.47
1	H	59	ALA	N-CA-C	5.27	119.55	113.18
1	E	102	ILE	C-N-CD	-5.21	103.65	125.00
1	B	104	ASN	CA-C-N	5.13	126.26	119.84
1	B	104	ASN	C-N-CA	5.13	126.26	119.84
1	F	104	ASN	CA-C-N	5.10	126.21	119.84
1	F	104	ASN	C-N-CA	5.10	126.21	119.84
1	E	139	GLU	N-CA-C	5.06	118.37	111.39
1	E	104	ASN	N-CA-C	-5.04	102.56	109.71
1	H	105	PRO	CB-CA-C	5.03	119.85	111.56

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Peptide
1	A	125	LYS	Peptide
1	A	127	ASN	Peptide
1	B	102	ILE	Peptide
1	C	102	ILE	Peptide
1	C	124	GLN	Peptide
1	C	125	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	D	102	ILE	Peptide
1	D	153	TYR	Peptide
1	D	154	LYS	Peptide
1	E	102	ILE	Peptide
1	E	150	PHE	Mainchain
1	F	102	ILE	Peptide
1	G	102	ILE	Peptide
1	H	102	ILE	Peptide
1	H	103	PRO	Peptide
1	H	142	ASP	Peptide

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	2505	0	2373	32	0
1	B	2515	0	2379	21	0
1	C	2521	0	2395	20	0
1	D	2506	0	2364	19	0
1	E	2474	0	2367	25	0
1	F	2533	0	2410	14	0
1	G	2519	0	2394	15	0
1	H	2513	0	2377	23	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
3	E	10	0	4	0	0
3	F	10	0	4	0	0
3	G	10	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	10	0	4	0	0
4	A	85	0	0	0	0
4	B	68	0	0	0	0
4	C	76	0	0	0	0
4	D	51	0	0	0	0
4	E	60	0	0	0	0
4	F	47	0	0	0	0
4	G	46	0	0	0	0
4	H	53	0	0	1	0
All	All	20660	0	19091	169	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 4.

All (169) 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:E:150:PHE:C	1:E:151:LEU:HD22	1.48	1.39
1:A:101:PHE:CD1	1:A:102:ILE:O	1.81	1.33
1:C:101:PHE:CD1	1:C:102:ILE:O	1.96	1.18
1:E:150:PHE:O	1:E:151:LEU:HD22	0.99	1.17
1:E:150:PHE:O	1:E:151:LEU:CD2	1.94	1.15
1:B:101:PHE:CD1	1:B:102:ILE:O	2.00	1.12
1:E:150:PHE:C	1:E:151:LEU:CD2	2.21	1.12
1:H:101:PHE:CD1	1:H:102:ILE:O	2.04	1.11
1:A:125:LYS:HA	1:A:126:PRO:O	1.53	1.07
1:D:101:PHE:CD1	1:D:102:ILE:O	2.08	1.05
1:G:101:PHE:CD1	1:G:102:ILE:O	2.15	0.99
1:A:101:PHE:HD1	1:A:102:ILE:O	1.44	0.98
1:C:103:PRO:O	1:C:105:PRO:HD3	1.63	0.96
1:E:103:PRO:O	1:E:105:PRO:HD3	1.69	0.92
1:F:83:GLN:HG2	1:F:105:PRO:O	1.72	0.88
1:A:83:GLN:HG2	1:A:105:PRO:O	1.74	0.87
1:E:83:GLN:HG2	1:E:105:PRO:O	1.75	0.86
1:A:103:PRO:O	1:A:105:PRO:HD3	1.76	0.86
1:H:101:PHE:HD1	1:H:102:ILE:O	1.56	0.86
1:D:151:LEU:HD22	1:D:152:ARG:CG	2.05	0.86
1:E:101:PHE:CD1	1:E:102:ILE:O	2.30	0.85
1:G:125:LYS:O	1:G:126:PRO:C	2.18	0.84
1:C:101:PHE:HD1	1:C:102:ILE:O	1.61	0.83
1:D:103:PRO:O	1:D:105:PRO:HD3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:PRO:O	1:B:105:PRO:HD3	1.78	0.82
1:B:101:PHE:HD1	1:B:102:ILE:O	1.60	0.80
1:F:101:PHE:CD1	1:F:102:ILE:O	2.36	0.78
1:A:124:GLN:O	1:A:126:PRO:O	2.03	0.76
1:A:101:PHE:CE1	1:A:102:ILE:O	2.41	0.74
1:B:83:GLN:CG	1:B:105:PRO:O	2.38	0.72
1:C:233:ASP:O	1:C:283:ARG:NH2	2.25	0.70
1:G:103:PRO:O	1:G:105:PRO:HD3	1.91	0.69
1:A:125:LYS:HA	1:A:126:PRO:C	2.17	0.69
1:D:149:GLU:O	1:D:151:LEU:N	2.28	0.66
1:B:83:GLN:HG3	1:B:105:PRO:O	1.96	0.65
1:F:103:PRO:O	1:F:105:PRO:HD3	1.97	0.65
1:B:83:GLN:HG2	1:B:105:PRO:O	1.98	0.64
1:C:101:PHE:CE1	1:C:102:ILE:O	2.51	0.64
1:C:83:GLN:HG2	1:C:105:PRO:O	1.99	0.62
1:B:115:VAL:HG21	1:B:334:LEU:HD11	1.80	0.62
1:A:218:ILE:HD12	1:A:344:ARG:NH2	2.15	0.61
1:H:103:PRO:O	1:H:105:PRO:HD3	2.00	0.61
1:C:243:LEU:HD21	1:C:342:THR:HG23	1.82	0.61
1:E:150:PHE:C	1:E:151:LEU:HD23	2.22	0.60
1:E:218:ILE:O	1:E:342:THR:HG22	2.01	0.59
1:G:83:GLN:HG2	1:G:105:PRO:O	2.03	0.59
1:D:340:ASN:HD21	1:D:342:THR:HG23	1.69	0.58
1:C:342:THR:HG22	1:C:344:ARG:HE	1.69	0.57
1:H:247:SER:HB2	1:H:270:MET:HE2	1.87	0.55
1:A:239:HIS:CD2	1:A:284:LEU:HD11	2.41	0.55
1:A:126:PRO:O	1:A:127:ASN:HB2	2.07	0.55
1:B:254:PHE:CZ	1:B:276:MET:HE1	2.42	0.55
1:H:342:THR:HG21	1:H:344:ARG:NH2	2.22	0.55
1:E:309:LEU:HD12	1:E:310:PRO:HD2	1.90	0.54
1:D:151:LEU:HD22	1:D:151:LEU:C	2.32	0.54
1:F:259:LEU:HD11	1:F:281:PHE:CZ	2.42	0.54
1:G:102:ILE:HG22	1:G:103:PRO:O	2.08	0.53
1:C:239:HIS:CD2	1:C:284:LEU:HD11	2.44	0.53
1:A:125:LYS:CA	1:A:126:PRO:O	2.42	0.53
1:A:83:GLN:CG	1:A:105:PRO:O	2.55	0.52
1:E:113:HIS:CG	1:E:319:VAL:HG13	2.44	0.52
1:D:142:ASP:O	1:D:146:GLN:HB2	2.10	0.52
1:D:101:PHE:CE1	1:D:102:ILE:O	2.61	0.52
1:D:243:LEU:HD22	1:D:344:ARG:HG3	1.92	0.52
1:H:132:ASP:OD1	1:H:140:THR:HG21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:LEU:HD11	1:H:342:THR:HG23	1.93	0.51
1:C:342:THR:HG21	1:C:344:ARG:HH21	1.74	0.51
1:D:101:PHE:HD1	1:D:102:ILE:O	1.85	0.51
1:G:101:PHE:CE1	1:G:102:ILE:O	2.61	0.51
1:D:309:LEU:HD12	1:D:310:PRO:HD2	1.92	0.51
1:D:247:SER:HB2	1:D:270:MET:HE2	1.93	0.50
1:A:126:PRO:HB2	1:A:190:THR:HG21	1.92	0.50
1:G:113:HIS:CG	1:G:319:VAL:HG13	2.47	0.50
1:A:67:LEU:HD11	1:A:90:ALA:HB2	1.93	0.50
1:A:254:PHE:CZ	1:A:276:MET:HE1	2.47	0.50
1:C:249:GLY:HA3	1:C:334:LEU:HD22	1.93	0.50
1:H:346:VAL:HG23	1:H:347:LEU:HG	1.93	0.50
1:F:113:HIS:CG	1:F:319:VAL:HG13	2.46	0.50
1:A:348:ALA:HB3	1:A:351:GLN:HB2	1.94	0.49
1:C:143:LEU:HD12	1:C:164:LEU:HB3	1.93	0.49
1:H:129:CYS:HB3	1:H:171:VAL:HG22	1.94	0.49
1:E:117:GLN:NE2	1:E:121:LEU:HD23	2.26	0.49
1:E:278:MET:O	1:E:283:ARG:HG2	2.12	0.49
1:E:122:TYR:O	1:E:171:VAL:HG11	2.12	0.49
1:E:83:GLN:CG	1:E:105:PRO:O	2.54	0.49
1:B:107:LEU:HB2	1:B:110:TYR:CD1	2.48	0.49
1:B:113:HIS:CG	1:B:319:VAL:HG13	2.48	0.49
1:E:247:SER:HB2	1:E:270:MET:HE2	1.95	0.49
1:G:233:ASP:O	1:G:283:ARG:NH2	2.46	0.48
1:G:338:ARG:NH1	3:G:401:AKG:O4	2.46	0.48
1:B:211:ASP:O	1:B:213:ARG:NH1	2.46	0.48
1:C:342:THR:CG2	1:C:344:ARG:HE	2.26	0.48
1:H:113:HIS:CG	1:H:319:VAL:HG13	2.49	0.48
1:C:115:VAL:HG11	1:C:334:LEU:HD11	1.96	0.48
1:E:233:ASP:O	1:E:283:ARG:NH2	2.48	0.47
1:G:257:GLY:HA2	1:G:265:PRO:HA	1.96	0.47
1:D:152:ARG:O	1:D:153:TYR:CB	2.62	0.47
1:A:100:ILE:HB	1:A:277:ILE:HB	1.96	0.47
1:B:175:TYR:HA	1:B:189:TYR:HB2	1.97	0.47
1:A:347:LEU:HD22	1:A:351:GLN:O	2.15	0.47
1:G:218:ILE:HD12	1:G:344:ARG:NH2	2.30	0.47
1:C:151:LEU:HD21	1:C:328:GLN:HB3	1.97	0.47
1:B:346:VAL:HG23	1:B:347:LEU:HG	1.96	0.46
1:F:342:THR:HG21	1:F:344:ARG:NH2	2.31	0.46
1:H:259:LEU:HG	1:H:285:LEU:HD23	1.97	0.46
1:B:114:TRP:CZ2	1:B:199:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:PHE:CE1	1:E:102:ILE:O	2.67	0.46
1:G:122:TYR:O	1:G:171:VAL:HG11	2.16	0.46
1:H:101:PHE:C	1:H:102:ILE:O	2.50	0.46
1:G:125:LYS:C	1:G:127:ASN:N	2.73	0.45
1:A:22:ALA:HB1	1:A:264:ALA:HB2	1.98	0.45
1:H:140:THR:HG22	1:H:140:THR:O	2.15	0.45
1:F:346:VAL:HG23	1:F:347:LEU:HD12	1.98	0.45
1:B:101:PHE:CE1	1:B:102:ILE:O	2.65	0.45
1:E:247:SER:OG	1:E:338:ARG:NH2	2.50	0.45
1:D:340:ASN:ND2	1:D:342:THR:HG23	2.30	0.44
1:E:93:LEU:HB2	1:E:96:TYR:HB2	1.98	0.44
1:C:67:LEU:HD11	1:C:90:ALA:HB2	1.99	0.44
1:F:309:LEU:HD12	1:F:310:PRO:HD2	2.00	0.44
1:A:119:LEU:HD21	1:A:333:TYR:CE2	2.53	0.44
1:B:243:LEU:CD2	1:B:342:THR:HG22	2.47	0.44
1:H:253:ILE:O	1:H:290:PRO:HD2	2.18	0.44
1:H:109:GLY:O	1:H:309:LEU:HA	2.18	0.44
1:A:277:ILE:HD12	1:A:277:ILE:N	2.33	0.44
1:A:272:SER:HB3	1:A:304:CYS:SG	2.58	0.43
1:F:83:GLN:CG	1:F:105:PRO:O	2.56	0.43
1:D:110:TYR:HA	1:D:309:LEU:HD13	1.99	0.43
1:B:102:ILE:HG22	1:B:103:PRO:O	2.19	0.43
1:A:115:VAL:HG21	1:A:334:LEU:HD11	2.00	0.43
1:F:248:PHE:HE2	1:F:341:MET:HE2	1.82	0.43
1:C:237:LEU:HD12	1:C:347:LEU:HD23	2.01	0.43
1:H:222:TYR:OH	1:H:228:LEU:HD12	2.19	0.43
1:G:107:LEU:O	1:G:108:PRO:C	2.62	0.42
1:H:318:MET:O	4:H:501:HOH:O	2.22	0.42
1:F:175:TYR:CD2	1:F:346:VAL:HG21	2.54	0.42
1:A:118:CYS:SG	1:A:341:MET:SD	3.17	0.42
1:D:178:ASN:HD22	1:D:178:ASN:C	2.27	0.42
1:A:190:THR:O	1:A:191:PRO:C	2.63	0.42
1:E:115:VAL:HG21	1:E:334:LEU:HD11	2.01	0.42
1:H:230:ILE:HA	1:H:288:ALA:HB2	2.01	0.42
1:B:172:THR:OG1	1:B:176:HIS:ND1	2.43	0.42
1:C:215:GLU:OE2	1:C:346:VAL:N	2.51	0.41
1:F:89:GLN:O	1:F:103:PRO:HD2	2.20	0.41
1:C:243:LEU:C	1:C:244:LEU:HD23	2.45	0.41
1:E:117:GLN:HE22	1:E:121:LEU:HD23	1.84	0.41
1:F:346:VAL:HG23	1:F:347:LEU:CD1	2.50	0.41
1:A:351:GLN:C	1:A:352:ASN:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HD13	1:C:294:PRO:HB3	2.01	0.41
1:H:82:LEU:HD13	1:H:88:TRP:CZ2	2.54	0.41
1:H:129:CYS:O	1:H:132:ASP:HB2	2.20	0.41
1:E:325:GLU:O	1:E:329:VAL:HG23	2.20	0.41
1:E:241:LYS:HG2	1:E:345:GLN:CD	2.45	0.41
1:H:243:LEU:HD21	1:H:344:ARG:NH1	2.36	0.41
1:D:150:PHE:CD1	1:D:150:PHE:N	2.88	0.41
1:D:151:LEU:CD2	1:D:152:ARG:CG	2.88	0.41
1:B:99:PHE:HE1	1:B:276:MET:HE3	1.86	0.41
1:B:198:PHE:CD2	1:B:318:MET:HG3	2.56	0.41
1:D:113:HIS:CG	1:D:319:VAL:HG13	2.56	0.41
1:H:247:SER:OG	1:H:338:ARG:NH2	2.54	0.41
1:H:309:LEU:O	1:H:310:PRO:C	2.64	0.41
1:B:119:LEU:HD21	1:B:333:TYR:CE2	2.56	0.40
1:E:244:LEU:O	1:E:342:THR:HA	2.21	0.40
1:F:259:LEU:HD11	1:F:281:PHE:CE1	2.56	0.40
1:A:119:LEU:HB3	1:A:165:LEU:HD11	2.02	0.40
1:A:119:LEU:HD22	1:A:165:LEU:HD11	2.03	0.40
1:A:244:LEU:O	1:A:342:THR:HA	2.22	0.40
1:G:176:HIS:HB2	1:G:188:HIS:ND1	2.37	0.40
1:A:101:PHE:C	1:A:102:ILE:O	2.49	0.40
1:A:222:TYR:HB3	1:A:292:VAL:HG21	2.03	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	315/389 (81%)	302 (96%)	13 (4%)	0	100	100
1	B	317/389 (82%)	300 (95%)	17 (5%)	0	100	100
1	C	317/389 (82%)	299 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	317/389 (82%)	301 (95%)	16 (5%)	0	100	100
1	E	311/389 (80%)	296 (95%)	15 (5%)	0	100	100
1	F	318/389 (82%)	307 (96%)	11 (4%)	0	100	100
1	G	317/389 (82%)	303 (96%)	14 (4%)	0	100	100
1	H	318/389 (82%)	302 (95%)	16 (5%)	0	100	100
All	All	2530/3112 (81%)	2410 (95%)	120 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	259/331 (78%)	245 (95%)	14 (5%)	20	51
1	B	259/331 (78%)	246 (95%)	13 (5%)	22	54
1	C	260/331 (78%)	245 (94%)	15 (6%)	18	49
1	D	257/331 (78%)	244 (95%)	13 (5%)	21	54
1	E	256/331 (77%)	244 (95%)	12 (5%)	23	57
1	F	261/331 (79%)	248 (95%)	13 (5%)	22	54
1	G	259/331 (78%)	247 (95%)	12 (5%)	24	58
1	H	257/331 (78%)	245 (95%)	12 (5%)	23	57
All	All	2068/2648 (78%)	1964 (95%)	104 (5%)	22	54

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	143	LEU
1	A	148	LYS
1	A	151	LEU
1	A	181	SER

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Mol	Chain	Res	Type
1	A	210	GLU
1	A	228	LEU
1	A	234	ARG
1	A	243	LEU
1	A	244	LEU
1	A	283	ARG
1	A	342	THR
1	A	349	THR
1	A	353	PHE
1	B	121	LEU
1	B	143	LEU
1	B	148	LYS
1	B	178	ASN
1	B	189	TYR
1	B	210	GLU
1	B	228	LEU
1	B	243	LEU
1	B	260	GLN
1	B	283	ARG
1	B	325	GLU
1	B	342	THR
1	B	346	VAL
1	C	24	ARG
1	C	121	LEU
1	C	140	THR
1	C	178	ASN
1	C	185	SER
1	C	187	ASP
1	C	189	TYR
1	C	210	GLU
1	C	228	LEU
1	C	244	LEU
1	C	283	ARG
1	C	299	GLU
1	C	325	GLU
1	C	342	THR
1	C	353	PHE
1	D	121	LEU
1	D	129	CYS
1	D	142	ASP
1	D	151	LEU
1	D	178	ASN

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Mol	Chain	Res	Type
1	D	219	LEU
1	D	228	LEU
1	D	243	LEU
1	D	244	LEU
1	D	283	ARG
1	D	297	GLU
1	D	325	GLU
1	D	346	VAL
1	E	32	GLN
1	E	64	LYS
1	E	100	ILE
1	E	116	LYS
1	E	125	LYS
1	E	140	THR
1	E	143	LEU
1	E	178	ASN
1	E	228	LEU
1	E	276	MET
1	E	283	ARG
1	E	340	ASN
1	F	24	ARG
1	F	32	GLN
1	F	41	GLU
1	F	124	GLN
1	F	125	LYS
1	F	148	LYS
1	F	187	ASP
1	F	200	SER
1	F	228	LEU
1	F	235	SER
1	F	276	MET
1	F	283	ARG
1	F	347	LEU
1	G	24	ARG
1	G	147	SER
1	G	194	SER
1	G	228	LEU
1	G	244	LEU
1	G	259	LEU
1	G	263	GLU
1	G	276	MET
1	G	283	ARG

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Mol	Chain	Res	Type
1	G	299	GLU
1	G	306	GLU
1	G	342	THR
1	H	32	GLN
1	H	61	LYS
1	H	65	SER
1	H	116	LYS
1	H	143	LEU
1	H	150	PHE
1	H	194	SER
1	H	210	GLU
1	H	260	GLN
1	H	272	SER
1	H	283	ARG
1	H	344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	328	GLN
1	B	113	HIS
1	B	260	GLN
1	C	127	ASN
1	C	134	HIS
1	C	146	GLN
1	C	178	ASN
1	C	188	HIS
1	C	220	ASN
1	C	239	HIS
1	C	250	GLN
1	D	124	GLN
1	D	127	ASN
1	D	146	GLN
1	D	178	ASN
1	D	220	ASN
1	D	250	GLN
1	D	340	ASN
1	D	351	GLN
1	E	220	ASN
1	E	340	ASN
1	F	32	GLN

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Mol	Chain	Res	Type
1	F	76	ASN
1	F	113	HIS
1	F	124	GLN
1	F	127	ASN
1	F	178	ASN
1	G	117	GLN
1	G	127	ASN
1	G	178	ASN
1	H	32	GLN
1	H	111	GLN
1	H	124	GLN
1	H	127	ASN
1	H	178	ASN
1	H	220	ASN
1	H	250	GLN
1	H	340	ASN

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AKG	C	401	2	9,9,9	1.76	1 (11%)	11,11,11	1.32	1 (9%)
3	AKG	F	401	2	9,9,9	1.74	1 (11%)	11,11,11	1.44	1 (9%)
3	AKG	E	401	2	9,9,9	1.80	1 (11%)	11,11,11	1.50	2 (18%)
3	AKG	A	401	2	9,9,9	1.83	1 (11%)	11,11,11	1.45	2 (18%)
3	AKG	D	401	2	9,9,9	2.00	2 (22%)	11,11,11	1.20	1 (9%)
3	AKG	B	401	2	9,9,9	1.99	1 (11%)	11,11,11	1.39	1 (9%)
3	AKG	G	401	2	9,9,9	1.71	1 (11%)	11,11,11	1.63	1 (9%)
3	AKG	H	401	2	9,9,9	1.83	1 (11%)	11,11,11	1.48	3 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AKG	C	401	2	-	6/9/9/9	-
3	AKG	F	401	2	-	3/9/9/9	-
3	AKG	E	401	2	-	3/9/9/9	-
3	AKG	A	401	2	-	3/9/9/9	-
3	AKG	D	401	2	-	2/9/9/9	-
3	AKG	B	401	2	-	3/9/9/9	-
3	AKG	G	401	2	-	6/9/9/9	-
3	AKG	H	401	2	-	5/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	AKG	C2-C1	-5.17	1.45	1.53
3	D	401	AKG	C2-C1	-5.04	1.45	1.53
3	H	401	AKG	C2-C1	-4.63	1.46	1.53
3	A	401	AKG	C2-C1	-4.54	1.46	1.53
3	E	401	AKG	C2-C1	-4.45	1.46	1.53
3	C	401	AKG	C2-C1	-4.44	1.46	1.53
3	F	401	AKG	C2-C1	-4.34	1.47	1.53
3	G	401	AKG	C2-C1	-4.23	1.47	1.53
3	D	401	AKG	O2-C1	-2.03	1.25	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	AKG	C3-C2-C1	3.58	121.95	115.86
3	C	401	AKG	C3-C2-C1	3.15	121.21	115.86
3	F	401	AKG	C3-C2-C1	3.14	121.20	115.86
3	B	401	AKG	C3-C2-C1	2.65	120.35	115.86
3	A	401	AKG	O1-C1-C2	-2.64	118.53	121.81
3	E	401	AKG	O1-C1-C2	-2.63	118.53	121.81
3	H	401	AKG	O3-C5-C4	-2.35	115.63	123.09
3	E	401	AKG	O2-C1-C2	2.20	119.70	113.59
3	D	401	AKG	C3-C2-C1	2.13	119.48	115.86
3	H	401	AKG	C3-C2-C1	2.12	119.46	115.86
3	H	401	AKG	O1-C1-C2	-2.04	119.27	121.81
3	A	401	AKG	C3-C2-C1	2.02	119.30	115.86

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	AKG	O2-C1-C2-C3
3	B	401	AKG	O2-C1-C2-C3
3	C	401	AKG	O2-C1-C2-C3
3	F	401	AKG	O2-C1-C2-C3
3	G	401	AKG	O2-C1-C2-C3
3	G	401	AKG	C1-C2-C3-C4
3	H	401	AKG	O1-C1-C2-O5
3	H	401	AKG	O1-C1-C2-C3
3	H	401	AKG	O2-C1-C2-C3
3	H	401	AKG	C1-C2-C3-C4
3	C	401	AKG	O1-C1-C2-O5
3	C	401	AKG	O1-C1-C2-C3
3	E	401	AKG	O2-C1-C2-O5
3	G	401	AKG	O5-C2-C3-C4
3	C	401	AKG	C3-C4-C5-O4
3	G	401	AKG	C2-C3-C4-C5
3	C	401	AKG	C3-C4-C5-O3
3	B	401	AKG	C3-C4-C5-O4
3	E	401	AKG	C3-C4-C5-O4
3	A	401	AKG	C3-C4-C5-O4
3	B	401	AKG	C3-C4-C5-O3
3	E	401	AKG	C3-C4-C5-O3
3	A	401	AKG	C3-C4-C5-O3
3	F	401	AKG	C3-C4-C5-O3
3	D	401	AKG	C3-C4-C5-O3
3	C	401	AKG	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	G	401	AKG	C3-C4-C5-O3
3	G	401	AKG	C3-C4-C5-O4
3	F	401	AKG	C3-C4-C5-O4
3	D	401	AKG	C3-C4-C5-O4
3	H	401	AKG	O5-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	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, 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	321/389 (82%)	0.15	9 (2%) 55 45	20, 40, 81, 105	0
1	B	323/389 (83%)	0.32	24 (7%) 20 15	20, 41, 102, 126	0
1	C	323/389 (83%)	0.31	19 (5%) 28 21	21, 46, 83, 106	0
1	D	323/389 (83%)	0.48	32 (9%) 13 9	19, 49, 107, 135	0
1	E	317/389 (81%)	0.43	22 (6%) 23 16	23, 48, 102, 143	0
1	F	324/389 (83%)	0.76	37 (11%) 10 7	32, 59, 114, 137	0
1	G	323/389 (83%)	0.67	27 (8%) 17 12	32, 59, 115, 133	0
1	H	324/389 (83%)	0.89	48 (14%) 5 4	28, 58, 130, 154	0
All	All	2578/3112 (82%)	0.50	218 (8%) 16 12	19, 51, 107, 154	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	152	ARG	7.2
1	B	142	ASP	6.9
1	H	132	ASP	6.4
1	C	19	GLY	5.5
1	B	150	PHE	5.0
1	H	19	GLY	4.9
1	B	146	GLN	4.8
1	D	59	ALA	4.7
1	H	141	GLN	4.6
1	H	102	ILE	4.5
1	E	131	LEU	4.5
1	B	151	LEU	4.4
1	H	147	SER	4.4
1	F	139	GLU	4.3
1	D	110	TYR	4.3
1	B	153	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	47	SER	4.2
1	F	143	LEU	4.1
1	G	296	PRO	3.9
1	H	164	LEU	3.9
1	E	153	TYR	3.9
1	H	131	LEU	3.8
1	E	141	GLN	3.8
1	E	151	LEU	3.8
1	D	311	ALA	3.8
1	H	181	SER	3.8
1	H	153	TYR	3.8
1	B	152	ARG	3.7
1	C	22	ALA	3.7
1	G	151	LEU	3.7
1	H	142	ASP	3.7
1	B	140	THR	3.7
1	F	189	TYR	3.6
1	F	354	PRO	3.6
1	D	19	GLY	3.6
1	G	147	SER	3.5
1	H	155	GLU	3.5
1	F	355	LEU	3.5
1	D	144	TRP	3.5
1	E	132	ASP	3.5
1	H	350	ASP	3.5
1	F	296	PRO	3.4
1	D	143	LEU	3.4
1	B	149	GLU	3.4
1	F	155	GLU	3.4
1	H	143	LEU	3.3
1	F	153	TYR	3.3
1	B	155	GLU	3.3
1	C	59	ALA	3.3
1	E	49	ALA	3.3
1	D	262	ASP	3.2
1	D	327	TRP	3.2
1	D	151	LEU	3.2
1	H	152	ARG	3.2
1	D	146	GLN	3.2
1	E	123	SER	3.2
1	B	164	LEU	3.1
1	B	166	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	68	ASN	3.1
1	B	141	GLN	3.0
1	C	155	GLU	3.0
1	G	355	LEU	3.0
1	F	174	GLY	3.0
1	D	310	PRO	3.0
1	H	149	GLU	3.0
1	E	135	MET	3.0
1	D	154	LYS	2.9
1	B	144	TRP	2.9
1	H	355	LEU	2.9
1	D	109	GLY	2.9
1	C	41	GLU	2.9
1	H	353	PHE	2.9
1	B	19	GLY	2.9
1	G	189	TYR	2.9
1	C	211	ASP	2.9
1	F	49	ALA	2.9
1	E	140	THR	2.9
1	C	20	GLU	2.9
1	B	59	ALA	2.8
1	H	91	TYR	2.8
1	E	58	GLY	2.8
1	H	179	TRP	2.8
1	D	107	LEU	2.8
1	F	124	GLN	2.8
1	H	173	VAL	2.8
1	F	237	LEU	2.8
1	B	147	SER	2.8
1	E	47	SER	2.8
1	F	163	SER	2.8
1	E	139	GLU	2.7
1	G	49	ALA	2.7
1	G	143	LEU	2.7
1	H	184	TYR	2.7
1	H	135	MET	2.7
1	G	139	GLU	2.7
1	F	210	GLU	2.7
1	F	47	SER	2.7
1	C	144	TRP	2.7
1	F	58	GLY	2.7
1	H	151	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	150	PHE	2.6
1	F	188	HIS	2.6
1	H	140	THR	2.6
1	A	138	GLU	2.6
1	B	143	LEU	2.6
1	D	75	GLN	2.6
1	H	146	GLN	2.6
1	H	48	ALA	2.6
1	D	153	TYR	2.6
1	B	324	MET	2.6
1	F	19	GLY	2.6
1	E	61	LYS	2.6
1	E	154	LYS	2.6
1	G	153	TYR	2.6
1	D	349	THR	2.6
1	E	70	SER	2.5
1	C	154	LYS	2.5
1	H	183	LYS	2.5
1	B	189	TYR	2.5
1	F	284	LEU	2.5
1	G	102	ILE	2.5
1	E	174	GLY	2.5
1	A	311	ALA	2.5
1	G	45	ASP	2.5
1	G	125	LYS	2.5
1	D	314	PRO	2.5
1	A	58	GLY	2.5
1	A	151	LEU	2.5
1	D	20	GLU	2.5
1	H	354	PRO	2.4
1	F	353	PHE	2.4
1	G	297	GLU	2.4
1	G	39	ASP	2.4
1	H	139	GLU	2.4
1	G	32	GLN	2.4
1	F	37	THR	2.4
1	F	140	THR	2.4
1	H	126	PRO	2.4
1	E	36	GLY	2.4
1	B	317	SER	2.4
1	H	90	ALA	2.4
1	C	58	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	36	GLY	2.4
1	G	34	ARG	2.4
1	B	145	GLU	2.4
1	D	138	GLU	2.4
1	B	134	HIS	2.4
1	A	19	GLY	2.3
1	G	60	GLN	2.3
1	D	147	SER	2.3
1	F	165	LEU	2.3
1	H	188	HIS	2.3
1	G	126	PRO	2.3
1	A	127	ASN	2.3
1	G	206	ALA	2.3
1	H	59	ALA	2.3
1	G	134	HIS	2.3
1	E	148	LYS	2.3
1	D	105	PRO	2.3
1	G	354	PRO	2.3
1	F	59	ALA	2.3
1	D	350	ASP	2.3
1	F	141	GLN	2.3
1	G	150	PHE	2.3
1	F	211	ASP	2.2
1	C	102	ILE	2.2
1	F	34	ARG	2.2
1	F	126	PRO	2.2
1	A	20	GLU	2.2
1	E	142	ASP	2.2
1	D	112	TRP	2.2
1	D	140	THR	2.2
1	F	147	SER	2.2
1	C	151	LEU	2.2
1	C	331	ALA	2.2
1	C	348	ALA	2.2
1	D	155	GLU	2.2
1	F	299	GLU	2.2
1	G	19	GLY	2.2
1	F	150	PHE	2.2
1	G	131	LEU	2.2
1	D	22	ALA	2.2
1	H	145	GLU	2.2
1	F	133	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	148	LYS	2.2
1	A	153	TYR	2.2
1	C	70	SER	2.2
1	D	356	GLU	2.2
1	E	149	GLU	2.2
1	A	261	ARG	2.1
1	C	298	GLY	2.1
1	F	298	GLY	2.1
1	F	138	GLU	2.1
1	H	178	ASN	2.1
1	B	148	LYS	2.1
1	D	141	GLN	2.1
1	D	134	HIS	2.1
1	C	319	VAL	2.1
1	H	125	LYS	2.1
1	B	58	GLY	2.1
1	D	121	LEU	2.1
1	H	58	GLY	2.1
1	D	136	SER	2.1
1	H	136	SER	2.1
1	H	235	SER	2.1
1	C	75	GLN	2.1
1	H	351	GLN	2.1
1	F	148	LYS	2.1
1	G	174	GLY	2.1
1	H	96	TYR	2.1
1	H	182	LYS	2.0
1	F	303	HIS	2.0
1	H	165	LEU	2.0
1	E	45	ASP	2.0
1	H	180	ASP	2.0
1	H	185	SER	2.0
1	C	21	ASP	2.0
1	H	20	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	AKG	H	401	10/10	0.86	0.15	52,59,63,65	0
3	AKG	G	401	10/10	0.92	0.14	64,67,72,73	0
3	AKG	F	401	10/10	0.95	0.09	62,67,68,69	0
3	AKG	D	401	10/10	0.95	0.08	34,35,37,37	0
3	AKG	E	401	10/10	0.95	0.10	42,53,59,62	0
3	AKG	A	401	10/10	0.96	0.11	28,29,31,31	0
3	AKG	C	401	10/10	0.97	0.07	24,27,28,28	0
3	AKG	B	401	10/10	0.97	0.08	25,28,28,30	0
2	MN	B	400	1/1	0.99	0.03	23,23,23,23	0
2	MN	D	400	1/1	0.99	0.02	19,19,19,19	0
2	MN	F	400	1/1	0.99	0.02	39,39,39,39	0
2	MN	G	400	1/1	0.99	0.04	38,38,38,38	0
2	MN	E	400	1/1	1.00	0.02	36,36,36,36	0
2	MN	C	400	1/1	1.00	0.01	19,19,19,19	0
2	MN	A	400	1/1	1.00	0.02	19,19,19,19	0
2	MN	H	400	1/1	1.00	0.05	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.