



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:55 AM UTC

PDB ID : 3U5O / pdb_00003u5o
Title : Crystal structure of the complex of TRIM33 PHD-Bromo and H3(1-22)K9me
3K14acK18ac histone peptide
Authors : Wang, Z.; Patel, D.J.
Deposited on : 2011-10-11
Resolution : 2.70 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

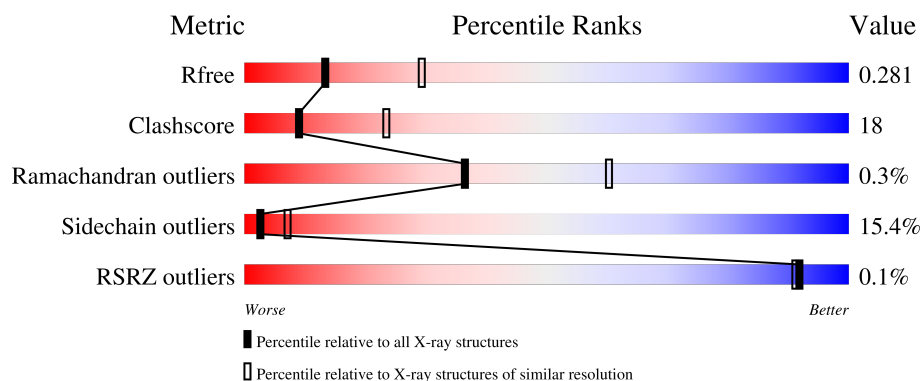
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	207	
1	B	207	
1	C	207	
1	D	207	
1	E	207	

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Mol	Chain	Length	Quality of chain
1	F	207	
1	G	207	
1	H	207	
2	I	22	
2	J	22	
2	K	22	
2	L	22	
2	M	22	
2	N	22	
2	O	22	
2	P	22	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	M3L	I	9	-	-	X	-
2	M3L	K	9	-	-	X	-
2	M3L	P	9	-	-	X	-
3	ZN	A	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13522 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 E3 ubiquitin-protein ligase TRIM33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1530	977	253	285	15			
1	B	189	Total	C	N	O	S	0	0	0
			1535	981	254	285	15			
1	C	195	Total	C	N	O	S	0	0	0
			1573	1003	262	293	15			
1	D	187	Total	C	N	O	S	0	0	0
			1517	969	250	283	15			
1	E	188	Total	C	N	O	S	0	0	0
			1526	975	252	284	15			
1	F	189	Total	C	N	O	S	0	0	0
			1530	977	253	285	15			
1	G	187	Total	C	N	O	S	0	0	0
			1515	968	250	282	15			
1	H	191	Total	C	N	O	S	0	0	0
			1548	988	257	288	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	881	SER	-	expression tag	UNP Q9UPN9
B	881	SER	-	expression tag	UNP Q9UPN9
C	881	SER	-	expression tag	UNP Q9UPN9
D	881	SER	-	expression tag	UNP Q9UPN9
E	881	SER	-	expression tag	UNP Q9UPN9
F	881	SER	-	expression tag	UNP Q9UPN9
G	881	SER	-	expression tag	UNP Q9UPN9
H	881	SER	-	expression tag	UNP Q9UPN9

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	J	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	K	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	L	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	M	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	N	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	O	20	Total	C	N	O	0	0	0
			154	93	34	27			
2	P	20	Total	C	N	O	0	0	0
			154	93	34	27			

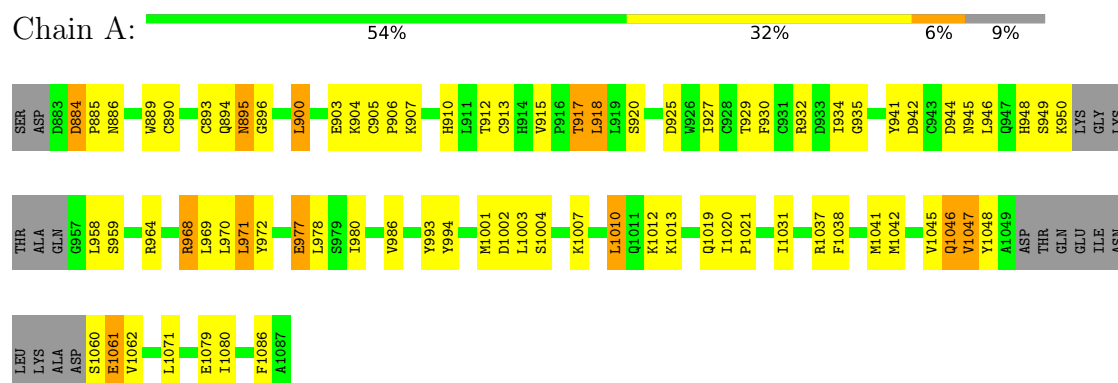
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		
3	G	2	Total	Zn	0	0
			2	2		
3	H	2	Total	Zn	0	0
			2	2		

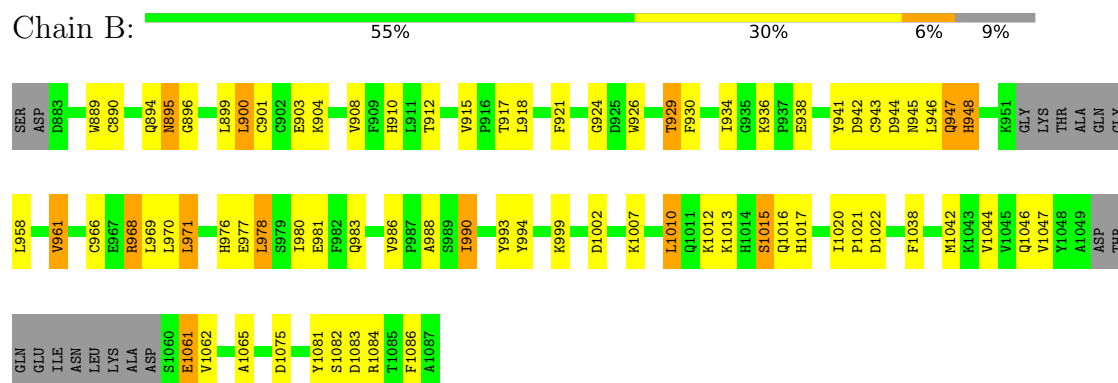
3 Residue-property plots [i](#)

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: E3 ubiquitin-protein ligase TRIM33



• Molecule 1: E3 ubiquitin-protein ligase TRIM33



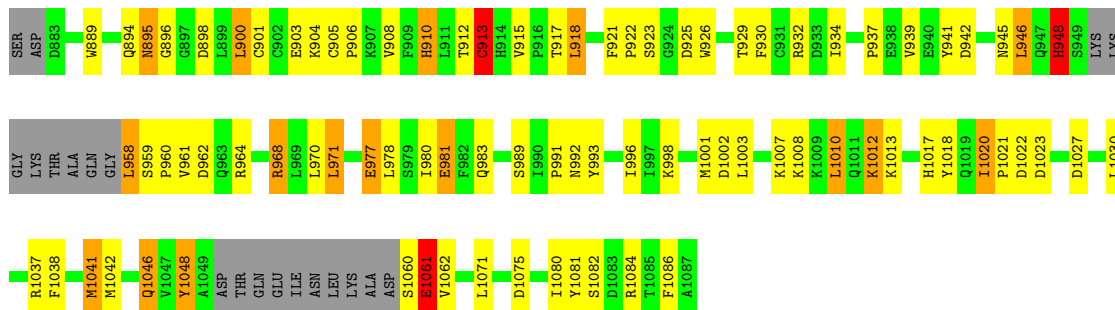
• Molecule 1: E3 ubiquitin-protein ligase TRIM33





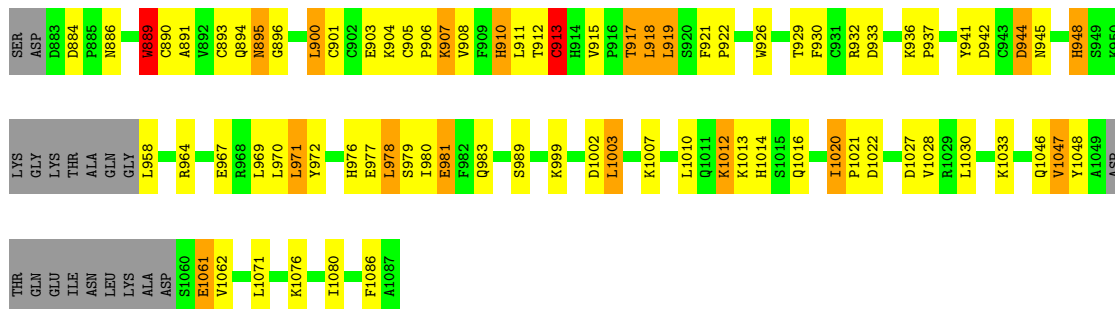
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain D: 49% 32% 8% 10%



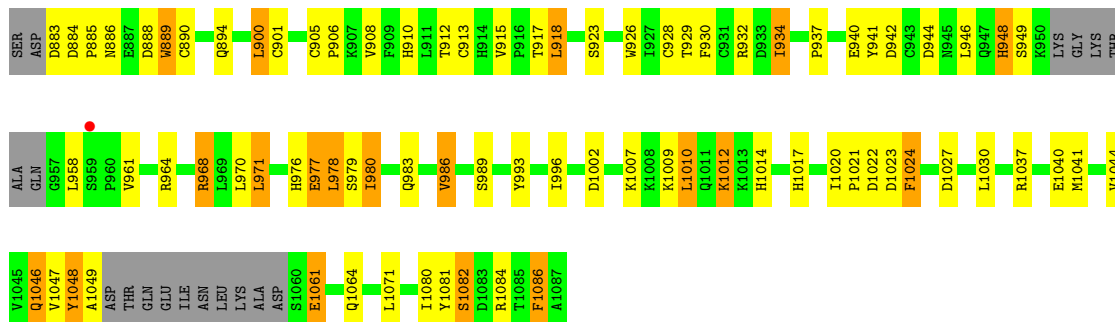
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain E: 53% 29% 8% 9%



• Molecule 1: E3 ubiquitin-protein ligase TRIM33

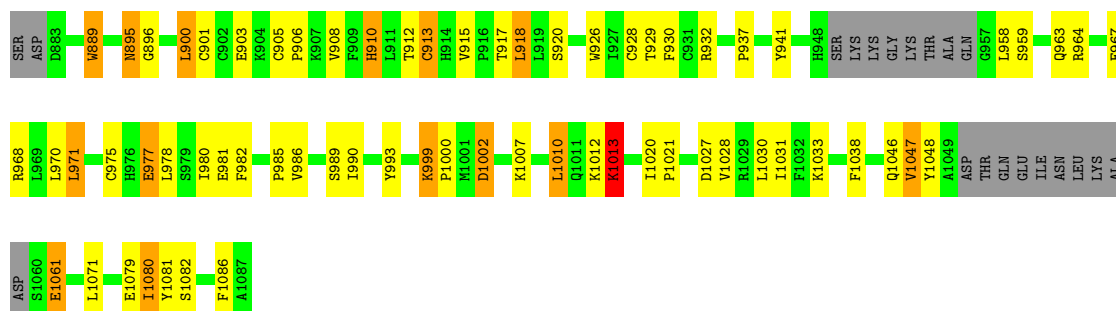
Chain F: 53% 29% 9% 9%



• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain G: 58% 25% 7% 10%

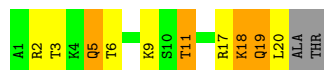




- Molecule 1: E3 ubiquitin-protein ligase TRIM33



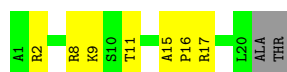
- Molecule 2: Histone H3.1



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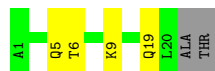
- Molecule 2: Histone H3.1



● Molecule 2: Histone H3.1

Chain M:  55% 32% 5% 9%

● Molecule 2: Histone H3.1

Chain N:  73% 18% 9%

● Molecule 2: Histone H3.1

Chain O:  45% 32% 14% 9%

● Molecule 2: Histone H3.1

Chain P:  50% 27% 9% 5% 9%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.64Å 63.65Å 125.19Å 90.05° 89.98° 89.93°	Depositor
Resolution (Å)	28.47 – 2.70 28.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (28.47-2.70) 92.9 (28.47-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.280 0.204 , 0.281	Depositor DCC
R_{free} test set	1932 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.470 for -k,h,l 0.470 for k,-h,l 0.477 for h,-k,-l 0.477 for -h,k,-l 0.477 for -h,-k,l 0.476 for -k,-h,-l 0.477 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13522	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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: M3L, ZN, ALY

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	0.97	0/1566	1.18	6/2116 (0.3%)
1	B	0.97	1/1571 (0.1%)	1.17	5/2122 (0.2%)
1	C	0.92	1/1610 (0.1%)	1.18	9/2175 (0.4%)
1	D	1.08	4/1553 (0.3%)	1.19	6/2100 (0.3%)
1	E	0.94	1/1562 (0.1%)	1.17	11/2111 (0.5%)
1	F	0.97	1/1566 (0.1%)	1.17	10/2116 (0.5%)
1	G	0.92	0/1551	1.20	9/2097 (0.4%)
1	H	0.96	2/1584 (0.1%)	1.19	11/2139 (0.5%)
2	I	0.78	0/123	1.45	2/160 (1.2%)
2	J	0.80	0/123	1.05	1/160 (0.6%)
2	K	0.79	0/123	0.94	0/160
2	L	0.73	0/123	0.88	0/160
2	M	0.87	0/123	1.01	0/160
2	N	0.76	0/123	0.98	0/160
2	O	0.74	0/123	0.93	0/160
2	P	0.85	0/123	1.18	1/160 (0.6%)
All	All	0.95	10/13547 (0.1%)	1.17	71/18256 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	948	HIS	ND1-CE1	15.46	1.48	1.32
1	E	948	HIS	CE1-NE2	8.33	1.40	1.32
1	D	948	HIS	CG-CD2	7.91	1.44	1.35
1	B	948	HIS	ND1-CE1	7.35	1.39	1.32
1	H	948	HIS	ND1-CE1	6.83	1.39	1.32
1	C	948	HIS	CE1-NE2	6.77	1.39	1.32
1	F	948	HIS	CE1-NE2	6.14	1.38	1.32
1	H	948	HIS	CG-CD2	5.61	1.42	1.35
1	D	948	HIS	CB-CG	5.23	1.57	1.50
1	D	948	HIS	CG-ND1	-5.23	1.32	1.38

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	11	THR	N-CA-C	11.10	122.95	111.07
1	D	913	CYS	N-CA-C	-8.51	103.48	114.04
1	F	986	VAL	CA-C-N	-8.46	112.02	120.31
1	F	986	VAL	C-N-CA	-8.46	112.02	120.31
1	D	1086	PHE	N-CA-C	7.76	121.17	108.52
1	B	983	GLN	N-CA-C	7.71	119.76	111.36
1	C	1086	PHE	N-CA-C	7.67	121.22	108.73
1	C	896	GLY	N-CA-C	7.49	122.12	110.96
1	G	959	SER	CA-C-N	7.43	126.97	119.24
1	G	959	SER	C-N-CA	7.43	126.97	119.24
1	E	913	CYS	N-CA-C	-7.20	104.13	113.12
1	H	896	GLY	N-CA-C	7.18	121.62	111.14
1	C	999	LYS	CA-C-N	7.16	127.12	120.03
1	C	999	LYS	C-N-CA	7.16	127.12	120.03
1	C	913	CYS	N-CA-C	-7.08	105.18	113.88
1	G	913	CYS	N-CA-C	-7.07	104.64	113.55
1	H	1086	PHE	N-CA-C	6.89	119.75	108.52
1	A	1086	PHE	N-CA-C	6.88	120.27	108.02
1	G	1086	PHE	N-CA-C	6.87	119.72	108.52
1	H	1020	ILE	CB-CA-C	6.85	116.04	109.33
1	H	913	CYS	N-CA-C	-6.78	104.01	112.90
1	F	910	HIS	N-CA-C	-6.64	101.14	110.50
1	G	999	LYS	CA-C-N	6.60	128.83	120.51
1	G	999	LYS	C-N-CA	6.60	128.83	120.51
1	B	1086	PHE	N-CA-C	6.54	119.12	107.80
1	A	910	HIS	N-CA-C	-6.53	101.30	110.50
1	H	910	HIS	N-CA-C	-6.49	101.97	110.53
1	E	1086	PHE	N-CA-C	6.41	118.96	108.52
1	E	889	TRP	N-CA-C	6.34	119.06	109.23
1	F	983	GLN	N-CA-C	6.25	118.17	111.36
1	D	1061	GLU	N-CA-C	6.13	118.75	111.33
1	D	1020	ILE	CB-CA-C	6.01	115.22	109.33
2	P	11	THR	N-CA-C	5.89	119.56	112.38
1	C	986	VAL	CA-C-N	-5.88	113.91	119.85
1	C	986	VAL	C-N-CA	-5.88	113.91	119.85
1	F	1082	SER	N-CA-C	-5.85	106.28	113.41
1	B	999	LYS	CA-C-N	5.75	126.23	120.14
1	B	999	LYS	C-N-CA	5.75	126.23	120.14
1	E	948	HIS	CG-CD2-NE2	-5.69	101.51	107.20
1	H	948	HIS	ND1-CG-CD2	-5.64	100.45	106.10
1	E	999	LYS	CA-C-N	5.63	126.11	120.14
1	E	999	LYS	C-N-CA	5.63	126.11	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	910	HIS	N-CA-C	-5.59	102.75	110.35
1	B	910	HIS	N-CA-C	-5.53	102.83	110.35
1	G	1033	LYS	N-CA-C	-5.51	104.97	110.97
1	A	913	CYS	N-CA-C	-5.50	107.11	113.88
1	D	910	HIS	N-CA-C	-5.44	102.95	110.35
1	F	886	ASN	N-CA-C	5.44	117.95	109.52
1	F	1024	PHE	N-CA-C	-5.38	105.05	111.03
1	E	886	ASN	N-CA-C	5.37	118.49	109.95
1	F	889	TRP	N-CA-C	5.35	118.15	109.06
1	F	888	ASP	N-CA-C	-5.32	106.47	113.17
1	A	959	SER	CA-C-N	5.30	124.75	119.24
1	A	959	SER	C-N-CA	5.30	124.75	119.24
1	E	884	ASP	N-CA-C	5.30	117.21	109.84
1	A	886	ASN	N-CA-C	5.27	118.59	110.42
1	C	910	HIS	N-CA-C	-5.26	103.19	110.35
1	F	1086	PHE	N-CA-C	5.26	116.99	108.41
1	E	910	HIS	N-CA-C	-5.22	102.55	110.28
1	C	886	ASN	N-CA-C	5.16	118.48	110.17
1	H	1003	LEU	N-CA-C	5.12	117.25	111.11
1	E	1003	LEU	N-CA-C	5.11	116.85	111.28
1	G	889	TRP	N-CA-C	5.10	117.13	109.23
1	H	884	ASP	CA-C-N	-5.09	115.64	120.83
1	H	884	ASP	C-N-CA	-5.09	115.64	120.83
1	H	986	VAL	CA-C-N	-5.09	114.75	120.14
1	H	986	VAL	C-N-CA	-5.09	114.75	120.14
2	I	11	THR	CB-CA-C	-5.08	102.91	110.88
1	D	1046	GLN	N-CA-C	5.03	117.66	111.82
1	E	981	GLU	N-CA-C	5.01	118.17	111.75
2	J	4	LYS	N-CA-C	5.01	116.45	108.79

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	1530	0	1491	63	0
1	B	1535	0	1500	51	0
1	C	1573	0	1540	56	0
1	D	1517	0	1475	66	0
1	E	1526	0	1488	52	0
1	F	1530	0	1491	71	0
1	G	1515	0	1472	52	0
1	H	1548	0	1511	50	0
2	I	154	0	169	22	0
2	J	154	0	170	12	0
2	K	154	0	168	14	0
2	L	154	0	168	8	0
2	M	154	0	170	10	0
2	N	154	0	169	7	0
2	O	154	0	168	10	0
2	P	154	0	170	30	0
3	A	2	0	0	2	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	1	0
3	F	2	0	0	1	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
All	All	13522	0	13320	495	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 18.

All (495) 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:F:1047:VAL:HG13	1:F:1048:TYR:CE1	1.59	1.35
1:F:1047:VAL:C	1:F:1048:TYR:HD1	1.57	1.12
1:G:895:ASN:HD22	1:G:896:GLY:N	1.55	1.04
1:F:1044:VAL:O	1:F:1047:VAL:HG12	1.59	1.00
1:A:895:ASN:HD22	1:A:896:GLY:H	1.03	0.99
1:E:890:CYS:HG	3:E:1:ZN:ZN	0.71	0.98
1:C:1061:GLU:H	1:C:1061:GLU:CD	1.70	0.98
1:H:895:ASN:HD22	1:H:896:GLY:H	1.00	0.97
1:E:895:ASN:HD22	1:E:896:GLY:H	1.09	0.97
1:F:1047:VAL:HG13	1:F:1048:TYR:HE1	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:ARG:HD3	1:D:941:TYR:CZ	2.01	0.96
1:C:895:ASN:HD22	1:C:896:GLY:N	1.65	0.94
1:F:890:CYS:HG	3:F:1:ZN:ZN	0.65	0.94
1:B:1013:LYS:O	1:B:1013:LYS:HG2	1.68	0.93
1:F:1047:VAL:C	1:F:1048:TYR:CD1	2.46	0.92
1:F:977:GLU:CD	1:F:977:GLU:H	1.78	0.92
1:G:895:ASN:ND2	1:G:896:GLY:H	1.69	0.91
2:K:9:M3L:O	2:K:9:M3L:HG2	1.68	0.90
1:D:895:ASN:HD22	1:D:896:GLY:N	1.68	0.89
1:C:895:ASN:ND2	1:C:896:GLY:H	1.70	0.89
1:E:895:ASN:HD22	1:E:896:GLY:N	1.68	0.89
1:D:895:ASN:HD22	1:D:896:GLY:H	0.90	0.89
1:D:959:SER:OG	1:D:960:PRO:HD2	1.71	0.88
1:F:889:TRP:CZ3	2:N:9:M3L:HD3	2.08	0.88
1:F:915:VAL:HG22	1:F:1007:LYS:HE3	1.56	0.87
1:F:1047:VAL:HG13	1:F:1048:TYR:CD1	2.11	0.86
1:F:1047:VAL:CG1	1:F:1048:TYR:CE1	2.53	0.86
1:B:901:CYS:HA	1:B:908:VAL:HG12	1.57	0.85
1:H:1020:ILE:HG13	1:H:1021:PRO:HD2	1.58	0.85
1:A:895:ASN:HD22	1:A:896:GLY:N	1.75	0.85
1:G:895:ASN:HD22	1:G:896:GLY:H	0.85	0.85
1:H:895:ASN:HD22	1:H:896:GLY:N	1.74	0.84
1:A:890:CYS:HG	3:A:1:ZN:ZN	0.88	0.84
1:H:895:ASN:ND2	1:H:896:GLY:H	1.74	0.84
1:A:895:ASN:ND2	1:A:896:GLY:H	1.75	0.83
1:C:944:ASP:O	1:C:948:HIS:HB2	1.77	0.83
1:D:895:ASN:ND2	1:D:896:GLY:H	1.74	0.82
1:F:1047:VAL:O	1:F:1048:TYR:HD1	1.62	0.82
1:E:894:GLN:O	2:M:9:M3L:HM23	1.80	0.81
1:D:915:VAL:HG22	1:D:1007:LYS:HE3	1.63	0.81
1:D:900:LEU:HD12	1:D:918:LEU:HD23	1.60	0.81
1:F:883:ASP:CG	1:F:884:ASP:H	1.88	0.81
1:B:936:LYS:HD3	1:B:938:GLU:OE1	1.81	0.81
2:P:20:LEU:O	2:P:20:LEU:HD23	1.82	0.80
1:A:889:TRP:CZ3	2:I:9:M3L:HD3	2.17	0.80
1:E:1061:GLU:CD	1:E:1061:GLU:H	1.89	0.80
1:B:912:THR:HA	1:B:917:THR:HG23	1.64	0.79
1:H:932:ARG:NH1	1:H:941:TYR:CD2	2.50	0.79
1:E:977:GLU:H	1:E:977:GLU:CD	1.89	0.79
1:H:932:ARG:CZ	1:H:941:TYR:CE2	2.65	0.79
1:F:1061:GLU:CD	1:F:1061:GLU:H	1.91	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:895:ASN:HD22	1:C:896:GLY:H	0.86	0.78
1:A:889:TRP:CZ3	2:I:9:M3L:CD	2.67	0.78
1:B:894:GLN:O	2:J:9:M3L:HM23	1.82	0.78
2:P:19:GLN:NE2	2:P:20:LEU:H	1.83	0.77
1:H:977:GLU:CD	1:H:977:GLU:H	1.91	0.76
1:B:930:PHE:HA	1:B:968:ARG:HD2	1.68	0.75
1:A:1061:GLU:CD	1:A:1061:GLU:H	1.95	0.75
2:I:5:GLN:HG3	2:I:6:THR:H	1.51	0.75
1:C:1061:GLU:CD	1:C:1061:GLU:N	2.45	0.74
1:D:959:SER:HB3	1:D:962:ASP:OD2	1.87	0.74
1:G:915:VAL:HG22	1:G:1007:LYS:HE3	1.70	0.73
1:A:889:TRP:CH2	2:I:9:M3L:HD3	2.24	0.73
2:P:9:M3L:CG	2:P:10:SER:H	2.01	0.73
1:E:895:ASN:ND2	1:E:896:GLY:H	1.86	0.72
1:G:912:THR:HA	1:G:917:THR:HG23	1.70	0.72
1:D:932:ARG:HD3	1:D:941:TYR:OH	1.89	0.72
1:C:889:TRP:CE2	2:K:9:M3L:CM2	2.73	0.72
1:B:1020:ILE:HG23	1:B:1022:ASP:HB2	1.72	0.71
1:A:889:TRP:CZ3	2:I:9:M3L:CG	2.74	0.71
2:L:11:THR:HG22	2:L:12:GLY:N	2.05	0.71
1:A:889:TRP:CZ3	2:I:9:M3L:HG2	2.26	0.70
1:A:977:GLU:CD	1:A:977:GLU:H	1.98	0.70
1:E:944:ASP:OD1	1:E:944:ASP:N	2.25	0.70
1:F:1048:TYR:CD1	1:F:1048:TYR:N	2.56	0.69
1:B:1020:ILE:CG2	1:B:1022:ASP:HB2	2.22	0.69
1:A:1019:GLN:HA	1:A:1019:GLN:OE1	1.92	0.69
1:H:894:GLN:HE21	2:P:9:M3L:CM2	2.05	0.69
1:F:889:TRP:CH2	2:N:9:M3L:HD3	2.27	0.69
1:F:1061:GLU:CD	1:F:1061:GLU:N	2.50	0.69
1:H:932:ARG:CZ	1:H:941:TYR:HE2	2.04	0.69
1:A:1045:VAL:CG1	1:D:1048:TYR:HD1	2.07	0.68
1:B:895:ASN:ND2	1:B:896:GLY:H	1.90	0.68
1:E:915:VAL:HG22	1:E:1007:LYS:HE3	1.76	0.68
1:B:895:ASN:HD22	1:B:896:GLY:N	1.92	0.68
1:A:930:PHE:HA	1:A:968:ARG:HD2	1.75	0.67
1:C:889:TRP:CD2	2:K:9:M3L:HM22	2.30	0.67
1:F:894:GLN:O	2:N:9:M3L:CM2	2.43	0.67
1:D:981:GLU:HG2	1:D:1062:VAL:HG22	1.77	0.66
1:C:958:LEU:HD23	1:C:1018:TYR:O	1.95	0.66
1:A:1037:ARG:HE	1:D:1037:ARG:HH21	1.43	0.66
1:E:912:THR:HA	1:E:917:THR:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:930:PHE:HA	1:F:968:ARG:HD2	1.77	0.66
1:C:930:PHE:CE2	1:C:971:LEU:HD13	2.30	0.66
1:D:900:LEU:HD22	1:D:926:TRP:CE3	2.31	0.65
1:E:981:GLU:HG3	1:E:1062:VAL:HG22	1.79	0.65
1:B:977:GLU:CD	1:B:977:GLU:H	2.02	0.65
1:D:1062:VAL:HG21	2:L:18:ALY:HG3	1.77	0.65
1:F:1020:ILE:HG13	1:F:1021:PRO:HD2	1.78	0.65
1:F:1047:VAL:CG1	1:F:1048:TYR:HE1	2.02	0.65
1:D:1022:ASP:OD1	1:D:1084:ARG:NH2	2.30	0.65
2:I:5:GLN:HG3	2:I:6:THR:N	2.10	0.65
1:A:912:THR:HA	1:A:917:THR:HG23	1.80	0.64
1:C:977:GLU:CD	1:C:977:GLU:H	2.04	0.64
1:D:977:GLU:CD	1:D:977:GLU:H	2.06	0.64
1:A:889:TRP:CE2	2:I:9:M3L:HM32	2.33	0.64
1:D:930:PHE:HA	1:D:968:ARG:HD2	1.81	0.63
1:E:937:PRO:HG3	1:E:964:ARG:CZ	2.28	0.63
1:F:1047:VAL:O	1:F:1048:TYR:CD1	2.50	0.63
1:F:932:ARG:NH2	1:F:964:ARG:HG2	2.14	0.62
1:A:1045:VAL:HG13	1:D:1048:TYR:HD1	1.63	0.62
1:C:932:ARG:NH2	1:C:964:ARG:HG2	2.14	0.62
1:E:930:PHE:CE2	1:E:971:LEU:HD13	2.33	0.62
1:F:900:LEU:HD12	1:F:918:LEU:HD23	1.80	0.62
1:F:977:GLU:CD	1:F:977:GLU:N	2.56	0.62
1:H:932:ARG:NH1	1:H:941:TYR:CE2	2.67	0.62
1:H:1020:ILE:HG13	1:H:1021:PRO:CD	2.30	0.62
1:D:946:LEU:O	1:D:946:LEU:HG	1.98	0.62
1:H:889:TRP:CE2	2:P:9:M3L:HM32	2.34	0.62
2:P:9:M3L:HG2	2:P:10:SER:H	1.65	0.62
1:B:1081:TYR:HB3	1:B:1084:ARG:HB3	1.82	0.61
1:F:1047:VAL:O	1:F:1047:VAL:HG22	2.00	0.61
1:H:1013:LYS:O	1:H:1013:LYS:HG2	1.98	0.61
1:E:1020:ILE:HG12	1:E:1022:ASP:OD1	2.00	0.61
1:A:890:CYS:SG	3:A:1:ZN:ZN	1.88	0.61
2:P:19:GLN:CG	2:P:20:LEU:H	2.12	0.61
1:D:937:PRO:HG3	1:D:964:ARG:CZ	2.31	0.61
1:D:932:ARG:NH2	1:D:964:ARG:HG2	2.15	0.61
1:D:1081:TYR:HB3	1:D:1084:ARG:HB3	1.83	0.61
1:B:990:ILE:HD12	2:J:18:ALY:HE3	1.81	0.61
1:C:919:LEU:HB2	1:C:942:ASP:OD1	2.01	0.61
1:D:959:SER:HG	1:D:960:PRO:HD2	1.66	0.60
1:F:937:PRO:HG3	1:F:964:ARG:NE	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:ALA:HB2	2:K:16:PRO:HG2	1.82	0.60
2:P:19:GLN:HE21	2:P:20:LEU:H	1.48	0.60
1:F:932:ARG:CZ	1:F:941:TYR:HE2	2.14	0.60
1:G:930:PHE:CE2	1:G:971:LEU:HD12	2.36	0.60
1:A:1061:GLU:CD	1:A:1061:GLU:N	2.57	0.60
1:C:905:CYS:HB2	1:C:906:PRO:HD2	1.84	0.60
1:H:957:GLY:HA3	1:H:1012:LYS:HG2	1.84	0.59
1:C:986:VAL:HG21	1:C:993:TYR:CZ	2.38	0.59
1:A:904:LYS:HD2	1:A:927:ILE:HD13	1.84	0.59
1:B:895:ASN:ND2	1:B:896:GLY:N	2.50	0.59
1:E:889:TRP:CE2	2:M:9:M3L:CM3	2.86	0.59
1:D:900:LEU:CD1	1:D:918:LEU:HD23	2.31	0.59
2:L:11:THR:CG2	2:L:12:GLY:N	2.66	0.59
1:D:945:ASN:OD1	1:D:1012:LYS:HB2	2.03	0.58
1:B:934:ILE:HG22	1:B:961:VAL:HG22	1.85	0.58
1:F:883:ASP:CG	1:F:884:ASP:N	2.61	0.58
1:A:903:GLU:OE2	1:A:925:ASP:HB3	2.02	0.58
1:B:1061:GLU:HG2	2:J:16:PRO:HB3	1.85	0.58
1:F:1048:TYR:O	1:F:1049:ALA:C	2.46	0.58
1:A:932:ARG:NH2	1:A:964:ARG:HD2	2.19	0.58
1:G:901:CYS:HA	1:G:908:VAL:HG12	1.85	0.58
2:P:19:GLN:CD	2:P:20:LEU:H	2.11	0.58
1:F:901:CYS:HA	1:F:908:VAL:HG12	1.85	0.58
1:G:977:GLU:CD	1:G:977:GLU:H	2.11	0.58
1:A:945:ASN:OD1	1:A:1012:LYS:HB2	2.04	0.57
1:E:1046:GLN:C	1:E:1048:TYR:H	2.11	0.57
1:E:1061:GLU:CD	1:E:1061:GLU:N	2.54	0.57
1:G:930:PHE:HA	1:G:968:ARG:HD2	1.86	0.57
2:K:9:M3L:O	2:K:9:M3L:CG	2.45	0.57
1:H:898:ASP:HB3	1:H:921:PHE:HZ	1.68	0.57
2:J:2:ARG:HG2	2:J:3:THR:N	2.19	0.57
1:A:935:GLY:H	1:A:964:ARG:NH2	2.02	0.57
1:F:1046:GLN:O	1:F:1046:GLN:HG3	2.04	0.57
1:G:889:TRP:CZ3	2:O:9:M3L:HD2	2.40	0.57
1:G:905:CYS:HB2	1:G:906:PRO:HD2	1.86	0.57
2:P:9:M3L:CG	2:P:10:SER:N	2.62	0.57
1:G:896:GLY:HA3	2:O:6:THR:HB	1.86	0.57
1:H:895:ASN:HD21	2:P:9:M3L:H	1.52	0.57
1:H:958:LEU:HD23	1:H:1018:TYR:O	2.05	0.57
1:E:891:ALA:HB2	1:E:907:LYS:HG2	1.87	0.56
1:G:1013:LYS:CG	1:G:1013:LYS:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:983:GLN:HG2	1:C:1003:LEU:HD12	1.88	0.56
1:D:1013:LYS:O	1:D:1013:LYS:CG	2.54	0.56
1:H:930:PHE:CE2	1:H:971:LEU:HD13	2.41	0.56
1:H:981:GLU:OE2	2:P:17:ARG:HD2	2.06	0.56
2:P:19:GLN:O	2:P:20:LEU:HB2	2.04	0.56
1:F:996:ILE:CD1	1:F:1041:MET:HG2	2.36	0.56
1:G:900:LEU:HD12	1:G:918:LEU:HD23	1.88	0.56
1:G:963:GLN:HG3	1:G:967:GLU:OE2	2.06	0.56
1:E:889:TRP:CD2	2:M:9:M3L:HM32	2.41	0.56
1:C:889:TRP:CE2	2:K:9:M3L:HM22	2.41	0.55
1:G:990:ILE:HD12	2:O:18:ALY:HD3	1.88	0.55
1:C:991:PRO:O	1:C:992:ASN:HB2	2.06	0.55
1:A:1046:GLN:C	1:A:1048:TYR:H	2.15	0.55
1:A:986:VAL:HG21	1:A:993:TYR:CZ	2.41	0.55
1:A:1037:ARG:HH21	1:D:1037:ARG:HE	1.55	0.55
1:F:912:THR:HA	1:F:917:THR:HG23	1.89	0.55
1:F:996:ILE:HD13	1:F:1041:MET:HG2	1.89	0.55
1:B:900:LEU:HD22	1:B:926:TRP:CE3	2.41	0.55
1:C:1014:HIS:CE1	1:C:1016:GLN:H	2.24	0.55
1:H:894:GLN:HE21	2:P:9:M3L:HM22	1.70	0.55
2:P:19:GLN:HE21	2:P:20:LEU:N	2.05	0.55
1:D:912:THR:HA	1:D:917:THR:HG23	1.89	0.55
1:F:884:ASP:OD1	1:F:885:PRO:HD2	2.07	0.55
1:A:889:TRP:HZ3	2:I:9:M3L:HG2	1.69	0.54
1:C:895:ASN:HD21	2:K:8:ARG:HA	1.71	0.54
1:D:939:VAL:HG23	1:D:941:TYR:CE1	2.42	0.54
1:C:953:LYS:O	1:C:953:LYS:HG3	2.08	0.54
1:C:900:LEU:HD22	1:C:926:TRP:CE3	2.42	0.54
1:D:901:CYS:HA	1:D:908:VAL:HG12	1.90	0.54
1:G:1013:LYS:O	1:G:1013:LYS:HG2	2.06	0.54
1:D:958:LEU:HD23	1:D:1018:TYR:O	2.08	0.54
1:D:930:PHE:CE2	1:D:971:LEU:HD12	2.42	0.54
1:B:926:TRP:NE1	1:B:941:TYR:CE1	2.77	0.53
1:H:991:PRO:O	1:H:992:ASN:HB2	2.08	0.53
1:G:986:VAL:HG21	1:G:993:TYR:CZ	2.44	0.53
1:B:966:CYS:HA	1:B:969:LEU:HD12	1.91	0.53
1:G:1061:GLU:HG2	2:O:16:PRO:HB3	1.91	0.53
1:E:905:CYS:HB2	1:E:906:PRO:HD2	1.90	0.53
1:E:1062:VAL:HG21	2:M:18:ALY:HG3	1.92	0.52
1:C:883:ASP:CG	1:C:884:ASP:H	2.18	0.52
1:B:1065:ALA:HB2	2:J:16:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:5:GLN:HG3	2:L:6:THR:N	2.25	0.52
1:A:1042:MET:O	1:A:1046:GLN:HB3	2.10	0.52
1:C:937:PRO:HG3	1:C:964:ARG:CZ	2.40	0.52
1:D:915:VAL:HB	1:D:971:LEU:HD23	1.92	0.52
1:D:942:ASP:CG	1:D:942:ASP:O	2.50	0.52
1:H:970:LEU:HD22	1:H:1010:LEU:HD23	1.91	0.52
1:E:895:ASN:HD21	2:M:8:ARG:HA	1.74	0.52
1:B:924:GLY:O	2:J:1:ALA:HB2	2.10	0.52
1:D:983:GLN:HG2	1:D:1003:LEU:HD12	1.92	0.51
1:G:895:ASN:ND2	1:G:896:GLY:N	2.40	0.51
1:B:1012:LYS:HA	1:B:1017:HIS:CD2	2.44	0.51
1:A:905:CYS:HB2	1:A:906:PRO:HD2	1.91	0.51
2:I:19:GLN:NE2	2:I:20:LEU:H	2.07	0.51
1:H:1012:LYS:HA	1:H:1017:HIS:CD2	2.44	0.51
1:H:947:GLN:O	1:H:950:LYS:HB3	2.10	0.51
1:C:886:ASN:OD1	2:K:2:ARG:NH1	2.44	0.51
1:E:912:THR:HA	1:E:917:THR:CG2	2.41	0.51
1:D:996:ILE:HD13	1:D:1041:MET:HB3	1.92	0.51
1:D:1020:ILE:HG13	1:D:1021:PRO:HD2	1.93	0.51
1:D:1027:ASP:O	1:D:1030:LEU:HB3	2.11	0.51
1:C:930:PHE:HA	1:C:968:ARG:HD2	1.92	0.51
2:P:19:GLN:NE2	2:P:20:LEU:N	2.58	0.51
1:C:1014:HIS:ND1	1:C:1016:GLN:N	2.57	0.51
1:A:970:LEU:HD22	1:A:1010:LEU:HD23	1.93	0.50
1:B:915:VAL:HB	1:B:971:LEU:HD23	1.93	0.50
1:D:942:ASP:OD1	1:D:942:ASP:N	2.30	0.50
1:D:998:LYS:CE	2:P:10:SER:OG	2.59	0.50
1:E:933:ASP:HB3	1:E:936:LYS:O	2.10	0.50
1:A:946:LEU:O	1:A:949:SER:HB2	2.11	0.50
1:C:1020:ILE:HG13	1:C:1021:PRO:HD2	1.92	0.50
1:A:1013:LYS:O	1:A:1013:LYS:HG3	2.11	0.50
1:G:889:TRP:CH2	2:O:9:M3L:HD2	2.45	0.50
2:I:2:ARG:HG2	2:I:3:THR:N	2.25	0.50
1:A:1020:ILE:HB	1:A:1021:PRO:HD2	1.93	0.50
1:A:1062:VAL:HG21	2:I:18:ALY:HG3	1.94	0.50
1:A:915:VAL:HG22	1:A:1007:LYS:HE3	1.94	0.50
1:G:895:ASN:HD21	2:O:8:ARG:HA	1.76	0.50
1:D:930:PHE:CE2	1:D:971:LEU:CD1	2.95	0.49
1:E:919:LEU:HD11	1:E:944:ASP:N	2.27	0.49
1:F:1046:GLN:C	1:F:1048:TYR:H	2.20	0.49
1:G:970:LEU:HD22	1:G:1010:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:905:CYS:HB2	1:H:906:PRO:CD	2.42	0.49
1:B:986:VAL:O	1:B:994:TYR:OH	2.28	0.49
1:C:889:TRP:CZ3	2:K:9:M3L:HD2	2.48	0.49
1:F:894:GLN:O	2:N:9:M3L:HM22	2.12	0.49
1:A:930:PHE:CE2	1:A:971:LEU:HD13	2.47	0.49
1:F:1081:TYR:HB3	1:F:1084:ARG:HB3	1.94	0.49
1:F:1012:LYS:HA	1:F:1017:HIS:CD2	2.47	0.49
1:G:985:PRO:HA	1:G:1002:ASP:OD1	2.11	0.49
2:P:19:GLN:CG	2:P:20:LEU:N	2.76	0.49
2:N:5:GLN:HG3	2:N:6:THR:N	2.27	0.49
1:D:981:GLU:OE1	2:L:18:ALY:HH31	2.12	0.49
1:E:889:TRP:CZ3	2:M:9:M3L:HD3	2.48	0.49
1:F:944:ASP:O	1:F:948:HIS:HB2	2.13	0.49
1:G:971:LEU:HD13	1:G:975:CYS:SG	2.53	0.49
1:C:889:TRP:CZ2	2:K:9:M3L:HM23	2.48	0.48
1:C:900:LEU:HD12	1:C:918:LEU:HD23	1.95	0.48
1:F:930:PHE:CE2	1:F:971:LEU:HD13	2.49	0.48
1:F:1010:LEU:HD13	1:F:1010:LEU:HA	1.65	0.48
1:H:895:ASN:HD21	2:P:8:ARG:HA	1.77	0.48
1:C:962:ASP:HB3	1:C:1021:PRO:HG3	1.95	0.48
1:E:983:GLN:HG2	1:E:1003:LEU:HD12	1.96	0.48
1:G:1020:ILE:HG13	1:G:1021:PRO:HD2	1.95	0.48
1:E:926:TRP:NE1	1:E:941:TYR:CE1	2.80	0.48
1:H:959:SER:HB2	1:H:962:ASP:HB2	1.95	0.48
1:B:970:LEU:HD22	1:B:1010:LEU:HD23	1.96	0.48
1:G:1080:ILE:HG22	1:G:1081:TYR:CD2	2.49	0.48
1:B:930:PHE:CE2	1:B:971:LEU:CD1	2.97	0.48
1:B:895:ASN:HD21	2:J:8:ARG:HA	1.79	0.48
1:G:930:PHE:CE2	1:G:971:LEU:CD1	2.97	0.48
1:F:934:ILE:HD11	1:F:968:ARG:NH2	2.30	0.47
1:A:884:ASP:OD1	1:A:885:PRO:HD2	2.14	0.47
1:D:981:GLU:HG3	2:L:18:ALY:HH32	1.96	0.47
1:G:937:PRO:HG3	1:G:964:ARG:CZ	2.43	0.47
1:C:889:TRP:CZ2	2:K:9:M3L:CM2	2.97	0.47
1:F:932:ARG:CZ	1:F:941:TYR:CE2	2.97	0.47
1:G:937:PRO:HG3	1:G:964:ARG:NE	2.29	0.47
1:A:993:TYR:HA	1:A:1038:PHE:CE1	2.49	0.47
1:B:988:ALA:HB1	2:I:6:THR:HG23	1.97	0.47
1:C:977:GLU:OE2	1:C:977:GLU:N	2.46	0.47
1:E:969:LEU:O	1:E:972:TYR:HB2	2.14	0.47
1:E:1020:ILE:HG13	1:E:1021:PRO:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:900:LEU:CD1	1:F:918:LEU:HD23	2.44	0.47
2:I:19:GLN:O	2:I:20:LEU:HB2	2.15	0.47
1:B:1044:VAL:O	1:B:1047:VAL:HG12	2.15	0.47
1:E:976:HIS:CE1	1:E:978:LEU:HB2	2.49	0.47
1:E:1046:GLN:C	1:E:1048:TYR:N	2.73	0.47
1:B:895:ASN:HD22	1:B:896:GLY:H	1.53	0.47
1:C:946:LEU:O	1:C:949:SER:HB2	2.15	0.47
1:H:986:VAL:HG21	1:H:993:TYR:CZ	2.49	0.47
1:F:942:ASP:OD1	1:F:942:ASP:N	2.40	0.46
1:G:932:ARG:HH22	1:G:964:ARG:HG2	1.80	0.46
1:D:934:ILE:HD11	1:D:968:ARG:CZ	2.45	0.46
1:D:1061:GLU:CD	1:D:1061:GLU:N	2.74	0.46
1:F:1020:ILE:HG22	1:F:1023:ASP:OD2	2.15	0.46
1:F:1041:MET:O	1:F:1044:VAL:HB	2.16	0.46
1:G:1027:ASP:O	1:G:1028:VAL:C	2.58	0.46
1:F:1021:PRO:O	1:F:1024:PHE:N	2.46	0.46
1:G:910:HIS:HB2	1:G:913:CYS:HB2	1.97	0.46
1:H:993:TYR:HA	1:H:1038:PHE:CE1	2.51	0.46
1:H:1042:MET:O	1:H:1046:GLN:HB3	2.16	0.46
1:A:1001:MET:HB3	1:A:1031:ILE:HG13	1.98	0.46
1:E:910:HIS:HB2	1:E:913:CYS:HB2	1.96	0.46
1:H:895:ASN:ND2	2:P:9:M3L:H	2.14	0.46
1:B:926:TRP:NE1	1:B:941:TYR:HE1	2.12	0.46
1:H:1062:VAL:HG21	2:P:18:ALY:N	2.29	0.46
1:C:1010:LEU:HD13	1:C:1010:LEU:HA	1.87	0.46
1:F:986:VAL:HG21	1:F:993:TYR:CZ	2.51	0.46
1:B:890:CYS:HB2	1:B:899:LEU:HD21	1.98	0.46
1:B:1020:ILE:HD12	1:B:1021:PRO:HD2	1.98	0.46
2:M:9:M3L:HM32	2:M:9:M3L:HD3	1.55	0.46
1:C:901:CYS:HA	1:C:908:VAL:HG12	1.98	0.45
1:G:889:TRP:CE2	2:O:9:M3L:HM32	2.51	0.45
1:H:933:ASP:HB3	1:H:936:LYS:O	2.16	0.45
1:D:1020:ILE:HG22	1:D:1023:ASP:CG	2.41	0.45
1:G:1046:GLN:C	1:G:1048:TYR:H	2.24	0.45
1:A:900:LEU:HD12	1:A:918:LEU:HD23	1.99	0.45
1:B:1013:LYS:O	1:B:1013:LYS:CG	2.52	0.45
1:D:970:LEU:HD22	1:D:1010:LEU:HD23	1.98	0.45
1:G:905:CYS:HB2	1:G:906:PRO:CD	2.46	0.45
1:D:958:LEU:HD13	1:D:962:ASP:HB2	1.97	0.45
1:G:981:GLU:OE2	2:O:17:ARG:HA	2.17	0.45
1:H:983:GLN:HG2	1:H:1003:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:979:SER:O	1:E:980:ILE:C	2.57	0.45
1:F:1014:HIS:O	1:F:1017:HIS:HB2	2.16	0.45
2:K:9:M3L:HM22	2:K:9:M3L:HD2	1.77	0.45
1:F:1037:ARG:O	1:F:1040:GLU:HB2	2.17	0.45
1:H:932:ARG:NH2	1:H:964:ARG:HG2	2.31	0.45
1:A:1037:ARG:NH2	1:D:1037:ARG:HE	2.13	0.45
1:C:911:LEU:HB3	1:C:918:LEU:HB3	1.98	0.45
1:F:905:CYS:HB2	1:F:906:PRO:HD2	1.99	0.45
1:G:915:VAL:HB	1:G:971:LEU:HD23	1.98	0.45
2:M:18:ALY:HE2	2:M:18:ALY:HH31	1.73	0.45
1:A:1045:VAL:CG1	1:D:1048:TYR:CD1	2.95	0.45
1:D:948:HIS:ND1	1:D:1012:LYS:HB3	2.32	0.45
1:D:1010:LEU:HD13	1:D:1010:LEU:HA	1.71	0.45
1:F:890:CYS:SG	1:F:913:CYS:SG	3.15	0.45
1:D:939:VAL:CG2	1:D:941:TYR:HE1	2.29	0.45
1:H:930:PHE:HA	1:H:968:ARG:HD2	1.99	0.45
1:E:948:HIS:CD2	1:E:1013:LYS:HB3	2.52	0.44
1:D:889:TRP:CE2	2:L:9:M3L:HM22	2.53	0.44
1:D:903:GLU:OE2	1:D:925:ASP:HB3	2.17	0.44
1:A:905:CYS:HB2	1:A:906:PRO:CD	2.47	0.44
1:E:977:GLU:CD	1:E:977:GLU:N	2.68	0.44
1:E:1027:ASP:O	1:E:1028:VAL:C	2.61	0.44
2:P:18:ALY:O	2:P:19:GLN:C	2.58	0.44
1:B:988:ALA:CB	2:I:6:THR:HG23	2.47	0.44
1:C:894:GLN:O	2:K:9:M3L:HM13	2.18	0.44
1:D:910:HIS:HB2	1:D:913:CYS:HB2	1.99	0.44
1:G:932:ARG:NH2	1:G:964:ARG:HG2	2.32	0.44
2:P:9:M3L:HG3	2:P:10:SER:N	2.33	0.44
1:D:921:PHE:HA	1:D:922:PRO:HD3	1.90	0.44
1:G:930:PHE:CZ	1:G:971:LEU:HD12	2.53	0.44
1:H:900:LEU:HD12	1:H:918:LEU:HD23	1.99	0.44
1:H:1027:ASP:O	1:H:1028:VAL:C	2.60	0.44
1:E:915:VAL:HG11	1:E:970:LEU:HD23	2.00	0.44
1:A:894:GLN:O	2:I:9:M3L:CM2	2.65	0.44
1:A:986:VAL:O	1:A:994:TYR:OH	2.30	0.44
1:B:948:HIS:CE1	1:B:1012:LYS:HB3	2.53	0.44
1:C:980:ILE:HG13	2:K:15:ALA:CB	2.47	0.44
1:C:1027:ASP:O	1:C:1028:VAL:C	2.58	0.44
1:B:944:ASP:O	1:B:947:GLN:HB2	2.18	0.43
1:B:976:HIS:CE1	1:B:978:LEU:HB2	2.53	0.43
1:A:977:GLU:CD	1:A:977:GLU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:911:LEU:HD22	1:E:918:LEU:HB3	2.00	0.43
1:A:932:ARG:HD3	1:A:941:TYR:CZ	2.54	0.43
1:F:1020:ILE:HG13	1:F:1021:PRO:CD	2.48	0.43
1:A:889:TRP:CZ2	2:I:9:M3L:HM32	2.53	0.43
1:B:945:ASN:OD1	1:B:1012:LYS:HB2	2.19	0.43
1:F:1082:SER:C	1:F:1084:ARG:H	2.25	0.43
1:C:900:LEU:HD12	1:C:918:LEU:CD2	2.48	0.43
1:B:1020:ILE:HG13	1:B:1022:ASP:H	1.84	0.43
1:E:900:LEU:HD22	1:E:926:TRP:CE3	2.54	0.43
2:I:9:M3L:HD3	2:I:9:M3L:HM32	1.68	0.43
1:A:900:LEU:CD1	1:A:918:LEU:HD23	2.49	0.43
1:B:1015:SER:O	1:B:1016:GLN:HG3	2.18	0.43
1:E:945:ASN:OD1	1:E:1012:LYS:HB2	2.18	0.43
1:A:895:ASN:ND2	1:A:896:GLY:N	2.51	0.43
1:D:1012:LYS:HG3	1:D:1017:HIS:NE2	2.33	0.43
2:O:2:ARG:HG2	2:O:3:THR:N	2.34	0.43
1:G:932:ARG:NH2	1:G:964:ARG:CD	2.81	0.42
1:G:993:TYR:HA	1:G:1038:PHE:CE1	2.53	0.42
1:G:999:LYS:HA	1:G:1000:PRO:HD3	1.78	0.42
1:A:1003:LEU:O	1:A:1004:SER:C	2.62	0.42
1:B:894:GLN:HE21	2:J:9:M3L:HM21	1.83	0.42
1:B:977:GLU:OE2	1:B:977:GLU:N	2.45	0.42
1:C:1022:ASP:OD1	1:C:1022:ASP:N	2.52	0.42
1:D:905:CYS:HB2	1:D:906:PRO:HD2	2.00	0.42
1:E:1076:LYS:HA	1:E:1076:LYS:HD3	1.86	0.42
1:H:981:GLU:HG2	1:H:1062:VAL:HG22	2.01	0.42
2:P:9:M3L:HG3	2:P:10:SER:H	1.79	0.42
2:P:11:THR:OG1	2:P:13:GLY:N	2.52	0.42
1:C:910:HIS:HB2	1:C:913:CYS:HB2	2.01	0.42
1:E:890:CYS:SG	1:E:893:CYS:SG	3.17	0.42
1:E:896:GLY:HA3	2:M:6:THR:HB	2.02	0.42
1:D:894:GLN:O	2:L:9:M3L:HE3	2.19	0.42
1:H:934:ILE:HD11	1:H:968:ARG:CZ	2.49	0.42
2:O:19:GLN:HG2	2:O:20:LEU:H	1.84	0.42
1:A:915:VAL:HG11	1:A:970:LEU:HB3	2.02	0.42
1:C:993:TYR:HA	1:C:1038:PHE:CE1	2.54	0.42
1:D:900:LEU:CD1	1:D:918:LEU:CD2	2.96	0.42
1:E:901:CYS:HA	1:E:908:VAL:HG12	2.01	0.42
2:P:10:SER:HB3	2:P:11:THR:H	1.70	0.42
1:A:907:LYS:HE3	1:A:930:PHE:CE2	2.55	0.42
1:B:912:THR:O	1:B:1007:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:926:TRP:NE1	1:G:941:TYR:CE1	2.87	0.42
2:I:18:ALY:HE3	2:I:18:ALY:HH31	1.88	0.42
1:A:969:LEU:O	1:A:972:TYR:HB2	2.19	0.42
1:C:970:LEU:HD22	1:C:1010:LEU:HD23	2.01	0.42
1:E:1014:HIS:CE1	1:E:1016:GLN:H	2.37	0.42
2:J:18:ALY:HH31	2:J:18:ALY:HE2	1.82	0.42
1:E:932:ARG:CZ	1:E:941:TYR:CE2	3.02	0.42
1:G:915:VAL:CG2	1:G:1007:LYS:HE3	2.44	0.42
1:H:894:GLN:NE2	2:P:9:M3L:CM2	2.78	0.42
1:B:921:PHE:CE2	1:C:961:VAL:HG21	2.55	0.42
1:E:889:TRP:CE2	2:M:9:M3L:HM32	2.54	0.42
1:H:959:SER:O	1:H:963:GLN:HB2	2.19	0.42
1:B:1062:VAL:HG21	2:J:18:ALY:HG3	2.01	0.41
1:C:895:ASN:ND2	1:C:896:GLY:N	2.47	0.41
1:D:1008:LYS:C	1:D:1010:LEU:N	2.78	0.41
1:E:967:GLU:HG3	1:E:1010:LEU:HD21	2.02	0.41
2:J:9:M3L:H	2:J:9:M3L:HG2	1.72	0.41
1:D:991:PRO:O	1:D:992:ASN:HB2	2.20	0.41
1:E:921:PHE:HA	1:E:922:PRO:HD3	1.88	0.41
1:E:926:TRP:NE1	1:E:941:TYR:HE1	2.17	0.41
1:F:926:TRP:CH2	1:F:928:CYS:HA	2.55	0.41
1:H:1008:LYS:O	1:H:1011:GLN:HG3	2.20	0.41
1:A:889:TRP:CE3	2:I:9:M3L:CD	3.02	0.41
1:A:1046:GLN:C	1:A:1048:TYR:N	2.76	0.41
1:C:1027:ASP:O	1:C:1030:LEU:HB3	2.21	0.41
1:C:1079:GLU:HG2	1:C:1079:GLU:O	2.21	0.41
1:H:889:TRP:CZ3	2:P:9:M3L:HB3	2.56	0.41
1:H:937:PRO:HG3	1:H:964:ARG:CZ	2.51	0.41
2:P:19:GLN:HG2	2:P:20:LEU:N	2.35	0.41
1:F:900:LEU:HD12	1:F:918:LEU:CD2	2.48	0.41
1:H:996:ILE:HD13	1:H:1041:MET:HB2	2.03	0.41
1:A:889:TRP:CE3	2:I:9:M3L:HD3	2.54	0.41
1:A:912:THR:HA	1:A:917:THR:CG2	2.50	0.41
1:E:1027:ASP:O	1:E:1030:LEU:HB3	2.21	0.41
2:N:5:GLN:HG3	2:N:6:THR:H	1.85	0.41
1:F:1022:ASP:HA	1:F:1086:PHE:CD2	2.55	0.41
1:G:982:PHE:CD2	1:G:982:PHE:N	2.88	0.41
1:B:929:THR:O	1:B:929:THR:CG2	2.68	0.41
1:F:915:VAL:CG2	1:F:1007:LYS:HE3	2.39	0.41
1:F:932:ARG:HH22	1:F:964:ARG:HG2	1.85	0.41
1:F:979:SER:O	1:F:980:ILE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1030:LEU:O	1:G:1031:ILE:C	2.64	0.41
1:G:1079:GLU:O	1:G:1079:GLU:HG3	2.21	0.41
1:B:901:CYS:SG	2:J:2:ARG:HD2	2.61	0.41
1:B:1083:ASP:OD2	1:B:1083:ASP:N	2.53	0.41
1:C:919:LEU:O	1:C:920:SER:HB3	2.21	0.41
1:C:926:TRP:NE1	1:C:941:TYR:CE1	2.88	0.41
1:C:932:ARG:HH21	1:C:964:ARG:HG2	1.86	0.41
1:C:1003:LEU:O	1:C:1004:SER:C	2.64	0.41
1:G:926:TRP:NE1	1:G:941:TYR:HE1	2.19	0.41
1:B:1010:LEU:HD13	1:B:1010:LEU:HA	1.72	0.40
1:D:900:LEU:CD2	1:D:926:TRP:CE3	3.03	0.40
1:F:937:PRO:HG3	1:F:964:ARG:CZ	2.51	0.40
1:G:900:LEU:HD12	1:G:918:LEU:CD2	2.51	0.40
1:G:928:CYS:SG	1:G:930:PHE:HB2	2.61	0.40
1:H:910:HIS:HB2	1:H:913:CYS:HB2	2.03	0.40
2:N:9:M3L:HM22	2:N:9:M3L:HD2	1.46	0.40
1:A:971:LEU:HD23	1:A:971:LEU:HA	1.93	0.40
1:B:993:TYR:HA	1:B:1038:PHE:CE1	2.56	0.40
1:C:911:LEU:HD21	1:C:921:PHE:CD1	2.57	0.40
1:D:993:TYR:HA	1:D:1038:PHE:CE1	2.56	0.40
1:F:900:LEU:HD22	1:F:901:CYS:O	2.21	0.40
1:F:976:HIS:CE1	1:F:978:LEU:HB2	2.56	0.40
1:G:1020:ILE:HG13	1:G:1021:PRO:CD	2.51	0.40
1:F:1027:ASP:O	1:F:1030:LEU:HB3	2.21	0.40
1:H:889:TRP:CZ2	2:P:9:M3L:HM32	2.56	0.40
1:H:990:ILE:HA	1:H:991:PRO:HD3	1.92	0.40
1:A:890:CYS:SG	1:A:893:CYS:SG	3.19	0.40
1:A:894:GLN:O	2:I:9:M3L:HM23	2.21	0.40
1:F:1047:VAL:O	1:F:1047:VAL:CG2	2.68	0.40
1:H:932:ARG:CZ	1:H:941:TYR:CD2	2.98	0.40
1:D:1013:LYS:O	1:D:1013:LYS:HG2	2.20	0.40
1:F:970:LEU:HD22	1:F:1010:LEU:HD23	2.04	0.40
1:F:1046:GLN:C	1:F:1048:TYR:N	2.79	0.40
1:F:1061:GLU:HA	1:F:1064:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	183/207 (88%)	167 (91%)	15 (8%)	1 (0%)	24	48
1	B	183/207 (88%)	170 (93%)	13 (7%)	0	100	100
1	C	191/207 (92%)	170 (89%)	21 (11%)	0	100	100
1	D	181/207 (87%)	169 (93%)	12 (7%)	0	100	100
1	E	182/207 (88%)	164 (90%)	17 (9%)	1 (0%)	24	48
1	F	183/207 (88%)	167 (91%)	16 (9%)	0	100	100
1	G	181/207 (87%)	169 (93%)	10 (6%)	2 (1%)	11	29
1	H	185/207 (89%)	166 (90%)	19 (10%)	0	100	100
2	I	15/22 (68%)	13 (87%)	2 (13%)	0	100	100
2	J	15/22 (68%)	13 (87%)	2 (13%)	0	100	100
2	K	15/22 (68%)	14 (93%)	1 (7%)	0	100	100
2	L	15/22 (68%)	14 (93%)	1 (7%)	0	100	100
2	M	15/22 (68%)	13 (87%)	2 (13%)	0	100	100
2	N	15/22 (68%)	14 (93%)	1 (7%)	0	100	100
2	O	15/22 (68%)	12 (80%)	3 (20%)	0	100	100
2	P	15/22 (68%)	14 (93%)	1 (7%)	0	100	100
All	All	1589/1832 (87%)	1449 (91%)	136 (9%)	4 (0%)	36	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	1013	LYS
1	A	1047	VAL
1	E	1047	VAL
1	G	1047	VAL

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	174/189 (92%)	146 (84%)	28 (16%)	2	6
1	B	175/189 (93%)	148 (85%)	27 (15%)	2	7
1	C	178/189 (94%)	151 (85%)	27 (15%)	3	7
1	D	173/189 (92%)	140 (81%)	33 (19%)	1	4
1	E	174/189 (92%)	149 (86%)	25 (14%)	3	8
1	F	174/189 (92%)	149 (86%)	25 (14%)	3	8
1	G	172/189 (91%)	151 (88%)	21 (12%)	5	12
1	H	176/189 (93%)	151 (86%)	25 (14%)	3	8
2	I	12/13 (92%)	8 (67%)	4 (33%)	0	1
2	J	12/13 (92%)	9 (75%)	3 (25%)	0	2
2	K	12/13 (92%)	10 (83%)	2 (17%)	2	6
2	L	12/13 (92%)	11 (92%)	1 (8%)	10	26
2	M	12/13 (92%)	8 (67%)	4 (33%)	0	1
2	N	12/13 (92%)	11 (92%)	1 (8%)	10	26
2	O	12/13 (92%)	10 (83%)	2 (17%)	2	6
2	P	12/13 (92%)	10 (83%)	2 (17%)	2	6
All	All	1492/1616 (92%)	1262 (85%)	230 (15%)	2	7

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	884	ASP
1	A	895	ASN
1	A	900	LEU
1	A	917	THR
1	A	918	LEU
1	A	920	SER
1	A	929	THR
1	A	934	ILE

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Mol	Chain	Res	Type
1	A	942	ASP
1	A	944	ASP
1	A	948	HIS
1	A	950	LYS
1	A	958	LEU
1	A	968	ARG
1	A	971	LEU
1	A	977	GLU
1	A	978	LEU
1	A	980	ILE
1	A	1002	ASP
1	A	1010	LEU
1	A	1041	MET
1	A	1046	GLN
1	A	1047	VAL
1	A	1060	SER
1	A	1061	GLU
1	A	1071	LEU
1	A	1079	GLU
1	A	1080	ILE
1	B	889	TRP
1	B	895	ASN
1	B	900	LEU
1	B	903	GLU
1	B	904	LYS
1	B	918	LEU
1	B	929	THR
1	B	942	ASP
1	B	943	CYS
1	B	946	LEU
1	B	947	GLN
1	B	958	LEU
1	B	961	VAL
1	B	968	ARG
1	B	971	LEU
1	B	978	LEU
1	B	980	ILE
1	B	981	GLU
1	B	990	ILE
1	B	1002	ASP
1	B	1010	LEU
1	B	1015	SER

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Mol	Chain	Res	Type
1	B	1042	MET
1	B	1046	GLN
1	B	1061	GLU
1	B	1075	ASP
1	B	1082	SER
1	C	895	ASN
1	C	899	LEU
1	C	900	LEU
1	C	903	GLU
1	C	904	LYS
1	C	917	THR
1	C	918	LEU
1	C	934	ILE
1	C	942	ASP
1	C	944	ASP
1	C	949	SER
1	C	958	LEU
1	C	961	VAL
1	C	971	LEU
1	C	977	GLU
1	C	978	LEU
1	C	980	ILE
1	C	981	GLU
1	C	989	SER
1	C	1002	ASP
1	C	1010	LEU
1	C	1022	ASP
1	C	1047	VAL
1	C	1060	SER
1	C	1061	GLU
1	C	1071	LEU
1	C	1082	SER
1	D	895	ASN
1	D	898	ASP
1	D	900	LEU
1	D	904	LYS
1	D	913	CYS
1	D	918	LEU
1	D	923	SER
1	D	929	THR
1	D	946	LEU
1	D	948	HIS

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Mol	Chain	Res	Type
1	D	958	LEU
1	D	961	VAL
1	D	968	ARG
1	D	971	LEU
1	D	977	GLU
1	D	978	LEU
1	D	980	ILE
1	D	981	GLU
1	D	989	SER
1	D	1001	MET
1	D	1002	ASP
1	D	1010	LEU
1	D	1012	LYS
1	D	1041	MET
1	D	1042	MET
1	D	1046	GLN
1	D	1048	TYR
1	D	1060	SER
1	D	1061	GLU
1	D	1071	LEU
1	D	1075	ASP
1	D	1080	ILE
1	D	1082	SER
1	E	889	TRP
1	E	895	ASN
1	E	900	LEU
1	E	903	GLU
1	E	904	LYS
1	E	907	LYS
1	E	913	CYS
1	E	917	THR
1	E	918	LEU
1	E	919	LEU
1	E	929	THR
1	E	942	ASP
1	E	944	ASP
1	E	958	LEU
1	E	971	LEU
1	E	978	LEU
1	E	989	SER
1	E	1002	ASP
1	E	1012	LYS

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Mol	Chain	Res	Type
1	E	1020	ILE
1	E	1033	LYS
1	E	1047	VAL
1	E	1061	GLU
1	E	1071	LEU
1	E	1080	ILE
1	F	900	LEU
1	F	918	LEU
1	F	923	SER
1	F	929	THR
1	F	934	ILE
1	F	940	GLU
1	F	946	LEU
1	F	949	SER
1	F	958	LEU
1	F	961	VAL
1	F	968	ARG
1	F	971	LEU
1	F	977	GLU
1	F	978	LEU
1	F	980	ILE
1	F	989	SER
1	F	1002	ASP
1	F	1009	LYS
1	F	1010	LEU
1	F	1012	LYS
1	F	1046	GLN
1	F	1048	TYR
1	F	1061	GLU
1	F	1071	LEU
1	F	1080	ILE
1	G	895	ASN
1	G	900	LEU
1	G	903	GLU
1	G	918	LEU
1	G	920	SER
1	G	929	THR
1	G	958	LEU
1	G	971	LEU
1	G	977	GLU
1	G	978	LEU
1	G	980	ILE

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Mol	Chain	Res	Type
1	G	989	SER
1	G	1002	ASP
1	G	1010	LEU
1	G	1012	LYS
1	G	1013	LYS
1	G	1047	VAL
1	G	1061	GLU
1	G	1071	LEU
1	G	1080	ILE
1	G	1082	SER
1	H	889	TRP
1	H	900	LEU
1	H	903	GLU
1	H	918	LEU
1	H	923	SER
1	H	929	THR
1	H	934	ILE
1	H	938	GLU
1	H	946	LEU
1	H	956	GLN
1	H	958	LEU
1	H	961	VAL
1	H	968	ARG
1	H	971	LEU
1	H	977	GLU
1	H	978	LEU
1	H	980	ILE
1	H	981	GLU
1	H	989	SER
1	H	1002	ASP
1	H	1009	LYS
1	H	1010	LEU
1	H	1046	GLN
1	H	1047	VAL
1	H	1071	LEU
2	I	5	GLN
2	I	11	THR
2	I	17	ARG
2	I	19	GLN
2	J	8	ARG
2	J	17	ARG
2	J	19	GLN

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Mol	Chain	Res	Type
2	K	11	THR
2	K	17	ARG
2	L	17	ARG
2	M	2	ARG
2	M	11	THR
2	M	19	GLN
2	M	20	LEU
2	N	19	GLN
2	O	17	ARG
2	O	19	GLN
2	P	11	THR
2	P	19	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	895	ASN
1	A	983	GLN
1	A	1064	GLN
1	B	894	GLN
1	B	895	ASN
1	B	948	HIS
1	B	983	GLN
1	C	895	ASN
1	C	956	GLN
1	C	983	GLN
1	D	895	ASN
1	D	983	GLN
1	D	1046	GLN
1	E	895	ASN
1	E	983	GLN
1	E	1039	ASN
1	F	983	GLN
1	F	1046	GLN
1	G	895	ASN
1	G	983	GLN
1	G	1064	GLN
1	H	894	GLN
1	H	895	ASN
1	H	983	GLN
1	H	992	ASN
1	H	1039	ASN

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Mol	Chain	Res	Type
1	H	1046	GLN
1	H	1064	GLN
2	I	19	GLN
2	J	5	GLN
2	J	19	GLN
2	L	5	GLN
2	M	5	GLN
2	O	5	GLN
2	O	19	GLN
2	P	5	GLN
2	P	19	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	M3L	O	9	2	10,11,12	0.72	0	9,14,16	1.24	0
2	ALY	P	18	2	10,11,12	0.82	0	7,12,14	0.90	0
2	ALY	M	14	2	3,4,12	0.67	0	2,4,14	0.75	0
2	ALY	L	18	2	10,11,12	0.67	0	7,12,14	2.36	3 (42%)
2	M3L	P	9	2	10,11,12	1.28	1 (10%)	9,14,16	1.49	1 (11%)
2	ALY	I	18	2	10,11,12	0.61	0	7,12,14	1.84	3 (42%)
2	M3L	J	9	2	10,11,12	0.78	0	9,14,16	0.99	0
2	M3L	K	9	2	10,11,12	0.99	0	9,14,16	0.71	0
2	ALY	I	14	2	3,4,12	0.70	0	2,4,14	0.79	0
2	ALY	N	18	2	10,11,12	0.62	0	7,12,14	0.83	0
2	ALY	P	14	2	3,4,12	0.61	0	2,4,14	0.90	0
2	ALY	O	18	2	10,11,12	0.58	0	7,12,14	1.10	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ALY	L	14	2	3,4,12	0.73	0	2,4,14	0.81	0
2	M3L	I	9	2	10,11,12	1.20	0	9,14,16	0.72	0
2	ALY	M	18	2	10,11,12	0.51	0	7,12,14	1.18	1 (14%)
2	M3L	M	9	2	10,11,12	1.00	0	9,14,16	0.77	0
2	ALY	N	14	2	3,4,12	0.73	0	2,4,14	0.85	0
2	M3L	L	9	2	10,11,12	0.78	0	9,14,16	0.64	0
2	ALY	K	18	2	10,11,12	0.56	0	7,12,14	1.07	0
2	ALY	J	18	2	10,11,12	0.66	0	7,12,14	1.74	1 (14%)
2	ALY	O	14	2	3,4,12	0.57	0	2,4,14	0.72	0
2	M3L	N	9	2	10,11,12	1.12	0	9,14,16	0.68	0
2	ALY	K	14	2	3,4,12	0.67	0	2,4,14	0.78	0
2	ALY	J	14	2	3,4,12	0.67	0	2,4,14	0.74	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
2	M3L	O	9	2	-	6/9/10/12	-
2	ALY	P	18	2	-	0/9/10/12	-
2	ALY	M	14	2	-	1/1/2/12	-
2	ALY	L	18	2	-	6/9/10/12	-
2	M3L	P	9	2	-	5/9/10/12	-
2	ALY	I	18	2	-	6/9/10/12	-
2	M3L	J	9	2	-	6/9/10/12	-
2	M3L	K	9	2	-	6/9/10/12	-
2	ALY	I	14	2	-	0/1/2/12	-
2	ALY	N	18	2	-	1/9/10/12	-
2	ALY	P	14	2	-	0/1/2/12	-
2	ALY	O	18	2	-	5/9/10/12	-
2	ALY	L	14	2	-	0/1/2/12	-
2	M3L	I	9	2	-	1/9/10/12	-
2	ALY	M	18	2	-	5/9/10/12	-
2	M3L	M	9	2	-	3/9/10/12	-
2	ALY	N	14	2	-	1/1/2/12	-
2	M3L	L	9	2	-	2/9/10/12	-
2	ALY	K	18	2	-	0/9/10/12	-
2	ALY	J	18	2	-	5/9/10/12	-
2	ALY	O	14	2	-	1/1/2/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	N	9	2	-	4/9/10/12	-
2	ALY	K	14	2	-	1/1/2/12	-
2	ALY	J	14	2	-	1/1/2/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	9	M3L	CE-NZ	-2.40	1.44	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	18	ALY	CE-NZ-CH	4.23	128.81	122.56
2	P	9	M3L	CD-CE-NZ	-3.94	101.52	115.97
2	J	18	ALY	CE-NZ-CH	3.79	128.16	122.56
2	L	18	ALY	OH-CH-CH3	-3.32	116.14	122.05
2	I	18	ALY	OH-CH-CH3	-3.26	116.26	122.05
2	L	18	ALY	CH3-CH-NZ	2.49	120.37	116.12
2	M	18	ALY	CE-NZ-CH	2.40	126.11	122.56
2	I	18	ALY	CH3-CH-NZ	2.14	119.77	116.12
2	I	18	ALY	CE-NZ-CH	2.10	125.66	122.56
2	O	18	ALY	CE-NZ-CH	2.02	125.54	122.56

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	18	ALY	N-CA-CB-CG
2	I	18	ALY	C-CA-CB-CG
2	J	14	ALY	O-C-CA-CB
2	J	18	ALY	O-C-CA-CB
2	K	9	M3L	O-C-CA-CB
2	K	14	ALY	O-C-CA-CB
2	L	18	ALY	N-CA-CB-CG
2	L	18	ALY	C-CA-CB-CG
2	M	14	ALY	O-C-CA-CB
2	N	14	ALY	O-C-CA-CB
2	O	9	M3L	N-CA-CB-CG
2	O	9	M3L	C-CA-CB-CG
2	O	14	ALY	O-C-CA-CB
2	O	18	ALY	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	I	18	ALY	CG-CD-CE-NZ
2	I	18	ALY	OH-CH-NZ-CE
2	I	18	ALY	CH3-CH-NZ-CE
2	J	18	ALY	OH-CH-NZ-CE
2	J	18	ALY	CH3-CH-NZ-CE
2	L	18	ALY	OH-CH-NZ-CE
2	L	18	ALY	CH3-CH-NZ-CE
2	M	18	ALY	OH-CH-NZ-CE
2	M	18	ALY	CH3-CH-NZ-CE
2	J	9	M3L	CE-CD-CG-CB
2	L	18	ALY	CG-CD-CE-NZ
2	O	18	ALY	CG-CD-CE-NZ
2	N	9	M3L	CG-CD-CE-NZ
2	K	9	M3L	CD-CE-NZ-CM1
2	J	18	ALY	CA-CB-CG-CD
2	K	9	M3L	CD-CE-NZ-CM2
2	J	18	ALY	CE-CD-CG-CB
2	M	18	ALY	CE-CD-CG-CB
2	L	18	ALY	CE-CD-CG-CB
2	J	9	M3L	CD-CE-NZ-CM1
2	O	9	M3L	CE-CD-CG-CB
2	K	9	M3L	CD-CE-NZ-CM3
2	J	9	M3L	CD-CE-NZ-CM2
2	J	9	M3L	CD-CE-NZ-CM3
2	O	18	ALY	CE-CD-CG-CB
2	O	9	M3L	CD-CE-NZ-CM3
2	I	9	M3L	CE-CD-CG-CB
2	N	9	M3L	CD-CE-NZ-CM2
2	P	9	M3L	CD-CE-NZ-CM3
2	N	9	M3L	CD-CE-NZ-CM1
2	O	9	M3L	CD-CE-NZ-CM1
2	O	9	M3L	CD-CE-NZ-CM2
2	P	9	M3L	CE-CD-CG-CB
2	I	18	ALY	CE-CD-CG-CB
2	L	9	M3L	CA-CB-CG-CD
2	M	18	ALY	CA-CB-CG-CD
2	N	9	M3L	CD-CE-NZ-CM3
2	K	9	M3L	CE-CD-CG-CB
2	P	9	M3L	CD-CE-NZ-CM2
2	P	9	M3L	CD-CE-NZ-CM1
2	M	9	M3L	CD-CE-NZ-CM3
2	M	9	M3L	CD-CE-NZ-CM1

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Mol	Chain	Res	Type	Atoms
2	M	9	M3L	CD-CE-NZ-CM2
2	L	9	M3L	CE-CD-CG-CB
2	J	9	M3L	C-CA-CB-CG
2	K	9	M3L	C-CA-CB-CG
2	O	18	ALY	C-CA-CB-CG
2	P	9	M3L	CG-CD-CE-NZ
2	J	9	M3L	N-CA-CB-CG
2	M	18	ALY	N-CA-CB-CG
2	N	18	ALY	N-CA-CB-CG
2	O	18	ALY	N-CA-CB-CG

There are no ring outliers.

14 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	9	M3L	3	0
2	P	18	ALY	2	0
2	L	18	ALY	3	0
2	P	9	M3L	13	0
2	I	18	ALY	2	0
2	J	9	M3L	3	0
2	K	9	M3L	10	0
2	O	18	ALY	1	0
2	I	9	M3L	13	0
2	M	18	ALY	2	0
2	M	9	M3L	6	0
2	L	9	M3L	2	0
2	J	18	ALY	3	0
2	N	9	M3L	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	189/207 (91%)	-0.78	0	100	100	51, 89, 141, 177	0
1	B	189/207 (91%)	-0.84	0	100	100	53, 91, 137, 182	0
1	C	195/207 (94%)	-0.85	0	100	100	51, 92, 150, 212	0
1	D	187/207 (90%)	-0.79	0	100	100	50, 89, 140, 154	0
1	E	188/207 (90%)	-0.86	0	100	100	49, 89, 138, 178	0
1	F	189/207 (91%)	-0.70	1 (0%)	87	86	49, 90, 139, 169	0
1	G	187/207 (90%)	-0.76	0	100	100	54, 90, 141, 166	0
1	H	191/207 (92%)	-0.75	0	100	100	50, 90, 136, 172	0
2	I	17/22 (77%)	-0.66	0	100	100	84, 114, 149, 151	0
2	J	17/22 (77%)	-0.60	0	100	100	87, 116, 174, 175	0
2	K	17/22 (77%)	-0.65	0	100	100	83, 109, 147, 152	0
2	L	17/22 (77%)	-0.82	0	100	100	80, 108, 152, 160	0
2	M	17/22 (77%)	-0.61	0	100	100	84, 115, 151, 161	0
2	N	17/22 (77%)	-0.67	0	100	100	81, 111, 148, 152	0
2	O	17/22 (77%)	-0.64	0	100	100	79, 107, 146, 155	0
2	P	17/22 (77%)	-0.67	0	100	100	82, 109, 140, 151	0
All	All	1651/1832 (90%)	-0.78	1 (0%)	92	91	49, 92, 143, 212	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	959	SER	2.2

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

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
2	ALY	J	14	5/13	0.94	0.10	146,150,152,154	0
2	ALY	L	14	5/13	0.94	0.11	120,124,131,133	0
2	ALY	M	14	5/13	0.94	0.10	137,141,148,152	0
2	ALY	K	14	5/13	0.95	0.08	123,125,138,140	0
2	ALY	O	14	5/13	0.95	0.11	136,138,143,144	0
2	ALY	I	14	5/13	0.96	0.12	138,141,144,145	0
2	ALY	O	18	12/13	0.96	0.06	52,82,105,114	0
2	ALY	P	14	5/13	0.96	0.09	121,126,129,130	0
2	ALY	N	18	12/13	0.97	0.06	55,77,98,101	0
2	ALY	P	18	12/13	0.97	0.11	56,78,101,102	0
2	M3L	M	9	12/13	0.98	0.05	70,80,118,120	0
2	ALY	J	18	12/13	0.98	0.05	58,76,95,96	0
2	ALY	M	18	12/13	0.98	0.06	53,84,100,101	0
2	ALY	N	14	5/13	0.98	0.09	136,136,137,143	0
2	M3L	J	9	12/13	0.98	0.05	72,85,105,109	0
2	M3L	O	9	12/13	0.98	0.05	65,84,109,112	0
2	ALY	K	18	12/13	0.98	0.08	47,73,104,109	0
2	M3L	L	9	12/13	0.98	0.07	61,81,110,118	0
2	M3L	P	9	12/13	0.98	0.06	77,88,110,116	0
2	ALY	I	18	12/13	0.98	0.08	53,75,95,101	0
2	ALY	L	18	12/13	0.98	0.08	58,82,109,116	0
2	M3L	N	9	12/13	0.99	0.05	74,80,110,111	0
2	M3L	I	9	12/13	0.99	0.04	64,78,108,114	0
2	M3L	K	9	12/13	0.99	0.05	68,86,121,130	0

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($\text{\AA}^2$)	Q<0.9
3	ZN	A	1	1/1	0.99	0.03	86,86,86,86	0
3	ZN	A	2	1/1	0.99	0.03	96,96,96,96	0
3	ZN	C	2	1/1	0.99	0.02	99,99,99,99	0
3	ZN	B	2	1/1	1.00	0.01	100,100,100,100	0
3	ZN	C	1	1/1	1.00	0.03	84,84,84,84	0
3	ZN	B	1	1/1	1.00	0.03	83,83,83,83	0
3	ZN	D	1	1/1	1.00	0.04	85,85,85,85	0
3	ZN	D	2	1/1	1.00	0.02	93,93,93,93	0
3	ZN	E	1	1/1	1.00	0.03	88,88,88,88	0
3	ZN	E	2	1/1	1.00	0.02	99,99,99,99	0
3	ZN	F	1	1/1	1.00	0.01	90,90,90,90	0
3	ZN	F	2	1/1	1.00	0.01	102,102,102,102	0
3	ZN	G	1	1/1	1.00	0.03	83,83,83,83	0
3	ZN	G	2	1/1	1.00	0.02	101,101,101,101	0
3	ZN	H	1	1/1	1.00	0.02	83,83,83,83	0
3	ZN	H	2	1/1	1.00	0.02	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.