Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID	:	3U5O
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

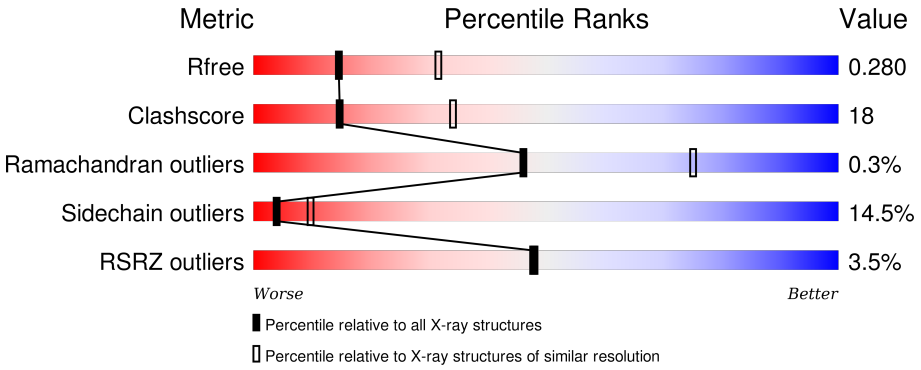
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 57% 28% 6% 9%
1	B	207	2% 57% 30% • 9%
1	C	207	3% 59% 29% 6% 6%
1	D	207	3% 51% 31% 8% 10%
1	E	207	3% 56% 29% 6% 9%

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Mol	Chain	Length	Quality of chain
1	F	207	3% 56% 30% 5% 9%
1	G	207	% 60% 25% 5% 10%
1	H	207	% 61% 26% 5% 8%
2	I	22	14% 45% 36% 9% 9%
2	J	22	18% 50% 36% 5% 9%
2	K	22	9% 55% 36% 9%
2	L	22	9% 64% 27% 9%
2	M	22	5% 55% 36% 9%
2	N	22	5% 73% 18% 9%
2	O	22	14% 45% 36% 9% 9%
2	P	22	9% 50% 32% 9% 9%

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	-
3	ZN	F	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 (three-letter code: ZN) (formula: Zn).

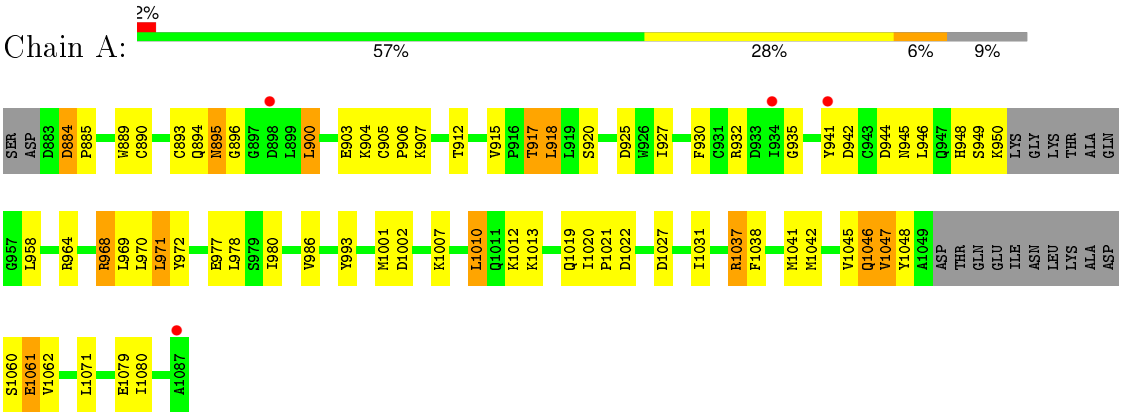
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	H	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

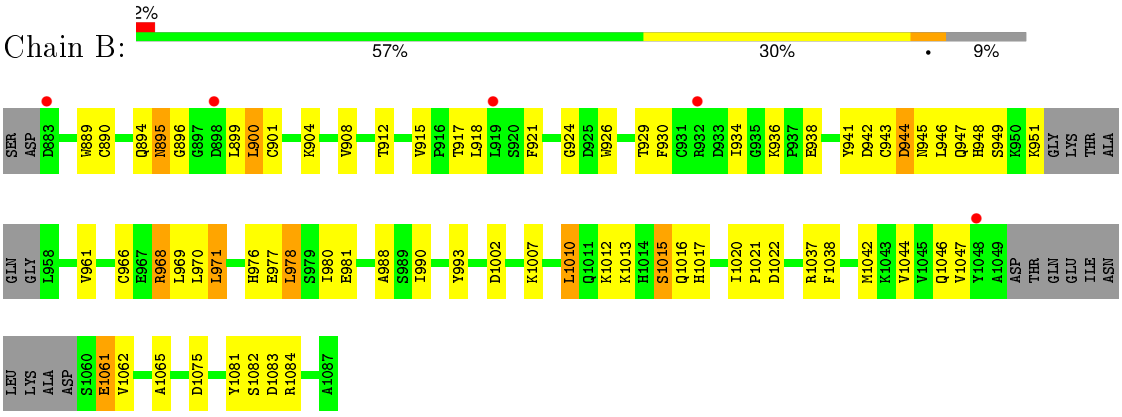
- Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain A:



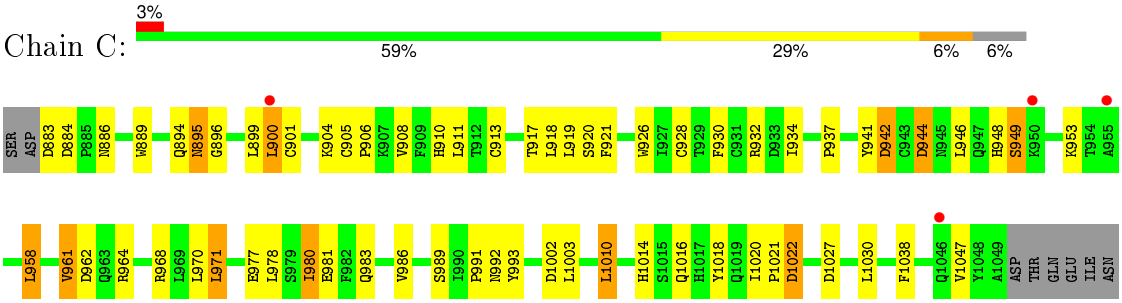
- Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain B:

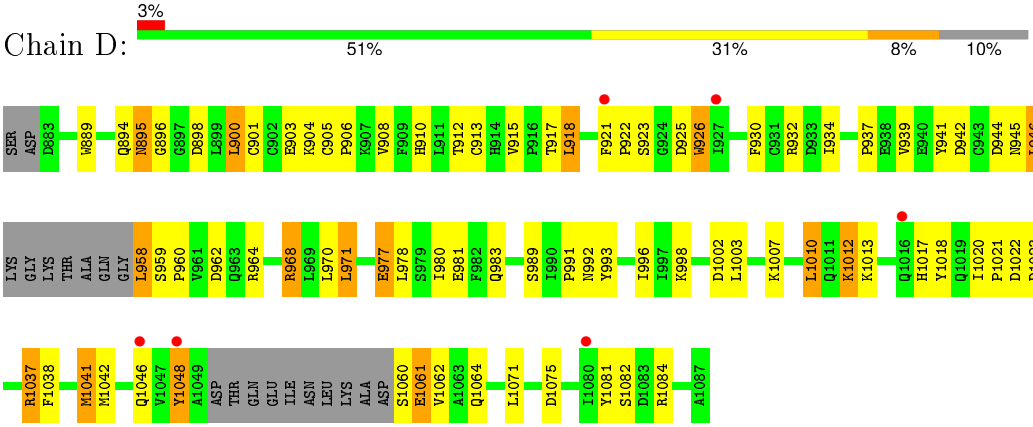


- Molecule 1: E3 ubiquitin-protein ligase TRIM33

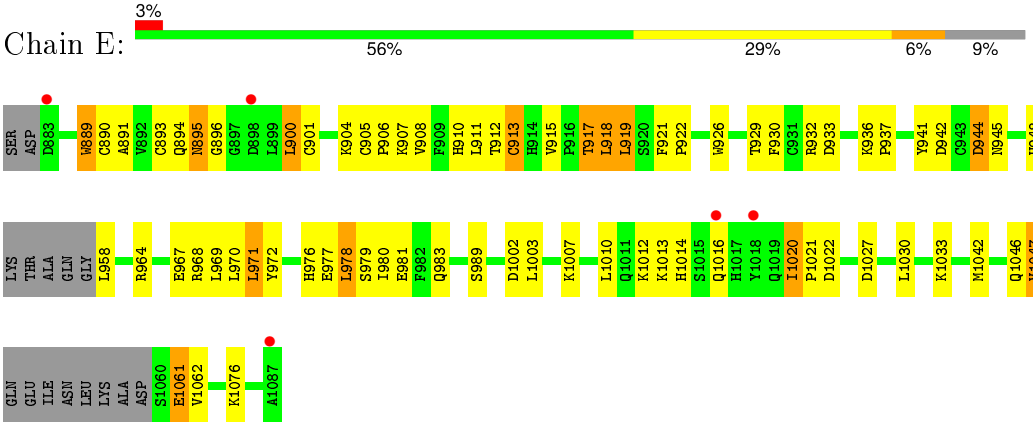
Chain C:



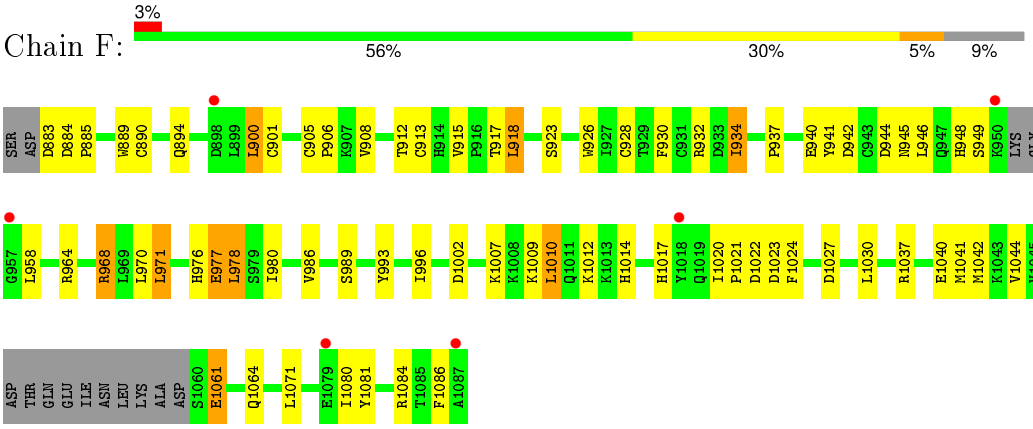
• Molecule 1: E3 ubiquitin-protein ligase TRIM33



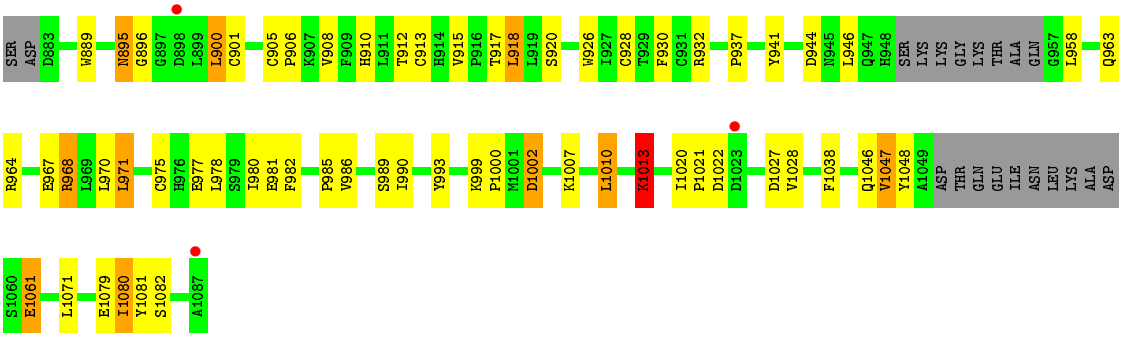
• Molecule 1: E3 ubiquitin-protein ligase TRIM33



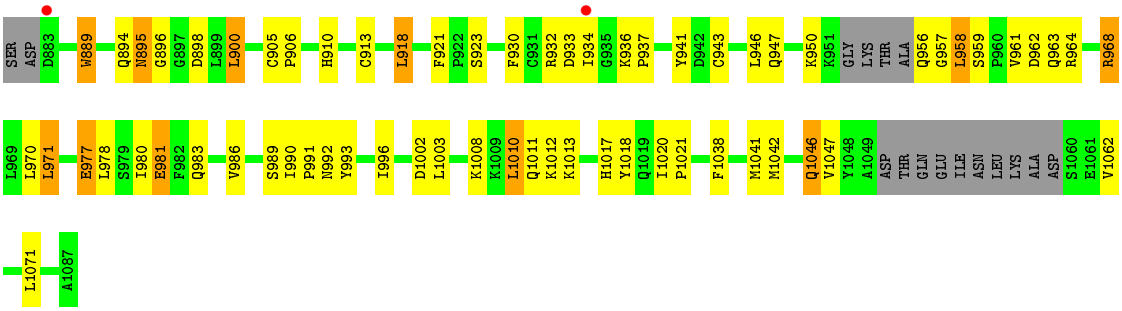
• Molecule 1: E3 ubiquitin-protein ligase TRIM33



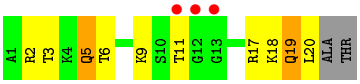
• Molecule 1: E3 ubiquitin-protein ligase TRIM33



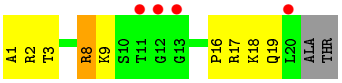
• Molecule 1: E3 ubiquitin-protein ligase TRIM33



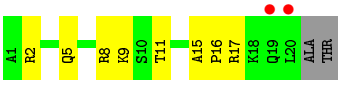
• Molecule 2: Histone H3.1



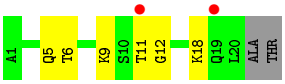
• Molecule 2: Histone H3.1



• Molecule 2: Histone H3.1

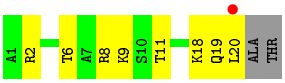


• Molecule 2: Histone H3.1



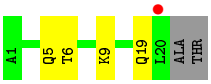
• Molecule 2: Histone H3.1

Chain M:



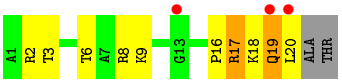
• Molecule 2: Histone H3.1

Chain N:



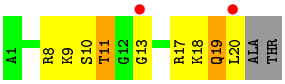
• Molecule 2: Histone H3.1

Chain O:



• Molecule 2: Histone H3.1

Chain P:



4 Data and refinement statistics (i)

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 28.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (28.47-2.70) 93.0 (28.48-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.280 0.204 , 0.280	Depositor DCC
R_{free} test set	1932 reflections (4.00%)	DCC
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.7	EDS
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
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 50209 reflections	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L, 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	0.74	0/1566	0.82	1/2116 (0.0%)
1	B	0.73	1/1571 (0.1%)	0.80	0/2122
1	C	0.70	0/1610	0.81	0/2175
1	D	0.78	3/1553 (0.2%)	0.80	0/2100
1	E	0.70	0/1562	0.81	0/2111
1	F	0.73	0/1566	0.77	0/2116
1	G	0.70	0/1551	0.81	0/2097
1	H	0.73	0/1584	0.84	0/2139
2	I	0.61	0/123	0.99	0/160
2	J	0.62	0/123	0.99	0/160
2	K	0.64	0/123	0.88	0/160
2	L	0.57	0/123	0.90	0/160
2	M	0.67	0/123	0.85	0/160
2	N	0.57	0/123	0.84	0/160
2	O	0.62	0/123	0.78	0/160
2	P	0.67	0/123	0.87	0/160
All	All	0.72	4/13547 (0.0%)	0.81	1/18256 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	949	SER	CB-OG	5.74	1.49	1.42
1	D	948	HIS	ND1-CE1	5.30	1.48	1.34
1	D	948	HIS	CG-CD2	5.18	1.44	1.35
1	D	926	TRP	CD2-CE2	5.04	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	958	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	59	0
1	B	1535	0	1500	50	0
1	C	1573	0	1540	54	0
1	D	1517	0	1475	65	0
1	E	1526	0	1488	50	0
1	F	1530	0	1491	69	0
1	G	1515	0	1472	51	0
1	H	1548	0	1511	47	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	168	10	0
2	N	154	0	168	7	0
2	O	154	0	168	10	0
2	P	154	0	169	27	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	2	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
All	All	13522	0	13316	478	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 (478) 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	1.07
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:F:890:CYS:HG	3:F:1:ZN:ZN	0.71	0.99
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: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
1:D:932:ARG:HD3	1:D:941:TYR:CZ	2.01	0.96
1:C:1061:GLU:H	1:C:1061:GLU:CD	1.70	0.95
1:C:895:ASN:HD22	1:C:896:GLY:N	1.65	0.94
1:B:1013:LYS:O	1:B:1013:LYS:HG2	1.68	0.93
1:G:895:ASN:ND2	1:G:896:GLY:H	1.69	0.91
2:K:9:M3L:HG2	2:K:9:M3L:O	1.68	0.90
1:D:895:ASN:HD22	1:D:896:GLY:N	1.68	0.89
1:E:895:ASN:HD22	1:E:896:GLY:N	1.68	0.89
1:C:895:ASN:ND2	1:C:896:GLY:H	1.70	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:1047:VAL:C	1:F:1048:TYR:CD1	2.46	0.88
1:F:977:GLU:CD	1:F:977:GLU:H	1.78	0.87
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:B:936:LYS:HD3	1:B:938:GLU:OE1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:LEU:HD23	2:P:20:LEU:O	1.82	0.80
1:A:889:TRP:CZ3	2:I:9:M3L:HD3	2.17	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:H:932:ARG:CZ	1:H:941:TYR:CE2	2.65	0.79
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:F:883:ASP:CG	1:F:884:ASP:H	1.88	0.76
1:B:930:PHE:HA	1:B:968:ARG:HD2	1.68	0.75
1:E:977:GLU:CD	1:E:977:GLU:H	1.89	0.75
1:E:1061:GLU:H	1:E:1061:GLU:CD	1.89	0.75
2:I:5:GLN:HG3	2:I:6:THR:H	1.51	0.75
1:F:1061:GLU:H	1:F:1061:GLU:CD	1.91	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:H:977:GLU:H	1:H:977:GLU:CD	1.91	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:E:944:ASP:N	1:E:944:ASP:OD1	2.25	0.70
1:A:1061:GLU:CD	1:A:1061:GLU:H	1.95	0.70
1:F:1048:TYR:N	1:F:1048:TYR:CD1	2.56	0.69
1:B:1020:ILE:CG2	1:B:1022:ASP:HB2	2.22	0.69
1:A:1019:GLN:OE1	1:A:1019:GLN:HA	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:H:932:ARG:CZ	1:H:941:TYR:HE2	2.04	0.69
1:B:895:ASN:ND2	1:B:896:GLY:H	1.90	0.68
1:A:1045:VAL:CG1	1:D:1048:TYR:HD1	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:977:GLU:H	1:A:977:GLU:CD	1.98	0.66
1:E:912:THR:HA	1:E:917:THR:HG23	1.78	0.66
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
2:I:5:GLN:HG3	2:I:6:THR:N	2.10	0.65
1:D:1062:VAL:HG21	2:L:18:ALY:HG3	1.77	0.65
1:F:1047:VAL:CG1	1:F:1048:TYR:HE1	2.02	0.65
1:F:1020:ILE:HG13	1:F:1021:PRO:HD2	1.78	0.65
1:D:1022:ASP:OD1	1:D:1084:ARG:NH2	2.30	0.65
1:A:912:THR:HA	1:A:917:THR:HG23	1.80	0.64
1:F:1061:GLU:N	1:F:1061:GLU:CD	2.50	0.64
1:A:889:TRP:CE2	2:I:9:M3L:HM32	2.33	0.64
1:F:1047:VAL:O	1:F:1048:TYR:CD1	2.50	0.63
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: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:1047:VAL:HG22	1:F:1047:VAL:O	2.00	0.62
1:H:1020:ILE:HG13	1:H:1021:PRO:CD	2.30	0.62
1:H:932:ARG:NH1	1:H:941:TYR:CE2	2.67	0.62
1:H:889:TRP:CE2	2:P:9:M3L:HM32	2.34	0.62
1:D:946:LEU:HG	1:D:946:LEU:O	1.98	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:H:1013:LYS:HG2	1:H:1013:LYS:O	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:E:1061:GLU:N	1:E:1061:GLU:CD	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:977:GLU:H	1:B:977:GLU:CD	2.02	0.60
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
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:C:905:CYS:HB2	1:C:906:PRO:HD2	1.84	0.60
1:C:977:GLU:H	1:C:977:GLU:CD	2.04	0.59
1:H:957:GLY:HA3	1:H:1012:LYS:HG2	1.84	0.59
1:C:1061:GLU:N	1:C:1061:GLU:CD	2.45	0.59
1:D:977:GLU:CD	1:D:977:GLU:H	2.06	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:E:889:TRP:CE2	2:M:9:M3L:CM3	2.86	0.59
1:B:895:ASN:ND2	1:B:896:GLY:N	2.50	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:A:1061:GLU:CD	1:A:1061:GLU:N	2.57	0.58
1:B:934:ILE:HG22	1:B:961:VAL:HG22	1.85	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: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
1:F:901:CYS:HA	1:F:908:VAL:HG12	1.85	0.58
1:F:890:CYS:SG	3:F:1:ZN:ZN	1.84	0.58
1:A:945:ASN:OD1	1:A:1012:LYS:HB2	2.04	0.57
2:K:9:M3L:O	2:K:9:M3L:CG	2.45	0.57
1:G:930:PHE:HA	1:G:968:ARG:HD2	1.86	0.57
2:J:2:ARG:HG2	2:J:3:THR:N	2.19	0.57
1:H:898:ASP:HB3	1:H:921:PHE:HZ	1.68	0.57
1:F:1046:GLN:O	1:F:1046:GLN:HG3	2.04	0.57
1:A:935:GLY:H	1:A:964:ARG:NH2	2.02	0.57
1:G:905:CYS:HB2	1:G:906:PRO:HD2	1.86	0.57
1:G:889:TRP:CZ3	2:O:9:M3L:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:G:1013:LYS:CG	2.52	0.56
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
2:P:19:GLN:O	2:P:20:LEU:HB2	2.04	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
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:F:996:ILE:HD13	1:F:1041:MET:HG2	1.89	0.55
1:A:1037:ARG:HH21	1:D:1037:ARG:HE	1.55	0.55
1:A:986:VAL:HG21	1:A:993:TYR:CZ	2.41	0.55
1:F:912:THR:HA	1:F:917:THR:HG23	1.89	0.55
2:P:19:GLN:HE21	2:P:20:LEU:N	2.05	0.55
1:H:894:GLN:HE21	2:P:9:M3L:HM22	1.70	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:F:884:ASP:OD1	1:F:885:PRO:HD2	2.07	0.55
1:D:912:THR:HA	1:D:917:THR:HG23	1.89	0.55
1:D:939:VAL:HG23	1:D:941:TYR:CE1	2.42	0.54
1:C:895:ASN:HD21	2:K:8:ARG:HA	1.71	0.54
1:A:889:TRP:HZ3	2:I:9:M3L:HG2	1.69	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:E:1046:GLN:C	1:E:1048:TYR:H	2.11	0.54
1:G:1013:LYS:O	1:G:1013:LYS:HG2	2.06	0.54
1:D:901:CYS:HA	1:D:908:VAL:HG12	1.90	0.54
1:D:958:LEU:HD23	1:D:1018:TYR:O	2.08	0.54
1:F:1048:TYR:O	1:F:1049:ALA:C	2.46	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:G:977:GLU:CD	1:G:977:GLU:H	2.11	0.53
2:P:19:GLN:CD	2:P:20:LEU:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1061:GLU:HG2	2:O:16:PRO:HB3	1.91	0.53
1:B:966:CYS:HA	1:B:969:LEU:HD12	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:B:1065:ALA:HB2	2:J:16:PRO:HG2	1.92	0.52
2:L:5:GLN:HG3	2:L:6:THR:N	2.25	0.52
1:D:915:VAL:HB	1:D:971:LEU:HD23	1.92	0.52
1:C:937:PRO:HG3	1:C:964:ARG:CZ	2.40	0.52
1:A:1042:MET:O	1:A:1046:GLN:HB3	2.10	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:G:895:ASN:ND2	1:G:896:GLY:N	2.40	0.51
1:D:983:GLN:HG2	1:D:1003:LEU:HD12	1.92	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:A:1013:LYS:HG3	1:A:1013:LYS:O	2.11	0.51
1:H:947:GLN:O	1:H:950:LYS:HB3	2.10	0.51
1:E:912:THR:HA	1:E:917:THR:CG2	2.41	0.51
1:C:886:ASN:OD1	2:K:2:ARG:NH1	2.44	0.51
1:D:1027:ASP:O	1:D:1030:LEU:HB3	2.11	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
2:P:19:GLN:NE2	2:P:20:LEU:N	2.58	0.51
1:C:930:PHE:HA	1:C:968:ARG:HD2	1.92	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:998:LYS:CE	2:P:10:SER:OG	2.59	0.50
1:D:942:ASP:OD1	1:D:942:ASP:N	2.30	0.50
1:A:1046:GLN:C	1:A:1048:TYR:H	2.15	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: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:G:895:ASN:HD21	2:O:8:ARG:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:VAL:HG22	1:A:1007:LYS:HE3	1.94	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:G:970:LEU:HD22	1:G:1010:LEU:HD23	1.93	0.49
1:H:905:CYS:HB2	1:H:906:PRO:CD	2.42	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
2:P:19:GLN:CG	2:P:20:LEU:N	2.76	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: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:G:971:LEU:HD13	1:G:975:CYS:SG	2.53	0.49
1:F:944:ASP:O	1:F:948:HIS:HB2	2.13	0.49
1:C:889:TRP:CZ2	2:K:9:M3L:HM23	2.48	0.48
1:H:895:ASN:HD21	2:P:8:ARG:HA	1.77	0.48
1:F:930:PHE:CE2	1:F:971:LEU:HD13	2.49	0.48
1:C:900:LEU:HD12	1:C:918:LEU:HD23	1.95	0.48
1:F:1010:LEU:HA	1:F:1010:LEU:HD13	1.65	0.48
1:C:962:ASP:HB3	1:C:1021:PRO:HG3	1.95	0.48
1:G:1020:ILE:HG13	1:G:1021:PRO:HD2	1.95	0.48
1:E:983:GLN:HG2	1:E:1003:LEU:HD12	1.96	0.48
1:H:959:SER:HB2	1:H:962:ASP:HB2	1.95	0.48
1:E:926:TRP:NE1	1:E:941:TYR:CE1	2.80	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:G:930:PHE:CE2	1:G:971:LEU:CD1	2.97	0.48
1:B:895:ASN:HD21	2:J:8:ARG:HA	1.79	0.48
1:F:934:ILE:HD11	1:F:968:ARG:NH2	2.30	0.47
1:C:883:ASP:CG	1:C:884:ASP:H	2.18	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:A:884:ASP:OD1	1:A:885:PRO:HD2	2.14	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:D:942:ASP:O	1:D:942:ASP:CG	2.50	0.47
1:F:977:GLU:CD	1:F:977:GLU:N	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:937:PRO:HG3	1:G:964:ARG:NE	2.29	0.47
1:F:883:ASP:CG	1:F:884:ASP:N	2.61	0.47
1:B:988:ALA:HB1	2:I:6:THR:HG23	1.97	0.47
1:F:900:LEU:CD1	1:F:918:LEU:HD23	2.44	0.47
1:E:1020:ILE:HG13	1:E:1021:PRO:N	2.28	0.47
1:C:977:GLU:N	1:C:977:GLU:OE2	2.46	0.47
1:A:993:TYR:HA	1:A:1038:PHE:CE1	2.49	0.47
2:I:19:GLN:O	2:I:20:LEU:HB2	2.15	0.47
1:E:969:LEU:O	1:E:972:TYR:HB2	2.14	0.47
1:E:976:HIS:CE1	1:E:978:LEU:HB2	2.49	0.47
1:B:1044:VAL:O	1:B:1047:VAL:HG12	2.15	0.47
1:B:895:ASN:HD22	1:B:896:GLY:H	1.53	0.47
1:H:986:VAL:HG21	1:H:993:TYR:CZ	2.49	0.47
1:C:946:LEU:O	1:C:949:SER:HB2	2.15	0.47
1:G:932:ARG:HH22	1:G:964:ARG:HG2	1.80	0.46
1:F:942:ASP:OD1	1:F:942:ASP:N	2.40	0.46
1:F:1041:MET:O	1:F:1044:VAL:HB	2.16	0.46
1:D:934:ILE:HD11	1:D:968:ARG:CZ	2.45	0.46
1:F:1020:ILE:HG22	1:F:1023:ASP:OD2	2.15	0.46
1:F:1021:PRO:O	1:F:1024:PHE:N	2.46	0.46
1:H:993:TYR:HA	1:H:1038:PHE:CE1	2.51	0.46
1:G:910:HIS:HB2	1:G:913:CYS:HB2	1.97	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:1062:VAL:HG21	2:P:18:ALY:N	2.29	0.46
1:B:926:TRP:NE1	1:B:941:TYR:HE1	2.12	0.46
1:C:1010:LEU:HA	1:C:1010:LEU:HD13	1.87	0.46
1:F:986:VAL:HG21	1:F:993:TYR:CZ	2.51	0.46
2:M:9:M3L:HM32	2:M:9:M3L:HD3	1.55	0.46
1:B:1020:ILE:HD12	1:B:1021:PRO:HD2	1.98	0.46
1:B:890:CYS:HB2	1:B:899:LEU:HD21	1.98	0.46
1:G:889:TRP:CE2	2:O:9:M3L:HM32	2.51	0.45
1:C:901:CYS:HA	1:C:908:VAL:HG12	1.98	0.45
1:H:933:ASP:HB3	1:H:936:LYS:O	2.16	0.45
1:F:1046:GLN:C	1:F:1048:TYR:H	2.20	0.45
1:B:1013:LYS:CG	1:B:1013:LYS:O	2.52	0.45
1:A:900:LEU:HD12	1:A:918:LEU:HD23	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:9:M3L:HD2	2:K:9:M3L:HM22	1.77	0.45
1:F:1014:HIS:O	1:F:1017:HIS:HB2	2.16	0.45
1:H:932:ARG:NH2	1:H:964:ARG:HG2	2.31	0.45
1:F:1037:ARG:O	1:F:1040:GLU:HB2	2.17	0.45
1:G:915:VAL:HB	1:G:971:LEU:HD23	1.98	0.45
1:A:1037:ARG:NH2	1:D:1037:ARG:HE	2.13	0.45
2:M:18:ALY:HH31	2:M:18:ALY:HE2	1.73	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:F:890:CYS:SG	1:F:913:CYS:SG	3.15	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:HA	1:D:1010:LEU:HD13	1.71	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:C:894:GLN:O	2:K:9:M3L:HM13	2.18	0.44
1:B:988:ALA:CB	2:I:6:THR:HG23	2.47	0.44
2:P:9:M3L:HG3	2:P:10:SER:N	2.33	0.44
1:G:932:ARG:NH2	1:G:964:ARG:HG2	2.32	0.44
1:D:910:HIS:HB2	1:D:913:CYS:HB2	1.99	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:D:921:PHE:HA	1:D:922:PRO:HD3	1.90	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: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: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:E:911:LEU:HD22	1:E:918:LEU:HB3	2.00	0.43
1:F:1020:ILE:HG13	1:F:1021:PRO:CD	2.48	0.43
1:A:932:ARG:HD3	1:A:941:TYR:CZ	2.54	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:C:900:LEU:HD12	1:C:918:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:M3L:HD3	2:I:9:M3L:HM32	1.68	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
1:A:900:LEU:CD1	1:A:918:LEU:HD23	2.49	0.43
1:E:945:ASN:OD1	1:E:1012:LYS:HB2	2.18	0.43
1:B:1015:SER:O	1:B:1016:GLN:HG3	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:993:TYR:HA	1:G:1038:PHE:CE1	2.53	0.42
1:G:932:ARG:NH2	1:G:964:ARG:CD	2.81	0.42
1:G:999:LYS:HA	1:G:1000:PRO:HD3	1.78	0.42
1:B:894:GLN:HE21	2:J:9:M3L:HM21	1.83	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:B:977:GLU:OE2	1:B:977:GLU:N	2.45	0.42
1:H:981:GLU:HG2	1:H:1062:VAL:HG22	2.01	0.42
1:D:905:CYS:HB2	1:D:906:PRO:HD2	2.00	0.42
1:E:1076:LYS:HD3	1:E:1076:LYS:HA	1.86	0.42
1:C:1022:ASP:OD1	1:C:1022:ASP:N	2.52	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:C:910:HIS:HB2	1:C:913:CYS:HB2	2.01	0.42
1:H:934:ILE:HD11	1:H:968:ARG:CZ	2.49	0.42
1:D:894:GLN:O	2:L:9:M3L:HE3	2.19	0.42
2:O:19:GLN:HG2	2:O:20:LEU:H	1.84	0.42
1:D:900:LEU:CD1	1:D:918:LEU:CD2	2.96	0.42
2:P:10:SER:HB3	2:P:11:THR:H	1.70	0.42
1:C:993:TYR:HA	1:C:1038:PHE:CE1	2.54	0.42
1:E:1046:GLN:C	1:E:1048:TYR:N	2.73	0.42
1:A:915:VAL:HG11	1:A:970:LEU:HB3	2.02	0.42
1:E:901:CYS:HA	1:E:908:VAL:HG12	2.01	0.42
1:A:907:LYS:HE3	1:A:930:PHE:CE2	2.55	0.42
2:I:18:ALY:HE3	2:I:18:ALY:HH31	1.88	0.42
1:G:926:TRP:NE1	1:G:941:TYR:CE1	2.87	0.42
2:J:18:ALY:HH31	2:J:18:ALY:HE2	1.82	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
1:A:969:LEU:O	1:A:972:TYR:HB2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:932:ARG:CZ	1:E:941:TYR:CE2	3.02	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:921:PHE:CE2	1:C:961:VAL:HG21	2.55	0.42
1:B:912:THR:O	1:B:1007:LYS:NZ	2.53	0.41
1:B:1062:VAL:HG21	2:J:18:ALY:HG3	2.01	0.41
1:G:1027:ASP:O	1:G:1028:VAL:C	2.58	0.41
1:D:1061:GLU:N	1:D:1061:GLU:CD	2.74	0.41
1:C:895:ASN:ND2	1:C:896:GLY:N	2.47	0.41
2:J:9:M3L:H	2:J:9:M3L:HG2	1.72	0.41
1:E:967:GLU:HG3	1:E:1010:LEU:HD21	2.02	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: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
2:P:19:GLN:HG2	2:P:20:LEU:N	2.35	0.41
1:A:889:TRP:CE3	2:I:9:M3L:CD	3.02	0.41
1:H:937:PRO:HG3	1:H:964:ARG:CZ	2.51	0.41
1:H:889:TRP:CZ3	2:P:9:M3L:HB3	2.56	0.41
1:C:1079:GLU:HG2	1:C:1079:GLU:O	2.21	0.41
1:C:1027:ASP:O	1:C:1030:LEU:HB3	2.21	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
2:N:5:GLN:HG3	2:N:6:THR:H	1.85	0.41
1:E:1027:ASP:O	1:E:1030:LEU:HB3	2.21	0.41
1:G:982:PHE:CD2	1:G:982:PHE:N	2.88	0.41
1:F:1022:ASP:HA	1:F:1086:PHE:CD2	2.55	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:D:1020:ILE:HG22	1:D:1023:ASP:CG	2.41	0.41
1:G:1079:GLU:HG3	1:G:1079:GLU:O	2.21	0.41
1:B:929:THR:O	1:B:929:THR:CG2	2.68	0.41
1:B:901:CYS:SG	2:J:2:ARG:HD2	2.61	0.41
1:C:932:ARG:HH21	1:C:964:ARG:HG2	1.86	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:G:926:TRP:NE1	1:G:941:TYR:HE1	2.19	0.41
1:B:1083:ASP:OD2	1:B:1083:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:9:M3L:HM22	2:N:9:M3L:HD2	1.46	0.40
1:D:900:LEU:CD2	1:D:926:TRP:CE3	3.03	0.40
1:G:928:CYS:SG	1:G:930:PHE:HB2	2.61	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:B:1010:LEU:HA	1:B:1010:LEU:HD13	1.72	0.40
1:H:910:HIS:HB2	1:H:913:CYS:HB2	2.03	0.40
1:A:971:LEU:HD23	1:A:971:LEU:HA	1.93	0.40
1:F:900:LEU:HD22	1:F:901:CYS:O	2.21	0.40
1:C:911:LEU:HD21	1:C:921:PHE:CD1	2.57	0.40
1:G:1020:ILE:HG13	1:G:1021:PRO:CD	2.51	0.40
1:D:993:TYR:HA	1:D:1038:PHE:CE1	2.56	0.40
1:B:993:TYR:HA	1:B:1038:PHE:CE1	2.56	0.40
1:F:976:HIS:CE1	1:F:978:LEU:HB2	2.56	0.40
1:G:1046:GLN:C	1:G:1048:TYR:H	2.24	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:F:1027:ASP:O	1:F:1030:LEU:HB3	2.21	0.40
1:E:979:SER:O	1:E:980:ILE:C	2.57	0.40
1:F:1047:VAL:CG2	1:F:1047:VAL:O	2.68	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:H:932:ARG:CZ	1:H:941:TYR:CD2	2.98	0.40
1:F:1061:GLU:HA	1:F:1064:GLN:HB2	2.03	0.40
1:D:1013:LYS:HG2	1:D:1013:LYS:O	2.20	0.40
1:F:970:LEU:HD22	1:F:1010:LEU:HD23	2.04	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	183/207 (88%)	167 (91%)	15 (8%)	1 (0%)	34 63
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%)	34 63
1	F	183/207 (88%)	167 (91%)	16 (9%)	0	100 100
1	G	181/207 (87%)	169 (93%)	10 (6%)	2 (1%)	17 42
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%)	46 75

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	174/189 (92%)	147 (84%)	27 (16%)	3 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	175/189 (93%)	151 (86%)	24 (14%)	4 11
1	C	178/189 (94%)	152 (85%)	26 (15%)	4 9
1	D	173/189 (92%)	142 (82%)	31 (18%)	2 5
1	E	174/189 (92%)	152 (87%)	22 (13%)	5 13
1	F	174/189 (92%)	150 (86%)	24 (14%)	4 10
1	G	172/189 (91%)	151 (88%)	21 (12%)	6 14
1	H	176/189 (93%)	154 (88%)	22 (12%)	6 13
2	I	12/13 (92%)	8 (67%)	4 (33%)	0 0
2	J	12/13 (92%)	9 (75%)	3 (25%)	1 2
2	K	12/13 (92%)	9 (75%)	3 (25%)	1 2
2	L	12/13 (92%)	12 (100%)	0	100 100
2	M	12/13 (92%)	8 (67%)	4 (33%)	0 0
2	N	12/13 (92%)	11 (92%)	1 (8%)	14 31
2	O	12/13 (92%)	10 (83%)	2 (17%)	3 7
2	P	12/13 (92%)	10 (83%)	2 (17%)	3 7
All	All	1492/1616 (92%)	1276 (86%)	216 (14%)	4 10

All (216) 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	942	ASP
1	A	944	ASP
1	A	948	HIS
1	A	950	LYS
1	A	968	ARG
1	A	971	LEU
1	A	978	LEU
1	A	980	ILE
1	A	1002	ASP
1	A	1010	LEU
1	A	1022	ASP

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Mol	Chain	Res	Type
1	A	1027	ASP
1	A	1037	ARG
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	904	LYS
1	B	918	LEU
1	B	942	ASP
1	B	943	CYS
1	B	944	ASP
1	B	946	LEU
1	B	951	LYS
1	B	968	ARG
1	B	971	LEU
1	B	978	LEU
1	B	980	ILE
1	B	981	GLU
1	B	1002	ASP
1	B	1010	LEU
1	B	1015	SER
1	B	1037	ARG
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	904	LYS
1	C	917	THR
1	C	928	CYS
1	C	934	ILE
1	C	942	ASP

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Mol	Chain	Res	Type
1	C	944	ASP
1	C	949	SER
1	C	958	LEU
1	C	961	VAL
1	C	971	LEU
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	1075	ASP
1	C	1082	SER
1	D	895	ASN
1	D	898	ASP
1	D	900	LEU
1	D	904	LYS
1	D	918	LEU
1	D	923	SER
1	D	944	ASP
1	D	946	LEU
1	D	948	HIS
1	D	958	LEU
1	D	968	ARG
1	D	971	LEU
1	D	977	GLU
1	D	978	LEU
1	D	980	ILE
1	D	989	SER
1	D	1002	ASP
1	D	1010	LEU
1	D	1012	LYS
1	D	1027	ASP
1	D	1037	ARG
1	D	1041	MET
1	D	1042	MET
1	D	1046	GLN

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Mol	Chain	Res	Type
1	D	1048	TYR
1	D	1060	SER
1	D	1061	GLU
1	D	1064	GLN
1	D	1071	LEU
1	D	1075	ASP
1	D	1082	SER
1	E	889	TRP
1	E	895	ASN
1	E	900	LEU
1	E	904	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	968	ARG
1	E	971	LEU
1	E	978	LEU
1	E	989	SER
1	E	1002	ASP
1	E	1020	ILE
1	E	1033	LYS
1	E	1042	MET
1	E	1047	VAL
1	E	1061	GLU
1	F	900	LEU
1	F	918	LEU
1	F	923	SER
1	F	934	ILE
1	F	940	GLU
1	F	945	ASN
1	F	946	LEU
1	F	949	SER
1	F	958	LEU
1	F	968	ARG
1	F	971	LEU
1	F	977	GLU
1	F	978	LEU

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Mol	Chain	Res	Type
1	F	980	ILE
1	F	989	SER
1	F	1002	ASP
1	F	1009	LYS
1	F	1010	LEU
1	F	1042	MET
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	918	LEU
1	G	920	SER
1	G	944	ASP
1	G	946	LEU
1	G	958	LEU
1	G	968	ARG
1	G	971	LEU
1	G	978	LEU
1	G	980	ILE
1	G	989	SER
1	G	1002	ASP
1	G	1010	LEU
1	G	1013	LYS
1	G	1022	ASP
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	895	ASN
1	H	900	LEU
1	H	918	LEU
1	H	923	SER
1	H	943	CYS
1	H	946	LEU
1	H	956	GLN
1	H	958	LEU
1	H	961	VAL

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Mol	Chain	Res	Type
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	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
2	K	5	GLN
2	K	11	THR
2	K	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	895	ASN
1	A	983	GLN
1	B	894	GLN
1	B	895	ASN
1	B	983	GLN
1	B	1046	GLN
1	C	895	ASN

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Mol	Chain	Res	Type
1	C	956	GLN
1	C	983	GLN
1	C	1016	GLN
1	D	895	ASN
1	D	983	GLN
1	D	1046	GLN
1	E	894	GLN
1	E	895	ASN
1	E	983	GLN
1	F	983	GLN
1	F	1046	GLN
1	G	894	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	1016	GLN
1	H	1046	GLN
2	I	19	GLN
2	M	5	GLN
2	O	19	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	ALY	I	14	2	3,4,12	0.61	0	0,4,14	0.00	-
2	ALY	I	18	2	10,11,12	0.60	0	10,12,14	1.62	3 (30%)
2	M3L	I	9	2	10,11,12	1.25	0	12,14,16	0.81	0
2	ALY	J	14	2	3,4,12	0.61	0	0,4,14	0.00	-
2	ALY	J	18	2	10,11,12	0.87	1 (10%)	10,12,14	1.62	2 (20%)
2	M3L	J	9	2	10,11,12	0.74	0	12,14,16	1.07	0
2	ALY	K	14	2	3,4,12	0.62	0	0,4,14	0.00	-
2	ALY	K	18	2	10,11,12	0.61	0	10,12,14	1.23	1 (10%)
2	M3L	K	9	2	10,11,12	0.95	0	12,14,16	0.94	1 (8%)
2	ALY	L	14	2	3,4,12	0.64	0	0,4,14	0.00	-
2	ALY	L	18	2	10,11,12	0.83	1 (10%)	10,12,14	2.07	4 (40%)
2	M3L	L	9	2	10,11,12	0.80	0	12,14,16	1.05	1 (8%)
2	ALY	M	14	2	3,4,12	0.60	0	0,4,14	0.00	-
2	ALY	M	18	2	10,11,12	0.60	0	10,12,14	1.23	2 (20%)
2	M3L	M	9	2	10,11,12	1.00	0	12,14,16	0.93	1 (8%)
2	ALY	N	14	2	3,4,12	0.63	0	0,4,14	0.00	-
2	ALY	N	18	2	10,11,12	0.83	1 (10%)	10,12,14	1.01	1 (10%)
2	M3L	N	9	2	10,11,12	1.08	0	12,14,16	1.77	2 (16%)
2	ALY	O	14	2	3,4,12	0.50	0	0,4,14	0.00	-
2	ALY	O	18	2	10,11,12	0.59	0	10,12,14	1.13	0
2	M3L	O	9	2	10,11,12	0.72	0	12,14,16	1.21	0
2	ALY	P	14	2	3,4,12	0.53	0	0,4,14	0.00	-
2	ALY	P	18	2	10,11,12	0.87	0	10,12,14	1.08	1 (10%)
2	M3L	P	9	2	10,11,12	1.38	2 (20%)	12,14,16	1.54	3 (25%)

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	ALY	I	14	2	-	0/0/2/12	0/0/0/0
2	ALY	I	18	2	-	2/8/10/12	0/0/0/0
2	M3L	I	9	2	-	0/8/10/12	0/0/0/0
2	ALY	J	14	2	-	0/0/2/12	0/0/0/0
2	ALY	J	18	2	-	2/8/10/12	0/0/0/0
2	M3L	J	9	2	-	0/8/10/12	0/0/0/0
2	ALY	K	14	2	-	0/0/2/12	0/0/0/0
2	ALY	K	18	2	-	0/8/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	K	9	2	-	0/8/10/12	0/0/0/0
2	ALY	L	14	2	-	0/0/2/12	0/0/0/0
2	ALY	L	18	2	-	2/8/10/12	0/0/0/0
2	M3L	L	9	2	-	0/8/10/12	0/0/0/0
2	ALY	M	14	2	-	0/0/2/12	0/0/0/0
2	ALY	M	18	2	-	2/8/10/12	0/0/0/0
2	M3L	M	9	2	-	0/8/10/12	0/0/0/0
2	ALY	N	14	2	-	0/0/2/12	0/0/0/0
2	ALY	N	18	2	-	0/8/10/12	0/0/0/0
2	M3L	N	9	2	-	0/8/10/12	0/0/0/0
2	ALY	O	14	2	-	0/0/2/12	0/0/0/0
2	ALY	O	18	2	-	0/8/10/12	0/0/0/0
2	M3L	O	9	2	-	0/8/10/12	0/0/0/0
2	ALY	P	14	2	-	0/0/2/12	0/0/0/0
2	ALY	P	18	2	-	0/8/10/12	0/0/0/0
2	M3L	P	9	2	-	0/8/10/12	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	9	M3L	CB-CA	-2.46	1.51	1.53
2	J	18	ALY	CB-CA	-2.36	1.51	1.53
2	N	18	ALY	CB-CA	-2.29	1.51	1.53
2	P	9	M3L	CE-NZ	-2.17	1.44	1.51
2	L	18	ALY	CB-CA	-2.04	1.51	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	9	M3L	CB-CA-N	-5.09	96.05	110.52
2	L	18	ALY	OH-CH-CH3	-3.22	116.14	122.06
2	I	18	ALY	OH-CH-CH3	-3.16	116.26	122.06
2	P	9	M3L	CD-CE-NZ	-3.14	101.52	116.08
2	P	9	M3L	CB-CA-N	-3.06	101.83	110.52
2	M	9	M3L	O-C-CA	-2.39	119.25	125.49
2	M	18	ALY	O-C-CA	-2.36	119.34	125.49
2	K	18	ALY	O-C-CA	-2.36	119.35	125.49
2	P	18	ALY	O-C-CA	-2.32	119.44	125.49
2	J	18	ALY	O-C-CA	-2.20	119.77	125.49
2	N	9	M3L	O-C-CA	-2.13	119.94	125.49
2	L	9	M3L	O-C-CA	-2.10	120.03	125.49
2	P	9	M3L	O-C-CA	-2.08	120.08	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	9	M3L	O-C-CA	-2.07	120.09	125.49
2	N	18	ALY	O-C-CA	-2.06	120.12	125.49
2	L	18	ALY	O-C-CA	-2.02	120.22	125.49
2	I	18	ALY	CE-NZ-CH	2.01	125.66	122.36
2	M	18	ALY	CE-NZ-CH	2.29	126.11	122.36
2	I	18	ALY	CH3-CH-NZ	2.35	119.77	116.19
2	L	18	ALY	CH3-CH-NZ	2.75	120.37	116.19
2	J	18	ALY	CE-NZ-CH	3.55	128.16	122.36
2	L	18	ALY	CE-NZ-CH	3.95	128.81	122.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	18	ALY	CH3-CH-NZ-CE
2	M	18	ALY	CH3-CH-NZ-CE
2	J	18	ALY	CH3-CH-NZ-CE
2	I	18	ALY	CH3-CH-NZ-CE
2	L	18	ALY	OH-CH-NZ-CE
2	J	18	ALY	OH-CH-NZ-CE
2	M	18	ALY	OH-CH-NZ-CE
2	I	18	ALY	OH-CH-NZ-CE

There are no ring outliers.

14 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	18	ALY	2	0
2	I	9	M3L	13	0
2	J	18	ALY	3	0
2	J	9	M3L	3	0
2	K	9	M3L	10	0
2	L	18	ALY	3	0
2	L	9	M3L	2	0
2	M	18	ALY	2	0
2	M	9	M3L	6	0
2	N	9	M3L	5	0
2	O	18	ALY	1	0
2	O	9	M3L	3	0
2	P	18	ALY	1	0
2	P	9	M3L	11	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	189/207 (91%)	0.15	4 (2%)	67	68	51, 89, 141, 177	0
1	B	189/207 (91%)	0.15	5 (2%)	59	59	53, 91, 137, 183	0
1	C	195/207 (94%)	0.21	6 (3%)	52	52	51, 92, 150, 212	0
1	D	187/207 (90%)	0.15	7 (3%)	45	45	50, 89, 140, 154	0
1	E	188/207 (90%)	0.18	6 (3%)	51	51	49, 89, 138, 178	0
1	F	189/207 (91%)	0.09	6 (3%)	51	51	49, 90, 139, 169	0
1	G	187/207 (90%)	0.22	3 (1%)	74	75	54, 90, 141, 166	0
1	H	191/207 (92%)	0.13	2 (1%)	84	85	50, 90, 136, 172	0
2	I	17/22 (77%)	0.62	3 (17%)	2	1	84, 114, 149, 151	0
2	J	17/22 (77%)	0.91	4 (23%)	1	1	87, 116, 174, 175	0
2	K	17/22 (77%)	0.65	2 (11%)	6	5	83, 109, 147, 152	0
2	L	17/22 (77%)	0.69	2 (11%)	6	5	80, 108, 152, 160	0
2	M	17/22 (77%)	0.79	1 (5%)	26	24	84, 115, 151, 161	0
2	N	17/22 (77%)	0.62	1 (5%)	26	24	81, 111, 148, 152	0
2	O	17/22 (77%)	0.70	3 (17%)	2	1	79, 107, 146, 155	0
2	P	17/22 (77%)	0.48	2 (11%)	6	5	82, 109, 140, 151	0
All	All	1651/1832 (90%)	0.20	57 (3%)	48	48	49, 92, 143, 212	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	7.2
1	G	1087	ALA	6.5
2	O	20	LEU	6.2
1	C	1087	ALA	5.1
1	C	955	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	1087	ALA	4.6
1	H	883	ASP	4.5
1	E	1087	ALA	4.1
2	K	20	LEU	3.8
2	N	20	LEU	3.7
2	J	13	GLY	3.6
1	D	948	HIS	3.6
1	E	1016	GLN	3.5
1	B	883	ASP	3.4
1	B	932	ARG	3.4
2	I	12	GLY	3.3
1	C	1046	GLN	3.2
2	O	13	GLY	3.2
2	L	19	GLN	3.1
1	D	1048	TYR	3.1
1	A	934	ILE	3.0
1	A	898	ASP	3.0
1	F	950	LYS	3.0
2	J	12	GLY	2.9
1	D	1080	ILE	2.8
1	D	927	ILE	2.8
1	A	941	TYR	2.7
1	G	1023	ASP	2.7
1	B	919	LEU	2.6
1	E	898	ASP	2.6
2	J	11	THR	2.6
2	P	20	LEU	2.6
1	F	898	ASP	2.6
1	B	898	ASP	2.6
2	L	11	THR	2.5
1	C	950	LYS	2.4
1	F	1018	TYR	2.4
2	M	20	LEU	2.3
1	C	1080	ILE	2.3
1	D	1046	GLN	2.3
1	F	957	GLY	2.3
1	E	883	ASP	2.2
1	G	898	ASP	2.2
2	P	13	GLY	2.2
1	C	900	LEU	2.2
2	J	20	LEU	2.2
2	I	13	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1016	GLN	2.1
1	E	1018	TYR	2.1
1	H	934	ILE	2.1
2	K	19	GLN	2.1
1	B	1048	TYR	2.1
2	O	19	GLN	2.0
1	D	921	PHE	2.0
1	E	1048	TYR	2.0
1	F	1079	GLU	2.0
2	I	11	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ALY	K	18	12/13	0.91	0.19	-	47,73,104,109	0
2	ALY	K	14	5/13	0.60	0.31	-	123,125,138,140	0
2	ALY	I	14	5/13	0.79	0.62	-	138,141,144,145	0
2	M3L	L	9	12/13	0.91	0.20	-	61,81,110,118	0
2	ALY	P	14	5/13	0.89	0.25	-	121,126,129,130	0
2	ALY	N	14	5/13	0.92	0.32	-	136,136,137,143	0
2	ALY	P	18	12/13	0.93	0.26	-	56,78,101,102	0
2	M3L	P	9	12/13	0.86	0.19	-	77,88,110,116	0
2	M3L	O	9	12/13	0.92	0.19	-	65,84,109,112	0
2	ALY	L	14	5/13	0.82	0.37	-	120,124,131,133	0
2	M3L	N	9	12/13	0.92	0.15	-	74,80,110,111	0
2	ALY	M	14	5/13	0.85	0.27	-	137,141,148,152	0
2	ALY	N	18	12/13	0.93	0.17	-	55,77,98,101	0
2	M3L	M	9	12/13	0.91	0.20	-	70,80,118,120	0
2	M3L	K	9	12/13	0.91	0.16	-	68,86,121,130	0
2	ALY	M	18	12/13	0.89	0.20	-	53,84,100,101	0
2	ALY	J	18	12/13	0.93	0.17	-	58,76,95,96	0
2	M3L	J	9	12/13	0.95	0.18	-	72,85,105,109	0
2	ALY	L	18	12/13	0.85	0.21	-	58,82,109,116	0
2	ALY	I	18	12/13	0.90	0.21	-	53,75,95,101	0
2	ALY	J	14	5/13	0.76	0.40	-	146,150,152,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ALY	O	14	5/13	0.75	0.45	-	136,138,143,144	0
2	M3L	I	9	12/13	0.89	0.16	-	64,78,108,114	0
2	ALY	O	18	12/13	0.93	0.15	-	52,82,105,114	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	H	1	1/1	0.98	0.17	1.81	83,83,83,83	0
3	ZN	B	1	1/1	0.99	0.19	1.08	83,83,83,83	0
3	ZN	C	1	1/1	0.99	0.18	1.05	84,84,84,84	0
3	ZN	G	2	1/1	0.98	0.18	0.82	101,101,101,101	0
3	ZN	H	2	1/1	0.95	0.18	0.46	99,99,99,99	0
3	ZN	A	1	1/1	0.99	0.15	0.39	86,86,86,86	0
3	ZN	D	2	1/1	0.96	0.16	0.20	93,93,93,93	0
3	ZN	F	2	1/1	0.93	0.17	0.19	102,102,102,102	0
3	ZN	C	2	1/1	0.92	0.17	0.12	99,99,99,99	0
3	ZN	E	2	1/1	0.84	0.16	-0.03	99,99,99,99	0
3	ZN	G	1	1/1	0.98	0.15	-0.07	83,83,83,83	0
3	ZN	A	2	1/1	0.97	0.17	-0.11	96,96,96,96	0
3	ZN	E	1	1/1	0.99	0.14	-0.47	88,88,88,88	0
3	ZN	B	2	1/1	0.98	0.13	-0.78	100,100,100,100	0
3	ZN	D	1	1/1	0.99	0.15	-	85,85,85,85	0
3	ZN	F	1	1/1	0.98	0.20	-	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.