Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2024 – 01:39 am GMT

PDB ID	:	4B09
Title	:	Structure of unphosphorylated BaeR dimer
Authors	:	Choudhury, H.; Beis, K.
Deposited on	:	2012-06-29
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

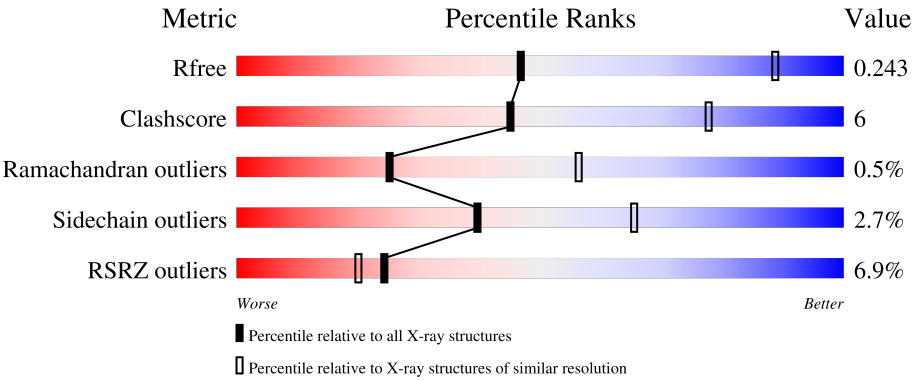
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.30 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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 <=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	240	4% 72% 18% • 9%
1	B	240	9% 74% 16% 10%
1	C	240	5% 72% 18% • 9%
1	D	240	8% 73% 15% • 10%
1	E	240	5% 75% 14% • 9%

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Mol	Chain	Length	Quality of chain
1	F	240	6% 77% 13% 10%
1	G	240	5% 74% 15% 9%
1	H	240	7% 76% 13% 10%
1	I	240	5% 75% 15% 9%
1	J	240	7% 71% 18% 10%
1	K	240	6% 72% 17% 9%
1	L	240	7% 74% 16% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21258 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 TRANSCRIPTIONAL REGULATORY PROTEIN BAER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	As	C	N	O	S	0	0	0
			1765	1	1127	309	321	7			
1	B	216	Total	As	C	N	O	S	0	0	0
			1751	2	1120	304	318	7			
1	C	218	Total	As	C	N	O	S	0	0	0
			1765	1	1127	309	321	7			
1	D	216	Total	As	C	N	O	S	0	0	0
			1751	2	1120	304	318	7			
1	E	218	Total	As	C	N	O	S	0	0	0
			1765	1	1127	309	321	7			
1	F	216	Total	As	C	N	O	S	0	0	0
			1751	2	1120	304	318	7			
1	G	218	Total	As	C	N	O	S	0	0	0
			1765	1	1127	309	321	7			
1	H	216	Total	As	C	N	O	S	0	0	0
			1751	2	1120	304	318	7			
1	I	218	Total	As	C	N	O	S	0	0	0
			1765	1	1127	309	321	7			
1	J	216	Total	As	C	N	O	S	0	0	0
			1751	2	1120	304	318	7			
1	K	218	Total	As	C	N	O	S	0	0	0
			1765	1	1127	309	321	7			
1	L	216	Total	As	C	N	O	S	0	0	0
			1751	2	1120	304	318	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	MET	THR	engineered mutation	UNP P69228
B	71	MET	THR	engineered mutation	UNP P69228
C	71	MET	THR	engineered mutation	UNP P69228
D	71	MET	THR	engineered mutation	UNP P69228
E	71	MET	THR	engineered mutation	UNP P69229

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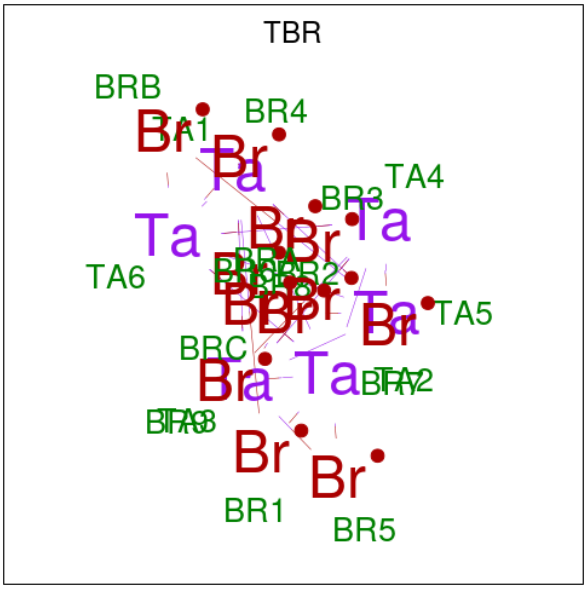
Chain	Residue	Modelled	Actual	Comment	Reference
F	71	MET	THR	engineered mutation	UNP P69228
G	71	MET	THR	engineered mutation	UNP P69228
H	71	MET	THR	engineered mutation	UNP P69228
I	71	MET	THR	engineered mutation	UNP P69228
J	71	MET	THR	engineered mutation	UNP P69228
K	71	MET	THR	engineered mutation	UNP P69228
L	71	MET	THR	engineered mutation	UNP P69228

- Molecule 2 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br Ta 18 12 6	0	0
2	B	1	Total Br Ta 18 12 6	0	0
2	C	1	Total Br Ta 18 12 6	0	0
2	D	1	Total Br Ta 18 12 6	0	0
2	E	1	Total Br Ta 18 12 6	0	0
2	F	1	Total Br Ta 18 12 6	0	0
2	G	1	Total Br Ta 18 12 6	0	0

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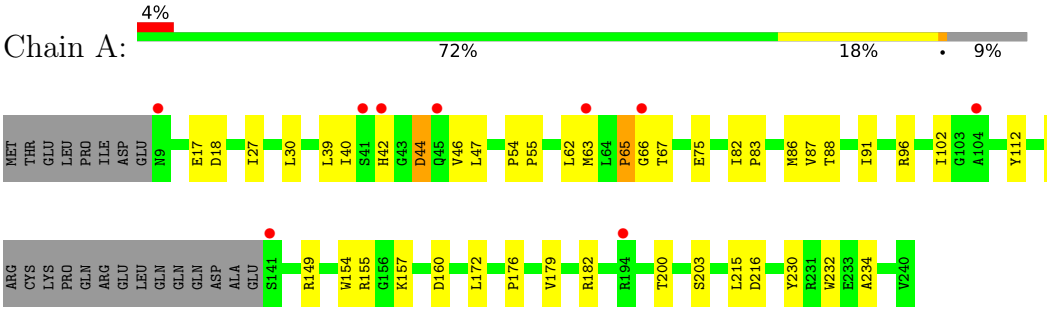
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total Br Ta 18 12 6	0	0
2	K	1	Total Br Ta 18 12 6	0	0

3 Residue-property plots

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

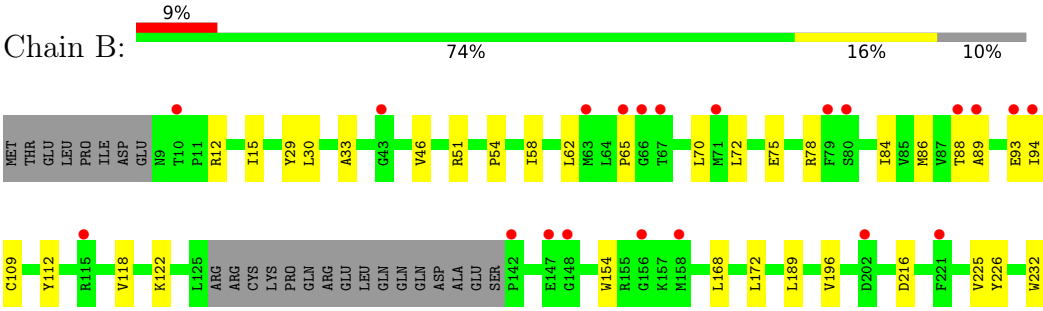
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain A:



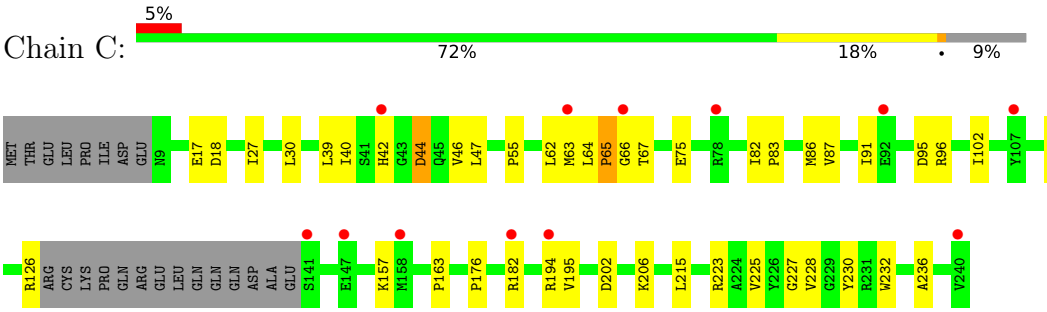
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain B:



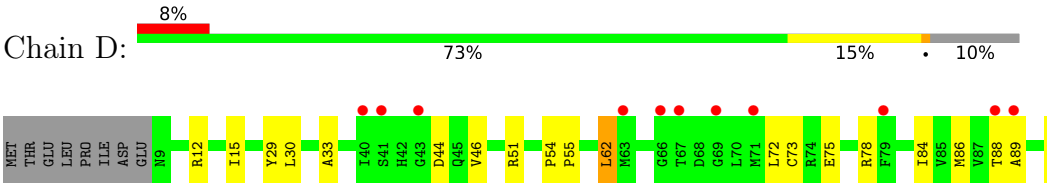
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

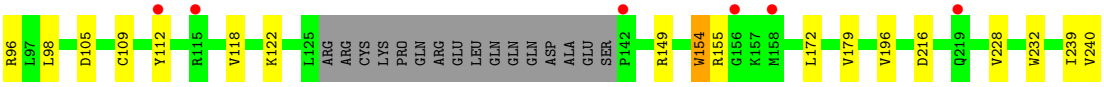
Chain C:



• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

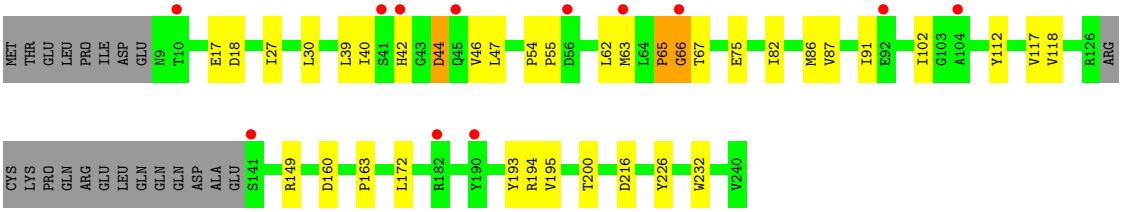
Chain D:





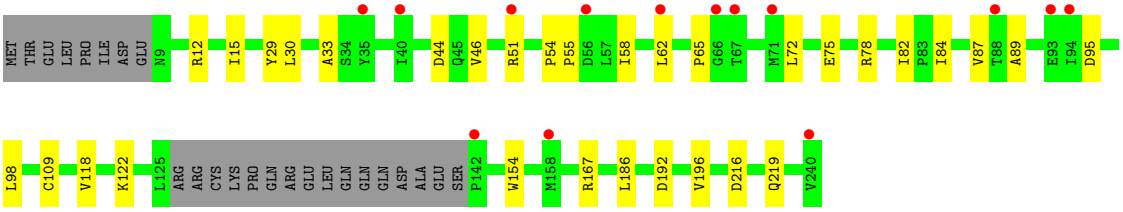
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain E:



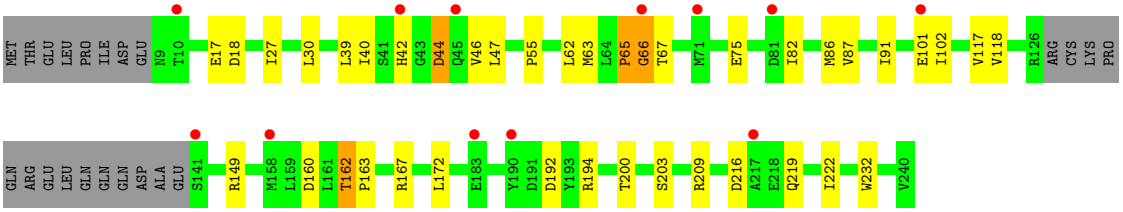
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain F:



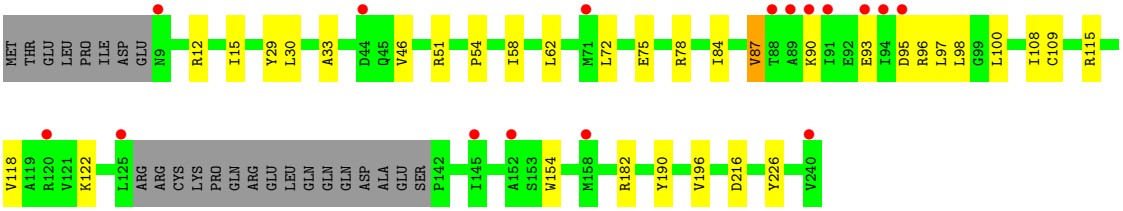
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain G:



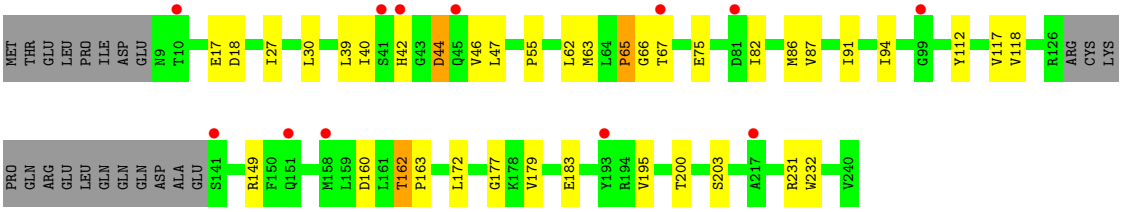
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain H:



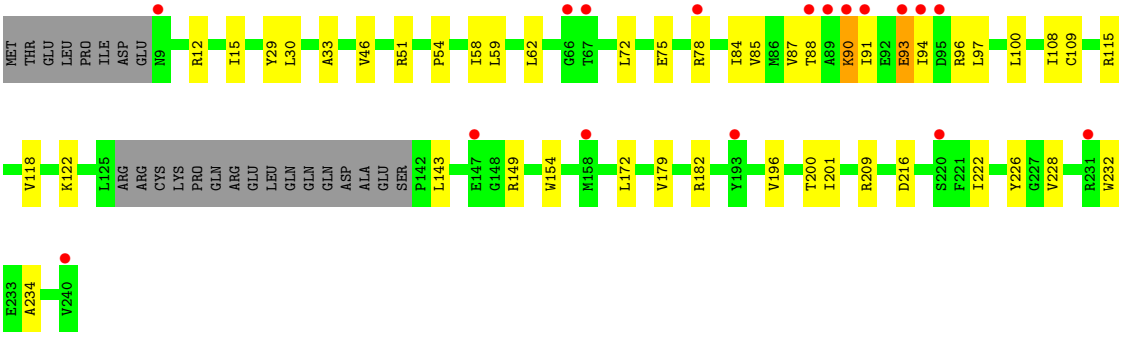
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain I:



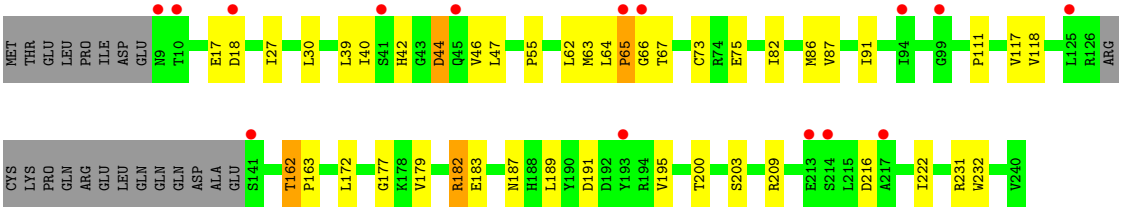
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain J:



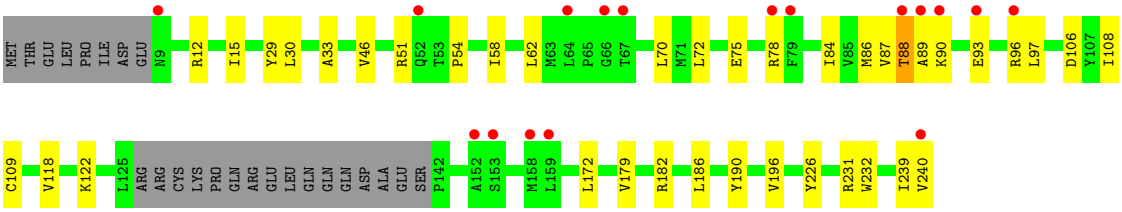
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain K:



• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN BAER

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	236.60Å 130.40Å 198.21Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	49.55 – 3.30 49.55 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.55-3.30) 98.6 (49.55-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.225 , 0.245 0.225 , 0.243	Depositor DCC
R_{free} test set	4488 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	109.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 91.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.019 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.063 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.056 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21258	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, 0.333 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: CAS, TBR

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	0.22	0/1781	0.42	0/2410
1	B	0.20	0/1764	0.39	0/2387
1	C	0.20	0/1781	0.39	0/2410
1	D	0.20	0/1764	0.39	0/2387
1	E	0.21	0/1781	0.40	0/2410
1	F	0.20	0/1764	0.39	0/2387
1	G	0.21	0/1781	0.40	0/2410
1	H	0.20	0/1764	0.39	0/2387
1	I	0.21	0/1781	0.40	0/2410
1	J	0.20	0/1764	0.39	0/2387
1	K	0.22	0/1781	0.42	0/2410
1	L	0.20	0/1764	0.39	0/2387
All	All	0.20	0/21270	0.40	0/28782

There are no bond length outliers.

There are no bond angle outliers.

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	1765	0	1807	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1751	0	1789	22	0
1	C	1765	0	1807	28	0
1	D	1751	0	1789	27	0
1	E	1765	0	1807	24	0
1	F	1751	0	1789	19	0
1	G	1765	0	1807	22	0
1	H	1751	0	1789	21	0
1	I	1765	0	1807	23	0
1	J	1751	0	1789	27	0
1	K	1765	0	1807	26	0
1	L	1751	0	1789	21	0
2	A	18	0	0	0	0
2	B	18	0	0	2	0
2	C	18	0	0	0	0
2	D	18	0	0	2	0
2	E	18	0	0	0	0
2	F	18	0	0	1	0
2	G	18	0	0	0	0
2	I	18	0	0	0	0
2	K	18	0	0	0	0
All	All	21258	0	21576	250	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 6.

All (250) 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:H:87:VAL:HG13	1:H:90:LYS:HE3	1.71	0.73
1:C:102:ILE:HD11	1:L:226:TYR:HD2	1.53	0.73
1:D:95:ASP:O	1:I:231:ARG:NH1	2.26	0.67
1:K:183:GLU:O	1:K:187:ASN:ND2	2.28	0.66
1:A:102:ILE:HD11	1:H:226:TYR:HD2	1.62	0.65
1:J:58:ILE:HB	1:J:84:ILE:HG12	1.79	0.65
1:F:75:GLU:OE2	1:F:78:ARG:NH2	2.31	0.64
1:J:75:GLU:OE2	1:J:78:ARG:NH2	2.29	0.64
1:B:75:GLU:OE2	1:B:78:ARG:NH2	2.31	0.63
1:D:75:GLU:OE2	1:D:78:ARG:NH2	2.31	0.62
1:K:62:LEU:HD11	1:K:86:MET:HB3	1.82	0.62
1:C:62:LEU:HD11	1:C:86:MET:HB3	1.82	0.62
1:I:62:LEU:HD11	1:I:86:MET:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:HD11	1:E:86:MET:HB3	1.82	0.61
1:C:163:PRO:HB2	1:C:195:VAL:HG22	1.83	0.61
1:H:154:TRP:HZ3	1:H:216:ASP:HB3	1.66	0.61
1:A:62:LEU:HD11	1:A:86:MET:HB3	1.82	0.61
1:G:62:LEU:HD11	1:G:86:MET:HB3	1.82	0.61
1:E:163:PRO:HB2	1:E:195:VAL:HG22	1.83	0.61
1:C:112:TYR:CD1	1:D:109:CAS:CE1	2.84	0.60
1:J:154:TRP:HZ3	1:J:216:ASP:HB3	1.65	0.60
1:L:75:GLU:OE2	1:L:78:ARG:NH2	2.30	0.60
1:E:102:ILE:HD11	1:J:226:TYR:HD2	1.65	0.60
1:C:65:PRO:O	1:C:67:THR:N	2.36	0.59
1:J:87:VAL:HG13	1:J:90:LYS:HE3	1.85	0.59
1:I:163:PRO:HB2	1:I:195:VAL:HG22	1.83	0.59
1:K:162:THR:HG22	1:K:163:PRO:HD2	1.85	0.59
1:E:65:PRO:O	1:E:67:THR:N	2.36	0.59
1:I:65:PRO:O	1:I:67:THR:N	2.36	0.58
1:E:112:TYR:CE1	1:F:109:CAS:CE2	2.86	0.58
1:I:162:THR:HG22	1:I:163:PRO:HD2	1.84	0.58
1:H:75:GLU:OE2	1:H:78:ARG:NH2	2.31	0.58
1:G:65:PRO:O	1:G:67:THR:N	2.36	0.58
1:K:65:PRO:O	1:K:67:THR:N	2.36	0.58
1:A:65:PRO:O	1:A:67:THR:N	2.36	0.57
1:J:209:ARG:NH1	1:J:222:ILE:O	2.35	0.57
1:B:239:ILE:HG22	1:B:240:VAL:HG23	1.85	0.57
1:F:154:TRP:HZ3	1:F:216:ASP:HB2	1.69	0.57
1:C:112:TYR:CE1	1:D:109:CAS:CE1	2.88	0.56
1:F:95:ASP:O	1:K:231:ARG:NH1	2.38	0.56
1:J:33:ALA:HB1	1:J:122:LYS:HE3	1.87	0.56
1:B:33:ALA:HB1	1:B:122:LYS:HE3	1.87	0.56
1:A:160:ASP:OD2	1:G:149:ARG:NH1	2.38	0.56
1:H:12:ARG:NH1	1:H:54:PRO:O	2.35	0.56
1:L:33:ALA:HB1	1:L:122:LYS:HE3	1.87	0.56
1:H:33:ALA:HB1	1:H:122:LYS:HE3	1.87	0.56
1:D:12:ARG:NH1	1:D:54:PRO:O	2.35	0.55
1:D:33:ALA:HB1	1:D:122:LYS:HE3	1.87	0.55
1:B:172:LEU:HB3	1:B:232:TRP:HB2	1.89	0.55
1:D:92:GLU:OE2	1:K:182:ARG:NH2	2.38	0.55
1:J:12:ARG:NH1	1:J:54:PRO:O	2.35	0.55
1:F:33:ALA:HB1	1:F:122:LYS:HE3	1.87	0.54
1:A:179:VAL:HG23	1:C:95:ASP:HB3	1.90	0.54
1:F:12:ARG:NH1	1:F:54:PRO:O	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:TYR:CD1	1:F:109:CAS:CE2	2.91	0.54
1:L:88:THR:OG1	1:L:89:ALA:N	2.41	0.54
1:B:12:ARG:NH1	1:B:54:PRO:O	2.35	0.54
1:B:226:TYR:HD2	1:G:102:ILE:HD11	1.72	0.54
1:D:154:TRP:HZ3	1:D:216:ASP:HB2	1.72	0.54
1:K:44:ASP:OD1	1:K:44:ASP:N	2.41	0.53
1:B:154:TRP:HZ3	1:B:216:ASP:HB2	1.73	0.53
1:C:44:ASP:N	1:C:44:ASP:OD1	2.42	0.53
1:E:149:ARG:NH1	1:I:160:ASP:OD2	2.37	0.53
1:G:44:ASP:OD1	1:G:44:ASP:N	2.42	0.53
1:I:44:ASP:OD1	1:I:44:ASP:N	2.42	0.53
1:K:111:PRO:HA	1:L:88:THR:HG21	1.90	0.53
1:B:58:ILE:HB	1:B:84:ILE:HG12	1.91	0.52
1:E:44:ASP:OD1	1:E:44:ASP:N	2.41	0.52
1:J:15:ILE:HD11	1:J:30:LEU:HD12	1.92	0.52
1:A:44:ASP:N	1:A:44:ASP:OD1	2.41	0.52
1:H:46:VAL:HG11	1:H:72:LEU:HD21	1.92	0.52
1:A:182:ARG:HG2	1:A:230:TYR:HE1	1.73	0.52
1:J:46:VAL:HG11	1:J:72:LEU:HD21	1.91	0.52
1:A:154:TRP:HB3	1:A:215:LEU:HD12	1.92	0.52
1:L:15:ILE:HD11	1:L:30:LEU:HD12	1.91	0.52
1:D:46:VAL:HG11	1:D:72:LEU:HD21	1.92	0.52
1:H:97:LEU:HD22	1:H:100:LEU:HD22	1.91	0.52
1:C:91:ILE:HD13	1:C:117:VAL:HG21	1.92	0.52
1:B:29:TYR:HB3	1:B:118:VAL:HG21	1.92	0.52
1:D:29:TYR:HB3	1:D:118:VAL:HG21	1.92	0.52
1:L:46:VAL:HG11	1:L:72:LEU:HD21	1.92	0.52
1:L:58:ILE:HB	1:L:84:ILE:HG12	1.90	0.52
1:D:15:ILE:HD11	1:D:30:LEU:HD12	1.92	0.51
1:G:91:ILE:HD13	1:G:117:VAL:HG21	1.93	0.51
1:B:65:PRO:HA	2:B:1241:TBR:BR5	2.65	0.51
1:H:15:ILE:HD11	1:H:30:LEU:HD12	1.91	0.51
1:J:97:LEU:HD22	1:J:100:LEU:HD22	1.91	0.51
1:G:162:THR:HG22	1:G:163:PRO:HD2	1.91	0.51
1:G:167:ARG:HE	1:G:192:ASP:HB2	1.75	0.51
1:B:15:ILE:HD11	1:B:30:LEU:HD12	1.91	0.51
1:H:29:TYR:HB3	1:H:118:VAL:HG21	1.92	0.51
1:C:176:PRO:HG3	1:C:236:ALA:HB2	1.93	0.51
1:L:29:TYR:HB3	1:L:118:VAL:HG21	1.92	0.51
1:G:87:VAL:HA	1:H:109:CAS:HB2	1.92	0.51
1:I:91:ILE:HD13	1:I:117:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:HD13	1:A:117:VAL:HG21	1.92	0.51
1:F:46:VAL:HG11	1:F:72:LEU:HD21	1.92	0.51
1:K:172:LEU:HB3	1:K:232:TRP:HB2	1.92	0.51
1:F:15:ILE:HD11	1:F:30:LEU:HD12	1.92	0.51
1:F:29:TYR:HB3	1:F:118:VAL:HG21	1.92	0.51
1:L:12:ARG:NH1	1:L:54:PRO:O	2.35	0.51
1:B:46:VAL:HG11	1:B:72:LEU:HD21	1.92	0.51
1:J:29:TYR:HB3	1:J:118:VAL:HG21	1.92	0.50
1:E:91:ILE:HD13	1:E:117:VAL:HG21	1.93	0.50
1:L:97:LEU:HD13	1:L:108:ILE:HD13	1.92	0.50
1:A:172:LEU:HB3	1:A:232:TRP:HB2	1.92	0.50
1:K:91:ILE:HD13	1:K:117:VAL:HG21	1.93	0.50
1:K:87:VAL:HA	1:L:109:CAS:HB2	1.93	0.50
1:E:226:TYR:OH	1:J:93:GLU:OE2	2.21	0.50
1:C:87:VAL:HA	1:D:109:CAS:HB2	1.93	0.50
1:G:172:LEU:HB3	1:G:232:TRP:HB2	1.94	0.49
1:C:225:VAL:HB	1:C:228:VAL:HB	1.95	0.49
1:I:87:VAL:HA	1:J:109:CAS:HB2	1.94	0.49
1:J:172:LEU:HB3	1:J:232:TRP:HB2	1.94	0.49
1:H:98:LEU:O	1:L:231:ARG:NH2	2.46	0.49
1:B:70:LEU:HD23	1:B:86:MET:HE2	1.95	0.48
1:D:62:LEU:HD12	1:D:86:MET:HE2	1.94	0.48
1:L:87:VAL:HG13	1:L:90:LYS:HE2	1.95	0.48
1:A:155:ARG:NH2	1:A:215:LEU:O	2.45	0.48
1:A:182:ARG:HG2	1:A:230:TYR:CE1	2.49	0.48
1:A:157:LYS:HB2	1:A:215:LEU:HD13	1.95	0.48
1:D:179:VAL:HG11	1:D:228:VAL:HG12	1.96	0.48
1:H:97:LEU:HD13	1:H:108:ILE:HD13	1.96	0.47
1:E:102:ILE:HD11	1:J:226:TYR:CD2	2.49	0.47
1:C:182:ARG:HH12	1:C:227:GLY:H	1.62	0.47
1:C:202:ASP:OD2	1:C:206:LYS:NZ	2.47	0.46
1:F:98:LEU:HD23	1:K:179:VAL:HG21	1.97	0.46
1:C:96:ARG:NH1	2:D:1241:TBR:BRB	3.03	0.46
1:H:58:ILE:HB	1:H:84:ILE:HG12	1.96	0.46
1:A:47:LEU:HD11	1:A:75:GLU:HG2	1.98	0.46
1:D:149:ARG:NH2	1:K:191:ASP:O	2.46	0.46
1:F:167:ARG:HE	1:F:192:ASP:HB2	1.80	0.46
1:D:94:ILE:O	1:D:96:ARG:N	2.44	0.46
1:A:126:ARG:HD2	1:H:190:TYR:CZ	2.50	0.46
1:F:65:PRO:HA	2:F:1241:TBR:BR6	2.71	0.46
1:A:200:THR:HG23	1:A:203:SER:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ILE:HG21	1:E:46:VAL:HG22	1.98	0.46
1:G:40:ILE:HG21	1:G:46:VAL:HG22	1.98	0.46
1:E:160:ASP:OD2	1:I:149:ARG:NH2	2.49	0.45
1:J:154:TRP:CZ3	1:J:216:ASP:HB3	2.50	0.45
1:C:40:ILE:HG21	1:C:46:VAL:HG22	1.99	0.45
1:C:47:LEU:HD11	1:C:75:GLU:HG2	1.98	0.45
1:A:87:VAL:HA	1:B:109:CAS:HB2	1.98	0.45
1:D:239:ILE:HG22	1:D:240:VAL:HG23	1.97	0.45
1:I:40:ILE:HG21	1:I:46:VAL:HG22	1.98	0.45
1:H:93:GLU:H	1:H:93:GLU:HG2	1.55	0.45
1:I:17:GLU:HB3	1:I:39:LEU:HD11	1.99	0.45
1:L:172:LEU:HB3	1:L:232:TRP:HB2	1.98	0.45
1:A:40:ILE:HG21	1:A:46:VAL:HG22	1.99	0.45
1:E:27:ILE:HD11	1:E:39:LEU:HB2	1.99	0.45
1:E:47:LEU:HD11	1:E:75:GLU:HG2	1.98	0.45
1:E:172:LEU:HB3	1:E:232:TRP:HB2	1.99	0.45
1:E:193:TYR:O	1:E:194:ARG:HB3	2.17	0.45
1:J:96:ARG:HA	1:J:96:ARG:HD3	1.85	0.45
1:A:17:GLU:HB3	1:A:39:LEU:HD11	1.99	0.45
1:G:17:GLU:HB3	1:G:39:LEU:HD11	1.99	0.45
1:G:27:ILE:HD11	1:G:39:LEU:HB2	1.99	0.45
1:E:87:VAL:HA	1:F:109:CAS:HB2	1.98	0.45
1:F:87:VAL:HG12	1:F:89:ALA:H	1.81	0.45
1:G:47:LEU:HD11	1:G:75:GLU:HG2	1.98	0.45
1:I:112:TYR:CD1	1:J:109:CAS:CE1	2.99	0.45
1:L:70:LEU:HD23	1:L:86:MET:HE2	1.99	0.45
1:C:157:LYS:HB2	1:C:215:LEU:HD13	1.99	0.45
1:I:27:ILE:HD11	1:I:39:LEU:HB2	1.99	0.45
1:I:47:LEU:HD11	1:I:75:GLU:HG2	1.98	0.45
1:K:47:LEU:HD11	1:K:75:GLU:HG2	1.98	0.45
1:G:18:ASP:OD1	1:G:42:HIS:HB2	2.17	0.44
1:A:83:PRO:HA	1:B:105:ASP:O	2.17	0.44
1:C:27:ILE:HD11	1:C:39:LEU:HB2	1.99	0.44
1:J:97:LEU:HD13	1:J:108:ILE:HD13	1.98	0.44
1:K:18:ASP:OD1	1:K:42:HIS:HB2	2.17	0.44
1:I:30:LEU:HD23	1:I:118:VAL:HG22	2.00	0.44
1:E:17:GLU:HB3	1:E:39:LEU:HD11	1.99	0.44
1:G:209:ARG:NH1	1:G:222:ILE:O	2.49	0.44
1:I:94:ILE:HD11	1:J:88:THR:HG21	2.00	0.44
1:K:40:ILE:HG21	1:K:46:VAL:HG22	1.99	0.44
1:K:55:PRO:HD2	1:K:82:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:OD1	1:A:42:HIS:HB2	2.17	0.44
1:D:95:ASP:HB3	1:I:177:GLY:O	2.18	0.44
1:D:98:LEU:HD23	1:I:179:VAL:HG21	2.00	0.44
1:C:182:ARG:HG2	1:C:230:TYR:HE2	1.83	0.44
1:K:17:GLU:HB3	1:K:39:LEU:HD11	1.99	0.44
1:K:30:LEU:HD23	1:K:118:VAL:HG22	2.00	0.44
1:C:18:ASP:OD1	1:C:42:HIS:HB2	2.17	0.44
1:C:55:PRO:HD2	1:C:82:ILE:HD13	1.99	0.44
1:E:18:ASP:OD1	1:E:42:HIS:HB2	2.18	0.44
1:I:18:ASP:OD1	1:I:42:HIS:HB2	2.17	0.44
1:I:55:PRO:HD2	1:I:82:ILE:HD13	2.00	0.44
1:A:176:PRO:HG2	2:D:1241:TBR:BR9	2.72	0.44
1:C:30:LEU:HD23	1:C:118:VAL:HG22	2.00	0.44
1:G:30:LEU:HD23	1:G:118:VAL:HG22	2.00	0.44
1:G:200:THR:HG23	1:G:203:SER:H	1.83	0.44
1:A:88:THR:HG21	1:B:93:GLU:HG3	2.00	0.43
1:G:55:PRO:HD2	1:G:82:ILE:HD13	1.99	0.43
1:I:200:THR:HG23	1:I:203:SER:H	1.82	0.43
1:K:27:ILE:HD11	1:K:39:LEU:HB2	1.99	0.43
1:K:209:ARG:NH1	1:K:222:ILE:O	2.50	0.43
1:B:168:LEU:HG	1:B:189:LEU:HD21	2.00	0.43
1:J:200:THR:OG1	1:J:201:ILE:N	2.51	0.43
1:C:17:GLU:HB3	1:C:39:LEU:HD11	1.99	0.43
1:A:30:LEU:HD23	1:A:118:VAL:HG22	2.00	0.43
1:C:126:ARG:HD2	1:L:190:TYR:CZ	2.53	0.43
1:A:55:PRO:HD2	1:A:82:ILE:HD13	1.99	0.43
1:A:96:ARG:NH1	2:B:1241:TBR:BR7	3.07	0.43
1:I:172:LEU:HB3	1:I:232:TRP:HB2	2.01	0.43
1:L:239:ILE:HG22	1:L:240:VAL:HG23	2.01	0.43
1:E:30:LEU:HD23	1:E:118:VAL:HG22	2.00	0.43
1:D:89:ALA:HB2	1:D:112:TYR:HB2	2.00	0.43
1:A:54:PRO:HA	1:A:55:PRO:HD3	1.84	0.43
1:H:96:ARG:HD3	1:H:96:ARG:HA	1.74	0.43
1:J:179:VAL:HG11	1:J:228:VAL:HG12	2.00	0.43
1:B:225:VAL:HG22	1:G:101:GLU:HG3	2.01	0.42
1:H:95:ASP:CG	1:L:179:VAL:H	2.22	0.42
1:H:154:TRP:CZ3	1:H:216:ASP:HB3	2.50	0.42
1:K:200:THR:HG23	1:K:203:SER:H	1.84	0.42
1:A:27:ILE:HD11	1:A:39:LEU:HB2	1.99	0.42
1:F:95:ASP:HB3	1:K:177:GLY:O	2.19	0.42
1:A:149:ARG:NH2	1:G:160:ASP:OD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:LEU:HD22	1:K:195:VAL:HG11	2.00	0.42
1:E:55:PRO:HD2	1:E:82:ILE:HD13	2.00	0.42
1:L:96:ARG:HA	1:L:96:ARG:HD3	1.87	0.42
1:A:176:PRO:HB3	1:A:232:TRP:HD1	1.85	0.42
1:C:83:PRO:HA	1:D:105:ASP:O	2.20	0.42
1:D:44:ASP:OD1	1:D:44:ASP:N	2.47	0.42
1:D:94:ILE:HG22	1:D:95:ASP:H	1.84	0.42
1:D:54:PRO:HA	1:D:55:PRO:HD3	1.95	0.42
1:A:102:ILE:HD11	1:H:226:TYR:CD2	2.48	0.41
1:A:112:TYR:CD1	1:B:109:CAS:CE2	3.03	0.41
1:B:94:ILE:HG22	1:B:95:ASP:H	1.85	0.41
1:A:232:TRP:CE2	1:A:234:ALA:HB3	2.56	0.41
1:F:58:ILE:HB	1:F:84:ILE:HG12	2.02	0.41
1:J:59:LEU:HD12	1:J:85:VAL:HB	2.02	0.41
1:J:115:ARG:HD2	1:J:115:ARG:HA	1.98	0.41
1:E:66:GLY:O	1:E:67:THR:OG1	2.34	0.41
1:B:89:ALA:HB2	1:B:112:TYR:HB2	2.01	0.41
1:C:62:LEU:O	1:C:64:LEU:N	2.53	0.41
1:C:176:PRO:HB3	1:C:232:TRP:HD1	1.86	0.41
1:D:172:LEU:HB3	1:D:232:TRP:HB2	2.02	0.41
1:E:54:PRO:HA	1:E:55:PRO:HD3	1.84	0.41
1:J:232:TRP:CZ2	1:J:234:ALA:HB3	2.56	0.41
1:D:73:CAS:SG	1:D:84:ILE:HG21	2.61	0.41
1:D:155:ARG:HE	1:D:155:ARG:HB3	1.65	0.41
1:G:66:GLY:O	1:G:67:THR:OG1	2.33	0.41
1:A:112:TYR:CE1	1:B:109:CAS:CE2	3.03	0.40
1:J:143:LEU:HB2	1:J:154:TRP:HD1	1.85	0.40
1:F:44:ASP:OD1	1:F:44:ASP:N	2.46	0.40
1:K:62:LEU:O	1:K:64:LEU:N	2.53	0.40
1:F:55:PRO:HD2	1:F:82:ILE:HD13	2.02	0.40
1:H:115:ARG:HD2	1:H:115:ARG:HA	1.97	0.40
1:K:73:CAS:CE2	1:L:106:ASP:CG	2.90	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	212/240 (88%)	200 (94%)	10 (5%)	2 (1%)	14 44
1	B	210/240 (88%)	201 (96%)	9 (4%)	0	100 100
1	C	212/240 (88%)	200 (94%)	10 (5%)	2 (1%)	14 44
1	D	210/240 (88%)	201 (96%)	9 (4%)	0	100 100
1	E	212/240 (88%)	200 (94%)	10 (5%)	2 (1%)	14 44
1	F	210/240 (88%)	204 (97%)	6 (3%)	0	100 100
1	G	212/240 (88%)	198 (93%)	12 (6%)	2 (1%)	14 44
1	H	210/240 (88%)	200 (95%)	10 (5%)	0	100 100
1	I	212/240 (88%)	199 (94%)	11 (5%)	2 (1%)	14 44
1	J	210/240 (88%)	201 (96%)	9 (4%)	0	100 100
1	K	212/240 (88%)	199 (94%)	11 (5%)	2 (1%)	14 44
1	L	210/240 (88%)	201 (96%)	9 (4%)	0	100 100
All	All	2532/2880 (88%)	2404 (95%)	116 (5%)	12 (0%)	25 56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLY
1	C	66	GLY
1	E	66	GLY
1	G	66	GLY
1	I	66	GLY
1	K	66	GLY
1	A	65	PRO
1	C	65	PRO
1	E	65	PRO
1	G	65	PRO
1	I	65	PRO
1	K	65	PRO

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	193/214 (90%)	190 (98%)	3 (2%)	58	76
1	B	191/214 (89%)	187 (98%)	4 (2%)	48	70
1	C	193/214 (90%)	189 (98%)	4 (2%)	48	70
1	D	191/214 (89%)	185 (97%)	6 (3%)	35	61
1	E	193/214 (90%)	189 (98%)	4 (2%)	48	70
1	F	191/214 (89%)	186 (97%)	5 (3%)	41	66
1	G	193/214 (90%)	187 (97%)	6 (3%)	35	61
1	H	191/214 (89%)	186 (97%)	5 (3%)	41	66
1	I	193/214 (90%)	189 (98%)	4 (2%)	48	70
1	J	191/214 (89%)	182 (95%)	9 (5%)	22	51
1	K	193/214 (90%)	188 (97%)	5 (3%)	41	66
1	L	191/214 (89%)	184 (96%)	7 (4%)	29	56
All	All	2304/2568 (90%)	2242 (97%)	62 (3%)	40	65

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	63	MET
1	A	216	ASP
1	B	51	ARG
1	B	62	LEU
1	B	88	THR
1	B	196	VAL
1	C	44	ASP
1	C	63	MET
1	C	194	ARG
1	C	223	ARG
1	D	51	ARG
1	D	62	LEU
1	D	88	THR
1	D	94	ILE
1	D	154	TRP
1	D	196	VAL
1	E	44	ASP

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Mol	Chain	Res	Type
1	E	63	MET
1	E	200	THR
1	E	216	ASP
1	F	51	ARG
1	F	62	LEU
1	F	186	LEU
1	F	196	VAL
1	F	219	GLN
1	G	44	ASP
1	G	63	MET
1	G	162	THR
1	G	194	ARG
1	G	216	ASP
1	G	219	GLN
1	H	51	ARG
1	H	62	LEU
1	H	87	VAL
1	H	182	ARG
1	H	196	VAL
1	I	44	ASP
1	I	63	MET
1	I	162	THR
1	I	183	GLU
1	J	51	ARG
1	J	62	LEU
1	J	90	LYS
1	J	91	ILE
1	J	93	GLU
1	J	94	ILE
1	J	149	ARG
1	J	182	ARG
1	J	196	VAL
1	K	44	ASP
1	K	63	MET
1	K	162	THR
1	K	182	ARG
1	K	216	ASP
1	L	51	ARG
1	L	62	LEU
1	L	88	THR
1	L	93	GLU
1	L	182	ARG

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Mol	Chain	Res	Type
1	L	186	LEU
1	L	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	187	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
1	CAS	H	109	1	5,8,9	0.69	0	1,9,11	0.24	0
1	CAS	J	73	1	5,8,9	0.63	0	1,9,11	0.08	0
1	CAS	K	73	1	5,8,9	0.67	0	1,9,11	0.06	0
1	CAS	E	109	1	4,5,9	0.61	0	1,5,11	0.13	0
1	CAS	I	73	1	5,8,9	0.65	0	1,9,11	0.06	0
1	CAS	B	73	1	5,8,9	0.64	0	1,9,11	0.02	0
1	CAS	F	73	1	5,8,9	0.68	0	1,9,11	0.11	0
1	CAS	L	109	1	5,8,9	0.69	0	1,9,11	0.33	0
1	CAS	D	73	1	5,8,9	0.63	0	1,9,11	0.02	0
1	CAS	L	73	1	5,8,9	0.61	0	1,9,11	0.08	0
1	CAS	J	109	1	5,8,9	0.67	0	1,9,11	0.28	0
1	CAS	K	109	1	4,5,9	0.62	0	1,5,11	0.18	0
1	CAS	G	109	1	4,5,9	0.61	0	1,5,11	0.20	0
1	CAS	A	73	1	5,8,9	0.63	0	1,9,11	0.10	0
1	CAS	I	109	1	4,5,9	0.62	0	1,5,11	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CAS	F	109	1	5,8,9	0.69	0	1,9,11	0.21	0
1	CAS	C	109	1	4,5,9	0.60	0	1,5,11	0.26	0
1	CAS	C	73	1	5,8,9	0.59	0	1,9,11	0.06	0
1	CAS	D	109	1	5,8,9	0.69	0	1,9,11	0.28	0
1	CAS	A	109	1	4,5,9	0.61	0	1,5,11	0.25	0
1	CAS	B	109	1	5,8,9	0.61	0	1,9,11	0.20	0
1	CAS	E	73	1	5,8,9	0.67	0	1,9,11	0.06	0
1	CAS	G	73	1	5,8,9	0.69	0	1,9,11	0.09	0
1	CAS	H	73	1	5,8,9	0.66	0	1,9,11	0.05	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
1	CAS	H	109	1	-	0/0/7/9	-
1	CAS	J	73	1	-	0/0/7/9	-
1	CAS	K	73	1	-	0/0/7/9	-
1	CAS	E	109	1	-	0/1/4/9	-
1	CAS	I	73	1	-	0/0/7/9	-
1	CAS	B	73	1	-	0/0/7/9	-
1	CAS	F	73	1	-	0/0/7/9	-
1	CAS	L	109	1	-	0/0/7/9	-
1	CAS	D	73	1	-	0/0/7/9	-
1	CAS	L	73	1	-	0/0/7/9	-
1	CAS	J	109	1	-	0/0/7/9	-
1	CAS	K	109	1	-	0/1/4/9	-
1	CAS	G	109	1	-	0/1/4/9	-
1	CAS	A	73	1	-	0/0/7/9	-
1	CAS	I	109	1	-	0/1/4/9	-
1	CAS	F	109	1	-	0/0/7/9	-
1	CAS	C	109	1	-	0/1/4/9	-
1	CAS	C	73	1	-	0/0/7/9	-
1	CAS	D	109	1	-	0/0/7/9	-
1	CAS	A	109	1	-	0/1/4/9	-
1	CAS	B	109	1	-	0/0/7/9	-
1	CAS	E	73	1	-	0/0/7/9	-
1	CAS	G	73	1	-	0/0/7/9	-
1	CAS	H	73	1	-	0/0/7/9	-

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.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	109	CAS	1	0
1	K	73	CAS	1	0
1	L	109	CAS	1	0
1	D	73	CAS	1	0
1	J	109	CAS	2	0
1	F	109	CAS	3	0
1	D	109	CAS	3	0
1	B	109	CAS	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands 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	TBR	D	1241	-	0,36,36	-	-	-		
2	TBR	A	1241	-	0,36,36	-	-	-		
2	TBR	E	1241	-	0,36,36	-	-	-		
2	TBR	B	1241	-	0,36,36	-	-	-		
2	TBR	K	1241	-	0,36,36	-	-	-		
2	TBR	C	1241	-	0,36,36	-	-	-		
2	TBR	F	1241	-	0,36,36	-	-	-		
2	TBR	G	1241	-	0,36,36	-	-	-		
2	TBR	I	1241	-	0,36,36	-	-	-		

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1241	TBR	2	0
2	B	1241	TBR	2	0
2	F	1241	TBR	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	216/240 (90%)	0.10	9 (4%) 41 31	48, 98, 147, 210	0
1	B	214/240 (89%)	0.42	22 (10%) 13 13	61, 121, 174, 251	0
1	C	216/240 (90%)	0.13	12 (5%) 31 25	66, 100, 150, 187	0
1	D	214/240 (89%)	0.57	19 (8%) 17 16	70, 135, 217, 274	0
1	E	216/240 (90%)	0.11	12 (5%) 31 25	60, 94, 145, 190	0
1	F	214/240 (89%)	0.36	14 (6%) 26 21	73, 116, 178, 235	0
1	G	216/240 (90%)	0.18	12 (5%) 31 25	62, 112, 163, 216	0
1	H	214/240 (89%)	0.40	16 (7%) 22 19	66, 116, 168, 258	0
1	I	216/240 (90%)	0.06	12 (5%) 31 25	67, 104, 153, 187	0
1	J	214/240 (89%)	0.43	17 (7%) 20 18	69, 125, 179, 265	0
1	K	216/240 (90%)	0.28	15 (6%) 24 20	70, 131, 187, 235	0
1	L	214/240 (89%)	0.55	17 (7%) 20 18	69, 131, 203, 248	0
All	All	2580/2880 (89%)	0.30	177 (6%) 24 20	48, 113, 178, 274	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	GLY	7.6
1	H	88	THR	7.2
1	L	88	THR	7.2
1	B	67	THR	6.4
1	J	88	THR	6.0
1	J	158	MET	5.8
1	L	93	GLU	5.6
1	C	66	GLY	5.0
1	G	141	SER	5.0
1	D	158	MET	5.0
1	L	152	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	L	96	ARG	4.9
1	H	93	GLU	4.9
1	D	67	THR	4.6
1	B	66	GLY	4.5
1	H	89	ALA	4.5
1	K	141	SER	4.3
1	B	71	MET	4.1
1	F	71	MET	4.1
1	H	158	MET	4.1
1	D	88	THR	4.1
1	D	93	GLU	4.0
1	E	45	GLN	4.0
1	D	71	MET	3.9
1	J	67	THR	3.9
1	B	65	PRO	3.8
1	L	67	THR	3.8
1	H	94	ILE	3.8
1	I	158	MET	3.8
1	B	88	THR	3.8
1	B	93	GLU	3.7
1	B	89	ALA	3.7
1	K	214	SER	3.7
1	I	141	SER	3.6
1	F	40	ILE	3.6
1	L	158	MET	3.6
1	A	42	HIS	3.6
1	G	101	GLU	3.6
1	J	95	ASP	3.6
1	J	93	GLU	3.6
1	F	158	MET	3.5
1	C	92	GLU	3.5
1	D	142	PRO	3.4
1	H	240	VAL	3.4
1	K	66	GLY	3.4
1	I	45	GLN	3.4
1	F	93	GLU	3.4
1	J	90	LYS	3.3
1	J	78	ARG	3.3
1	F	66	GLY	3.3
1	C	42	HIS	3.3
1	L	90	LYS	3.2
1	K	18	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	43	GLY	3.2
1	B	94	ILE	3.2
1	D	69	GLY	3.1
1	K	41	SER	3.1
1	E	10	THR	3.1
1	B	240	VAL	3.1
1	B	148	GLY	3.1
1	K	65	PRO	3.1
1	D	115	ARG	3.1
1	D	94	ILE	3.0
1	L	89	ALA	3.0
1	K	45	GLN	3.0
1	E	92	GLU	3.0
1	A	141	SER	3.0
1	E	42	HIS	3.0
1	L	79	PHE	3.0
1	J	91	ILE	2.9
1	A	63	MET	2.9
1	B	43	GLY	2.9
1	I	193	TYR	2.9
1	D	40	ILE	2.9
1	K	217	ALA	2.9
1	K	10	THR	2.9
1	E	182	ARG	2.9
1	B	158	MET	2.9
1	K	193	TYR	2.9
1	H	91	ILE	2.9
1	J	66	GLY	2.8
1	B	63	MET	2.8
1	F	67	THR	2.8
1	B	79	PHE	2.8
1	F	88	THR	2.8
1	C	78	ARG	2.7
1	F	35	TYR	2.7
1	I	99	GLY	2.7
1	A	41	SER	2.7
1	E	41	SER	2.7
1	I	10	THR	2.7
1	E	104	ALA	2.7
1	F	240	VAL	2.7
1	L	153	SER	2.6
1	B	80	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	71	MET	2.6
1	F	56	ASP	2.6
1	C	194	ARG	2.6
1	H	145	ILE	2.6
1	C	141	SER	2.6
1	H	9	ASN	2.6
1	J	9	ASN	2.6
1	K	94	ILE	2.5
1	L	52	GLN	2.5
1	K	99	GLY	2.5
1	B	115	ARG	2.5
1	F	51	ARG	2.5
1	L	240	VAL	2.5
1	G	81	ASP	2.5
1	L	64	LEU	2.5
1	D	66	GLY	2.5
1	G	42	HIS	2.5
1	B	156	GLY	2.5
1	L	66	GLY	2.5
1	J	220	SER	2.5
1	G	45	GLN	2.5
1	H	95	ASP	2.5
1	E	66	GLY	2.5
1	B	142	PRO	2.5
1	D	156	GLY	2.5
1	H	90	LYS	2.5
1	J	193	TYR	2.4
1	F	94	ILE	2.4
1	L	78	ARG	2.4
1	C	63	MET	2.4
1	H	120	ARG	2.4
1	K	125	LEU	2.4
1	G	158	MET	2.4
1	D	219	GLN	2.4
1	F	142	PRO	2.3
1	K	213	GLU	2.3
1	I	81	ASP	2.3
1	J	240	VAL	2.3
1	E	190	TYR	2.3
1	F	62	LEU	2.3
1	A	45	GLN	2.3
1	G	190	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	2.3
1	G	183	GLU	2.3
1	K	9	ASN	2.3
1	D	79	PHE	2.3
1	I	42	HIS	2.2
1	G	217	ALA	2.2
1	J	147	GLU	2.2
1	B	202	ASP	2.2
1	L	9	ASN	2.2
1	J	89	ALA	2.2
1	C	182	ARG	2.2
1	J	231	ARG	2.2
1	H	71	MET	2.2
1	L	159	LEU	2.2
1	D	89	ALA	2.2
1	D	41	SER	2.2
1	E	63	MET	2.2
1	B	147	GLU	2.2
1	I	151	GLN	2.2
1	J	94	ILE	2.1
1	C	107	TYR	2.1
1	G	66	GLY	2.1
1	C	240	VAL	2.1
1	A	104	ALA	2.1
1	D	112	TYR	2.1
1	G	10	THR	2.1
1	A	9	ASN	2.1
1	H	125	LEU	2.1
1	C	147	GLU	2.1
1	B	10	THR	2.1
1	I	41	SER	2.1
1	E	56	ASP	2.1
1	H	44	ASP	2.1
1	H	152	ALA	2.0
1	C	158	MET	2.0
1	D	63	MET	2.0
1	I	217	ALA	2.0
1	I	67	THR	2.0
1	B	221	PHE	2.0
1	E	141	SER	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. 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	B-factors(Å^2)	Q<0.9
1	CAS	G	109	6/10	0.61	0.21	100,103,103,105	0
1	CAS	I	109	6/10	0.74	0.18	92,95,97,98	0
1	CAS	K	109	6/10	0.75	0.20	116,118,120,121	0
1	CAS	C	109	6/10	0.78	0.16	69,72,74,78	0
1	CAS	J	73	9/10	0.83	0.21	148,152,165,168	0
1	CAS	A	109	6/10	0.84	0.14	68,74,78,79	0
1	CAS	F	109	9/10	0.88	0.17	47,108,113,163	0
1	CAS	E	109	6/10	0.88	0.12	71,74,77,78	0
1	CAS	H	73	9/10	0.88	0.20	129,156,161,161	0
1	CAS	L	73	9/10	0.88	0.18	147,154,161,167	0
1	CAS	B	109	9/10	0.89	0.17	30,86,94,159	0
1	CAS	H	109	9/10	0.89	0.16	106,110,129,130	0
1	CAS	B	73	9/10	0.91	0.20	116,122,125,125	0
1	CAS	C	73	9/10	0.92	0.15	27,108,113,173	0
1	CAS	D	73	9/10	0.92	0.19	121,143,149,151	0
1	CAS	D	109	9/10	0.92	0.15	106,109,113,114	0
1	CAS	L	109	9/10	0.92	0.13	103,105,124,138	0
1	CAS	J	109	9/10	0.94	0.13	100,102,120,140	0
1	CAS	A	73	9/10	0.94	0.14	52,92,96,111	0
1	CAS	I	73	9/10	0.95	0.12	98,120,125,127	0
1	CAS	F	73	9/10	0.95	0.15	112,119,125,125	0
1	CAS	K	73	9/10	0.95	0.12	118,152,159,164	0
1	CAS	E	73	9/10	0.96	0.11	106,108,123,136	0
1	CAS	G	73	9/10	0.97	0.10	119,143,148,154	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	TBR	K	1241	18/18	0.89	0.15	140,191,214,224	18
2	TBR	D	1241	18/18	0.92	0.08	230,263,300,302	18
2	TBR	G	1241	18/18	0.93	0.08	179,223,246,246	18
2	TBR	I	1241	18/18	0.94	0.11	138,182,219,220	18
2	TBR	F	1241	18/18	0.96	0.10	89,147,155,168	18
2	TBR	B	1241	18/18	0.97	0.06	101,157,182,183	18
2	TBR	A	1241	18/18	0.98	0.05	138,167,184,184	0
2	TBR	E	1241	18/18	0.98	0.05	175,197,219,223	0
2	TBR	C	1241	18/18	0.99	0.04	152,186,198,209	0

6.5 Other polymers (i)

There are no such residues in this entry.