Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 08:08 AM EDT

PDB ID	:	3H4E
Title	:	X-ray Structure of Hexameric HIV-1 CA
Authors	:	Pornillos, O.
Deposited on	:	2009-04-19
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

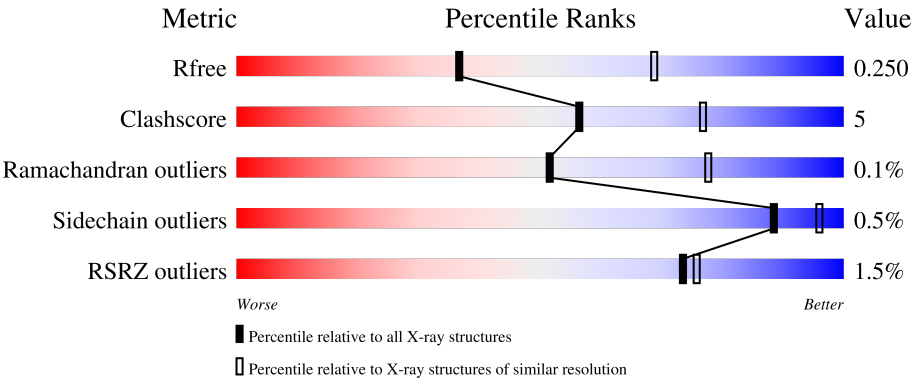
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	231	83% 11% 6%
1	B	231	% 72% 16% 12%
1	C	231	% 83% 9% 8%
1	D	231	2% 74% 13% 13%
1	E	231	81% 9% 10%

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Mol	Chain	Length	Quality of chain
1	F	231	82% 12% 5%
1	G	231	81% 13% 6%
1	H	231	78% 12% 10%
1	I	231	78% 13% 9%
1	J	231	76% 16% 7%
1	K	231	76% 10% 14%
1	L	231	80% 9% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19082 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 Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1632	1028	284	306	14			
1	B	204	Total	C	N	O	S	0	0	0
			1564	986	271	293	14			
1	C	212	Total	C	N	O	S	0	0	0
			1618	1015	283	306	14			
1	D	200	Total	C	N	O	S	0	0	0
			1522	955	266	287	14			
1	E	207	Total	C	N	O	S	0	0	0
			1574	991	273	297	13			
1	F	219	Total	C	N	O	S	0	0	0
			1661	1044	290	313	14			
1	G	218	Total	C	N	O	S	0	0	0
			1652	1037	288	313	14			
1	H	208	Total	C	N	O	S	0	0	0
			1587	999	278	296	14			
1	I	211	Total	C	N	O	S	0	0	0
			1588	1005	273	296	14			
1	J	214	Total	C	N	O	S	0	0	0
			1630	1022	286	308	14			
1	K	198	Total	C	N	O	S	0	0	0
			1509	950	262	283	14			
1	L	205	Total	C	N	O	S	0	0	0
			1545	973	265	294	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12497
A	45	CYS	GLU	engineered mutation	UNP P12497
A	184	ALA	TRP	engineered mutation	UNP P12497
A	185	ALA	MET	engineered mutation	UNP P12497
B	14	CYS	ALA	engineered mutation	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12497
B	184	ALA	TRP	engineered mutation	UNP P12497
B	185	ALA	MET	engineered mutation	UNP P12497
C	14	CYS	ALA	engineered mutation	UNP P12497
C	45	CYS	GLU	engineered mutation	UNP P12497
C	184	ALA	TRP	engineered mutation	UNP P12497
C	185	ALA	MET	engineered mutation	UNP P12497
D	14	CYS	ALA	engineered mutation	UNP P12497
D	45	CYS	GLU	engineered mutation	UNP P12497
D	184	ALA	TRP	engineered mutation	UNP P12497
D	185	ALA	MET	engineered mutation	UNP P12497
E	14	CYS	ALA	engineered mutation	UNP P12497
E	45	CYS	GLU	engineered mutation	UNP P12497
E	184	ALA	TRP	engineered mutation	UNP P12497
E	185	ALA	MET	engineered mutation	UNP P12497
F	14	CYS	ALA	engineered mutation	UNP P12497
F	45	CYS	GLU	engineered mutation	UNP P12497
F	184	ALA	TRP	engineered mutation	UNP P12497
F	185	ALA	MET	engineered mutation	UNP P12497
G	14	CYS	ALA	engineered mutation	UNP P12497
G	45	CYS	GLU	engineered mutation	UNP P12497
G	184	ALA	TRP	engineered mutation	UNP P12497
G	185	ALA	MET	engineered mutation	UNP P12497
H	14	CYS	ALA	engineered mutation	UNP P12497
H	45	CYS	GLU	engineered mutation	UNP P12497
H	184	ALA	TRP	engineered mutation	UNP P12497
H	185	ALA	MET	engineered mutation	UNP P12497
I	14	CYS	ALA	engineered mutation	UNP P12497
I	45	CYS	GLU	engineered mutation	UNP P12497
I	184	ALA	TRP	engineered mutation	UNP P12497
I	185	ALA	MET	engineered mutation	UNP P12497
J	14	CYS	ALA	engineered mutation	UNP P12497
J	45	CYS	GLU	engineered mutation	UNP P12497
J	184	ALA	TRP	engineered mutation	UNP P12497
J	185	ALA	MET	engineered mutation	UNP P12497
K	14	CYS	ALA	engineered mutation	UNP P12497
K	45	CYS	GLU	engineered mutation	UNP P12497
K	184	ALA	TRP	engineered mutation	UNP P12497
K	185	ALA	MET	engineered mutation	UNP P12497
L	14	CYS	ALA	engineered mutation	UNP P12497
L	45	CYS	GLU	engineered mutation	UNP P12497
L	184	ALA	TRP	engineered mutation	UNP P12497

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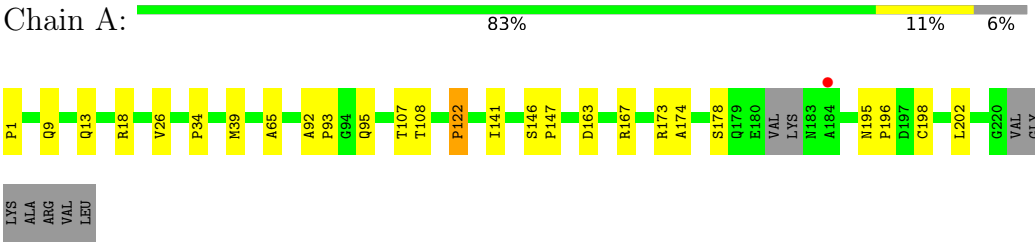
Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12497

3 Residue-property plots (i)

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

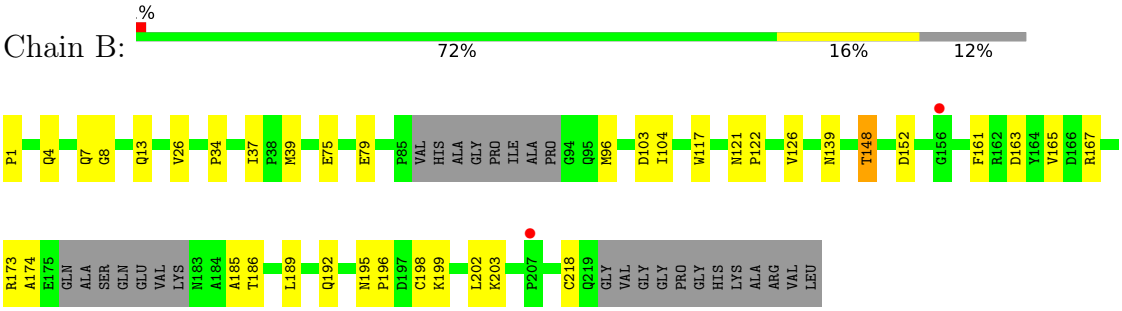
• Molecule 1: Capsid protein p24

Chain A:



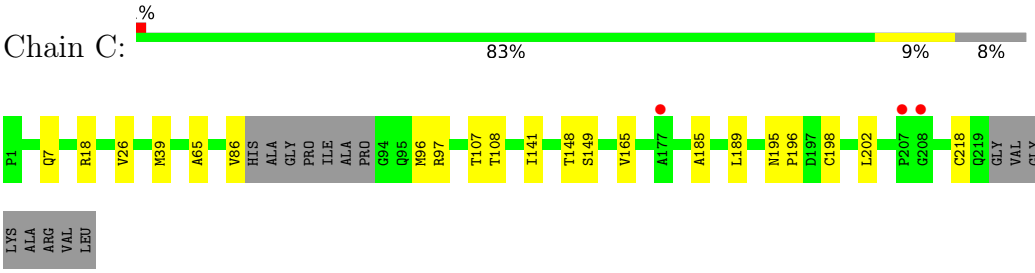
• Molecule 1: Capsid protein p24

Chain B:



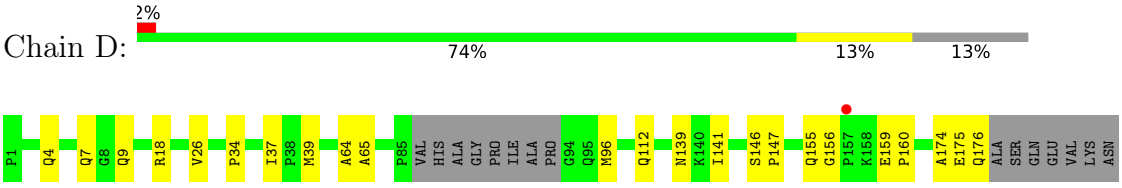
• Molecule 1: Capsid protein p24

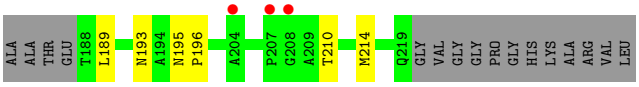
Chain C:



• Molecule 1: Capsid protein p24

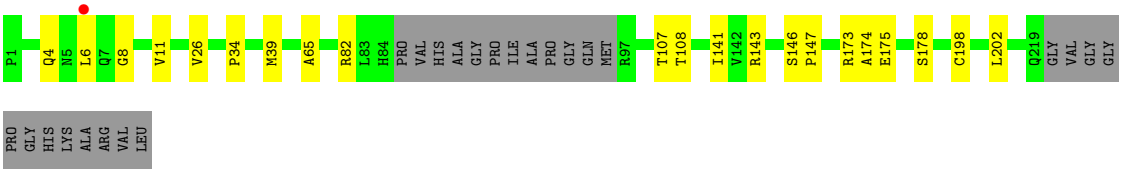
Chain D:





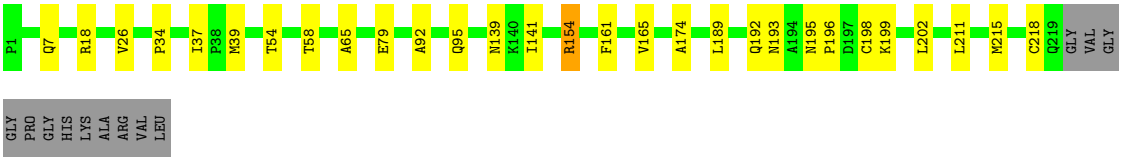
• Molecule 1: Capsid protein p24

Chain E:



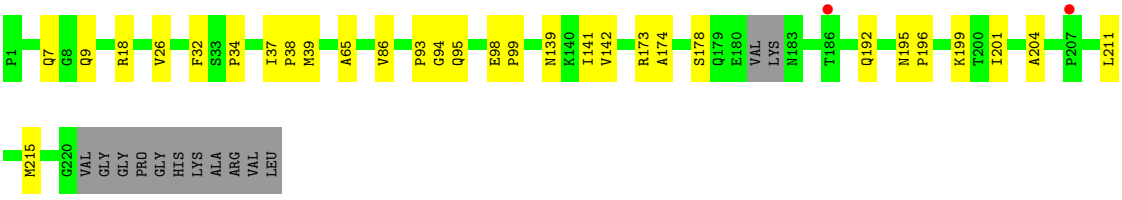
• Molecule 1: Capsid protein p24

Chain F:



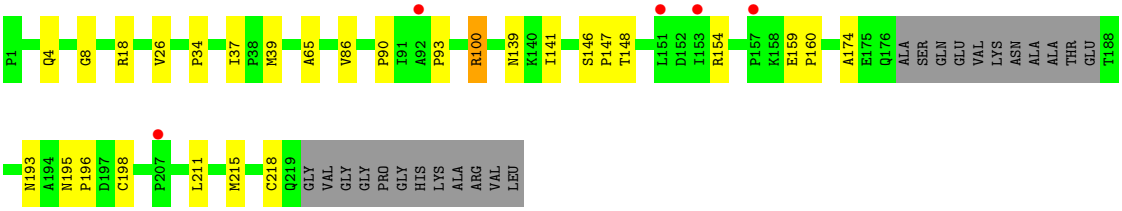
• Molecule 1: Capsid protein p24

Chain G:



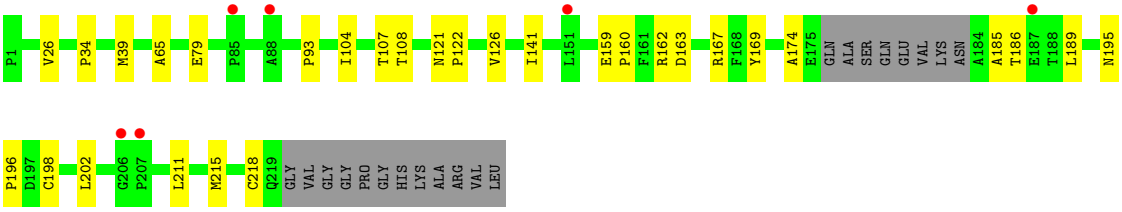
• Molecule 1: Capsid protein p24

Chain H:

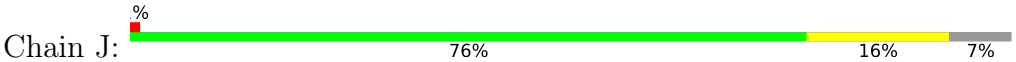


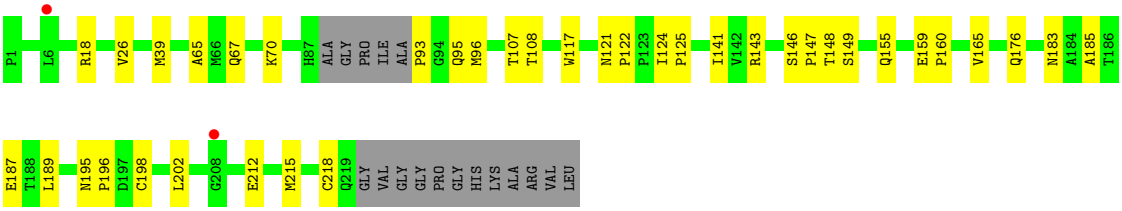
• Molecule 1: Capsid protein p24

Chain I:

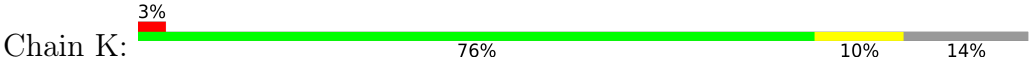


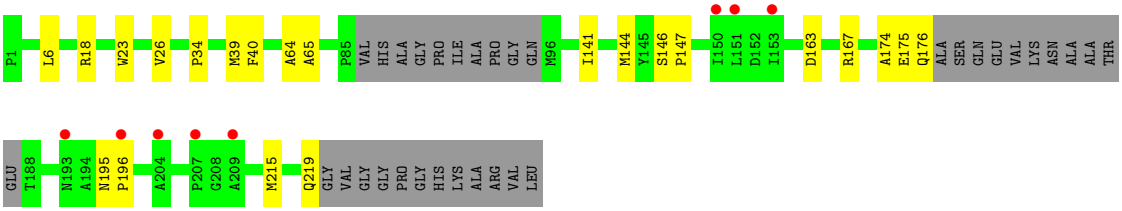
• Molecule 1: Capsid protein p24



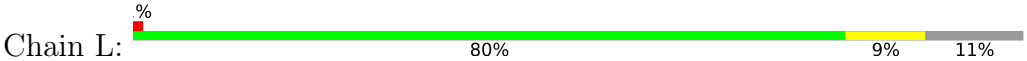


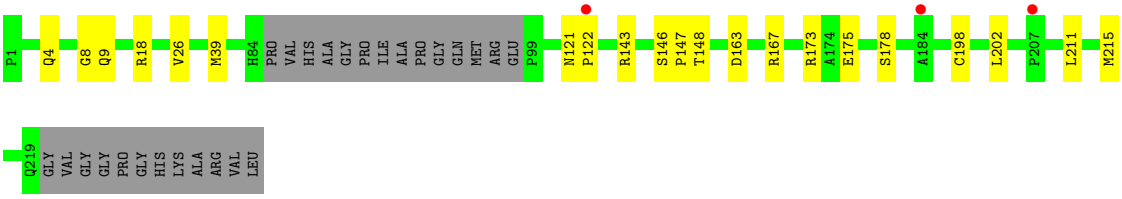
• Molecule 1: Capsid protein p24





• Molecule 1: Capsid protein p24





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.06Å 136.66Å 208.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.74 – 2.70 35.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (34.74-2.70) 95.9 (35.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.238 , 0.263 0.224 , 0.250	Depositor DCC
R_{free} test set	2565 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19082	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

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	0.37	0/1668	0.49	0/2273
1	B	0.37	0/1596	0.50	0/2168
1	C	0.36	0/1651	0.49	0/2246
1	D	0.35	0/1554	0.50	0/2112
1	E	0.36	0/1606	0.49	0/2185
1	F	0.35	0/1697	0.49	0/2310
1	G	0.36	0/1687	0.49	0/2297
1	H	0.35	0/1623	0.50	0/2210
1	I	0.35	0/1624	0.50	0/2213
1	J	0.36	0/1664	0.50	0/2263
1	K	0.35	0/1541	0.49	0/2096
1	L	0.35	0/1577	0.47	0/2148
All	All	0.36	0/19488	0.49	0/26521

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	1632	0	1575	18	0
1	B	1564	0	1533	25	0
1	C	1618	0	1573	14	0
1	D	1522	0	1455	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1574	0	1532	12	1
1	F	1661	0	1612	18	0
1	G	1652	0	1604	20	0
1	H	1587	0	1546	18	0
1	I	1588	0	1544	20	0
1	J	1630	0	1583	25	1
1	K	1509	0	1452	17	0
1	L	1545	0	1483	11	0
All	All	19082	0	18492	186	1

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 5.

All (186) 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:J:212:GLU:HG3	1:K:144:MET:SD	2.10	0.91
1:H:4:GLN:NE2	1:H:8:GLY:HA2	1.89	0.88
1:B:199:LYS:O	1:B:203:LYS:HG3	1.76	0.84
1:H:154:ARG:HG2	1:H:193:ASN:HB3	1.68	0.75
1:C:96:MET:HE2	1:H:93:PRO:HA	1.68	0.74
1:G:18:ARG:NH2	1:H:18:ARG:HH11	1.88	0.70
1:G:18:ARG:HH22	1:H:18:ARG:HH11	1.42	0.68
1:L:4:GLN:HE21	1:L:8:GLY:HA2	1.58	0.67
1:C:185:ALA:O	1:C:189:LEU:HB2	1.94	0.67
1:B:4:GLN:NE2	1:B:8:GLY:HA2	2.10	0.66
1:G:192:GLN:O	1:G:199:LYS:HE2	1.96	0.66
1:J:215:MET:HB2	1:K:144:MET:HE1	1.78	0.66
1:B:4:GLN:HE21	1:B:8:GLY:HA2	1.62	0.65
1:B:96:MET:HE2	1:I:93:PRO:HA	1.79	0.64
1:K:175:GLU:O	1:K:176:GLN:HG2	1.97	0.64
1:H:86:VAL:HG21	1:H:100:ARG:HG2	1.80	0.63
1:D:175:GLU:O	1:D:176:GLN:HG2	1.98	0.63
1:E:6:LEU:HD13	1:F:7:GLN:NE2	2.13	0.62
1:A:93:PRO:HB3	1:J:96:MET:HE2	1.82	0.61
1:I:34:PRO:HG3	1:I:174:ALA:HA	1.83	0.61
1:E:6:LEU:HD22	1:F:7:GLN:HE21	1.64	0.61
1:K:18:ARG:NH2	1:L:18:ARG:HG2	2.18	0.59
1:J:185:ALA:O	1:J:189:LEU:HB2	2.02	0.59
1:H:154:ARG:HG2	1:H:193:ASN:CB	2.33	0.58
1:A:18:ARG:HG3	1:F:18:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.86	0.58
1:G:34:PRO:HG3	1:G:174:ALA:HA	1.85	0.58
1:B:7:GLN:HE22	1:C:7:GLN:HE21	1.52	0.56
1:B:148:THR:HG22	1:B:152:ASP:HB2	1.87	0.56
1:I:162:ARG:HG3	1:I:215:MET:HE1	1.89	0.55
1:L:173:ARG:HA	1:L:178:SER:O	2.06	0.55
1:J:18:ARG:CZ	1:K:18:ARG:HD3	2.36	0.55
1:E:4:GLN:NE2	1:E:8:GLY:HA2	2.23	0.54
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.90	0.54
1:C:202:LEU:HD21	1:C:218:CYS:SG	2.47	0.54
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.90	0.54
1:A:34:PRO:HG3	1:A:174:ALA:HA	1.90	0.53
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.89	0.53
1:H:37:ILE:HD13	1:H:139:ASN:OD1	2.09	0.53
1:J:165:VAL:HG12	1:K:64:ALA:HB2	1.89	0.53
1:J:183:ASN:O	1:J:187:GLU:HG3	2.09	0.52
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.92	0.52
1:C:198:CYS:O	1:C:202:LEU:HG	2.10	0.52
1:G:94:GLY:O	1:G:95:GLN:HG2	2.09	0.51
1:A:198:CYS:O	1:A:202:LEU:HG	2.11	0.51
1:C:97:ARG:HB2	1:H:90:PRO:HB2	1.92	0.51
1:B:7:GLN:NE2	1:B:7:GLN:HA	2.26	0.51
1:A:122:PRO:HG3	1:I:122:PRO:HB3	1.91	0.51
1:B:198:CYS:HB3	1:B:218:CYS:SG	2.51	0.51
1:E:198:CYS:O	1:E:202:LEU:HG	2.11	0.51
1:J:202:LEU:HD21	1:J:218:CYS:SG	2.51	0.50
1:H:34:PRO:HG3	1:H:174:ALA:HA	1.94	0.50
1:I:198:CYS:O	1:I:202:LEU:HG	2.11	0.50
1:J:107:THR:HG22	1:J:108:THR:HG23	1.93	0.50
1:E:143:ARG:HG2	1:E:175:GLU:O	2.11	0.50
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.92	0.50
1:B:198:CYS:O	1:B:202:LEU:HG	2.13	0.49
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.93	0.49
1:E:26:VAL:HG21	1:E:39:MET:HG2	1.95	0.49
1:J:198:CYS:SG	1:J:218:CYS:HB3	2.52	0.49
1:J:198:CYS:O	1:J:202:LEU:HG	2.12	0.49
1:I:185:ALA:O	1:I:189:LEU:HB2	2.13	0.49
1:B:75:GLU:O	1:B:79:GLU:HG3	2.13	0.49
1:I:163:ASP:O	1:I:167:ARG:HG3	2.13	0.49
1:B:148:THR:CG2	1:B:152:ASP:HB2	2.43	0.49
1:F:92:ALA:HB3	1:F:95:GLN:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:PRO:HD2	1:J:95:GLN:HE21	1.78	0.48
1:B:103:ASP:HB3	1:B:117:TRP:CH2	2.49	0.48
1:A:146:SER:HA	1:A:147:PRO:HD3	1.62	0.48
1:K:34:PRO:HG3	1:K:174:ALA:HA	1.95	0.48
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.95	0.48
1:A:195:ASN:HB2	1:A:196:PRO:CD	2.43	0.48
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.96	0.47
1:G:32:PHE:O	1:G:142:VAL:HG22	2.14	0.47
1:A:107:THR:HG22	1:A:108:THR:HG23	1.97	0.47
1:G:195:ASN:HB2	1:G:196:PRO:CD	2.44	0.47
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.95	0.47
1:G:173:ARG:HA	1:G:178:SER:O	2.14	0.47
1:A:122:PRO:HG3	1:I:122:PRO:HG3	1.97	0.47
1:E:34:PRO:HG3	1:E:174:ALA:HA	1.96	0.47
1:F:192:GLN:HA	1:F:199:LYS:HE3	1.97	0.46
1:I:107:THR:HG22	1:I:108:THR:HG23	1.97	0.46
1:B:104:ILE:HG12	1:B:126:VAL:HG12	1.96	0.46
1:D:34:PRO:HG3	1:D:174:ALA:HA	1.96	0.46
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.97	0.46
1:J:146:SER:HA	1:J:147:PRO:HD3	1.58	0.46
1:I:79:GLU:HA	1:I:79:GLU:OE1	2.15	0.46
1:G:201:ILE:O	1:G:204:ALA:HB3	2.16	0.46
1:F:211:LEU:O	1:F:215:MET:HG3	2.16	0.46
1:D:195:ASN:HB2	1:D:196:PRO:CD	2.46	0.45
1:J:195:ASN:HB2	1:J:196:PRO:CD	2.46	0.45
1:J:215:MET:CB	1:K:144:MET:HE1	2.45	0.45
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.97	0.45
1:K:23:TRP:CZ3	1:K:40:PHE:HB2	2.52	0.45
1:B:26:VAL:HG21	1:B:39:MET:HG2	1.99	0.45
1:B:34:PRO:HG3	1:B:174:ALA:HA	1.99	0.45
1:G:86:VAL:HG13	1:G:98:GLU:HB2	1.98	0.45
1:B:185:ALA:O	1:B:189:LEU:HB2	2.16	0.45
1:K:18:ARG:HH21	1:L:18:ARG:HG2	1.79	0.45
1:D:9:GLN:HE22	1:G:9:GLN:HE21	1.63	0.44
1:F:189:LEU:HD11	1:F:193:ASN:ND2	2.31	0.44
1:J:143:ARG:HD3	1:J:176:GLN:OE1	2.16	0.44
1:A:92:ALA:O	1:A:95:GLN:HB2	2.17	0.44
1:C:148:THR:HG22	1:C:149:SER:O	2.17	0.44
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.97	0.44
1:B:161:PHE:O	1:B:165:VAL:HG23	2.16	0.44
1:D:159:GLU:HA	1:D:160:PRO:HD3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:ARG:HG3	1:F:193:ASN:HB3	1.99	0.44
1:G:211:LEU:O	1:G:215:MET:HG3	2.17	0.44
1:K:146:SER:HA	1:K:147:PRO:HD3	1.85	0.44
1:A:93:PRO:CB	1:J:96:MET:HE2	2.45	0.44
1:F:198:CYS:O	1:F:202:LEU:HG	2.17	0.44
1:J:26:VAL:HG21	1:J:39:MET:HG2	2.00	0.44
1:E:173:ARG:HA	1:E:178:SER:O	2.18	0.44
1:F:79:GLU:HA	1:F:79:GLU:OE1	2.18	0.44
1:K:6:LEU:HD23	1:K:6:LEU:HA	1.75	0.44
1:D:96:MET:HE3	1:G:94:GLY:H	1.81	0.44
1:D:7:GLN:HB3	1:G:7:GLN:NE2	2.32	0.43
1:C:86:VAL:O	1:C:86:VAL:HG23	2.19	0.43
1:F:34:PRO:HG3	1:F:174:ALA:HA	2.00	0.43
1:K:163:ASP:O	1:K:167:ARG:HG3	2.18	0.43
1:A:1:PRO:HD2	1:A:13:GLN:O	2.18	0.43
1:A:9:GLN:HA	1:A:9:GLN:OE1	2.18	0.43
1:L:211:LEU:O	1:L:215:MET:HG3	2.19	0.43
1:C:26:VAL:HG21	1:C:39:MET:HG2	2.00	0.43
1:F:37:ILE:HD13	1:F:139:ASN:OD1	2.19	0.43
1:H:146:SER:HA	1:H:147:PRO:HD3	1.75	0.43
1:L:26:VAL:HG21	1:L:39:MET:HG2	2.01	0.43
1:B:34:PRO:HB2	1:B:173:ARG:HD3	2.01	0.42
1:D:189:LEU:HD11	1:D:193:ASN:ND2	2.34	0.42
1:J:121:ASN:HA	1:J:122:PRO:HA	1.93	0.42
1:C:107:THR:HG22	1:C:108:THR:HG23	1.99	0.42
1:H:198:CYS:SG	1:H:218:CYS:HB3	2.60	0.42
1:I:121:ASN:HA	1:I:122:PRO:HA	1.83	0.42
1:K:195:ASN:HB2	1:K:196:PRO:CD	2.48	0.42
1:D:210:THR:O	1:D:214:MET:HG3	2.19	0.42
1:C:65:ALA:HB1	1:C:141:ILE:HD13	2.01	0.42
1:G:65:ALA:HB1	1:G:141:ILE:HD13	2.02	0.42
1:J:124:ILE:HA	1:J:125:PRO:HD3	1.91	0.42
1:K:215:MET:O	1:K:219:GLN:HG3	2.20	0.42
1:D:155:GLN:HG2	1:D:156:GLY:O	2.20	0.42
1:E:107:THR:HG22	1:E:108:THR:HG23	2.01	0.42
1:F:202:LEU:HD21	1:F:218:CYS:SG	2.59	0.42
1:G:37:ILE:HD13	1:G:139:ASN:OD1	2.18	0.42
1:A:173:ARG:HA	1:A:178:SER:O	2.20	0.42
1:C:195:ASN:HB2	1:C:196:PRO:CD	2.50	0.42
1:B:1:PRO:HD2	1:B:13:GLN:O	2.19	0.42
1:J:148:THR:HG22	1:J:149:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:THR:O	1:F:58:THR:HG23	2.18	0.42
1:I:211:LEU:O	1:I:215:MET:HG3	2.19	0.42
1:L:163:ASP:O	1:L:167:ARG:HG3	2.20	0.42
1:A:93:PRO:HG3	1:J:117:TRP:CE2	2.55	0.42
1:D:4:GLN:HE21	1:E:11:VAL:HG11	1.84	0.42
1:G:98:GLU:HA	1:G:99:PRO:HD3	1.83	0.42
1:B:117:TRP:CE2	1:I:93:PRO:HG2	2.55	0.41
1:F:195:ASN:HB2	1:F:196:PRO:CD	2.50	0.41
1:H:159:GLU:HA	1:H:160:PRO:HD3	1.92	0.41
1:L:143:ARG:HG2	1:L:175:GLU:O	2.19	0.41
1:E:146:SER:HA	1:E:147:PRO:HD3	1.87	0.41
1:F:161:PHE:O	1:F:165:VAL:HG23	2.20	0.41
1:B:37:ILE:HD13	1:B:139:ASN:OD1	2.20	0.41
1:G:37:ILE:HB	1:G:38:PRO:HD3	2.03	0.41
1:I:195:ASN:HB2	1:I:196:PRO:CD	2.50	0.41
1:A:65:ALA:HB1	1:A:141:ILE:HD13	2.02	0.41
1:C:18:ARG:HH21	1:D:18:ARG:HH21	1.69	0.41
1:D:146:SER:HA	1:D:147:PRO:HD3	1.82	0.41
1:H:195:ASN:HB2	1:H:196:PRO:CD	2.50	0.41
1:B:192:GLN:HA	1:B:199:LYS:HE3	2.02	0.41
1:H:211:LEU:O	1:H:215:MET:HG3	2.21	0.41
1:L:198:CYS:O	1:L:202:LEU:HG	2.21	0.41
1:I:26:VAL:HG21	1:I:39:MET:HG2	2.01	0.41
1:B:195:ASN:HB2	1:B:196:PRO:CD	2.51	0.41
1:C:165:VAL:HG12	1:D:64:ALA:HB2	2.02	0.41
1:H:198:CYS:HB3	1:H:218:CYS:SG	2.61	0.41
1:I:104:ILE:HG12	1:I:126:VAL:HG12	2.01	0.41
1:I:198:CYS:SG	1:I:218:CYS:HB3	2.60	0.41
1:A:163:ASP:O	1:A:167:ARG:HG3	2.21	0.41
1:B:121:ASN:HA	1:B:122:PRO:HA	1.92	0.40
1:J:159:GLU:HA	1:J:160:PRO:HD3	1.89	0.40
1:D:37:ILE:HD13	1:D:139:ASN:OD1	2.21	0.40
1:L:121:ASN:HA	1:L:122:PRO:HA	1.90	0.40
1:I:169:TYR:CZ	1:J:67:GLN:HG2	2.56	0.40
1:B:163:ASP:O	1:B:167:ARG:HG3	2.22	0.40
1:D:96:MET:CE	1:G:93:PRO:HA	2.51	0.40
1:I:159:GLU:HA	1:I:160:PRO:HD3	1.96	0.40
1:L:146:SER:HA	1:L:147:PRO:HD3	1.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ARG:NH1	1:J:155:GLN:O[3_454]	2.16	0.04

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	214/231 (93%)	212 (99%)	2 (1%)	0	100	100
1	B	198/231 (86%)	194 (98%)	3 (2%)	1 (0%)	29	54
1	C	208/231 (90%)	205 (99%)	3 (1%)	0	100	100
1	D	194/231 (84%)	191 (98%)	3 (2%)	0	100	100
1	E	203/231 (88%)	197 (97%)	6 (3%)	0	100	100
1	F	217/231 (94%)	210 (97%)	7 (3%)	0	100	100
1	G	214/231 (93%)	209 (98%)	5 (2%)	0	100	100
1	H	204/231 (88%)	201 (98%)	3 (2%)	0	100	100
1	I	207/231 (90%)	203 (98%)	3 (1%)	1 (0%)	29	54
1	J	210/231 (91%)	206 (98%)	4 (2%)	0	100	100
1	K	192/231 (83%)	190 (99%)	2 (1%)	0	100	100
1	L	201/231 (87%)	197 (98%)	4 (2%)	0	100	100
All	All	2462/2772 (89%)	2415 (98%)	45 (2%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	186	THR
1	B	186	THR

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	168/193 (87%)	167 (99%)	1 (1%)	86 95
1	B	166/193 (86%)	165 (99%)	1 (1%)	86 95
1	C	171/193 (89%)	171 (100%)	0	100 100
1	D	158/193 (82%)	157 (99%)	1 (1%)	86 95
1	E	165/193 (86%)	165 (100%)	0	100 100
1	F	172/193 (89%)	171 (99%)	1 (1%)	86 95
1	G	173/193 (90%)	173 (100%)	0	100 100
1	H	168/193 (87%)	166 (99%)	2 (1%)	71 88
1	I	165/193 (86%)	165 (100%)	0	100 100
1	J	172/193 (89%)	171 (99%)	1 (1%)	86 95
1	K	158/193 (82%)	158 (100%)	0	100 100
1	L	160/193 (83%)	158 (99%)	2 (1%)	69 87
All	All	1996/2316 (86%)	1987 (100%)	9 (0%)	88 96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	PRO
1	B	148	THR
1	D	112	GLN
1	F	154	ARG
1	H	100	ARG
1	H	148	THR
1	J	70	LYS
1	L	9	GLN
1	L	148	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	B	7	GLN
1	B	120	HIS
1	C	120	HIS
1	D	4	GLN
1	D	7	GLN
1	E	4	GLN
1	E	50	GLN
1	F	7	GLN
1	G	9	GLN
1	L	4	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	218/231 (94%)	-0.19	1 (0%) 91 92	31, 51, 88, 116	0
1	B	204/231 (88%)	-0.12	2 (0%) 82 83	31, 53, 84, 116	0
1	C	212/231 (91%)	-0.16	3 (1%) 75 77	32, 51, 88, 117	0
1	D	200/231 (86%)	-0.06	4 (2%) 65 67	33, 51, 89, 119	0
1	E	207/231 (89%)	-0.19	1 (0%) 91 92	33, 52, 85, 113	0
1	F	219/231 (94%)	-0.26	0 100 100	33, 51, 89, 115	0
1	G	218/231 (94%)	-0.14	2 (0%) 84 85	34, 53, 91, 116	0
1	H	208/231 (90%)	-0.23	5 (2%) 59 60	35, 53, 89, 119	0
1	I	211/231 (91%)	-0.02	6 (2%) 53 54	35, 52, 86, 116	0
1	J	214/231 (92%)	-0.25	2 (0%) 84 85	32, 52, 88, 116	0
1	K	198/231 (85%)	-0.03	8 (4%) 38 37	33, 52, 88, 116	0
1	L	205/231 (88%)	-0.11	3 (1%) 73 76	33, 53, 89, 117	0
All	All	2514/2772 (90%)	-0.15	37 (1%) 73 76	31, 52, 89, 119	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	PRO	5.8
1	H	207	PRO	4.5
1	D	208	GLY	4.5
1	G	207	PRO	4.0
1	L	207	PRO	3.9
1	L	184	ALA	3.7
1	D	157	PRO	3.6
1	I	207	PRO	3.5
1	C	208	GLY	3.5
1	K	193	ASN	3.5
1	J	208	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	196	PRO	3.2
1	L	122	PRO	3.2
1	K	153	ILE	3.1
1	H	153	ILE	3.0
1	J	6	LEU	2.9
1	K	151	LEU	2.7
1	K	207	PRO	2.7
1	C	207	PRO	2.7
1	C	177	ALA	2.6
1	B	156	GLY	2.6
1	I	85	PRO	2.5
1	A	184	ALA	2.5
1	H	151	LEU	2.5
1	E	6	LEU	2.4
1	H	157	PRO	2.4
1	K	150	ILE	2.4
1	I	88	ALA	2.3
1	G	186	THR	2.3
1	I	206	GLY	2.2
1	I	187	GLU	2.2
1	I	151	LEU	2.1
1	K	204	ALA	2.1
1	K	209	ALA	2.1
1	B	207	PRO	2.1
1	D	204	ALA	2.0
1	H	92	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.