



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:47 AM UTC

PDB ID : 9DIV / pdb_00009div
Title : The crystal structure of de novo designed ChuA binding protein C8
Authors : Fox, D.; Grinter, R.
Deposited on : 2024-09-06
Resolution : 2.46 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

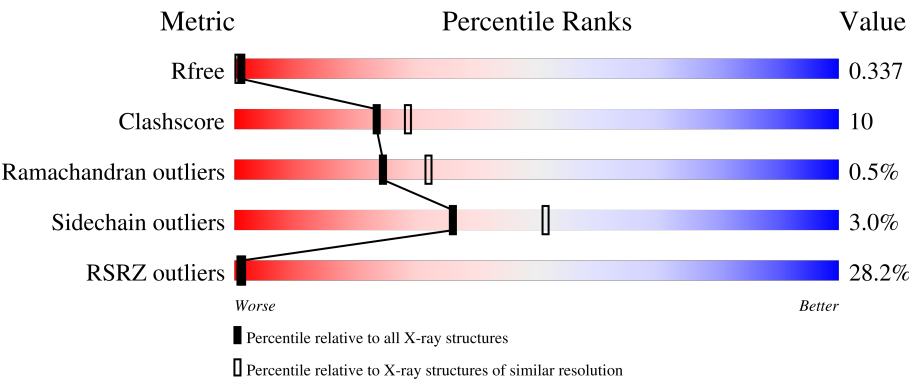
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	152	19% 75% 14% • 10%
1	B	152	26% 69% 20% • 11%
1	C	152	25% 82% 11% •• 5%
1	D	152	23% 76% 19% • 5%
1	E	152	24% 64% 21% 14%

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Mol	Chain	Length	Quality of chain
1	F	152	24% 69% 16% •• 13%
1	G	152	24% 64% 20% 15%
1	H	152	35% 65% 18% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7525 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 De novo designed ChuA binding protein C8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			952	605	159	186	2			
1	B	136	Total	C	N	O	S	0	0	0
			944	599	158	185	2			
1	C	145	Total	C	N	O	S	0	0	0
			1010	639	172	197	2			
1	D	145	Total	C	N	O	S	0	0	0
			1010	639	172	197	2			
1	E	130	Total	C	N	O	S	0	0	0
			904	572	152	178	2			
1	F	132	Total	C	N	O	S	0	0	0
			918	581	154	181	2			
1	G	129	Total	C	N	O	S	0	0	0
			896	571	150	173	2			
1	H	128	Total	C	N	O	S	0	0	0
			890	567	151	171	1			

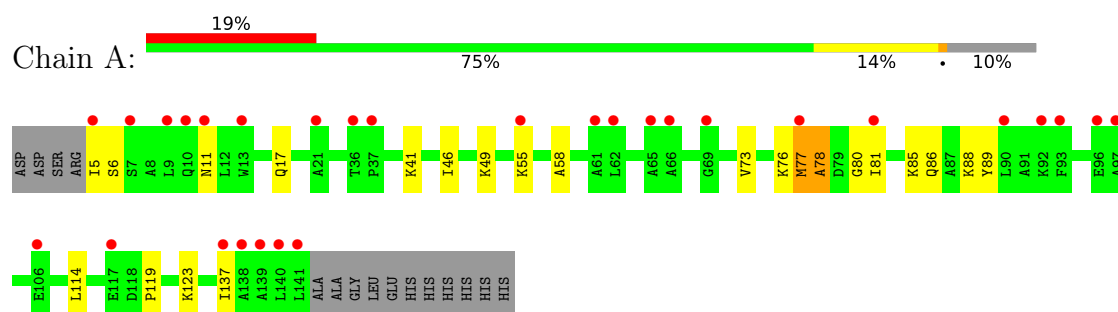
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		

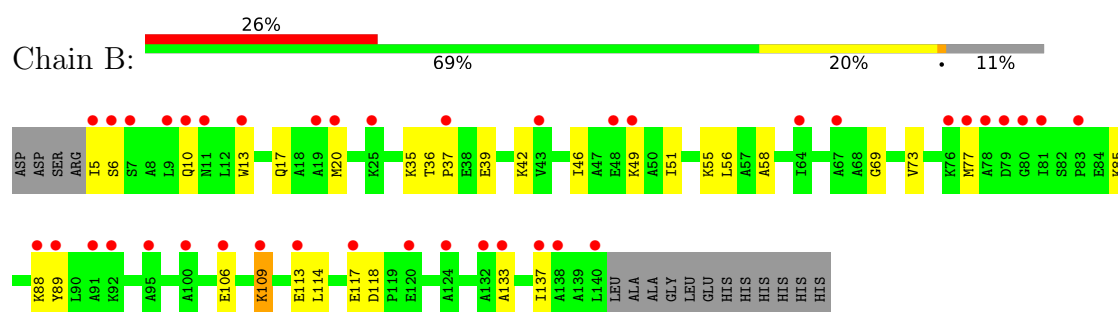
3 Residue-property plots [i](#)

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.

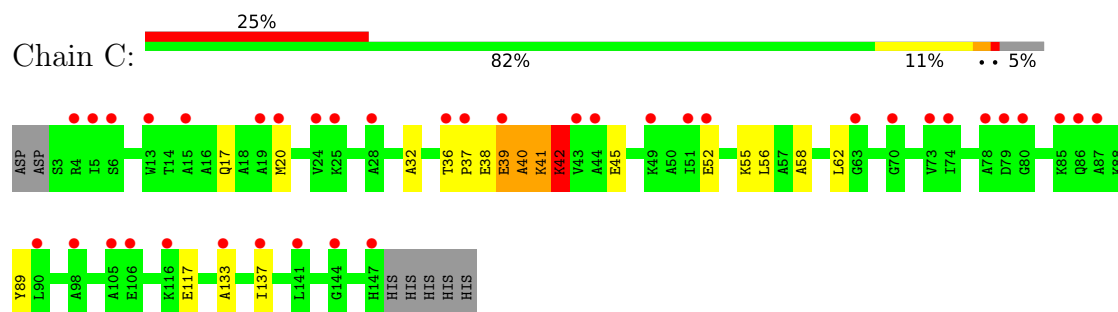
- Molecule 1: De novo designed ChuA binding protein C8



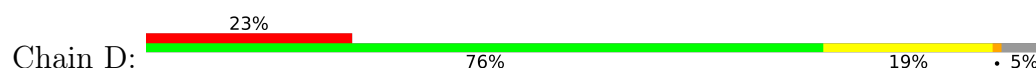
- Molecule 1: De novo designed ChuA binding protein C8

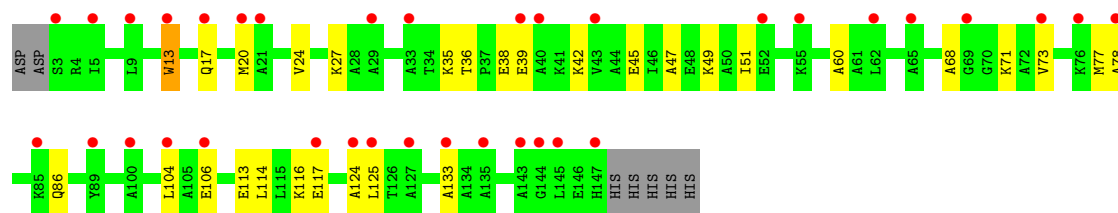


- Molecule 1: De novo designed ChuA binding protein C8

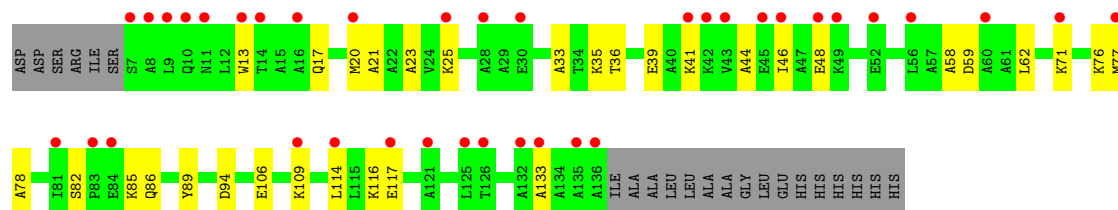


- Molecule 1: De novo designed ChuA binding protein C8

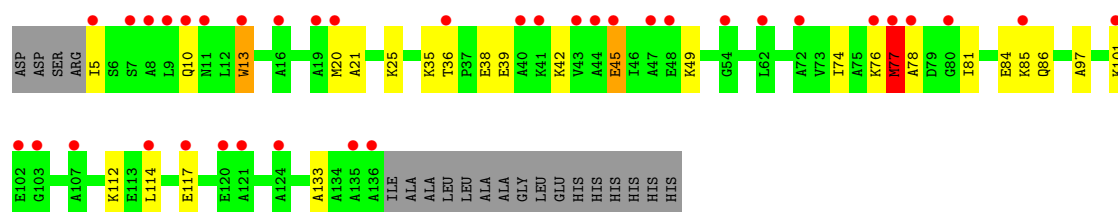




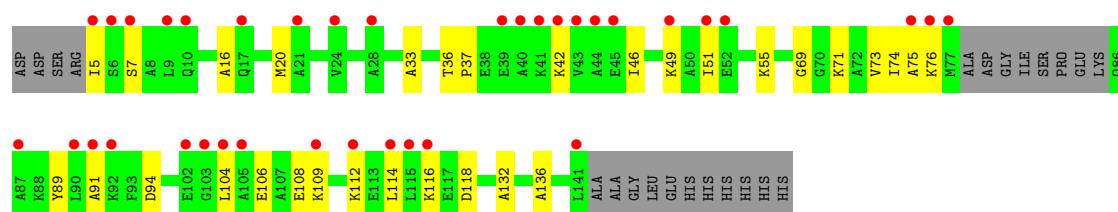
- Molecule 1: De novo designed ChuA binding protein C8



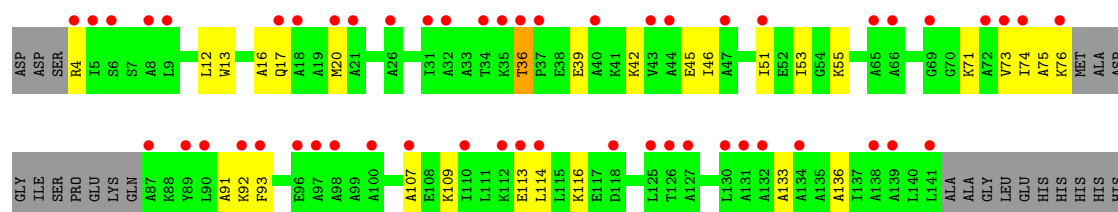
- Molecule 1: De novo designed ChuA binding protein C8



- Molecule 1: De novo designed ChuA binding protein C8



- Molecule 1: De novo designed ChuA binding protein C8



HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.37Å 110.30Å 127.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.46 46.32 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.32-2.46) 99.1 (46.32-2.46)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.301 , 0.324 0.314 , 0.337	Depositor DCC
R_{free} test set	2165 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7525	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1947e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/958	0.49	0/1293
1	B	0.27	0/950	0.64	0/1282
1	C	0.25	0/1017	0.57	2/1372 (0.1%)
1	D	0.35	0/1017	0.65	0/1372
1	E	0.36	0/910	0.72	2/1227 (0.2%)
1	F	0.36	0/924	0.72	0/1246
1	G	0.29	0/900	0.55	0/1213
1	H	0.39	0/894	0.62	0/1205
All	All	0.32	0/7570	0.62	4/10210 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	ALA	N-CA-C	-9.24	102.00	113.18
1	C	42	LYS	N-CA-C	-5.95	104.70	111.07
1	E	116	LYS	CA-C-N	-5.63	111.11	121.41
1	E	116	LYS	C-N-CA	-5.63	111.11	121.41

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	952	0	1015	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	944	0	1004	20	0
1	C	1010	0	1070	17	0
1	D	1010	0	1070	19	0
1	E	904	0	956	27	0
1	F	918	0	972	22	0
1	G	896	0	960	24	0
1	H	890	0	956	21	0
2	B	1	0	0	0	0
All	All	7525	0	8003	158	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 10.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:LYS:HB3	1:E:39:GLU:HB2	1.56	0.87
1:E:35:LYS:HB3	1:E:39:GLU:CB	2.11	0.80
1:F:35:LYS:HB3	1:F:39:GLU:HB2	1.64	0.79
1:E:36:THR:H	1:E:39:GLU:HG3	1.49	0.78
1:H:20:MET:HE2	1:H:133:ALA:HA	1.68	0.75
1:B:49:LYS:HD2	1:B:114:LEU:HD21	1.71	0.72
1:D:42:LYS:HD2	1:D:117:GLU:OE2	1.90	0.70
1:G:74:ILE:C	1:G:76:LYS:H	1.98	0.70
1:B:42:LYS:HE2	1:B:118:ASP:HB2	1.75	0.69
1:H:75:ALA:O	1:H:76:LYS:C	2.37	0.68
1:H:13:TRP:CD1	1:H:17:GLN:HE21	2.11	0.68
1:D:35:LYS:HD3	1:D:39:GLU:HG3	1.76	0.68
1:F:35:LYS:HB3	1:F:39:GLU:CB	2.23	0.67
1:A:58:ALA:HA	1:A:137:ILE:HD11	1.76	0.67
1:G:42:LYS:NZ	1:G:118:ASP:HB2	2.11	0.66
1:F:77:MET:O	1:F:81:ILE:HG12	1.95	0.66
1:D:78:ALA:O	1:D:86:GLN:NE2	2.29	0.65
1:E:13:TRP:CH2	1:E:62:LEU:HD13	2.31	0.65
1:C:17:GLN:HA	1:C:20:MET:HE3	1.78	0.65
1:C:58:ALA:HB1	1:C:137:ILE:HD11	1.79	0.64
1:G:5:ILE:HG22	1:G:7:SER:H	1.62	0.64
1:B:5:ILE:HG23	1:B:6:SER:H	1.62	0.64
1:B:58:ALA:HA	1:B:137:ILE:HD11	1.78	0.64
1:A:5:ILE:HG22	1:A:6:SER:H	1.63	0.64
1:D:20:MET:HE2	1:D:133:ALA:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:MET:HE2	1:E:133:ALA:HA	1.79	0.63
1:H:91:ALA:O	1:H:92:LYS:HB3	2.00	0.62
1:E:13:TRP:HD1	1:E:17:GLN:HE21	1.47	0.62
1:E:36:THR:N	1:E:39:GLU:HG3	2.16	0.61
1:B:10:GLN:O	1:B:10:GLN:HG3	2.00	0.60
1:E:13:TRP:CD1	1:E:17:GLN:HE21	2.19	0.60
1:B:46:ILE:HG23	1:B:114:LEU:HD22	1.83	0.60
1:F:20:MET:HE2	1:F:133:ALA:HA	1.83	0.60
1:H:74:ILE:HG12	1:H:93:PHE:HE2	1.66	0.60
1:H:42:LYS:O	1:H:45:GLU:HG2	2.02	0.60
1:F:36:THR:OG1	1:F:39:GLU:HG3	2.02	0.60
1:D:68:ALA:HA	1:D:71:LYS:HZ1	1.67	0.60
1:B:13:TRP:NE1	1:B:17:GLN:HE21	2.00	0.59
1:E:13:TRP:O	1:E:17:GLN:HG3	2.02	0.59
1:E:106:GLU:HA	1:E:109:LYS:HD3	1.83	0.59
1:A:78:ALA:O	1:A:86:GLN:NE2	2.36	0.59
1:G:74:ILE:O	1:G:76:LYS:N	2.36	0.58
1:B:35:LYS:HD3	1:B:39:GLU:HB3	1.86	0.58
1:D:113:GLU:HA	1:D:116:LYS:HZ3	1.69	0.57
1:G:42:LYS:HZ1	1:G:118:ASP:HB2	1.68	0.57
1:H:46:ILE:HG23	1:H:114:LEU:HD22	1.87	0.57
1:F:42:LYS:HA	1:F:45:GLU:HG3	1.87	0.57
1:D:35:LYS:HD3	1:D:39:GLU:CG	2.35	0.56
1:G:74:ILE:HD13	1:G:76:LYS:HZ1	1.70	0.56
1:B:35:LYS:HB3	1:B:39:GLU:HB2	1.87	0.55
1:B:51:ILE:HG22	1:B:55:LYS:HE2	1.87	0.55
1:B:13:TRP:CD1	1:B:17:GLN:HE21	2.24	0.55
1:C:32:ALA:HB1	1:C:40:ALA:HB1	1.87	0.55
1:C:89:TYR:CG	1:H:76:LYS:HD2	2.43	0.54
1:E:71:LYS:NZ	1:E:94:ASP:OD1	2.40	0.54
1:G:106:GLU:O	1:G:109:LYS:HB3	2.08	0.54
1:D:73:VAL:HG12	1:D:77:MET:HE2	1.91	0.53
1:H:13:TRP:O	1:H:17:GLN:HG3	2.08	0.53
1:H:51:ILE:HG22	1:H:55:LYS:HE2	1.91	0.53
1:G:36:THR:HB	1:G:37:PRO:HD2	1.91	0.52
1:H:73:VAL:O	1:H:76:LYS:HB2	2.09	0.52
1:D:27:LYS:HE2	1:D:124:ALA:HB1	1.90	0.52
1:C:133:ALA:O	1:C:137:ILE:HG12	2.10	0.52
1:E:82:SER:H	1:E:85:LYS:NZ	2.09	0.51
1:A:73:VAL:HG12	1:A:77:MET:HE2	1.91	0.51
1:G:74:ILE:C	1:G:76:LYS:N	2.61	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG12	1:B:77:MET:HE2	1.91	0.51
1:G:71:LYS:NZ	1:G:94:ASP:OD1	2.32	0.50
1:E:13:TRP:HZ2	1:E:59:ASP:OD1	1.93	0.50
1:C:36:THR:HG23	1:C:38:GLU:HB2	1.94	0.50
1:D:42:LYS:HD3	1:D:45:GLU:OE2	2.11	0.50
1:F:76:LYS:C	1:F:78:ALA:H	2.20	0.50
1:F:97:ALA:O	1:F:101:LYS:HG3	2.11	0.50
1:C:42:LYS:O	1:C:45:GLU:HG2	2.11	0.50
1:F:77:MET:HG3	1:F:81:ILE:HD13	1.93	0.50
1:A:49:LYS:HD2	1:A:114:LEU:HD21	1.93	0.49
1:C:36:THR:OG1	1:C:38:GLU:OE1	2.27	0.49
1:A:88:LYS:NZ	1:A:89:TYR:CZ	2.81	0.49
1:E:44:ALA:O	1:E:48:GLU:HG2	2.12	0.49
1:A:89:TYR:CD2	1:E:77:MET:HE3	2.48	0.49
1:A:11:ASN:OD1	1:F:10:GLN:HG2	2.12	0.49
1:C:62:LEU:HG	1:C:137:ILE:HD12	1.93	0.49
1:C:36:THR:OG1	1:C:37:PRO:HD2	2.13	0.49
1:F:5:ILE:HD11	1:G:33:ALA:HB2	1.93	0.49
1:F:10:GLN:NE2	1:F:13:TRP:CZ2	2.80	0.49
1:E:46:ILE:HG23	1:E:114:LEU:HD11	1.95	0.48
1:G:46:ILE:HG23	1:G:114:LEU:HD22	1.95	0.48
1:H:13:TRP:NE1	1:H:17:GLN:HE21	2.11	0.48
1:A:41:LYS:HE2	1:G:49:LYS:HZ1	1.78	0.48
1:E:13:TRP:CD1	1:E:17:GLN:NE2	2.80	0.48
1:H:36:THR:HG22	1:H:39:GLU:H	1.78	0.48
1:F:21:ALA:O	1:F:25:LYS:HD3	2.14	0.48
1:G:51:ILE:HG22	1:G:55:LYS:HE2	1.95	0.48
1:F:13:TRP:HE3	1:F:13:TRP:C	2.22	0.48
1:G:49:LYS:HD3	1:G:114:LEU:HD21	1.96	0.48
1:F:78:ALA:O	1:F:86:GLN:NE2	2.46	0.47
1:F:13:TRP:C	1:F:13:TRP:CE3	2.93	0.47
1:E:46:ILE:HA	1:E:114:LEU:HD11	1.95	0.47
1:A:76:LYS:O	1:A:78:ALA:N	2.48	0.47
1:A:88:LYS:NZ	1:A:89:TYR:OH	2.47	0.47
1:G:89:TYR:C	1:G:91:ALA:H	2.23	0.46
1:B:88:LYS:HD3	1:B:89:TYR:CE2	2.50	0.46
1:G:69:GLY:O	1:G:73:VAL:HG23	2.16	0.46
1:H:17:GLN:HB3	1:H:55:LYS:NZ	2.31	0.46
1:E:33:ALA:HA	1:H:4:ARG:HH21	1.81	0.46
1:E:78:ALA:O	1:E:86:GLN:NE2	2.49	0.46
1:F:49:LYS:HB2	1:F:114:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ILE:HG13	1:A:85:LYS:HB2	1.98	0.45
1:D:113:GLU:HA	1:D:116:LYS:NZ	2.30	0.45
1:G:76:LYS:HE2	1:G:76:LYS:HB2	1.56	0.45
1:B:56:LEU:HD11	1:B:106:GLU:OE2	2.17	0.45
1:C:20:MET:SD	1:C:133:ALA:HA	2.57	0.45
1:C:41:LYS:HD2	1:C:41:LYS:N	2.32	0.45
1:C:42:LYS:HA	1:C:45:GLU:HG2	1.99	0.45
1:H:74:ILE:CG1	1:H:93:PHE:HE2	2.30	0.45
1:B:20:MET:HE3	1:B:133:ALA:HB2	1.98	0.45
1:D:36:THR:OG1	1:D:38:GLU:OE1	2.30	0.45
1:C:52:GLU:O	1:C:56:LEU:HG	2.17	0.44
1:A:46:ILE:HG23	1:A:114:LEU:HD22	2.00	0.44
1:G:16:ALA:HB1	1:G:136:ALA:HB1	2.00	0.44
1:C:55:LYS:HB3	1:C:55:LYS:HE2	1.68	0.44
1:D:35:LYS:CD	1:D:39:GLU:HG3	2.44	0.44
1:D:68:ALA:HA	1:D:71:LYS:NZ	2.32	0.44
1:G:20:MET:HA	1:G:132:ALA:HB1	1.99	0.44
1:E:58:ALA:O	1:E:62:LEU:HD12	2.17	0.44
1:G:104:LEU:O	1:G:108:GLU:HG3	2.18	0.44
1:D:24:VAL:HG11	1:D:51:ILE:HG13	2.00	0.44
1:H:74:ILE:HG12	1:H:93:PHE:CE2	2.49	0.43
1:H:113:GLU:HA	1:H:116:LYS:HG2	2.00	0.43
1:A:17:GLN:HB3	1:A:55:LYS:HE3	1.99	0.43
1:E:41:LYS:HE2	1:E:41:LYS:HB3	1.71	0.43
1:G:73:VAL:HG12	1:G:76:LYS:NZ	2.34	0.43
1:E:23:ALA:N	1:H:12:LEU:HD13	2.33	0.43
1:A:41:LYS:CE	1:G:49:LYS:HZ1	2.30	0.43
1:H:16:ALA:HB1	1:H:136:ALA:HB1	2.01	0.43
1:B:36:THR:HB	1:B:37:PRO:HD2	2.01	0.43
1:F:42:LYS:HE2	1:F:117:GLU:CD	2.45	0.42
1:C:42:LYS:HB3	1:C:42:LYS:HE2	1.51	0.42
1:F:77:MET:HG3	1:F:81:ILE:CD1	2.50	0.42
1:F:84:GLU:OE2	1:F:85:LYS:HG3	2.19	0.42
1:C:39:GLU:HA	1:C:42:LYS:HG3	2.02	0.42
1:D:49:LYS:HB2	1:D:114:LEU:HD11	2.02	0.42
1:E:21:ALA:O	1:E:25:LYS:HG3	2.20	0.42
1:D:47:ALA:HA	1:D:125:LEU:HD13	2.01	0.41
1:A:80:GLY:HA3	1:E:89:TYR:OH	2.20	0.41
1:F:77:MET:HE3	1:F:77:MET:HB3	1.85	0.41
1:A:119:PRO:O	1:A:123:LYS:HG3	2.20	0.41
1:B:85:LYS:O	1:B:88:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ILE:HA	1:F:77:MET:HG2	2.03	0.41
1:G:42:LYS:HZ2	1:G:118:ASP:HB2	1.83	0.41
1:B:42:LYS:CE	1:B:118:ASP:HB2	2.48	0.41
1:D:60:ALA:HB1	1:D:104:LEU:HD12	2.03	0.41
1:B:106:GLU:O	1:B:109:LYS:HE2	2.21	0.40
1:E:76:LYS:C	1:E:78:ALA:H	2.29	0.40
1:B:69:GLY:O	1:B:73:VAL:HG23	2.22	0.40
1:E:36:THR:H	1:E:39:GLU:CG	2.25	0.40
1:D:13:TRP:O	1:D:17:GLN:HG3	2.21	0.40
1:H:53:ILE:HG23	1:H:107:ALA:HB1	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	135/152 (89%)	130 (96%)	3 (2%)	2 (2%)	8	7
1	B	134/152 (88%)	129 (96%)	5 (4%)	0	100	100
1	C	143/152 (94%)	140 (98%)	2 (1%)	1 (1%)	18	24
1	D	143/152 (94%)	141 (99%)	2 (1%)	0	100	100
1	E	128/152 (84%)	126 (98%)	2 (2%)	0	100	100
1	F	130/152 (86%)	128 (98%)	1 (1%)	1 (1%)	16	20
1	G	125/152 (82%)	121 (97%)	3 (2%)	1 (1%)	16	20
1	H	124/152 (82%)	121 (98%)	3 (2%)	0	100	100
All	All	1062/1216 (87%)	1036 (98%)	21 (2%)	5 (0%)	24	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	75	ALA
1	A	78	ALA
1	C	117	GLU
1	A	77	MET
1	F	77	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/93 (87%)	81 (100%)	0	100	100
1	B	80/93 (86%)	77 (96%)	3 (4%)	29	43
1	C	86/93 (92%)	83 (96%)	3 (4%)	32	46
1	D	86/93 (92%)	84 (98%)	2 (2%)	44	59
1	E	76/93 (82%)	75 (99%)	1 (1%)	61	73
1	F	78/93 (84%)	73 (94%)	5 (6%)	16	22
1	G	75/93 (81%)	73 (97%)	2 (3%)	39	54
1	H	74/93 (80%)	71 (96%)	3 (4%)	27	40
All	All	636/744 (86%)	617 (97%)	19 (3%)	36	51

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	109	LYS
1	B	113	GLU
1	B	117	GLU
1	C	39	GLU
1	C	41	LYS
1	C	42	LYS
1	D	13	TRP
1	D	106	GLU
1	E	117	GLU
1	F	13	TRP
1	F	38	GLU

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Mol	Chain	Res	Type
1	F	45	GLU
1	F	77	MET
1	F	112	LYS
1	G	112	LYS
1	G	116	LYS
1	H	36	THR
1	H	71	LYS
1	H	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	137/152 (90%)	1.42	29 (21%) 2 2	39, 54, 81, 107	0
1	B	136/152 (89%)	1.61	40 (29%) 1 1	41, 60, 91, 102	0
1	C	145/152 (95%)	1.39	38 (26%) 1 1	41, 57, 92, 109	0
1	D	145/152 (95%)	1.44	35 (24%) 2 1	43, 57, 88, 104	0
1	E	130/152 (85%)	1.68	37 (28%) 1 1	42, 59, 96, 118	0
1	F	132/152 (86%)	1.58	37 (28%) 1 1	43, 59, 94, 119	0
1	G	129/152 (84%)	1.59	36 (27%) 1 1	40, 58, 94, 118	0
1	H	128/152 (84%)	1.94	53 (41%) 0 0	46, 64, 98, 126	0
All	All	1082/1216 (88%)	1.58	305 (28%) 1 1	39, 58, 94, 126	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	49	LYS	6.2
1	A	140	LEU	5.8
1	B	138	ALA	5.8
1	E	13	TRP	5.6
1	E	42	LYS	5.4
1	D	13	TRP	5.3
1	A	138	ALA	5.3
1	C	141	LEU	5.3
1	B	10	GLN	5.2
1	H	76	LYS	5.2
1	C	13	TRP	5.1
1	G	75	ALA	5.1
1	H	90	LEU	5.0
1	A	5	ILE	4.9
1	G	6	SER	4.9
1	B	13	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	13	TRP	4.8
1	H	87	ALA	4.8
1	A	62	LEU	4.8
1	G	39	GLU	4.7
1	A	139	ALA	4.6
1	A	141	LEU	4.6
1	E	117	GLU	4.5
1	H	139	ALA	4.5
1	D	55	LYS	4.5
1	F	40	ALA	4.5
1	F	117	GLU	4.4
1	D	78	ALA	4.3
1	H	89	TYR	4.3
1	D	85	LYS	4.2
1	G	28	ALA	4.2
1	F	43	VAL	4.2
1	H	36	THR	4.2
1	H	74	ILE	4.1
1	A	96	GLU	4.1
1	A	9	LEU	4.1
1	A	92	LYS	4.1
1	G	90	LEU	4.1
1	B	137	ILE	4.1
1	G	105	ALA	4.0
1	H	114	LEU	4.0
1	A	13	TRP	4.0
1	B	37	PRO	4.0
1	C	105	ALA	4.0
1	A	10	GLN	3.9
1	G	5	ILE	3.9
1	G	109	LYS	3.9
1	H	92	LYS	3.9
1	H	4	ARG	3.8
1	B	80	GLY	3.8
1	A	65	ALA	3.8
1	D	100	ALA	3.8
1	B	140	LEU	3.7
1	D	29	ALA	3.7
1	H	127	ALA	3.6
1	G	116	LYS	3.6
1	C	137	ILE	3.6
1	H	73	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	3.6
1	B	9	LEU	3.5
1	B	91	ALA	3.5
1	C	5	ILE	3.5
1	A	61	ALA	3.5
1	C	49	LYS	3.5
1	G	43	VAL	3.5
1	B	78	ALA	3.4
1	F	107	ALA	3.4
1	F	136	ALA	3.4
1	H	93	PHE	3.4
1	B	113	GLU	3.4
1	E	48	GLU	3.4
1	C	144	GLY	3.4
1	H	8	ALA	3.3
1	G	10	GLN	3.3
1	C	43	VAL	3.3
1	E	136	ALA	3.3
1	G	102	GLU	3.3
1	E	132	ALA	3.3
1	A	93	PHE	3.3
1	A	37	PRO	3.2
1	B	77	MET	3.2
1	B	124	ALA	3.2
1	F	44	ALA	3.2
1	H	141	LEU	3.2
1	F	20	MET	3.2
1	B	88	LYS	3.2
1	H	43	VAL	3.2
1	C	74	ILE	3.2
1	E	28	ALA	3.2
1	F	5	ILE	3.2
1	E	121	ALA	3.1
1	F	45	GLU	3.1
1	H	37	PRO	3.1
1	E	9	LEU	3.1
1	E	43	VAL	3.1
1	G	24	VAL	3.1
1	H	69	GLY	3.1
1	C	116	LYS	3.1
1	G	9	LEU	3.1
1	A	97	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	98	ALA	3.1
1	E	20	MET	3.1
1	G	141	LEU	3.1
1	E	126	THR	3.1
1	D	133	ALA	3.1
1	H	6	SER	3.1
1	H	51	ILE	3.1
1	G	112	LYS	3.0
1	H	138	ALA	3.0
1	G	77	MET	3.0
1	B	95	ALA	3.0
1	D	43	VAL	3.0
1	B	64	ILE	2.9
1	D	33	ALA	2.9
1	H	40	ALA	2.9
1	G	41	LYS	2.9
1	E	114	LEU	2.9
1	B	89	TYR	2.9
1	G	45	GLU	2.9
1	B	49	LYS	2.9
1	H	9	LEU	2.9
1	D	3	SER	2.9
1	C	147	HIS	2.9
1	F	41	LYS	2.8
1	B	117	GLU	2.8
1	G	49	LYS	2.8
1	C	28	ALA	2.8
1	H	96	GLU	2.8
1	B	81	ILE	2.8
1	A	66	ALA	2.8
1	F	11	ASN	2.7
1	E	16	ALA	2.7
1	D	62	LEU	2.7
1	D	117	GLU	2.7
1	G	52	GLU	2.7
1	G	76	LYS	2.7
1	H	35	LYS	2.7
1	H	125	LEU	2.7
1	G	91	ALA	2.7
1	H	65	ALA	2.7
1	H	66	ALA	2.7
1	A	137	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	11	ASN	2.7
1	D	145	LEU	2.7
1	B	109	LYS	2.6
1	G	42	LYS	2.6
1	B	43	VAL	2.6
1	G	114	LEU	2.6
1	C	78	ALA	2.6
1	F	72	ALA	2.6
1	D	144	GLY	2.6
1	B	25	LYS	2.6
1	B	19	ALA	2.6
1	F	36	THR	2.6
1	G	87	ALA	2.6
1	H	130	LEU	2.6
1	D	17	GLN	2.6
1	H	17	GLN	2.6
1	H	21	ALA	2.6
1	F	54	GLY	2.5
1	D	5	ILE	2.5
1	A	106	GLU	2.5
1	D	39	GLU	2.5
1	E	10	GLN	2.5
1	E	133	ALA	2.5
1	G	92	LYS	2.5
1	H	97	ALA	2.5
1	C	20	MET	2.5
1	E	46	ILE	2.5
1	C	24	VAL	2.5
1	C	73	VAL	2.5
1	G	7	SER	2.5
1	E	77	MET	2.5
1	C	70	GLY	2.5
1	F	103	GLY	2.5
1	C	90	LEU	2.5
1	G	21	ALA	2.5
1	F	7	SER	2.5
1	C	106	GLU	2.5
1	D	147	HIS	2.5
1	F	121	ALA	2.5
1	G	44	ALA	2.5
1	H	47	ALA	2.5
1	D	106	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	80	GLY	2.4
1	F	76	LYS	2.4
1	D	104	LEU	2.4
1	F	19	ALA	2.4
1	H	44	ALA	2.4
1	C	63	GLY	2.4
1	E	71	LYS	2.4
1	H	5	ILE	2.4
1	G	17	GLN	2.4
1	D	40	ALA	2.4
1	F	135	ALA	2.4
1	B	6	SER	2.4
1	C	80	GLY	2.4
1	E	8	ALA	2.4
1	H	26	ALA	2.4
1	B	83	PRO	2.4
1	E	41	LYS	2.4
1	H	107	ALA	2.4
1	H	132	ALA	2.4
1	E	83	PRO	2.3
1	C	52	GLU	2.3
1	D	52	GLU	2.3
1	F	48	GLU	2.3
1	H	113	GLU	2.3
1	H	126	THR	2.3
1	E	81	ILE	2.3
1	G	104	LEU	2.3
1	H	118	ASP	2.3
1	A	55	LYS	2.3
1	D	73	VAL	2.3
1	C	39	GLU	2.3
1	E	45	GLU	2.3
1	E	84	GLU	2.3
1	B	133	ALA	2.3
1	F	8	ALA	2.3
1	H	100	ALA	2.3
1	E	14	THR	2.3
1	B	7	SER	2.3
1	C	6	SER	2.3
1	F	10	GLN	2.3
1	F	9	LEU	2.3
1	G	115	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	31	ILE	2.3
1	H	20	MET	2.3
1	C	98	ALA	2.3
1	E	135	ALA	2.3
1	F	47	ALA	2.3
1	H	72	ALA	2.3
1	D	20	MET	2.3
1	B	67	ALA	2.2
1	H	131	ALA	2.2
1	D	9	LEU	2.2
1	C	37	PRO	2.2
1	D	89	TYR	2.2
1	B	20	MET	2.2
1	C	19	ALA	2.2
1	D	127	ALA	2.2
1	F	124	ALA	2.2
1	H	18	ALA	2.2
1	E	25	LYS	2.2
1	A	36	THR	2.2
1	F	114	LEU	2.2
1	G	103	GLY	2.2
1	F	120	GLU	2.2
1	C	15	ALA	2.2
1	F	16	ALA	2.2
1	F	85	LYS	2.2
1	F	101	LYS	2.2
1	F	77	MET	2.2
1	A	69	GLY	2.2
1	D	69	GLY	2.2
1	B	48	GLU	2.2
1	H	112	LYS	2.2
1	C	133	ALA	2.1
1	G	40	ALA	2.1
1	C	51	ILE	2.1
1	G	51	ILE	2.1
1	A	117	GLU	2.1
1	C	25	LYS	2.1
1	C	85	LYS	2.1
1	D	76	LYS	2.1
1	A	90	LEU	2.1
1	E	125	LEU	2.1
1	A	81	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	110	ILE	2.1
1	C	4	ARG	2.1
1	C	86	GLN	2.1
1	D	21	ALA	2.1
1	D	124	ALA	2.1
1	E	60	ALA	2.1
1	H	32	ALA	2.1
1	B	11	ASN	2.1
1	E	56	LEU	2.1
1	B	92	LYS	2.1
1	C	79	ASP	2.1
1	E	7	SER	2.1
1	A	77	MET	2.1
1	A	21	ALA	2.1
1	D	135	ALA	2.1
1	D	143	ALA	2.1
1	H	134	ALA	2.1
1	E	52	GLU	2.1
1	H	34	THR	2.1
1	C	87	ALA	2.0
1	D	65	ALA	2.0
1	F	78	ALA	2.0
1	A	11	ASN	2.0
1	B	106	GLU	2.0
1	B	120	GLU	2.0
1	B	76	LYS	2.0
1	B	100	ALA	2.0
1	B	132	ALA	2.0
1	C	44	ALA	2.0
1	D	125	LEU	2.0
1	E	30	GLU	2.0
1	F	62	LEU	2.0
1	E	109	LYS	2.0
1	F	102	GLU	2.0
1	C	36	THR	2.0
1	B	79	ASP	2.0
1	A	7	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.