



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:15 PM UTC

PDB ID : 6J4A / pdb_00006j4a
Title : Human H chain ferritin with an extension peptide
Authors : Zhang, X.; Zang, J.; Zhou, K.; Zhao, G.
Deposited on : 2019-01-08
Resolution : 3.99 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

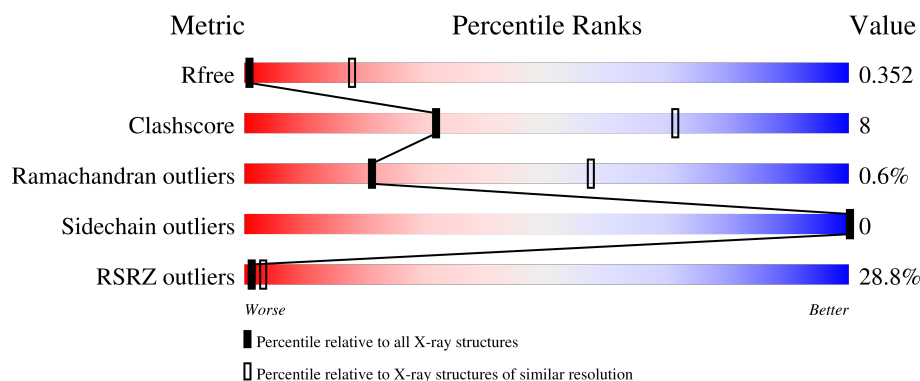
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	183	29% 68% 26% 6%
1	B	183	28% 70% 23% 6%
1	C	183	23% 79% 15% 6%
1	D	183	25% 78% 16% 6%
1	E	183	38% 70% 24% 6%

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Mol	Chain	Length	Quality of chain
1	F	183	
1	G	183	
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16972 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	B	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	C	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	D	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	E	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	F	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	G	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	H	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	I	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	J	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	K	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	L	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	conflict	UNP P02794
B	86	GLN	LYS	conflict	UNP P02794
C	86	GLN	LYS	conflict	UNP P02794
D	86	GLN	LYS	conflict	UNP P02794
E	86	GLN	LYS	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	86	GLN	LYS	conflict	UNP P02794
G	86	GLN	LYS	conflict	UNP P02794
H	86	GLN	LYS	conflict	UNP P02794
I	86	GLN	LYS	conflict	UNP P02794
J	86	GLN	LYS	conflict	UNP P02794
K	86	GLN	LYS	conflict	UNP P02794
L	86	GLN	LYS	conflict	UNP P02794

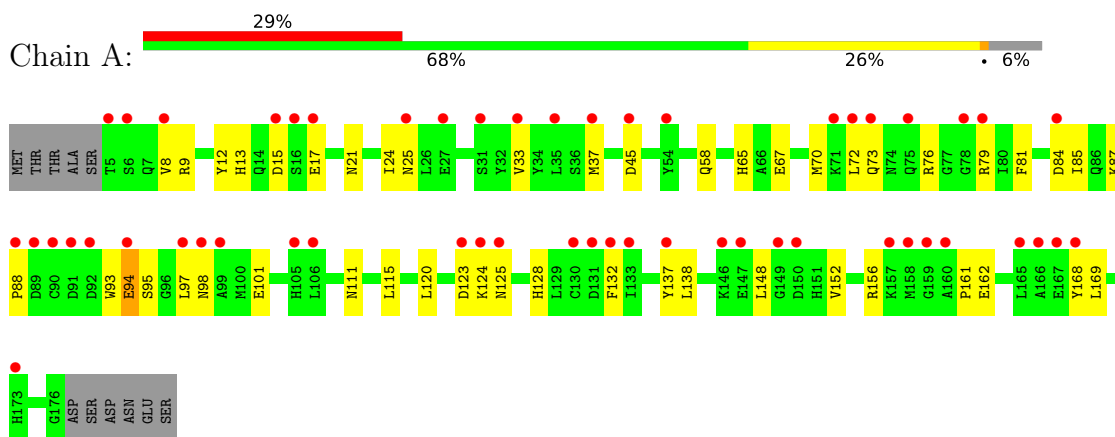
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	1	Total O 1 1	0	0
2	D	2	Total O 2 2	0	0
2	E	1	Total O 1 1	0	0
2	F	2	Total O 2 2	0	0
2	G	1	Total O 1 1	0	0
2	H	2	Total O 2 2	0	0
2	I	1	Total O 1 1	0	0
2	J	2	Total O 2 2	0	0
2	L	1	Total O 1 1	0	0

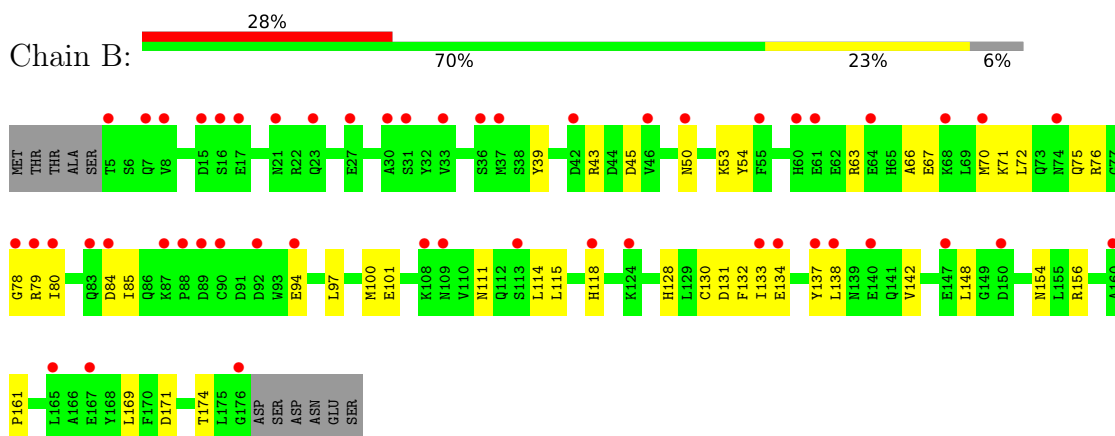
3 Residue-property plots [i](#)

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.

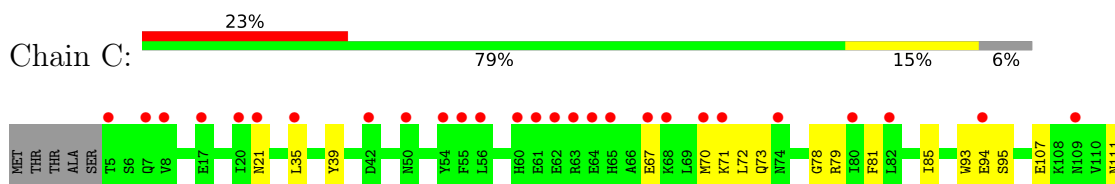
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain

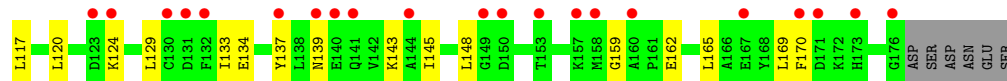
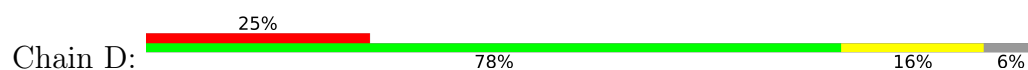


• Molecule 1: Ferritin heavy chain

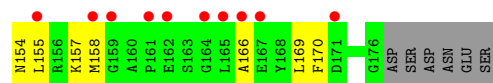
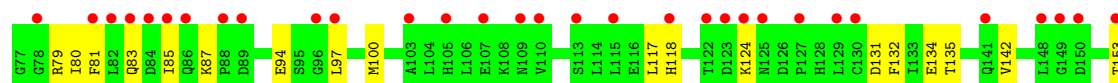
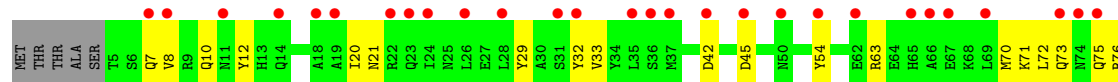
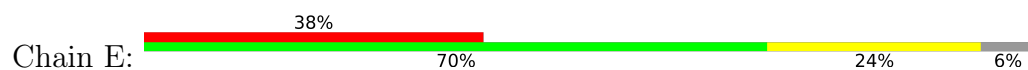




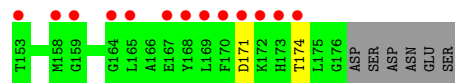
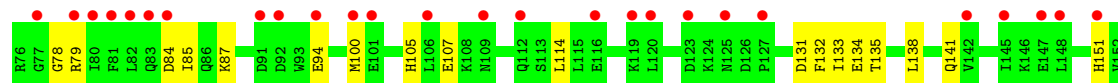
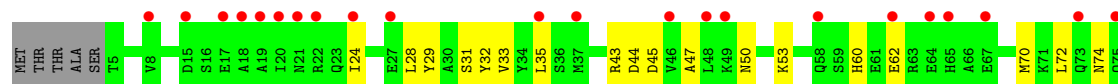
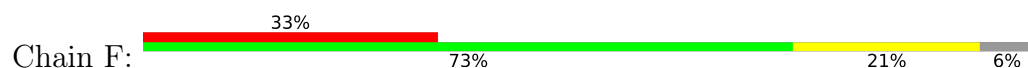
• Molecule 1: Ferritin heavy chain



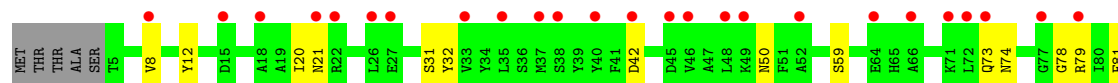
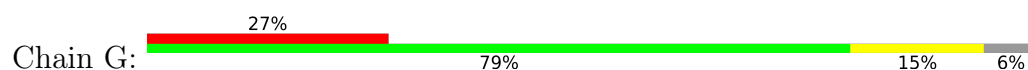
• Molecule 1: Ferritin heavy chain

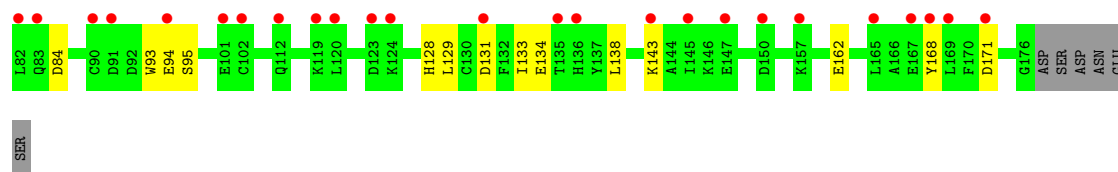


• Molecule 1: Ferritin heavy chain



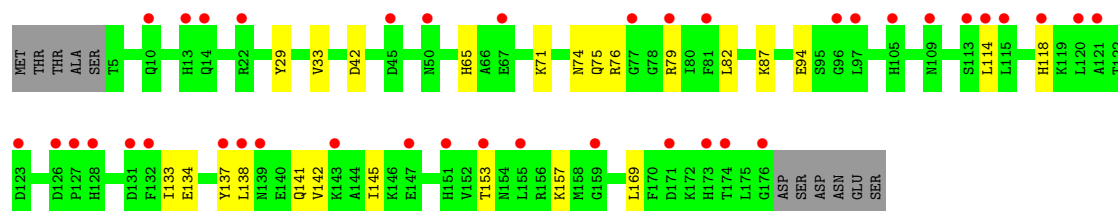
• Molecule 1: Ferritin heavy chain





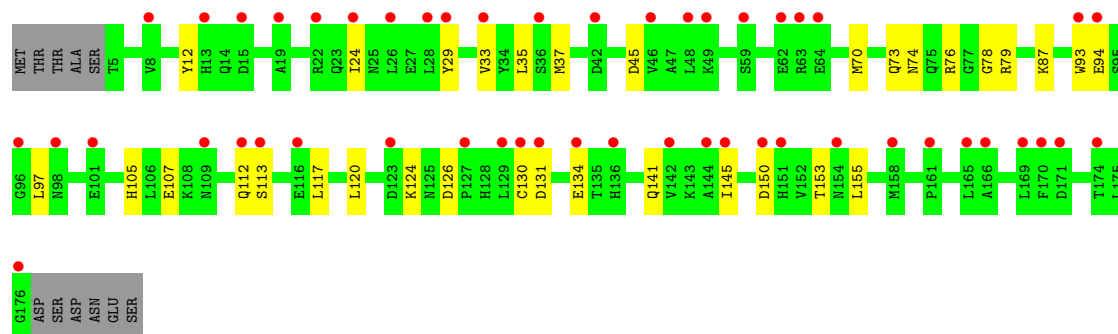
● Molecule 1: Ferritin heavy chain

Chain H: 21% 81% 13% 6%



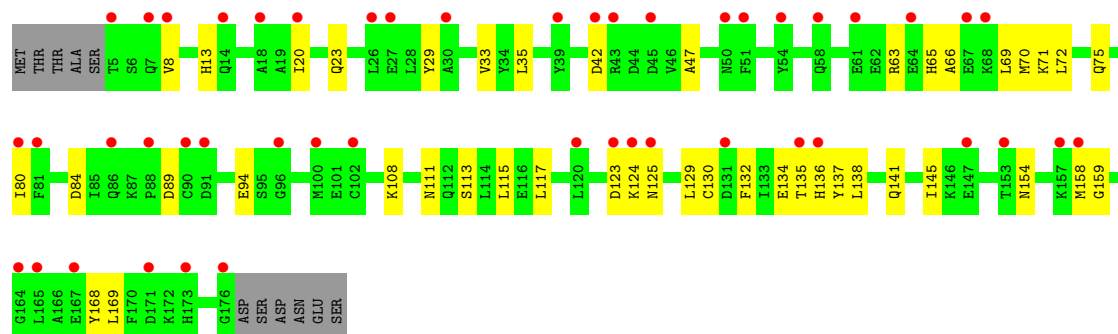
● Molecule 1: Ferritin heavy chain

Chain I: 27% 76% 18% 6%



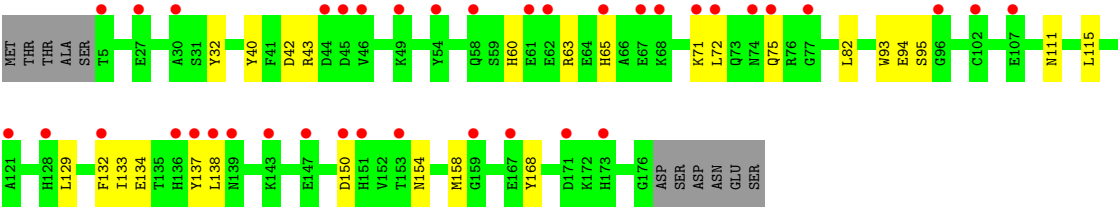
● Molecule 1: Ferritin heavy chain

Chain J: 26% 70% 24% 6%

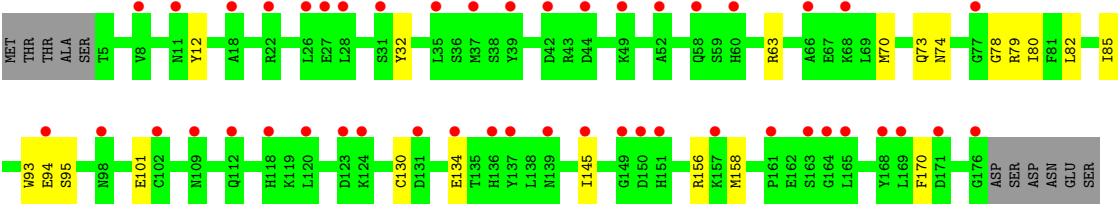
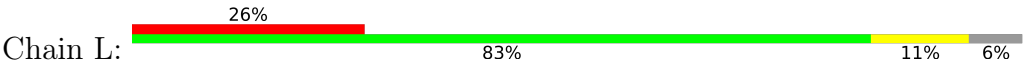


● Molecule 1: Ferritin heavy chain

Chain K: 21% 80% 14% 6%



● Molecule 1: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	219.80Å 219.80Å 148.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.31 – 3.99 107.31 – 3.99	Depositor EDS
% Data completeness (in resolution range)	95.1 (107.31-3.99) 79.5 (107.31-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 4.01Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.283 , 0.351 0.285 , 0.352	Depositor DCC
R_{free} test set	1536 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtrriage
Anisotropy	0.439	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16972	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.66 % 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 6.2702e-05. 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	0.17	0/1442	0.42	0/1943
1	B	0.17	0/1442	0.36	0/1943
1	C	0.17	0/1442	0.34	0/1943
1	D	0.13	0/1442	0.30	0/1943
1	E	0.15	0/1442	0.37	0/1943
1	F	0.14	0/1442	0.32	0/1943
1	G	0.13	0/1442	0.32	0/1943
1	H	0.13	0/1442	0.31	0/1943
1	I	0.14	0/1442	0.32	0/1943
1	J	0.14	0/1442	0.31	0/1943
1	K	0.15	0/1442	0.32	0/1943
1	L	0.13	0/1442	0.33	0/1943
All	All	0.15	0/17304	0.34	0/23316

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 [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	1413	0	1352	37	0
1	B	1413	0	1352	38	0
1	C	1413	0	1352	20	0
1	D	1413	0	1352	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1413	0	1352	43	0
1	F	1413	0	1352	30	1
1	G	1413	0	1352	23	1
1	H	1413	0	1352	17	0
1	I	1413	0	1352	25	0
1	J	1413	0	1352	34	0
1	K	1413	0	1352	21	0
1	L	1413	0	1352	14	0
2	A	3	0	0	1	0
2	B	1	0	0	0	0
2	D	2	0	0	1	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	L	1	0	0	0	0
All	All	16972	0	16224	268	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 8.

All (268) 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:158:MET:HE1	1:E:170:PHE:HB2	1.63	0.81
1:A:33:VAL:HG12	1:A:88:PRO:HB3	1.63	0.80
1:C:21:ASN:HD21	1:C:81:PHE:H	1.30	0.79
1:F:107:GLU:OE1	1:F:141:GLN:NE2	2.18	0.77
1:B:174:THR:HG1	1:J:168:TYR:HH	1.33	0.77
1:B:67:GLU:O	1:B:71:LYS:N	2.16	0.74
1:C:21:ASN:OD1	1:C:73:GLN:NE2	2.24	0.71
1:C:78:GLY:O	1:C:79:ARG:NH1	2.24	0.70
1:D:78:GLY:O	1:D:79:ARG:NH1	2.21	0.70
1:B:63:ARG:HE	1:B:67:GLU:CD	2.00	0.70
1:E:63:ARG:HH22	1:F:60:HIS:CD2	2.10	0.69
1:B:78:GLY:O	1:B:79:ARG:NH1	2.26	0.69
1:A:21:ASN:OD1	1:A:73:GLN:NE2	2.27	0.68
1:A:101:GLU:OE1	1:A:156:ARG:NH2	2.29	0.66
1:K:42:ASP:HB3	1:L:74:ASN:HD22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LEU:HD21	1:J:169:LEU:HD13	1.79	0.65
1:A:85:ILE:HD11	1:B:85:ILE:HD12	1.77	0.65
1:B:174:THR:OG1	1:J:168:TYR:OH	2.08	0.64
1:L:101:GLU:OE1	1:L:156:ARG:NH2	2.30	0.64
1:G:134:GLU:HA	1:G:138:LEU:HB2	1.80	0.64
1:A:79:ARG:NH1	1:B:45:ASP:OD2	2.29	0.64
1:I:74:ASN:HD22	1:J:42:ASP:HB3	1.63	0.64
1:C:21:ASN:ND2	1:C:81:PHE:H	1.95	0.63
1:A:9:ARG:NH2	1:A:17:GLU:OE2	2.32	0.62
1:A:93:TRP:O	1:A:95:SER:N	2.33	0.62
1:J:65:HIS:O	1:J:137:TYR:OH	2.17	0.62
1:A:21:ASN:ND2	1:A:81:PHE:H	1.98	0.61
1:L:78:GLY:O	1:L:79:ARG:NH1	2.33	0.61
1:A:8:VAL:HG23	1:H:145:ILE:HG22	1.81	0.61
1:B:97:LEU:HD23	1:B:161:PRO:HD3	1.82	0.61
1:F:134:GLU:HA	1:F:138:LEU:HB2	1.82	0.60
1:G:21:ASN:HD21	1:G:81:PHE:HB2	1.66	0.59
1:K:65:HIS:O	1:K:137:TYR:OH	2.20	0.59
1:E:87:LYS:H	1:E:87:LYS:HD3	1.67	0.59
1:A:169:LEU:HD21	1:E:169:LEU:HD13	1.83	0.59
1:E:42:ASP:HB3	1:F:74:ASN:HD22	1.67	0.59
1:K:40:TYR:HD1	1:K:43:ARG:HD3	1.67	0.58
1:C:174:THR:HG1	1:K:168:TYR:HH	1.51	0.58
1:J:154:ASN:O	1:J:158:MET:HG2	2.03	0.58
1:G:131:ASP:HA	1:G:134:GLU:HG2	1.86	0.58
1:I:12:TYR:OH	1:I:73:GLN:OE1	2.22	0.57
1:E:118:HIS:NE2	1:E:134:GLU:OE2	2.37	0.57
1:F:31:SER:HB2	1:F:62:GLU:HB2	1.86	0.57
1:I:35:LEU:HD11	1:J:70:MET:SD	2.45	0.57
1:E:155:LEU:HA	1:E:158:MET:HE2	1.87	0.56
1:B:101:GLU:OE1	1:B:156:ARG:NH2	2.38	0.56
1:E:131:ASP:O	1:E:135:THR:N	2.39	0.56
1:I:24:ILE:HD13	1:I:70:MET:HG3	1.88	0.56
1:J:130:CYS:O	1:J:134:GLU:HG3	2.06	0.56
1:G:31:SER:O	1:G:59:SER:OG	2.23	0.56
1:B:72:LEU:HB2	1:B:132:PHE:HE2	1.71	0.55
1:E:131:ASP:HA	1:E:134:GLU:HB2	1.87	0.55
1:I:97:LEU:HD13	1:I:155:LEU:HB2	1.89	0.55
1:E:12:TYR:OH	1:E:73:GLN:OE1	2.23	0.55
1:I:45:ASP:N	1:I:45:ASP:OD1	2.37	0.55
1:I:76:ARG:HH22	1:I:126:ASP:CG	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:GLU:OE1	1:I:141:GLN:NE2	2.34	0.55
1:A:12:TYR:HD1	1:A:76:ARG:HE	1.53	0.54
1:I:130:CYS:O	1:I:134:GLU:HG3	2.07	0.54
1:F:134:GLU:HG3	1:F:138:LEU:HD12	1.90	0.54
1:A:45:ASP:C	1:E:153:THR:HG21	2.32	0.54
1:C:131:ASP:HA	1:C:134:GLU:HB2	1.90	0.54
1:E:10:GLN:HE21	1:I:112:GLN:HE22	1.56	0.54
1:H:118:HIS:NE2	1:H:134:GLU:OE2	2.37	0.54
1:J:20:ILE:HG23	1:J:69:LEU:HD22	1.90	0.54
1:K:150:ASP:O	1:K:154:ASN:ND2	2.41	0.53
1:G:12:TYR:OH	1:G:73:GLN:OE1	2.23	0.53
1:J:63:ARG:HG2	1:J:63:ARG:HH11	1.72	0.53
1:C:114:LEU:HD13	1:C:137:TYR:HB3	1.91	0.53
1:C:133:ILE:HG22	1:C:138:LEU:HG	1.90	0.52
1:C:174:THR:OG1	1:K:168:TYR:OH	2.21	0.52
1:B:114:LEU:HD13	1:B:137:TYR:HB3	1.91	0.52
1:F:50:ASN:ND2	1:F:171:ASP:OD1	2.43	0.52
1:D:20:ILE:HD13	1:D:117:LEU:HD11	1.90	0.52
1:A:79:ARG:HH22	1:B:43:ARG:CZ	2.23	0.52
1:D:134:GLU:OE1	2:D:201:HOH:O	2.19	0.51
1:E:87:LYS:H	1:E:87:LYS:CD	2.22	0.51
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.46	0.51
1:A:120:LEU:O	1:A:124:LYS:HG2	2.10	0.51
1:L:130:CYS:O	1:L:134:GLU:HG3	2.10	0.51
1:D:139:ASN:O	1:D:143:LYS:HG3	2.10	0.51
1:A:58:GLN:NE2	2:A:201:HOH:O	2.35	0.51
1:F:43:ARG:NH2	1:F:45:ASP:OD2	2.44	0.51
1:I:29:TYR:O	1:I:33:VAL:HG23	2.10	0.51
1:K:71:LYS:O	1:K:75:GLN:HG3	2.11	0.51
1:D:129:LEU:O	1:D:133:ILE:HG12	2.11	0.51
1:E:8:VAL:HB	1:I:145:ILE:HG22	1.92	0.51
1:G:133:ILE:HG22	1:G:138:LEU:HG	1.93	0.50
1:I:87:LYS:N	1:J:84:ASP:OD1	2.44	0.50
1:L:158:MET:HE1	1:L:170:PHE:HB2	1.93	0.50
1:F:47:ALA:HB1	1:I:150:ASP:OD1	2.11	0.50
1:C:70:MET:HE1	1:D:35:LEU:HG	1.92	0.50
1:A:98:ASN:O	1:A:98:ASN:ND2	2.26	0.50
1:G:20:ILE:HD11	1:G:129:LEU:HD11	1.94	0.50
1:B:70:MET:HE3	1:B:80:ILE:HG21	1.93	0.50
1:J:66:ALA:O	1:J:70:MET:HG3	2.11	0.50
1:A:25:ASN:ND2	1:A:84:ASP:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASN:ND2	1:J:47:ALA:O	2.45	0.50
1:B:66:ALA:O	1:B:70:MET:HG3	2.12	0.50
1:G:21:ASN:ND2	1:G:81:PHE:HB2	2.26	0.49
1:A:13:HIS:CE1	1:A:15:ASP:HB2	2.47	0.49
1:A:65:HIS:O	1:A:137:TYR:OH	2.26	0.49
1:D:108:LYS:HG3	1:D:145:ILE:HD13	1.94	0.49
1:B:133:ILE:HG22	1:B:138:LEU:HG	1.94	0.49
1:K:63:ARG:HH11	1:L:63:ARG:HH11	1.61	0.49
1:I:105:HIS:O	1:I:105:HIS:ND1	2.44	0.48
1:D:93:TRP:O	1:D:95:SER:N	2.47	0.48
1:F:78:GLY:O	1:F:79:ARG:NH1	2.46	0.48
1:A:168:TYR:CE2	1:E:158:MET:SD	3.07	0.48
1:G:21:ASN:HD21	1:G:81:PHE:H	1.61	0.48
1:I:78:GLY:O	1:I:79:ARG:NH1	2.47	0.48
1:A:94:GLU:HG2	1:A:95:SER:H	1.78	0.48
1:B:118:HIS:NE2	1:B:134:GLU:OE2	2.47	0.48
1:C:85:ILE:HD12	1:D:85:ILE:HD12	1.95	0.48
1:F:45:ASP:OD1	1:F:45:ASP:N	2.40	0.48
1:K:82:LEU:HD13	1:L:32:TYR:CE1	2.49	0.48
1:C:79:ARG:HD3	1:C:79:ARG:HA	1.70	0.48
1:K:72:LEU:HD21	1:K:129:LEU:HD13	1.95	0.48
1:K:133:ILE:HG22	1:K:138:LEU:HG	1.95	0.48
1:G:42:ASP:HB3	1:H:74:ASN:HD22	1.79	0.47
1:L:12:TYR:OH	1:L:73:GLN:OE1	2.30	0.47
1:E:83:GLN:HA	1:F:87:LYS:HD2	1.95	0.47
1:F:131:ASP:OD1	1:F:135:THR:OG1	2.32	0.47
1:A:37:MET:HG2	1:A:93:TRP:CE2	2.50	0.47
1:A:94:GLU:HG2	1:A:95:SER:N	2.30	0.47
1:E:154:ASN:O	1:E:157:LYS:N	2.48	0.47
1:L:70:MET:HE3	1:L:80:ILE:HG21	1.97	0.47
1:B:169:LEU:HD21	1:H:169:LEU:HD13	1.97	0.47
1:J:89:ASP:OD1	1:J:89:ASP:N	2.44	0.47
1:B:76:ARG:HD2	1:E:142:VAL:HG11	1.96	0.47
1:E:32:TYR:HE2	1:F:85:ILE:HG13	1.80	0.47
1:F:24:ILE:HD13	1:F:70:MET:HG2	1.97	0.47
1:J:71:LYS:O	1:J:75:GLN:HG3	2.14	0.47
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.50	0.46
1:A:67:GLU:HG2	1:B:39:TYR:OH	2.14	0.46
1:A:97:LEU:HD23	1:A:161:PRO:HD3	1.97	0.46
1:C:107:GLU:OE1	1:C:141:GLN:NE2	2.38	0.46
1:J:72:LEU:HD21	1:J:129:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:O	1:A:115:LEU:HG	2.14	0.46
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.51	0.46
1:F:50:ASN:HA	1:F:53:LYS:HB2	1.97	0.46
1:G:78:GLY:O	1:G:79:ARG:NH1	2.40	0.46
1:J:8:VAL:HB	1:L:145:ILE:HG22	1.97	0.46
1:B:131:ASP:HA	1:B:134:GLU:HG3	1.97	0.46
1:B:134:GLU:HB3	1:I:131:ASP:HB2	1.97	0.46
1:A:24:ILE:HD13	1:A:70:MET:HG3	1.98	0.46
1:D:65:HIS:HB3	1:D:137:TYR:HE2	1.81	0.46
1:E:154:ASN:O	1:E:158:MET:HG3	2.16	0.46
1:E:21:ASN:ND2	1:E:81:PHE:O	2.49	0.45
1:A:128:HIS:HD1	1:H:142:VAL:HG21	1.81	0.45
1:B:63:ARG:NE	1:B:67:GLU:OE2	2.43	0.45
1:J:29:TYR:O	1:J:33:VAL:HG23	2.16	0.45
1:E:158:MET:HB2	1:E:166:ALA:HB1	1.99	0.45
1:E:71:LYS:O	1:E:75:GLN:HG3	2.17	0.45
1:I:37:MET:HA	1:I:93:TRP:CD1	2.51	0.45
1:B:71:LYS:O	1:B:75:GLN:HG3	2.16	0.45
1:G:162:GLU:H	1:G:162:GLU:HG3	1.58	0.45
1:E:10:GLN:NE2	1:I:112:GLN:HE22	2.14	0.45
1:E:45:ASP:OD2	1:F:79:ARG:NH2	2.47	0.45
1:J:141:GLN:O	1:J:145:ILE:HG13	2.17	0.45
1:A:72:LEU:HD13	1:A:132:PHE:CD2	2.52	0.45
1:A:21:ASN:HD21	1:A:81:PHE:H	1.64	0.44
1:B:54:TYR:CE2	1:B:100:MET:HE1	2.52	0.44
1:E:10:GLN:O	1:E:76:ARG:NH2	2.46	0.44
1:E:79:ARG:HD2	1:F:43:ARG:HD2	1.99	0.44
1:K:129:LEU:O	1:K:133:ILE:HG12	2.18	0.44
1:E:70:MET:HE1	1:F:35:LEU:HG	1.99	0.44
1:E:155:LEU:HD23	1:E:158:MET:HE2	1.99	0.44
1:F:28:LEU:HB3	1:F:85:ILE:HD13	1.99	0.44
1:B:111:ASN:O	1:B:115:LEU:HG	2.16	0.44
1:E:79:ARG:HD3	1:E:79:ARG:HA	1.73	0.44
1:F:100:MET:HE1	1:F:151:HIS:ND1	2.31	0.44
1:D:79:ARG:HA	1:D:79:ARG:HD3	1.77	0.44
1:E:20:ILE:HD13	1:E:117:LEU:HD11	2.00	0.44
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.87	0.44
1:E:54:TYR:CE2	1:E:100:MET:HE1	2.53	0.44
1:A:148:LEU:O	1:A:152:VAL:HG23	2.17	0.44
1:C:93:TRP:O	1:C:95:SER:N	2.51	0.44
1:E:63:ARG:HH22	1:F:60:HIS:HD2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:THR:O	1:H:157:LYS:HG2	2.18	0.43
1:J:123:ASP:C	1:J:125:ASN:H	2.24	0.43
1:H:65:HIS:O	1:H:137:TYR:OH	2.32	0.43
1:J:70:MET:HE2	1:J:80:ILE:HD13	1.99	0.43
1:J:108:LYS:HG3	1:J:145:ILE:HD13	2.00	0.43
1:L:93:TRP:O	1:L:95:SER:N	2.51	0.43
1:G:32:TYR:CE1	1:H:82:LEU:HD13	2.54	0.43
1:J:23:GLN:OE1	1:J:113:SER:OG	2.36	0.43
1:J:63:ARG:HG2	1:J:63:ARG:NH1	2.33	0.43
1:J:111:ASN:O	1:J:115:LEU:HG	2.18	0.43
1:L:79:ARG:HA	1:L:79:ARG:HD3	1.73	0.43
1:K:154:ASN:O	1:K:158:MET:HG3	2.19	0.43
1:D:170:PHE:CD1	1:D:170:PHE:C	2.97	0.43
1:F:114:LEU:HD22	1:F:133:ILE:HG23	2.01	0.43
1:J:20:ILE:HD13	1:J:117:LEU:HD11	1.99	0.43
1:K:32:TYR:CZ	1:L:82:LEU:HD13	2.53	0.43
1:A:87:LYS:N	1:B:84:ASP:OD1	2.47	0.43
1:B:76:ARG:HD3	1:B:128:HIS:HD1	1.84	0.43
1:B:79:ARG:HA	1:B:79:ARG:HD3	1.82	0.43
1:H:76:ARG:HH11	1:H:76:ARG:HG3	1.83	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.43
1:B:53:LYS:HB2	1:B:53:LYS:HE3	1.91	0.43
1:D:139:ASN:HA	1:G:128:HIS:CD2	2.54	0.43
1:H:141:GLN:O	1:H:145:ILE:HG13	2.19	0.42
1:J:135:THR:HB	1:J:136:HIS:CD2	2.53	0.42
1:C:67:GLU:O	1:C:71:LYS:N	2.36	0.42
1:D:120:LEU:O	1:D:124:LYS:HG2	2.19	0.42
1:F:105:HIS:ND1	1:F:105:HIS:O	2.53	0.42
1:G:79:ARG:HD3	1:G:79:ARG:HA	1.73	0.42
1:G:93:TRP:O	1:G:95:SER:N	2.51	0.42
1:J:124:LYS:HD2	1:J:124:LYS:N	2.33	0.42
1:K:134:GLU:HA	1:K:138:LEU:HD12	2.01	0.42
1:K:111:ASN:O	1:K:115:LEU:HG	2.18	0.42
1:J:13:HIS:CG	1:J:124:LYS:HG2	2.54	0.42
1:J:134:GLU:HA	1:J:138:LEU:HD12	2.01	0.42
1:C:39:TYR:OH	1:D:67:GLU:HB3	2.18	0.42
1:D:148:LEU:HD23	1:D:148:LEU:HA	1.92	0.42
1:E:29:TYR:O	1:E:33:VAL:HG23	2.20	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.55	0.42
1:G:129:LEU:O	1:G:133:ILE:HG12	2.20	0.42
1:D:145:ILE:HG22	1:G:8:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:32:TYR:CE1	1:L:85:ILE:HD11	2.55	0.42
1:K:93:TRP:O	1:K:95:SER:N	2.53	0.42
1:A:123:ASP:C	1:A:125:ASN:H	2.27	0.41
1:A:162:GLU:OE1	1:A:162:GLU:HA	2.20	0.41
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.20	0.41
1:E:7:GLN:HG3	1:E:8:VAL:HG13	2.01	0.41
1:E:73:GLN:HG2	1:E:80:ILE:HG12	2.02	0.41
1:A:84:ASP:OD1	1:A:84:ASP:N	2.53	0.41
1:C:72:LEU:HD22	1:C:132:PHE:CE2	2.55	0.41
1:I:113:SER:O	1:I:117:LEU:HB2	2.20	0.41
1:K:134:GLU:HA	1:K:138:LEU:HB2	2.01	0.41
1:D:114:LEU:HD13	1:D:137:TYR:HB3	2.02	0.41
1:D:159:GLY:O	1:D:162:GLU:HG2	2.20	0.41
1:E:21:ASN:ND2	1:E:81:PHE:HB2	2.35	0.41
1:H:71:LYS:O	1:H:75:GLN:HG3	2.20	0.41
1:D:65:HIS:O	1:D:137:TYR:OH	2.32	0.41
1:I:120:LEU:O	1:I:124:LYS:HG2	2.20	0.41
1:E:97:LEU:HD13	1:E:155:LEU:HB3	2.03	0.41
1:D:70:MET:HE3	1:D:82:LEU:HD21	2.02	0.41
1:E:87:LYS:HD2	1:F:84:ASP:OD1	2.21	0.41
1:G:21:ASN:HD21	1:G:81:PHE:N	2.18	0.41
1:H:133:ILE:O	1:H:138:LEU:HG	2.21	0.41
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.95	0.41
1:F:45:ASP:HA	1:I:153:THR:HG21	2.02	0.41
1:G:50:ASN:HB2	1:G:171:ASP:CG	2.46	0.41
1:H:29:TYR:O	1:H:33:VAL:HG23	2.20	0.41
1:J:72:LEU:HD22	1:J:132:PHE:CE2	2.55	0.41
1:C:35:LEU:HD21	1:D:70:MET:SD	2.61	0.41
1:K:60:HIS:O	1:K:63:ARG:HB3	2.21	0.41
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.84	0.40
1:E:124:LYS:HA	1:E:124:LYS:HD3	1.82	0.40
1:I:70:MET:HE1	1:J:35:LEU:HD11	2.03	0.40
1:I:124:LYS:HA	1:I:124:LYS:HD2	1.89	0.40
1:B:132:PHE:C	1:B:132:PHE:CD1	2.99	0.40
1:H:79:ARG:HA	1:H:79:ARG:HD3	1.81	0.40
1:B:72:LEU:HD13	1:B:132:PHE:CE2	2.56	0.40
1:G:143:LYS:N	1:G:143:LYS:HD3	2.37	0.40
1:H:114:LEU:HD12	1:H:141:GLN:HG3	2.04	0.40
1:B:130:CYS:O	1:B:134:GLU:HG3	2.21	0.40
1:D:165:LEU:HD11	1:J:169:LEU:HD12	2.04	0.40
1:E:79:ARG:NH2	1:F:44:ASP:OD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ILE:HG13	1:F:32:TYR:CE2	2.57	0.40
1:A:85:ILE:CD1	1:B:85:ILE:HD12	2.49	0.40
1:B:142:VAL:HG21	1:I:76:ARG:HD3	2.03	0.40
1:C:111:ASN:O	1:C:115:LEU:HG	2.22	0.40
1:F:29:TYR:O	1:F:33:VAL:HG23	2.21	0.40
1:G:74:ASN:HD22	1:H:42:ASP:HB3	1.86	0.40
1:G:84:ASP:OD1	1:H:87:LYS:N	2.55	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:F:174:THR:OG1	1:G:168:TYR:OH[8_777]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/183 (93%)	158 (93%)	11 (6%)	1 (1%)	21	57
1	B	170/183 (93%)	161 (95%)	8 (5%)	1 (1%)	21	57
1	C	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	21	57
1	D	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	21	57
1	E	170/183 (93%)	160 (94%)	9 (5%)	1 (1%)	21	57
1	F	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	21	57
1	G	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	21	57
1	H	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	21	57
1	I	170/183 (93%)	168 (99%)	1 (1%)	1 (1%)	21	57
1	J	170/183 (93%)	163 (96%)	5 (3%)	2 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	170/183 (93%)	161 (95%)	8 (5%)	1 (1%)	21	57
1	L	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	21	57
All	All	2040/2196 (93%)	1958 (96%)	69 (3%)	13 (1%)	21	57

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	D	94	GLU
1	H	94	GLU
1	B	94	GLU
1	E	94	GLU
1	G	94	GLU
1	I	94	GLU
1	K	94	GLU
1	C	94	GLU
1	F	94	GLU
1	L	94	GLU
1	J	159	GLY
1	J	94	GLU

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	153/163 (94%)	153 (100%)	0	100	100
1	B	153/163 (94%)	153 (100%)	0	100	100
1	C	153/163 (94%)	153 (100%)	0	100	100
1	D	153/163 (94%)	153 (100%)	0	100	100
1	E	153/163 (94%)	153 (100%)	0	100	100
1	F	153/163 (94%)	153 (100%)	0	100	100
1	G	153/163 (94%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	153/163 (94%)	153 (100%)	0	100	100
1	I	153/163 (94%)	153 (100%)	0	100	100
1	J	153/163 (94%)	153 (100%)	0	100	100
1	K	153/163 (94%)	153 (100%)	0	100	100
1	L	153/163 (94%)	153 (100%)	0	100	100
All	All	1836/1956 (94%)	1836 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	136	HIS
1	B	60	HIS
1	B	112	GLN
1	B	141	GLN
1	C	75	GLN
1	C	105	HIS
1	C	111	ASN
1	D	139	ASN
1	D	141	GLN
1	E	10	GLN
1	E	141	GLN
1	F	50	ASN
1	F	60	HIS
1	F	74	ASN
1	F	139	ASN
1	G	21	ASN
1	G	60	HIS
1	G	111	ASN
1	H	136	HIS
1	H	139	ASN
1	I	74	ASN
1	I	86	GLN
1	I	111	ASN
1	J	125	ASN
1	J	139	ASN
1	J	154	ASN
1	L	74	ASN

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Mol	Chain	Res	Type
1	L	118	HIS

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	172/183 (93%)	1.62	53 (30%) 1 3	27, 44, 61, 77	0
1	B	172/183 (93%)	1.62	51 (29%) 1 3	28, 44, 65, 75	0
1	C	172/183 (93%)	1.51	43 (25%) 2 4	28, 44, 66, 91	0
1	D	172/183 (93%)	1.56	46 (26%) 1 3	27, 43, 64, 78	0
1	E	172/183 (93%)	1.77	69 (40%) 0 1	22, 42, 63, 83	0
1	F	172/183 (93%)	1.75	61 (35%) 1 2	21, 40, 59, 68	0
1	G	172/183 (93%)	1.57	50 (29%) 1 3	21, 40, 60, 70	0
1	H	172/183 (93%)	1.45	39 (22%) 2 4	21, 41, 62, 84	0
1	I	172/183 (93%)	1.54	50 (29%) 1 3	23, 39, 57, 71	0
1	J	172/183 (93%)	1.56	47 (27%) 1 3	21, 40, 59, 75	0
1	K	172/183 (93%)	1.41	38 (22%) 2 4	20, 41, 59, 68	0
1	L	172/183 (93%)	1.54	47 (27%) 1 3	20, 41, 60, 70	0
All	All	2064/2196 (93%)	1.58	594 (28%) 1 3	20, 42, 62, 91	0

All (594) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ALA	7.3
1	E	150	ASP	6.0
1	I	158	MET	5.5
1	D	149	GLY	5.4
1	C	137	TYR	5.3
1	H	121	ALA	5.2
1	C	64	GLU	5.1
1	K	137	TYR	5.0
1	D	17	GLU	4.9
1	F	81	PHE	4.9
1	J	167	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	64	GLU	4.8
1	D	35	LEU	4.7
1	G	165	LEU	4.7
1	E	148	LEU	4.6
1	F	158	MET	4.6
1	I	131	ASP	4.6
1	L	150	ASP	4.6
1	I	154	ASN	4.6
1	K	147	GLU	4.6
1	F	21	ASN	4.5
1	A	165	LEU	4.5
1	G	169	LEU	4.5
1	E	123	ASP	4.5
1	G	8	VAL	4.5
1	E	42	ASP	4.4
1	L	149	GLY	4.4
1	B	147	GLU	4.3
1	G	48	LEU	4.3
1	C	94	GLU	4.2
1	K	58	GLN	4.2
1	F	94	GLU	4.2
1	G	168	TYR	4.1
1	L	27	GLU	4.1
1	D	150	ASP	4.1
1	K	159	GLY	4.1
1	K	128	HIS	4.1
1	K	67	GLU	4.0
1	L	131	ASP	4.0
1	K	45	ASP	4.0
1	B	5	THR	3.9
1	J	45	ASP	3.9
1	A	98	ASN	3.9
1	L	8	VAL	3.9
1	H	131	ASP	3.9
1	G	49	LYS	3.9
1	F	101	GLU	3.9
1	C	5	THR	3.9
1	E	122	THR	3.9
1	B	94	GLU	3.9
1	K	171	ASP	3.8
1	B	134	GLU	3.8
1	J	147	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	170	PHE	3.8
1	I	94	GLU	3.8
1	K	71	LYS	3.8
1	A	90	CYS	3.8
1	L	109	ASN	3.8
1	C	140	GLU	3.8
1	C	175	LEU	3.7
1	J	67	GLU	3.7
1	K	138	LEU	3.7
1	F	48	LEU	3.7
1	B	89	ASP	3.7
1	J	171	ASP	3.7
1	D	37	MET	3.6
1	F	20	ILE	3.6
1	J	54	TYR	3.6
1	L	137	TYR	3.6
1	K	132	PHE	3.6
1	A	166	ALA	3.6
1	F	79	ARG	3.6
1	A	78	GLY	3.6
1	C	8	VAL	3.6
1	I	116	GLU	3.6
1	F	46	VAL	3.6
1	J	153	THR	3.6
1	B	160	ALA	3.5
1	L	165	LEU	3.5
1	C	74	ASN	3.5
1	L	49	LYS	3.5
1	C	129	LEU	3.5
1	J	125	ASN	3.5
1	D	171	ASP	3.5
1	F	92	ASP	3.5
1	H	126	ASP	3.5
1	A	84	ASP	3.5
1	A	133	ILE	3.5
1	D	46	VAL	3.5
1	F	73	GLN	3.5
1	H	137	TYR	3.4
1	L	68	LYS	3.4
1	D	141	GLN	3.4
1	A	106	LEU	3.4
1	L	112	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	90	CYS	3.4
1	D	83	GLN	3.4
1	G	45	ASP	3.4
1	J	42	ASP	3.4
1	L	66	ALA	3.4
1	K	77	GLY	3.3
1	A	130	CYS	3.3
1	C	171	ASP	3.3
1	G	26	LEU	3.3
1	G	33	VAL	3.3
1	F	67	GLU	3.3
1	D	131	ASP	3.3
1	D	109	ASN	3.3
1	C	65	HIS	3.3
1	G	120	LEU	3.2
1	A	159	GLY	3.2
1	H	147	GLU	3.2
1	F	116	GLU	3.2
1	E	130	CYS	3.2
1	D	68	LYS	3.2
1	B	50	ASN	3.2
1	H	171	ASP	3.2
1	A	88	PRO	3.2
1	I	26	LEU	3.2
1	C	50	ASN	3.2
1	E	74	ASN	3.2
1	E	54	TYR	3.2
1	F	151	HIS	3.2
1	B	138	LEU	3.2
1	H	14	GLN	3.2
1	K	74	ASN	3.2
1	D	91	ASP	3.2
1	D	137	TYR	3.2
1	J	88	PRO	3.2
1	C	176	GLY	3.1
1	D	65	HIS	3.1
1	A	124	LYS	3.1
1	H	45	ASP	3.1
1	B	7	GLN	3.1
1	E	7	GLN	3.1
1	J	58	GLN	3.1
1	E	11	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	64	GLU	3.1
1	G	15	ASP	3.1
1	B	108	LYS	3.1
1	B	176	GLY	3.1
1	E	171	ASP	3.1
1	H	143	LYS	3.1
1	I	129	LEU	3.1
1	F	112	GLN	3.1
1	J	135	THR	3.1
1	F	8	VAL	3.1
1	G	27	GLU	3.1
1	A	150	ASP	3.1
1	D	123	ASP	3.1
1	J	8	VAL	3.0
1	A	168	TYR	3.0
1	E	167	GLU	3.0
1	I	48	LEU	3.0
1	E	149	GLY	3.0
1	F	173	HIS	3.0
1	C	68	LYS	3.0
1	F	22	ARG	3.0
1	F	35	LEU	3.0
1	F	169	LEU	3.0
1	F	24	ILE	3.0
1	A	158	MET	3.0
1	C	144	ALA	3.0
1	J	39	TYR	3.0
1	A	147	GLU	3.0
1	I	151	HIS	3.0
1	L	39	TYR	3.0
1	B	78	GLY	3.0
1	I	142	VAL	3.0
1	F	167	GLU	2.9
1	A	132	PHE	2.9
1	L	42	ASP	2.9
1	A	94	GLU	2.9
1	H	81	PHE	2.9
1	E	158	MET	2.9
1	B	8	VAL	2.9
1	B	68	LYS	2.9
1	I	171	ASP	2.9
1	K	173	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	136	HIS	2.9
1	D	132	PHE	2.9
1	A	157	LYS	2.9
1	B	124	LYS	2.9
1	K	153	THR	2.9
1	G	35	LEU	2.9
1	B	137	TYR	2.9
1	I	161	PRO	2.9
1	E	78	GLY	2.9
1	G	73	GLN	2.9
1	I	8	VAL	2.9
1	J	14	GLN	2.9
1	K	68	LYS	2.9
1	F	174	THR	2.9
1	C	21	ASN	2.9
1	A	91	ASP	2.8
1	G	94	GLU	2.9
1	L	123	ASP	2.8
1	J	164	GLY	2.8
1	E	153	THR	2.8
1	L	22	ARG	2.8
1	I	150	ASP	2.8
1	E	113	SER	2.8
1	C	173	HIS	2.8
1	I	130	CYS	2.8
1	J	26	LEU	2.8
1	A	149	GLY	2.8
1	E	50	ASN	2.8
1	G	83	GLN	2.8
1	J	102	CYS	2.8
1	I	28	LEU	2.8
1	K	54	TYR	2.8
1	A	17	GLU	2.8
1	B	16	SER	2.8
1	B	113	SER	2.8
1	D	61	GLU	2.8
1	D	75	GLN	2.8
1	E	159	GLY	2.8
1	F	153	THR	2.8
1	E	26	LEU	2.7
1	H	115	LEU	2.7
1	A	123	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	145	ILE	2.7
1	E	37	MET	2.7
1	E	124	LYS	2.7
1	G	124	LYS	2.7
1	G	101	GLU	2.7
1	H	173	HIS	2.7
1	E	36	SER	2.7
1	I	49	LYS	2.7
1	J	124	LYS	2.7
1	J	158	MET	2.7
1	B	83	GLN	2.7
1	F	15	ASP	2.7
1	I	33	VAL	2.7
1	E	32	TYR	2.7
1	H	96	GLY	2.7
1	K	75	GLN	2.7
1	F	18	ALA	2.7
1	C	61	GLU	2.7
1	I	13	HIS	2.7
1	E	18	ALA	2.7
1	J	96	GLY	2.7
1	B	33	VAL	2.7
1	E	83	GLN	2.7
1	E	84	ASP	2.7
1	B	61	GLU	2.7
1	D	140	GLU	2.7
1	K	102	CYS	2.7
1	B	55	PHE	2.7
1	A	16	SER	2.7
1	H	151	HIS	2.6
1	F	91	ASP	2.6
1	G	150	ASP	2.6
1	E	81	PHE	2.6
1	I	165	LEU	2.6
1	C	80	ILE	2.6
1	E	22	ARG	2.6
1	E	105	HIS	2.6
1	E	73	GLN	2.6
1	B	42	ASP	2.6
1	F	84	ASP	2.6
1	C	67	GLU	2.6
1	G	167	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	82	LEU	2.6
1	L	145	ILE	2.6
1	L	77	GLY	2.6
1	A	35	LEU	2.6
1	B	150	ASP	2.6
1	C	150	ASP	2.6
1	E	155	LEU	2.6
1	H	138	LEU	2.6
1	L	44	ASP	2.6
1	A	25	ASN	2.6
1	D	139	ASN	2.6
1	I	112	GLN	2.6
1	L	58	GLN	2.6
1	B	27	GLU	2.6
1	D	45	ASP	2.6
1	G	171	ASP	2.6
1	I	15	ASP	2.6
1	H	22	ARG	2.6
1	A	75	GLN	2.6
1	D	144	ALA	2.6
1	F	19	ALA	2.6
1	K	27	GLU	2.6
1	A	71	LYS	2.6
1	B	46	VAL	2.6
1	F	125	ASN	2.6
1	I	109	ASN	2.6
1	L	139	ASN	2.6
1	B	60	HIS	2.5
1	J	136	HIS	2.5
1	E	31	SER	2.5
1	F	119	LYS	2.5
1	H	79	ARG	2.5
1	I	46	VAL	2.5
1	A	15	ASP	2.5
1	L	35	LEU	2.5
1	C	55	PHE	2.5
1	L	164	GLY	2.5
1	C	54	TYR	2.5
1	F	168	TYR	2.5
1	F	142	VAL	2.5
1	H	67	GLU	2.5
1	A	72	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	114	LEU	2.5
1	D	158	MET	2.5
1	K	44	ASP	2.5
1	L	18	ALA	2.5
1	G	119	LYS	2.5
1	A	167	GLU	2.5
1	I	101	GLU	2.5
1	B	21	ASN	2.5
1	E	89	ASP	2.5
1	J	131	ASP	2.5
1	E	161	PRO	2.5
1	E	69	LEU	2.5
1	L	60	HIS	2.5
1	B	17	GLU	2.5
1	L	37	MET	2.5
1	B	74	ASN	2.5
1	E	109	ASN	2.5
1	E	88	PRO	2.5
1	D	5	THR	2.5
1	F	65	HIS	2.5
1	E	23	GLN	2.5
1	H	120	LEU	2.5
1	L	102	CYS	2.5
1	G	64	GLU	2.4
1	L	134	GLU	2.4
1	A	73	GLN	2.4
1	D	30	ALA	2.4
1	I	127	PRO	2.4
1	J	5	THR	2.4
1	E	62	GLU	2.4
1	J	7	GLN	2.4
1	F	164	GLY	2.4
1	A	131	ASP	2.4
1	J	90	CYS	2.4
1	J	20	ILE	2.4
1	C	35	LEU	2.4
1	E	35	LEU	2.4
1	H	10	GLN	2.4
1	I	63	ARG	2.4
1	A	37	MET	2.4
1	D	157	LYS	2.4
1	K	143	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	80	ILE	2.4
1	B	165	LEU	2.4
1	G	72	LEU	2.4
1	D	94	GLU	2.4
1	L	118	HIS	2.4
1	B	70	MET	2.4
1	F	75	GLN	2.4
1	G	52	ALA	2.4
1	G	37	MET	2.4
1	D	176	GLY	2.4
1	H	159	GLY	2.4
1	I	113	SER	2.4
1	G	123	ASP	2.4
1	B	79	ARG	2.4
1	A	173	HIS	2.4
1	G	102	CYS	2.4
1	E	127	PRO	2.4
1	G	143	LYS	2.4
1	B	31	SER	2.4
1	C	133	ILE	2.4
1	E	97	LEU	2.4
1	J	80	ILE	2.4
1	G	131	ASP	2.4
1	I	22	ARG	2.4
1	G	66	ALA	2.4
1	I	19	ALA	2.4
1	E	141	GLN	2.3
1	J	173	HIS	2.3
1	L	151	HIS	2.3
1	D	21	ASN	2.3
1	D	93	TRP	2.3
1	J	176	GLY	2.3
1	L	120	LEU	2.3
1	L	169	LEU	2.3
1	E	8	VAL	2.3
1	C	63	ARG	2.3
1	L	171	ASP	2.3
1	B	167	GLU	2.3
1	E	75	GLN	2.3
1	B	133	ILE	2.3
1	H	118	HIS	2.3
1	I	59	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	169	LEU	2.3
1	C	157	LYS	2.3
1	F	49	LYS	2.3
1	J	157	LYS	2.3
1	J	18	ALA	2.3
1	A	45	ASP	2.3
1	D	15	ASP	2.3
1	F	62	GLU	2.3
1	G	91	ASP	2.3
1	K	61	GLU	2.3
1	E	65	HIS	2.3
1	E	164	GLY	2.3
1	H	113	SER	2.3
1	H	127	PRO	2.3
1	K	136	HIS	2.3
1	J	43	ARG	2.3
1	D	170	PHE	2.3
1	F	120	LEU	2.3
1	H	132	PHE	2.3
1	L	26	LEU	2.3
1	J	123	ASP	2.3
1	G	38	SER	2.3
1	G	46	VAL	2.3
1	H	50	ASN	2.3
1	H	139	ASN	2.3
1	H	153	THR	2.3
1	L	98	ASN	2.3
1	G	82	LEU	2.3
1	J	81	PHE	2.3
1	F	17	GLU	2.3
1	F	37	MET	2.3
1	J	100	MET	2.3
1	K	5	THR	2.3
1	K	65	HIS	2.3
1	E	129	LEU	2.3
1	K	72	LEU	2.3
1	D	160	ALA	2.3
1	D	130	CYS	2.3
1	J	27	GLU	2.3
1	L	163	SER	2.3
1	A	33	VAL	2.3
1	B	88	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	123	ASP	2.3
1	I	123	ASP	2.3
1	B	109	ASN	2.2
1	F	109	ASN	2.2
1	C	148	LEU	2.2
1	F	82	LEU	2.2
1	J	165	LEU	2.2
1	C	132	PHE	2.2
1	E	85	ILE	2.2
1	K	30	ALA	2.2
1	C	62	GLU	2.2
1	D	90	CYS	2.2
1	I	176	GLY	2.2
1	C	42	ASP	2.2
1	F	171	ASP	2.2
1	H	123	ASP	2.2
1	J	50	ASN	2.2
1	J	30	ALA	2.2
1	J	68	LYS	2.2
1	I	134	GLU	2.2
1	E	165	LEU	2.2
1	J	120	LEU	2.2
1	D	153	THR	2.2
1	B	15	ASP	2.2
1	A	99	ALA	2.2
1	G	71	LYS	2.2
1	L	157	LYS	2.2
1	E	28	LEU	2.2
1	L	161	PRO	2.2
1	B	92	ASP	2.2
1	D	124	LYS	2.2
1	G	42	ASP	2.2
1	I	42	ASP	2.2
1	K	150	ASP	2.2
1	E	166	ALA	2.2
1	K	121	ALA	2.2
1	A	6	SER	2.2
1	E	14	GLN	2.2
1	H	155	LEU	2.2
1	I	29	TYR	2.2
1	A	8	VAL	2.2
1	E	67	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	64	GLU	2.2
1	F	147	GLU	2.2
1	G	147	GLU	2.2
1	J	61	GLU	2.2
1	J	51	PHE	2.2
1	L	11	ASN	2.2
1	A	105	HIS	2.2
1	C	131	ASP	2.2
1	H	13	HIS	2.2
1	I	136	HIS	2.2
1	F	106	LEU	2.2
1	F	165	LEU	2.2
1	E	110	VAL	2.2
1	L	176	GLY	2.2
1	F	172	LYS	2.2
1	L	124	LYS	2.2
1	E	19	ALA	2.1
1	I	144	ALA	2.1
1	L	52	ALA	2.1
1	C	60	HIS	2.1
1	E	45	ASP	2.1
1	G	90	CYS	2.1
1	J	91	ASP	2.1
1	A	137	TYR	2.1
1	G	145	ILE	2.1
1	I	96	GLY	2.1
1	K	49	LYS	2.1
1	H	97	LEU	2.1
1	A	125	ASN	2.1
1	B	36	SER	2.1
1	D	36	SER	2.1
1	L	31	SER	2.1
1	G	157	LYS	2.1
1	C	147	GLU	2.1
1	D	167	GLU	2.1
1	E	107	GLU	2.1
1	J	64	GLU	2.1
1	K	167	GLU	2.1
1	G	135	THR	2.1
1	I	174	THR	2.1
1	C	56	LEU	2.1
1	C	109	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	125	ASN	2.1
1	G	21	ASN	2.1
1	K	139	ASN	2.1
1	B	23	GLN	2.1
1	A	92	ASP	2.1
1	B	84	ASP	2.1
1	D	173	HIS	2.1
1	E	118	HIS	2.1
1	K	46	VAL	2.1
1	E	96	GLY	2.1
1	F	77	GLY	2.1
1	H	176	GLY	2.1
1	A	27	GLU	2.1
1	C	82	LEU	2.1
1	H	174	THR	2.1
1	B	30	ALA	2.1
1	C	20	ILE	2.1
1	I	98	ASN	2.1
1	J	86	GLN	2.1
1	B	118	HIS	2.1
1	A	89	ASP	2.1
1	A	97	LEU	2.1
1	F	159	GLY	2.1
1	G	40	TYR	2.1
1	L	28	LEU	2.1
1	F	100	MET	2.1
1	F	127	PRO	2.1
1	I	64	GLU	2.1
1	L	94	GLU	2.1
1	E	103	ALA	2.1
1	F	80	ILE	2.1
1	I	145	ILE	2.1
1	F	58	GLN	2.1
1	F	148	LEU	2.1
1	K	96	GLY	2.1
1	I	62	GLU	2.1
1	K	62	GLU	2.1
1	K	107	GLU	2.1
1	A	79	ARG	2.1
1	E	66	ALA	2.1
1	G	18	ALA	2.1
1	G	112	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	170	PHE	2.1
1	H	109	ASN	2.1
1	B	37	MET	2.1
1	C	70	MET	2.1
1	A	54	TYR	2.0
1	C	128	HIS	2.0
1	G	77	GLY	2.0
1	H	105	HIS	2.0
1	L	168	TYR	2.0
1	A	5	THR	2.0
1	D	92	ASP	2.0
1	A	146	LYS	2.0
1	B	87	LYS	2.0
1	E	24	ILE	2.0
1	F	27	GLU	2.0
1	G	22	ARG	2.0
1	G	79	ARG	2.0
1	A	31	SER	2.0
1	I	166	ALA	2.0
1	C	7	GLN	2.0
1	D	56	LEU	2.0
1	E	115	LEU	2.0
1	D	39	TYR	2.0
1	B	140	GLU	2.0
1	C	17	GLU	2.0
1	I	93	TRP	2.0
1	I	36	SER	2.0
1	E	86	GLN	2.0
1	F	83	GLN	2.0
1	C	71	LYS	2.0
1	D	71	LYS	2.0
1	H	77	GLY	2.0
1	I	24	ILE	2.0
1	G	136	HIS	2.0
1	H	128	HIS	2.0
1	K	151	HIS	2.0
1	E	162	GLU	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.