



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:18 AM EDT

PDB ID : 4HFO / pdb_00004hfo
Title : Biogenic amine-binding protein selenomethionine derivative
Authors : Andersen, J.F.; Xu, X.; Chang, B.; Mans, B.J.; Ribeiro, J.M.
Deposited on : 2012-10-05
Resolution : 3.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

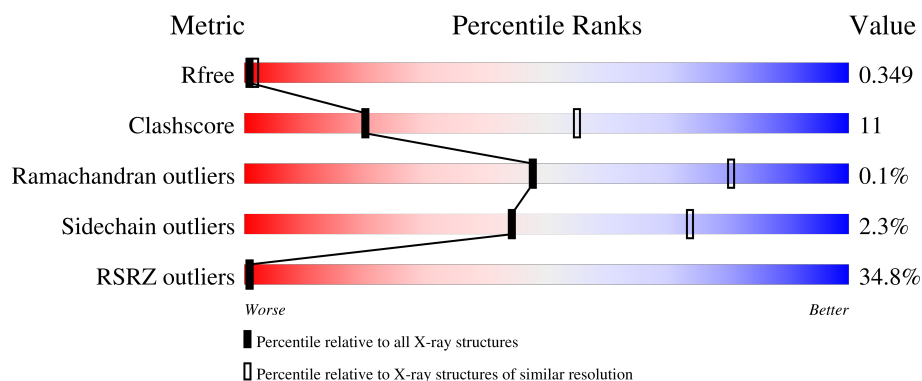
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	195	22% 75% 24% .
1	B	195	24% 72% 28% .
1	C	195	38% 74% 25% ..
1	D	195	25% 81% 18% ..
1	I	195	36% 77% 22% .

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Mol	Chain	Length	Quality of chain
1	J	195	31%70%30%.
1	K	195	40%73%25%..
1	L	195	58%79%19%..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12360 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 Biogenic amine-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1552	980	253	313	4	2			
1	B	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			
1	C	193	Total	C	N	O	S	Se	0	0	0
			1542	975	251	310	4	2			
1	D	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			
1	I	195	Total	C	N	O	S	Se	0	0	0
			1552	980	253	313	4	2			
1	J	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			
1	K	193	Total	C	N	O	S	Se	0	0	0
			1542	975	251	310	4	2			
1	L	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MSE	ILE	conflict	UNP Q86PT9
A	134	MSE	LEU	conflict	UNP Q86PT9
B	25	MSE	ILE	conflict	UNP Q86PT9
B	134	MSE	LEU	conflict	UNP Q86PT9
C	25	MSE	ILE	conflict	UNP Q86PT9
C	134	MSE	LEU	conflict	UNP Q86PT9
D	25	MSE	ILE	conflict	UNP Q86PT9
D	134	MSE	LEU	conflict	UNP Q86PT9
I	25	MSE	ILE	conflict	UNP Q86PT9
I	134	MSE	LEU	conflict	UNP Q86PT9
J	25	MSE	ILE	conflict	UNP Q86PT9
J	134	MSE	LEU	conflict	UNP Q86PT9
K	25	MSE	ILE	conflict	UNP Q86PT9

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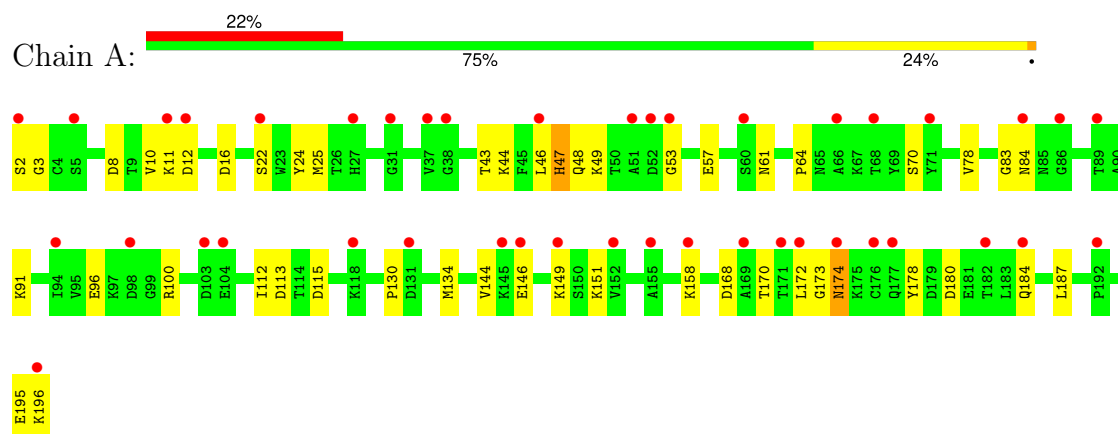
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Chain	Residue	Modelled	Actual	Comment	Reference
K	134	MSE	LEU	conflict	UNP Q86PT9
L	25	MSE	ILE	conflict	UNP Q86PT9
L	134	MSE	LEU	conflict	UNP Q86PT9

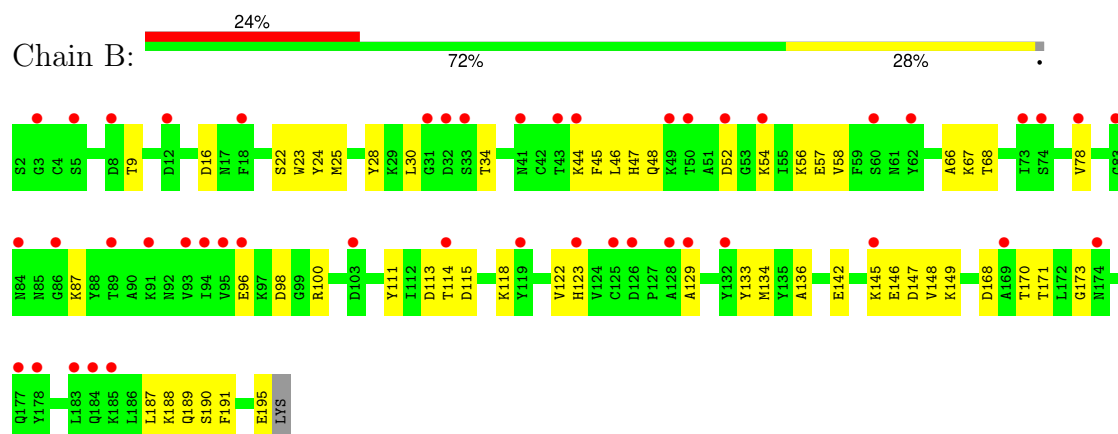
3 Residue-property plots [i](#)

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.

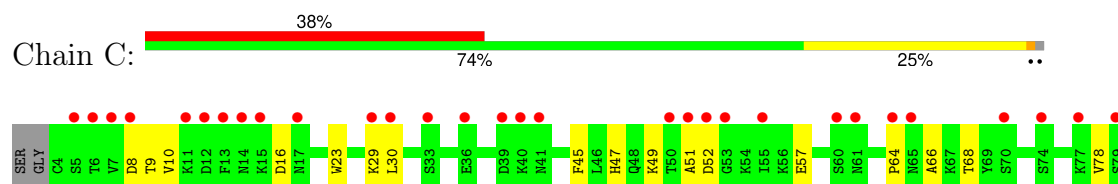
• Molecule 1: Biogenic amine-binding protein

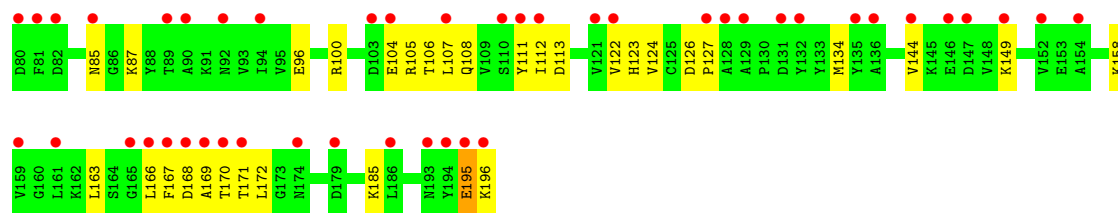


• Molecule 1: Biogenic amine-binding protein

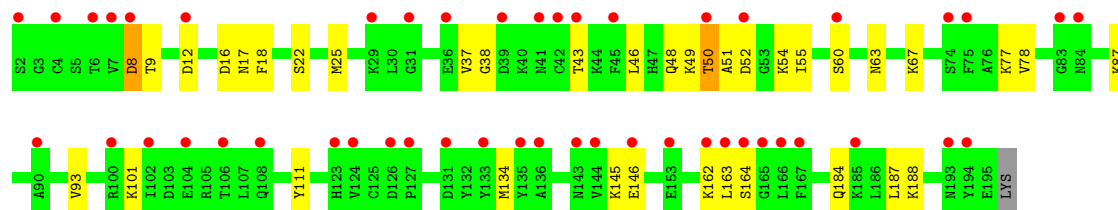
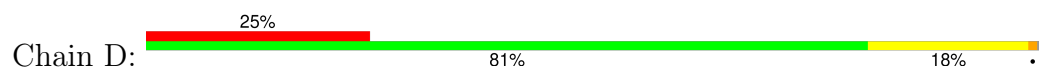


• Molecule 1: Biogenic amine-binding protein

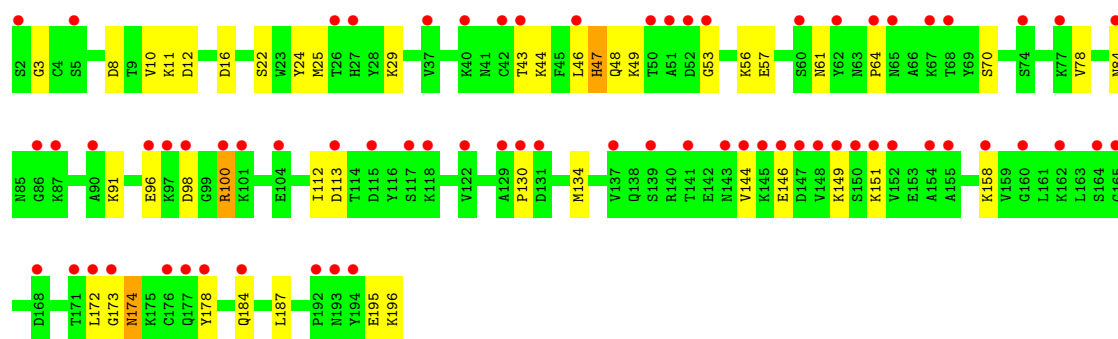
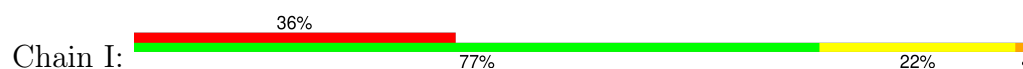




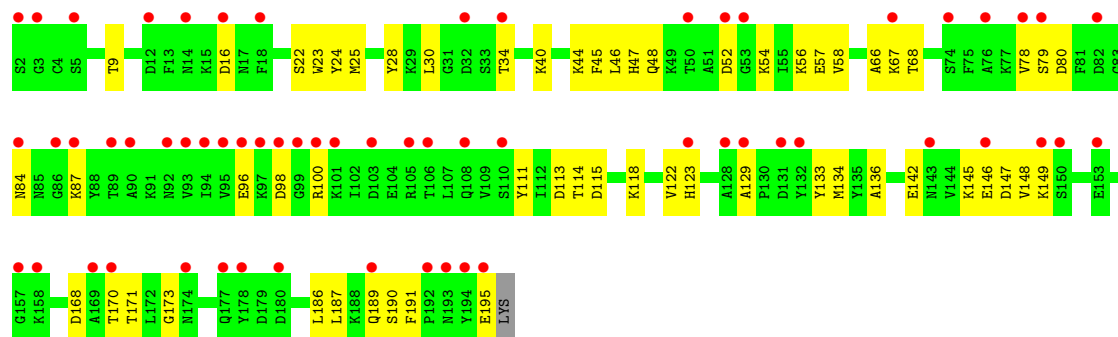
• Molecule 1: Biogenic amine-binding protein



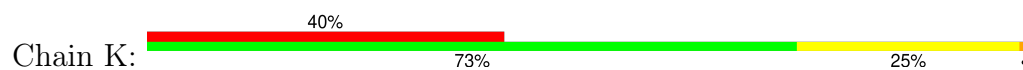
• Molecule 1: Biogenic amine-binding protein

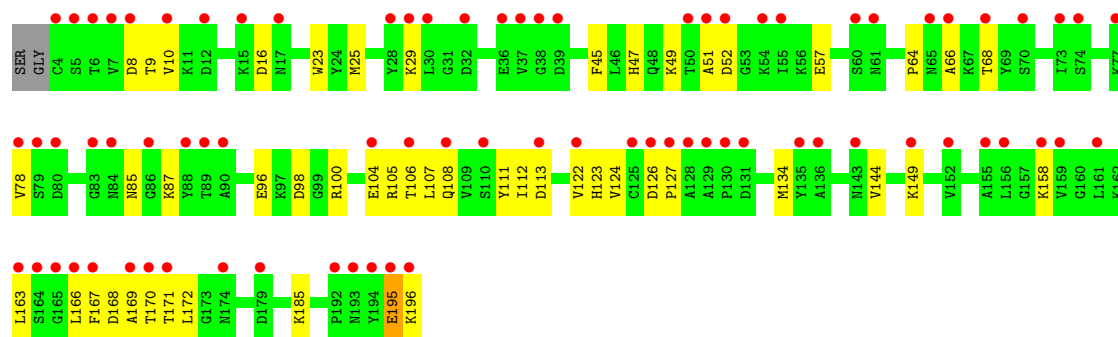


• Molecule 1: Biogenic amine-binding protein

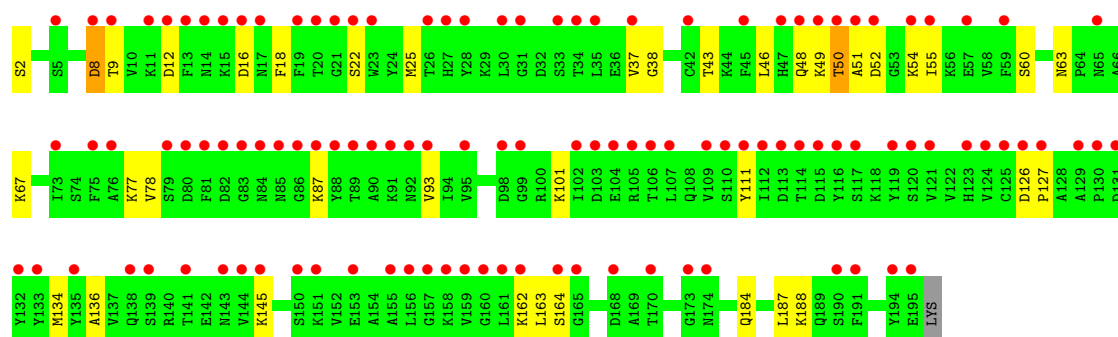
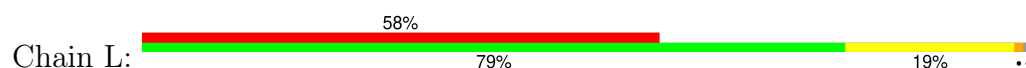


• Molecule 1: Biogenic amine-binding protein





● Molecule 1: Biogenic amine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.16Å 70.66Å 108.41Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	42.66 – 3.00 42.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.66-3.00) 99.5 (42.66-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.321 , 0.349 0.323 , 0.349	Depositor DCC
R_{free} test set	1541 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.1	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	0.84	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å ²)	83.0	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 66.02 % 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 6.4577e-06. 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

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	0.38	0/1581	0.71	0/2129
1	B	0.33	0/1572	0.75	2/2118 (0.1%)
1	C	0.36	0/1571	0.74	1/2116 (0.0%)
1	D	0.41	0/1572	0.76	0/2118
1	I	0.38	0/1581	0.71	0/2129
1	J	0.33	0/1572	0.76	2/2118 (0.1%)
1	K	0.35	0/1571	0.74	1/2116 (0.0%)
1	L	0.40	0/1572	0.76	0/2118
All	All	0.37	0/12592	0.74	6/16962 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	CA-C-N	6.01	125.63	119.56
1	B	129	ALA	C-N-CA	6.01	125.63	119.56
1	J	129	ALA	CA-C-N	5.98	125.60	119.56
1	J	129	ALA	C-N-CA	5.98	125.60	119.56
1	K	195	GLU	N-CA-C	-5.03	103.08	110.52
1	C	195	GLU	N-CA-C	-5.00	103.12	110.52

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	1552	0	1497	49	6
1	B	1543	0	1484	39	10
1	C	1542	0	1489	42	1
1	D	1543	0	1484	32	0
1	I	1552	0	1497	37	8
1	J	1543	0	1484	47	2
1	K	1542	0	1489	36	6
1	L	1543	0	1484	30	1
All	All	12360	0	11908	277	19

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 11.

All (277) 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:A:11:LYS:NZ	1:J:80:ASP:HA	1.59	1.17
1:C:112:ILE:HG23	1:C:158:LYS:HE3	1.23	1.16
1:L:25:MSE:HE1	1:L:134:MSE:SE	2.00	1.11
1:K:112:ILE:HG23	1:K:158:LYS:HE3	1.23	1.11
1:A:11:LYS:NZ	1:J:80:ASP:OD1	1.88	1.06
1:C:168:ASP:O	1:C:171:THR:HG22	1.63	0.99
1:K:168:ASP:O	1:K:171:THR:HG22	1.63	0.98
1:A:83:GLY:HA2	1:I:98:ASP:OD2	1.64	0.96
1:A:11:LYS:HZ1	1:J:80:ASP:CA	1.80	0.95
1:A:11:LYS:HZ1	1:J:80:ASP:HA	1.26	0.95
1:A:11:LYS:CE	1:J:80:ASP:HA	1.97	0.94
1:A:11:LYS:HZ3	1:J:80:ASP:CG	1.77	0.92
1:D:162:LYS:HZ2	1:D:164:SER:H	1.09	0.92
1:L:162:LYS:HZ2	1:L:164:SER:H	1.19	0.89
1:K:112:ILE:CG2	1:K:158:LYS:HE3	2.06	0.86
1:A:25:MSE:HE1	1:A:134:MSE:SE	2.25	0.85
1:A:11:LYS:NZ	1:J:80:ASP:CA	2.35	0.85
1:B:25:MSE:HE1	1:B:134:MSE:SE	2.26	0.85
1:K:112:ILE:HG23	1:K:158:LYS:CE	2.07	0.84
1:C:112:ILE:HG23	1:C:158:LYS:CE	2.08	0.84
1:J:25:MSE:HE1	1:J:134:MSE:SE	2.28	0.83
1:C:112:ILE:CG2	1:C:158:LYS:HE3	2.06	0.83
1:I:25:MSE:HE1	1:I:134:MSE:SE	2.32	0.78
1:A:11:LYS:HE2	1:J:80:ASP:HA	1.66	0.77
1:L:16:ASP:OD1	1:L:49:LYS:HE2	1.83	0.77
1:D:16:ASP:OD1	1:D:49:LYS:HE2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:TYR:CE1	1:B:44:LYS:HD2	2.20	0.76
1:J:24:TYR:CE1	1:J:44:LYS:HD2	2.20	0.75
1:J:9:THR:HG21	1:J:87:LYS:HB2	1.69	0.73
1:D:25:MSE:HE1	1:D:134:MSE:SE	2.38	0.73
1:L:50:THR:HG21	1:L:52:ASP:CG	2.13	0.73
1:D:50:THR:HG21	1:D:52:ASP:CG	2.13	0.73
1:D:50:THR:CG2	1:D:52:ASP:CG	2.63	0.71
1:B:9:THR:HG21	1:B:87:LYS:HB2	1.69	0.71
1:L:50:THR:HG21	1:L:52:ASP:OD2	1.91	0.71
1:A:11:LYS:NZ	1:J:80:ASP:CB	2.54	0.71
1:I:22:SER:HB3	1:I:46:LEU:HD23	1.73	0.70
1:L:50:THR:CG2	1:L:52:ASP:CG	2.64	0.70
1:A:83:GLY:CA	1:I:98:ASP:OD2	2.37	0.70
1:D:50:THR:HG21	1:D:52:ASP:OD2	1.91	0.70
1:A:22:SER:HB3	1:A:46:LEU:HD23	1.73	0.69
1:L:52:ASP:OD1	1:L:54:LYS:HG3	1.93	0.69
1:J:66:ALA:O	1:J:68:THR:HG23	1.92	0.69
1:K:29:LYS:HB2	1:K:166:LEU:CD2	2.22	0.69
1:D:52:ASP:OD1	1:D:54:LYS:HG3	1.92	0.69
1:B:34:THR:HG21	1:C:185:LYS:NZ	2.08	0.69
1:B:66:ALA:O	1:B:68:THR:HG23	1.92	0.69
1:C:29:LYS:HB2	1:C:166:LEU:CD2	2.22	0.69
1:I:8:ASP:H	1:I:158:LYS:HZ1	1.41	0.68
1:A:11:LYS:HZ1	1:J:80:ASP:CB	2.08	0.67
1:A:11:LYS:HE3	1:A:12:ASP:OD2	1.96	0.66
1:B:25:MSE:HE2	1:B:136:ALA:CB	2.25	0.66
1:C:51:ALA:HB2	1:I:184:GLN:HG2	1.78	0.66
1:B:34:THR:HG21	1:C:185:LYS:HZ3	1.60	0.65
1:D:162:LYS:HD2	1:D:163:LEU:N	2.12	0.65
1:I:11:LYS:HE3	1:I:12:ASP:OD2	1.96	0.65
1:L:162:LYS:HD2	1:L:163:LEU:N	2.12	0.64
1:B:147:ASP:OD1	1:B:148:VAL:HG13	1.97	0.64
1:C:52:ASP:OD2	1:I:44:LYS:NZ	2.30	0.64
1:J:147:ASP:OD1	1:J:148:VAL:HG13	1.97	0.64
1:J:145:LYS:O	1:J:148:VAL:HG22	1.98	0.63
1:K:105:ARG:HG3	1:K:107:LEU:CD1	2.29	0.63
1:D:162:LYS:HZ2	1:D:164:SER:N	1.89	0.63
1:L:162:LYS:NZ	1:L:164:SER:H	1.95	0.63
1:B:145:LYS:O	1:B:148:VAL:HG22	1.98	0.63
1:J:191:PHE:O	1:J:195:GLU:HG2	1.98	0.63
1:C:105:ARG:HG3	1:C:107:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ASP:OD1	1:L:8:ASP:N	2.24	0.62
1:B:191:PHE:O	1:B:195:GLU:HG2	1.99	0.62
1:A:195:GLU:O	1:A:196:LYS:HB2	2.00	0.62
1:A:8:ASP:H	1:A:158:LYS:HZ1	1.48	0.62
1:C:106:THR:O	1:C:127:PRO:HD2	2.01	0.61
1:K:106:THR:O	1:K:127:PRO:HD2	2.01	0.61
1:A:83:GLY:C	1:I:100:ARG:CZ	2.73	0.61
1:I:195:GLU:O	1:I:196:LYS:HB2	2.00	0.61
1:K:111:TYR:CE2	1:K:122:VAL:HB	2.36	0.60
1:C:111:TYR:CE2	1:C:122:VAL:HB	2.35	0.60
1:J:54:LYS:HE2	1:J:195:GLU:HA	1.84	0.60
1:B:142:GLU:O	1:B:170:THR:HG21	2.02	0.60
1:I:8:ASP:O	1:I:158:LYS:HE2	2.02	0.59
1:J:142:GLU:O	1:J:170:THR:HG21	2.02	0.59
1:A:8:ASP:O	1:A:158:LYS:HE2	2.02	0.59
1:A:83:GLY:O	1:I:100:ARG:CZ	2.50	0.59
1:B:54:LYS:HE2	1:B:195:GLU:HA	1.84	0.59
1:A:174:ASN:OD1	1:A:174:ASN:N	2.36	0.59
1:J:25:MSE:CE	1:J:134:MSE:SE	3.01	0.58
1:J:25:MSE:HE2	1:J:136:ALA:CB	2.34	0.58
1:A:115:ASP:HB2	1:J:84:ASN:ND2	2.18	0.58
1:K:25:MSE:HE1	1:K:134:MSE:SE	2.52	0.58
1:L:162:LYS:HZ2	1:L:164:SER:N	1.97	0.58
1:I:174:ASN:OD1	1:I:174:ASN:N	2.36	0.58
1:C:29:LYS:HB2	1:C:166:LEU:HD22	1.86	0.57
1:I:3:GLY:HA2	1:I:130:PRO:CB	2.34	0.57
1:L:22:SER:HB3	1:L:46:LEU:HD23	1.86	0.57
1:A:11:LYS:HE2	1:J:79:SER:O	2.05	0.57
1:A:47:HIS:HB3	1:A:57:GLU:HA	1.86	0.57
1:B:25:MSE:CE	1:B:134:MSE:SE	3.01	0.57
1:D:8:ASP:OD1	1:D:8:ASP:N	2.24	0.57
1:A:195:GLU:O	1:A:196:LYS:CB	2.53	0.57
1:I:47:HIS:HB3	1:I:57:GLU:HA	1.86	0.57
1:D:50:THR:HG23	1:D:52:ASP:H	1.70	0.57
1:I:10:VAL:HG22	1:I:113:ASP:HA	1.87	0.57
1:L:162:LYS:HD2	1:L:163:LEU:H	1.68	0.57
1:A:10:VAL:HG22	1:A:113:ASP:HA	1.87	0.56
1:D:22:SER:HB3	1:D:46:LEU:HD23	1.86	0.56
1:K:29:LYS:HB2	1:K:166:LEU:HD22	1.86	0.56
1:C:8:ASP:HB2	1:C:158:LYS:NZ	2.20	0.56
1:K:8:ASP:HB2	1:K:158:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLY:HA2	1:A:130:PRO:CB	2.34	0.56
1:I:195:GLU:O	1:I:196:LYS:CB	2.53	0.56
1:J:40:LYS:NZ	1:K:98:ASP:OD2	2.32	0.56
1:D:162:LYS:HD2	1:D:163:LEU:H	1.69	0.56
1:L:25:MSE:CE	1:L:134:MSE:SE	2.92	0.56
1:C:9:THR:HG21	1:C:87:LYS:HB2	1.89	0.55
1:K:9:THR:HG21	1:K:87:LYS:HB2	1.89	0.55
1:L:50:THR:HG23	1:L:52:ASP:H	1.70	0.54
1:B:98:ASP:OD2	1:B:100:ARG:NH2	2.32	0.54
1:A:12:ASP:HA	1:A:84:ASN:ND2	2.23	0.53
1:K:104:GLU:HG2	1:K:105:ARG:N	2.23	0.53
1:I:12:ASP:HA	1:I:84:ASN:ND2	2.23	0.53
1:J:146:GLU:HA	1:J:149:LYS:HG3	1.90	0.53
1:C:104:GLU:HG2	1:C:105:ARG:N	2.23	0.53
1:B:96:GLU:HB2	1:B:98:ASP:OD1	2.08	0.53
1:J:115:ASP:OD2	1:J:118:LYS:HB2	2.09	0.53
1:B:146:GLU:HA	1:B:149:LYS:HG3	1.90	0.53
1:K:158:LYS:O	1:K:158:LYS:HG3	2.09	0.53
1:C:158:LYS:O	1:C:158:LYS:HG3	2.09	0.53
1:K:64:PRO:HG2	1:K:172:LEU:HD13	1.92	0.52
1:B:115:ASP:OD2	1:B:118:LYS:HB2	2.09	0.52
1:J:96:GLU:HB2	1:J:98:ASP:OD1	2.09	0.52
1:A:2:SER:CB	1:D:17:ASN:OD1	2.58	0.52
1:I:48:GLN:HG2	1:I:187:LEU:HD11	1.92	0.52
1:C:64:PRO:HG2	1:C:172:LEU:HD13	1.92	0.52
1:C:104:GLU:CG	1:C:105:ARG:N	2.73	0.52
1:K:104:GLU:CG	1:K:105:ARG:N	2.73	0.51
1:A:48:GLN:HG2	1:A:187:LEU:HD11	1.92	0.51
1:K:167:PHE:CE2	1:K:169:ALA:HA	2.46	0.51
1:J:98:ASP:OD2	1:J:100:ARG:NH2	2.32	0.51
1:I:146:GLU:HA	1:I:149:LYS:HG3	1.92	0.51
1:D:48:GLN:HG2	1:D:187:LEU:HD11	1.93	0.51
1:C:167:PHE:CE2	1:C:169:ALA:HA	2.46	0.51
1:J:48:GLN:HG2	1:J:187:LEU:HD11	1.94	0.50
1:A:146:GLU:HA	1:A:149:LYS:HG3	1.92	0.50
1:B:48:GLN:HG2	1:B:187:LEU:HD11	1.94	0.50
1:D:63:ASN:O	1:D:67:LYS:N	2.44	0.50
1:B:47:HIS:HB3	1:B:57:GLU:HA	1.93	0.50
1:I:25:MSE:HE1	1:I:134:MSE:CE	2.41	0.50
1:A:11:LYS:NZ	1:J:80:ASP:CG	2.50	0.50
1:L:9:THR:HG21	1:L:87:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:THR:CG2	1:L:52:ASP:OD1	2.60	0.50
1:D:50:THR:CG2	1:D:52:ASP:OD1	2.60	0.50
1:J:47:HIS:HB3	1:J:57:GLU:HA	1.93	0.50
1:L:48:GLN:HG2	1:L:187:LEU:HD11	1.93	0.49
1:D:9:THR:HG21	1:D:87:LYS:HB2	1.93	0.49
1:K:9:THR:OG1	1:K:85:ASN:HB3	2.12	0.49
1:C:23:TRP:HB2	1:C:45:PHE:CZ	2.47	0.49
1:K:23:TRP:HB2	1:K:45:PHE:CZ	2.47	0.49
1:B:52:ASP:OD2	1:B:54:LYS:HB2	2.13	0.49
1:B:111:TYR:CE2	1:B:122:VAL:HB	2.47	0.49
1:J:52:ASP:OD2	1:J:54:LYS:HB2	2.13	0.49
1:B:190:SER:HA	1:B:195:GLU:OE2	2.12	0.49
1:J:111:TYR:CE2	1:J:122:VAL:HB	2.47	0.48
1:A:53:GLY:O	1:A:78:VAL:HG23	2.13	0.48
1:J:25:MSE:SE	1:J:28:TYR:CD2	3.16	0.48
1:D:25:MSE:CE	1:D:134:MSE:SE	3.11	0.48
1:L:63:ASN:O	1:L:67:LYS:N	2.44	0.48
1:J:190:SER:HA	1:J:195:GLU:OE2	2.12	0.48
1:I:53:GLY:O	1:I:78:VAL:HG23	2.14	0.48
1:C:9:THR:OG1	1:C:85:ASN:HB3	2.12	0.48
1:I:25:MSE:SE	1:I:43:THR:HG21	2.63	0.48
1:K:167:PHE:CZ	1:K:169:ALA:HA	2.50	0.47
1:B:34:THR:HG21	1:C:185:LYS:HD3	1.97	0.47
1:I:24:TYR:CE2	1:I:44:LYS:HD2	2.49	0.47
1:B:133:TYR:CZ	1:D:146:GLU:HB2	2.50	0.47
1:A:24:TYR:CE2	1:A:44:LYS:HD2	2.50	0.47
1:C:144:VAL:O	1:C:149:LYS:HE3	2.15	0.46
1:I:112:ILE:HG23	1:I:158:LYS:HD3	1.98	0.46
1:C:167:PHE:CZ	1:C:169:ALA:HA	2.50	0.46
1:K:144:VAL:O	1:K:149:LYS:HE3	2.15	0.46
1:C:16:ASP:OD1	1:C:49:LYS:HE2	2.16	0.46
1:C:66:ALA:O	1:C:68:THR:HG23	2.16	0.46
1:K:16:ASP:OD1	1:K:49:LYS:HE2	2.16	0.46
1:A:112:ILE:HG23	1:A:158:LYS:HD3	1.98	0.46
1:C:195:GLU:O	1:C:196:LYS:HB2	2.16	0.46
1:A:8:ASP:H	1:A:158:LYS:NZ	2.11	0.46
1:K:195:GLU:O	1:K:196:LYS:HB2	2.16	0.46
1:B:23:TRP:HB2	1:B:45:PHE:CZ	2.50	0.46
1:C:30:LEU:HD13	1:C:134:MSE:HE3	1.96	0.46
1:J:171:THR:C	1:J:173:GLY:H	2.24	0.46
1:B:171:THR:C	1:B:173:GLY:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:CG2	1:C:113:ASP:HA	2.46	0.45
1:I:8:ASP:H	1:I:158:LYS:NZ	2.11	0.45
1:K:10:VAL:CG2	1:K:113:ASP:HA	2.46	0.45
1:K:66:ALA:O	1:K:68:THR:HG23	2.16	0.45
1:I:16:ASP:OD1	1:I:49:LYS:CE	2.64	0.45
1:K:8:ASP:HB2	1:K:158:LYS:HZ1	1.81	0.45
1:L:184:GLN:O	1:L:188:LYS:HG2	2.17	0.45
1:B:25:MSE:HE2	1:B:136:ALA:HB2	1.98	0.45
1:J:23:TRP:HB2	1:J:45:PHE:CZ	2.50	0.45
1:D:184:GLN:O	1:D:188:LYS:HG2	2.17	0.45
1:A:16:ASP:OD1	1:A:49:LYS:CE	2.64	0.45
1:J:168:ASP:O	1:J:171:THR:HG22	2.16	0.45
1:A:2:SER:HB2	1:D:17:ASN:OD1	2.17	0.45
1:B:168:ASP:O	1:B:171:THR:HG22	2.16	0.45
1:B:25:MSE:SE	1:B:28:TYR:CD2	3.20	0.44
1:J:30:LEU:HD12	1:J:133:TYR:O	2.17	0.44
1:J:34:THR:HG21	1:K:185:LYS:HD3	1.99	0.44
1:C:122:VAL:HG22	1:C:123:HIS:N	2.32	0.44
1:K:108:GLN:CG	1:K:127:PRO:HG3	2.47	0.44
1:K:122:VAL:HG22	1:K:123:HIS:N	2.32	0.44
1:B:30:LEU:HD12	1:B:133:TYR:O	2.17	0.44
1:J:56:LYS:NZ	1:J:189:GLN:O	2.51	0.44
1:C:108:GLN:CG	1:C:127:PRO:HG3	2.48	0.44
1:B:56:LYS:NZ	1:B:189:GLN:O	2.51	0.44
1:L:37:VAL:HG13	1:L:38:GLY:N	2.33	0.44
1:L:145:LYS:HE2	1:L:145:LYS:HB3	1.79	0.44
1:J:113:ASP:O	1:J:114:THR:HB	2.18	0.43
1:A:11:LYS:HZ3	1:J:80:ASP:CB	2.24	0.43
1:B:113:ASP:O	1:B:114:THR:HB	2.18	0.43
1:A:61:ASN:HB2	1:A:70:SER:OG	2.19	0.43
1:B:34:THR:HG21	1:C:185:LYS:CE	2.48	0.43
1:A:2:SER:HB3	1:D:17:ASN:OD1	2.18	0.43
1:L:25:MSE:HE3	1:L:136:ALA:CB	2.49	0.43
1:A:151:LYS:HE3	1:A:151:LYS:HB2	1.87	0.43
1:I:61:ASN:HB2	1:I:70:SER:OG	2.19	0.43
1:B:22:SER:HB3	1:B:46:LEU:CD2	2.49	0.43
1:C:96:GLU:OE2	1:C:100:ARG:NH2	2.47	0.43
1:D:37:VAL:HG13	1:D:38:GLY:N	2.33	0.43
1:B:133:TYR:CE1	1:D:146:GLU:HB2	2.54	0.43
1:J:22:SER:HB3	1:J:46:LEU:CD2	2.49	0.43
1:I:151:LYS:HE3	1:I:151:LYS:HB2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:CG2	1:A:113:ASP:HA	2.49	0.42
1:I:10:VAL:CG2	1:I:113:ASP:HA	2.49	0.42
1:I:64:PRO:HG2	1:I:172:LEU:HD22	2.01	0.42
1:L:43:THR:HA	1:L:60:SER:O	2.19	0.42
1:C:8:ASP:HB2	1:C:158:LYS:HZ1	1.83	0.42
1:C:51:ALA:HB2	1:I:184:GLN:CG	2.48	0.42
1:D:43:THR:HA	1:D:60:SER:O	2.19	0.42
1:C:126:ASP:C	1:C:126:ASP:OD1	2.63	0.42
1:J:122:VAL:HG22	1:J:123:HIS:N	2.35	0.42
1:C:96:GLU:CD	1:C:100:ARG:HE	2.28	0.42
1:K:96:GLU:OE2	1:K:100:ARG:NH2	2.47	0.41
1:K:126:ASP:OD1	1:K:126:ASP:C	2.63	0.41
1:A:64:PRO:HG2	1:A:172:LEU:HD22	2.01	0.41
1:B:34:THR:CG2	1:C:185:LYS:NZ	2.82	0.41
1:L:50:THR:HG21	1:L:52:ASP:OD1	2.21	0.41
1:A:25:MSE:SE	1:A:43:THR:HG21	2.70	0.41
1:A:83:GLY:O	1:I:100:ARG:NH2	2.54	0.41
1:D:93:VAL:CG1	1:D:101:LYS:HG3	2.51	0.41
1:A:44:LYS:HB2	1:A:178:TYR:CD1	2.55	0.41
1:D:50:THR:HG22	1:D:52:ASP:OD1	2.21	0.41
1:I:44:LYS:HB2	1:I:178:TYR:CD1	2.55	0.41
1:L:93:VAL:CG1	1:L:101:LYS:HG3	2.50	0.41
1:B:122:VAL:HG22	1:B:123:HIS:N	2.35	0.41
1:I:29:LYS:O	1:I:134:MSE:HA	2.21	0.41
1:C:107:LEU:HD23	1:C:124:VAL:HG11	2.02	0.41
1:D:18:PHE:CZ	1:D:111:TYR:CZ	3.08	0.41
1:D:50:THR:HG23	1:D:51:ALA:N	2.35	0.41
1:L:50:THR:HG23	1:L:51:ALA:N	2.35	0.41
1:B:45:PHE:CB	1:B:58:VAL:O	2.69	0.41
1:L:18:PHE:CZ	1:L:111:TYR:CZ	3.08	0.40
1:I:47:HIS:CB	1:I:56:LYS:O	2.70	0.40
1:J:58:VAL:HG11	1:J:186:LEU:HB2	2.03	0.40
1:K:96:GLU:CD	1:K:100:ARG:HE	2.28	0.40
1:B:100:ARG:HE	1:B:100:ARG:HB2	1.69	0.40
1:C:47:HIS:CD2	1:C:57:GLU:HG2	2.57	0.40
1:K:47:HIS:CD2	1:K:57:GLU:HG2	2.57	0.40
1:C:107:LEU:HD23	1:C:124:VAL:CG1	2.52	0.40
1:D:162:LYS:NZ	1:D:164:SER:H	1.95	0.40
1:J:45:PHE:CB	1:J:58:VAL:O	2.70	0.40
1:L:50:THR:HG22	1:L:52:ASP:OD1	2.21	0.40
1:A:83:GLY:HA2	1:I:100:ARG:NE	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD1	1:A:170:THR:OG1	2.33	0.40
1:D:145:LYS:HE2	1:D:145:LYS:HB3	1.80	0.40
1:K:107:LEU:HD23	1:K:124:VAL:HG11	2.02	0.40
1:K:124:VAL:O	1:K:134:MSE:N	2.51	0.40
1:L:126:ASP:HA	1:L:127:PRO:HD2	1.84	0.40

All (19) 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:J:16:ASP:O	1:J:67:LYS:NZ[2_546]	1.00	1.20
1:B:142:GLU:CD	1:I:146:GLU:OE2[2_645]	1.08	1.12
1:B:142:GLU:OE2	1:I:146:GLU:OE1[2_645]	1.26	0.94
1:A:184:GLN:CG	1:K:51:ALA:CB[1_545]	1.32	0.88
1:B:142:GLU:OE2	1:I:146:GLU:CD[2_645]	1.35	0.85
1:B:142:GLU:OE2	1:I:146:GLU:OE2[2_645]	1.41	0.79
1:B:142:GLU:CG	1:I:146:GLU:OE2[2_645]	1.65	0.55
1:B:188:LYS:NZ	1:C:106:THR:OG1[2_645]	1.78	0.42
1:A:184:GLN:CD	1:K:51:ALA:CB[1_545]	1.81	0.39
1:A:44:LYS:NZ	1:K:52:ASP:OD2[1_545]	1.87	0.33
1:A:184:GLN:NE2	1:K:51:ALA:CB[1_545]	1.92	0.28
1:A:180:ASP:OD1	1:K:52:ASP:OD2[1_545]	1.95	0.25
1:I:8:ASP:OD1	1:L:2:SER:O[2_656]	1.96	0.24
1:J:16:ASP:C	1:J:67:LYS:NZ[2_546]	1.96	0.24
1:B:142:GLU:CD	1:I:146:GLU:CD[2_645]	1.97	0.23
1:B:142:GLU:OE1	1:I:146:GLU:OE2[2_645]	2.02	0.18
1:B:16:ASP:CA	1:B:67:LYS:NZ[2_645]	2.09	0.11
1:A:44:LYS:NZ	1:K:52:ASP:CG[1_545]	2.16	0.04
1:B:16:ASP:CB	1:B:67:LYS:NZ[2_645]	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	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	60
1	B	192/195 (98%)	184 (96%)	8 (4%)	0	100	100
1	C	191/195 (98%)	185 (97%)	6 (3%)	0	100	100
1	D	192/195 (98%)	187 (97%)	5 (3%)	0	100	100
1	I	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	60
1	J	192/195 (98%)	184 (96%)	8 (4%)	0	100	100
1	K	191/195 (98%)	185 (97%)	6 (3%)	0	100	100
1	L	192/195 (98%)	187 (97%)	5 (3%)	0	100	100
All	All	1536/1560 (98%)	1484 (97%)	50 (3%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLY
1	I	173	GLY

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	173/171 (101%)	167 (96%)	6 (4%)	32	65
1	B	172/171 (101%)	171 (99%)	1 (1%)	78	88
1	C	172/171 (101%)	169 (98%)	3 (2%)	53	78
1	D	172/171 (101%)	166 (96%)	6 (4%)	32	65
1	I	173/171 (101%)	167 (96%)	6 (4%)	32	65
1	J	172/171 (101%)	171 (99%)	1 (1%)	78	88
1	K	172/171 (101%)	169 (98%)	3 (2%)	53	78
1	L	172/171 (101%)	166 (96%)	6 (4%)	32	65
All	All	1378/1368 (101%)	1346 (98%)	32 (2%)	44	74

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	91	LYS
1	A	96	GLU
1	A	100	ARG
1	A	144	VAL
1	A	174	ASN
1	B	78	VAL
1	C	78	VAL
1	C	163	LEU
1	C	170	THR
1	D	8	ASP
1	D	12	ASP
1	D	50	THR
1	D	55	ILE
1	D	77	LYS
1	D	78	VAL
1	I	47	HIS
1	I	91	LYS
1	I	96	GLU
1	I	100	ARG
1	I	144	VAL
1	I	174	ASN
1	J	78	VAL
1	K	78	VAL
1	K	163	LEU
1	K	170	THR
1	L	8	ASP
1	L	12	ASP
1	L	50	THR
1	L	55	ILE
1	L	77	LYS
1	L	78	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	B	123	HIS
1	C	85	ASN
1	C	108	GLN
1	C	138	GLN
1	D	123	HIS
1	I	123	HIS

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Mol	Chain	Res	Type
1	I	184	GLN
1	J	84	ASN
1	J	123	HIS
1	K	108	GLN
1	K	138	GLN
1	L	17	ASN
1	L	123	HIS
1	L	138	GLN

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	193/195 (98%)	1.39	42 (21%) 2 1	16, 56, 166, 320	0
1	B	192/195 (98%)	1.56	46 (23%) 2 1	21, 72, 172, 556	0
1	C	191/195 (97%)	1.77	75 (39%) 1 1	15, 69, 185, 315	0
1	D	192/195 (98%)	1.56	48 (25%) 2 1	19, 62, 181, 342	0
1	I	193/195 (98%)	1.71	70 (36%) 1 1	18, 66, 185, 392	0
1	J	192/195 (98%)	1.63	61 (31%) 1 1	12, 57, 207, 522	0
1	K	191/195 (97%)	2.12	78 (40%) 0 1	17, 62, 241, 558	0
1	L	192/195 (98%)	2.43	114 (59%) 0 0	19, 77, 244, 554	0
All	All	1536/1560 (98%)	1.77	534 (34%) 1 1	12, 65, 199, 558	0

All (534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	SER	11.3
1	K	60	SER	11.2
1	K	89	THR	8.7
1	K	90	ALA	8.4
1	K	128	ALA	8.2
1	B	73	ILE	7.9
1	A	31	GLY	7.4
1	L	89	THR	7.3
1	L	57	GLU	7.1
1	C	60	SER	7.1
1	J	95	VAL	7.0
1	K	169	ALA	6.9
1	J	169	ALA	6.8
1	K	127	PRO	6.8
1	D	166	LEU	6.6
1	K	166	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	J	99	GLY	6.6
1	B	169	ALA	6.5
1	J	94	ILE	6.4
1	C	55	ILE	6.3
1	C	132	TYR	6.3
1	K	171	THR	6.3
1	D	136	ALA	6.3
1	L	86	GLY	6.3
1	A	86	GLY	6.2
1	K	159	VAL	6.2
1	K	50	THR	6.2
1	D	163	LEU	6.1
1	A	60	SER	6.1
1	B	119	TYR	6.0
1	L	194	TYR	6.0
1	A	46	LEU	5.9
1	I	115	ASP	5.8
1	K	30	LEU	5.8
1	B	178	TYR	5.7
1	L	116	TYR	5.7
1	K	126	ASP	5.6
1	B	94	ILE	5.6
1	L	173	GLY	5.5
1	K	108	GLN	5.5
1	I	165	GLY	5.4
1	L	79	SER	5.4
1	L	107	LEU	5.4
1	L	13	PHE	5.3
1	K	61	ASN	5.3
1	C	89	THR	5.3
1	A	5	SER	5.2
1	I	155	ALA	5.1
1	L	37	VAL	5.1
1	C	128	ALA	5.1
1	J	106	THR	5.1
1	L	90	ALA	5.0
1	C	7	VAL	5.0
1	B	129	ALA	4.9
1	K	152	VAL	4.9
1	A	66	ALA	4.9
1	D	90	ALA	4.9
1	C	149	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	K	51	ALA	4.9
1	I	118	LYS	4.8
1	L	92	ASN	4.8
1	C	30	LEU	4.8
1	C	70	SER	4.8
1	L	17	ASN	4.7
1	C	166	LEU	4.7
1	K	86	GLY	4.7
1	A	104	GLU	4.7
1	L	195	GLU	4.7
1	I	46	LEU	4.7
1	L	103	ASP	4.6
1	L	119	TYR	4.6
1	D	102	ILE	4.6
1	D	135	TYR	4.6
1	I	145	LYS	4.6
1	A	131	ASP	4.6
1	A	184	GLN	4.6
1	D	45	PHE	4.6
1	L	160	GLY	4.5
1	D	52	ASP	4.5
1	L	52	ASP	4.5
1	K	164	SER	4.5
1	D	124	VAL	4.5
1	K	52	ASP	4.5
1	I	74	SER	4.5
1	D	127	PRO	4.5
1	J	192	PRO	4.5
1	L	8	ASP	4.4
1	C	146	GLU	4.4
1	A	53	GLY	4.4
1	A	149	LYS	4.4
1	K	192	PRO	4.4
1	I	117	SER	4.4
1	I	171	THR	4.3
1	J	12	ASP	4.3
1	K	156	LEU	4.3
1	C	179	ASP	4.3
1	J	3	GLY	4.3
1	I	147	ASP	4.3
1	L	82	ASP	4.3
1	J	157	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	156	LEU	4.2
1	L	157	GLY	4.2
1	I	52	ASP	4.2
1	L	76	ALA	4.2
1	J	178	TYR	4.2
1	L	85	ASN	4.2
1	K	161	LEU	4.2
1	I	184	GLN	4.2
1	L	112	ILE	4.2
1	K	70	SER	4.1
1	I	164	SER	4.1
1	I	86	GLY	4.1
1	I	37	VAL	4.1
1	I	5	SER	4.1
1	I	62	TYR	4.1
1	J	128	ALA	4.1
1	B	62	TYR	4.1
1	C	74	SER	4.0
1	K	179	ASP	4.0
1	L	115	ASP	4.0
1	K	77	LYS	4.0
1	C	135	TYR	4.0
1	L	35	LEU	4.0
1	A	2	SER	4.0
1	B	84	ASN	4.0
1	J	132	TYR	4.0
1	L	51	ALA	4.0
1	L	111	TYR	4.0
1	A	146	GLU	4.0
1	D	164	SER	4.0
1	I	141	THR	3.9
1	I	139	SER	3.9
1	J	123	HIS	3.9
1	A	152	VAL	3.9
1	A	171	THR	3.9
1	I	176	CYS	3.9
1	J	14	ASN	3.9
1	J	86	GLY	3.9
1	L	153	GLU	3.8
1	C	77	LYS	3.8
1	L	159	VAL	3.8
1	K	80	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	108	GLN	3.8
1	L	91	LYS	3.8
1	L	104	GLU	3.8
1	L	55	ILE	3.7
1	C	194	TYR	3.7
1	B	74	SER	3.7
1	L	135	TYR	3.7
1	D	108	GLN	3.7
1	J	110	SER	3.7
1	L	49	LYS	3.7
1	C	90	ALA	3.7
1	B	177	GLN	3.7
1	J	193	ASN	3.7
1	J	158	LYS	3.7
1	D	8	ASP	3.7
1	B	95	VAL	3.7
1	B	93	VAL	3.6
1	J	194	TYR	3.6
1	K	12	ASP	3.6
1	I	27	HIS	3.6
1	K	125	CYS	3.6
1	C	131	ASP	3.6
1	J	131	ASP	3.6
1	L	23	TRP	3.6
1	L	164	SER	3.6
1	J	170	THR	3.6
1	A	94	ILE	3.6
1	K	74	SER	3.6
1	K	106	THR	3.6
1	C	40	LYS	3.6
1	I	104	GLU	3.6
1	B	89	THR	3.6
1	L	84	ASN	3.5
1	C	147	ASP	3.5
1	L	12	ASP	3.5
1	L	16	ASP	3.5
1	I	151	LYS	3.5
1	K	66	ALA	3.5
1	C	104	GLU	3.5
1	I	65	ASN	3.5
1	C	170	THR	3.5
1	L	30	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	167	PHE	3.5
1	C	159	VAL	3.5
1	A	103	ASP	3.5
1	C	17	ASN	3.5
1	J	174	ASN	3.5
1	K	17	ASN	3.5
1	L	26	THR	3.5
1	K	5	SER	3.5
1	C	52	ASP	3.5
1	I	98	ASP	3.5
1	K	165	GLY	3.4
1	C	161	LEU	3.4
1	I	2	SER	3.4
1	J	79	SER	3.4
1	B	54	LYS	3.4
1	J	53	GLY	3.4
1	L	162	LYS	3.4
1	D	104	GLU	3.4
1	D	162	LYS	3.4
1	L	161	LEU	3.4
1	C	51	ALA	3.4
1	C	121	VAL	3.4
1	K	113	ASP	3.4
1	K	163	LEU	3.4
1	L	88	TYR	3.4
1	C	171	THR	3.4
1	I	84	ASN	3.3
1	A	27	HIS	3.3
1	I	146	GLU	3.3
1	L	42	CYS	3.3
1	B	3	GLY	3.3
1	C	152	VAL	3.3
1	K	10	VAL	3.3
1	L	65	ASN	3.3
1	I	90	ALA	3.3
1	K	194	TYR	3.2
1	L	133	TYR	3.2
1	A	98	ASP	3.2
1	C	82	ASP	3.2
1	L	54	LYS	3.2
1	A	37	VAL	3.2
1	I	152	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	100	ARG	3.2
1	B	123	HIS	3.2
1	K	4	CYS	3.2
1	L	132	TYR	3.2
1	L	158	LYS	3.2
1	J	76	ALA	3.2
1	D	144	VAL	3.2
1	L	114	THR	3.2
1	B	128	ALA	3.2
1	D	42	CYS	3.2
1	L	45	PHE	3.2
1	J	52	ASP	3.1
1	I	87	LYS	3.1
1	A	52	ASP	3.1
1	J	103	ASP	3.1
1	L	75	PHE	3.1
1	B	132	TYR	3.1
1	A	51	ALA	3.1
1	L	22	SER	3.1
1	K	104	GLU	3.1
1	C	127	PRO	3.1
1	C	193	ASN	3.1
1	D	50	THR	3.1
1	D	39	ASP	3.1
1	C	92	ASN	3.1
1	C	8	ASP	3.1
1	L	80	ASP	3.1
1	C	64	PRO	3.1
1	I	143	ASN	3.0
1	K	136	ALA	3.0
1	L	20	THR	3.0
1	D	167	PHE	3.0
1	L	87	LYS	3.0
1	K	130	PRO	3.0
1	A	12	ASP	3.0
1	J	143	ASN	3.0
1	L	144	VAL	3.0
1	C	50	THR	3.0
1	J	5	SER	3.0
1	C	129	ALA	3.0
1	D	123	HIS	3.0
1	L	59	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	60	SER	3.0
1	A	11	LYS	3.0
1	C	15	LYS	3.0
1	I	137	VAL	3.0
1	K	193	ASN	3.0
1	I	96	GLU	2.9
1	L	155	ALA	2.9
1	C	5	SER	2.9
1	B	83	GLY	2.9
1	C	168	ASP	2.9
1	L	109	VAL	2.9
1	L	47	HIS	2.9
1	L	126	ASP	2.9
1	D	193	ASN	2.9
1	I	26	THR	2.9
1	K	84	ASN	2.9
1	C	79	SER	2.9
1	L	31	GLY	2.9
1	I	113	ASP	2.9
1	K	8	ASP	2.9
1	L	81	PHE	2.9
1	J	2	SER	2.9
1	C	61	ASN	2.9
1	I	150	SER	2.8
1	K	129	ALA	2.8
1	B	43	THR	2.8
1	L	130	PRO	2.8
1	C	11	LYS	2.8
1	K	158	LYS	2.8
1	B	183	LEU	2.8
1	L	5	SER	2.8
1	B	96	GLU	2.8
1	C	65	ASN	2.8
1	K	149	LYS	2.8
1	K	38	GLY	2.8
1	L	124	VAL	2.8
1	L	113	ASP	2.8
1	I	154	ALA	2.8
1	A	118	LYS	2.8
1	A	192	PRO	2.8
1	C	196	LYS	2.8
1	D	60	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	195	GLU	2.8
1	I	193	ASN	2.8
1	A	196	LYS	2.8
1	K	196	LYS	2.8
1	J	150	SER	2.8
1	A	84	ASN	2.7
1	C	169	ALA	2.7
1	I	67	LYS	2.7
1	I	148	VAL	2.7
1	L	95	VAL	2.7
1	L	83	GLY	2.7
1	B	103	ASP	2.7
1	C	80	ASP	2.7
1	C	103	ASP	2.7
1	I	178	TYR	2.7
1	I	144	VAL	2.7
1	B	125	CYS	2.7
1	J	34	THR	2.7
1	A	172	LEU	2.7
1	K	174	ASN	2.7
1	K	15	LYS	2.7
1	L	170	THR	2.7
1	D	84	ASN	2.7
1	J	93	VAL	2.6
1	L	120	SER	2.6
1	B	8	ASP	2.6
1	L	191	PHE	2.6
1	B	114	THR	2.6
1	B	78	VAL	2.6
1	I	40	LYS	2.6
1	B	174	ASN	2.6
1	J	177	GLN	2.6
1	J	96	GLU	2.6
1	J	195	GLU	2.6
1	A	182	THR	2.6
1	K	170	THR	2.6
1	L	73	ILE	2.6
1	B	33	SER	2.6
1	B	126	ASP	2.6
1	A	158	LYS	2.6
1	D	185	LYS	2.6
1	K	110	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	117	SER	2.5
1	L	190	SER	2.5
1	L	21	GLY	2.5
1	B	49	LYS	2.5
1	C	14	ASN	2.5
1	C	174	ASN	2.5
1	I	158	LYS	2.5
1	L	15	LYS	2.5
1	L	145	LYS	2.5
1	K	6	THR	2.5
1	L	106	THR	2.5
1	K	88	TYR	2.5
1	L	121	VAL	2.5
1	D	131	ASP	2.5
1	I	64	PRO	2.5
1	C	107	LEU	2.5
1	B	86	GLY	2.5
1	J	67	LYS	2.5
1	L	11	LYS	2.5
1	A	177	GLN	2.5
1	C	33	SER	2.5
1	K	79	SER	2.5
1	K	131	ASP	2.5
1	L	9	THR	2.5
1	I	101	LYS	2.5
1	I	149	LYS	2.5
1	K	155	ALA	2.5
1	K	39	ASP	2.5
1	K	28	TYR	2.5
1	L	48	GLN	2.5
1	I	51	ALA	2.4
1	D	36	GLU	2.4
1	J	105	ARG	2.4
1	I	172	LEU	2.4
1	I	173	GLY	2.4
1	L	93	VAL	2.4
1	A	169	ALA	2.4
1	J	146	GLU	2.4
1	J	100	ARG	2.4
1	K	29	LYS	2.4
1	J	98	ASP	2.4
1	D	165	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	36	GLU	2.4
1	A	68	THR	2.4
1	K	7	VAL	2.4
1	L	131	ASP	2.4
1	J	97	LYS	2.4
1	J	149	LYS	2.4
1	B	18	PHE	2.4
1	L	150	SER	2.4
1	A	89	THR	2.4
1	D	43	THR	2.4
1	D	12	ASP	2.4
1	J	32	ASP	2.4
1	D	41	ASN	2.3
1	B	52	ASP	2.3
1	I	100	ARG	2.3
1	K	36	GLU	2.3
1	I	122	VAL	2.3
1	L	110	SER	2.3
1	C	6	THR	2.3
1	C	165	GLY	2.3
1	L	105	ARG	2.3
1	K	65	ASN	2.3
1	C	122	VAL	2.3
1	C	29	LYS	2.3
1	D	31	GLY	2.3
1	K	83	GLY	2.3
1	D	6	THR	2.3
1	D	106	THR	2.3
1	I	129	ALA	2.3
1	L	27	HIS	2.3
1	K	143	ASN	2.3
1	L	168	ASP	2.3
1	L	138	GLN	2.3
1	B	31	GLY	2.3
1	J	89	THR	2.3
1	A	176	CYS	2.3
1	L	98	ASP	2.3
1	D	153	GLU	2.3
1	K	195	GLU	2.3
1	I	192	PRO	2.3
1	L	127	PRO	2.3
1	I	68	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	141	THR	2.3
1	L	33	SER	2.3
1	A	145	LYS	2.3
1	L	14	ASN	2.3
1	D	146	GLU	2.2
1	A	38	GLY	2.2
1	L	123	HIS	2.2
1	K	122	VAL	2.2
1	J	16	ASP	2.2
1	C	136	ALA	2.2
1	L	129	ALA	2.2
1	K	54	LYS	2.2
1	D	7	VAL	2.2
1	I	177	GLN	2.2
1	I	42	CYS	2.2
1	C	12	ASP	2.2
1	D	126	ASP	2.2
1	C	53	GLY	2.2
1	I	130	PRO	2.2
1	D	29	LYS	2.2
1	I	97	LYS	2.2
1	C	111	TYR	2.2
1	K	37	VAL	2.2
1	B	5	SER	2.2
1	C	112	ILE	2.2
1	L	143	ASN	2.2
1	I	160	GLY	2.2
1	I	131	ASP	2.2
1	I	168	ASP	2.2
1	J	87	LYS	2.2
1	L	19	PHE	2.2
1	B	50	THR	2.2
1	J	50	THR	2.2
1	D	133	TYR	2.2
1	K	73	ILE	2.2
1	B	91	LYS	2.2
1	D	143	ASN	2.2
1	J	90	ALA	2.2
1	D	83	GLY	2.2
1	J	18	PHE	2.2
1	J	82	ASP	2.2
1	I	43	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	194	TYR	2.1
1	B	145	LYS	2.1
1	J	153	GLU	2.1
1	L	99	GLY	2.1
1	A	174	ASN	2.1
1	B	41	ASN	2.1
1	C	81	PHE	2.1
1	C	39	ASP	2.1
1	L	34	THR	2.1
1	J	101	LYS	2.1
1	D	2	SER	2.1
1	I	53	GLY	2.1
1	C	167	PHE	2.1
1	J	84	ASN	2.1
1	J	78	VAL	2.1
1	J	180	ASP	2.1
1	A	71	TYR	2.1
1	I	162	LYS	2.1
1	J	189	GLN	2.1
1	A	22	SER	2.1
1	C	110	SER	2.1
1	J	74	SER	2.1
1	C	41	ASN	2.1
1	C	85	ASN	2.1
1	K	78	VAL	2.1
1	B	12	ASP	2.1
1	D	4	CYS	2.1
1	K	55	ILE	2.1
1	I	50	THR	2.1
1	K	68	THR	2.1
1	K	135	TYR	2.1
1	L	28	TYR	2.1
1	C	154	ALA	2.1
1	L	151	LYS	2.1
1	C	94	ILE	2.1
1	L	125	CYS	2.1
1	B	184	GLN	2.1
1	D	75	PHE	2.1
1	B	185	LYS	2.0
1	L	174	ASN	2.0
1	I	194	TYR	2.0
1	K	32	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	13	PHE	2.0
1	L	165	GLY	2.0
1	C	144	VAL	2.0
1	C	186	LEU	2.0
1	B	60	SER	2.0
1	L	102	ILE	2.0
1	L	139	SER	2.0
1	J	92	ASN	2.0
1	A	155	ALA	2.0
1	J	129	ALA	2.0
1	L	50	THR	2.0
1	B	32	ASP	2.0
1	B	44	LYS	2.0
1	I	77	LYS	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 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.