



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:20 AM UTC

PDB ID : 1AVO / pdb_00001avo
Title : PROTEASOME ACTIVATOR REG(ALPHA)
Authors : Hill, C.P.; Knowlton, J.R.
Deposited on : 1997-09-18
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

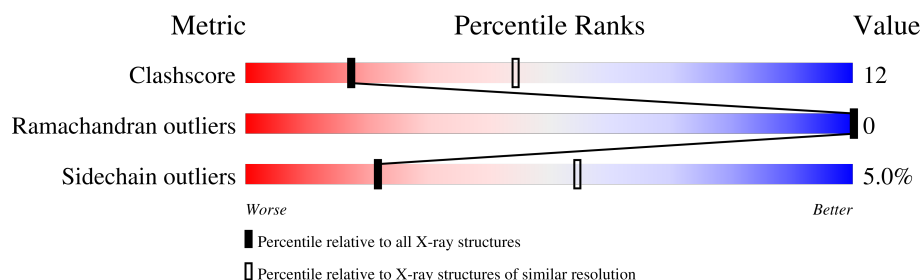
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	60	58% 33% 8%
1	C	60	65% 28% 5% •
1	E	60	60% 33% 5% •
1	G	60	62% 32% 5% •
1	I	60	63% 30% 5% •
1	K	60	62% 32% 5% •
1	M	60	63% 30% 5% •
2	B	140	66% 30% •

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Mol	Chain	Length	Quality of chain
2	D	140	66%31%..
2	F	140	66%30%..
2	H	140	70%28%..
2	J	140	62%34%..
2	L	140	73%24%..
2	N	140	67%31%..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11361 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 11S REGULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			
1	C	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			
1	E	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			
1	G	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			
1	I	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			
1	K	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			
1	M	60	Total	C	N	O	S	0	0	0
			475	303	78	93	1			

- Molecule 2 is a protein called 11S REGULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			
2	D	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			
2	F	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			
2	H	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			
2	J	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			
2	L	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			
2	N	140	Total	C	N	O	S	0	0	0
			1148	734	200	210	4			

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 11S REGULATOR

Chain A: 



• Molecule 1: 11S REGULATOR

Chain C: 



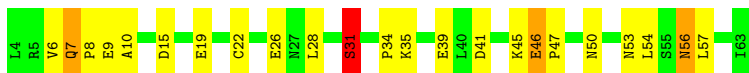
• Molecule 1: 11S REGULATOR

Chain E: 



• Molecule 1: 11S REGULATOR

Chain G: 



• Molecule 1: 11S REGULATOR

Chain I: 



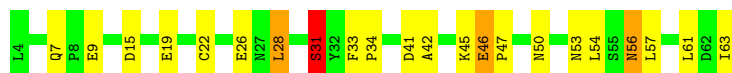
• Molecule 1: 11S REGULATOR

Chain K: 



• Molecule 1: 11S REGULATOR

Chain M: 63% 30% 5% •



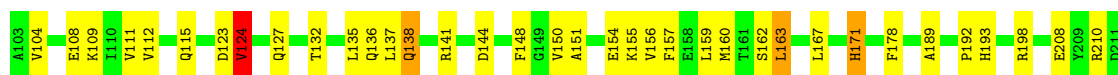
• Molecule 2: 11S REGULATOR

Chain B: 66% 30% •



• Molecule 2: 11S REGULATOR

Chain D: 66% 31% ••



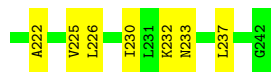
• Molecule 2: 11S REGULATOR

Chain F: 66% 30% ••



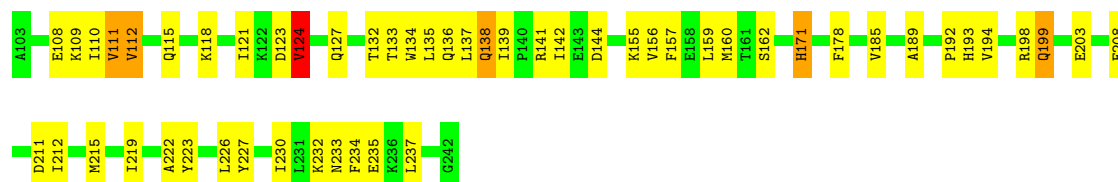
• Molecule 2: 11S REGULATOR

Chain H: 70% 28% ••



- Molecule 2: 11S REGULATOR

Chain J:  62% 34% ..



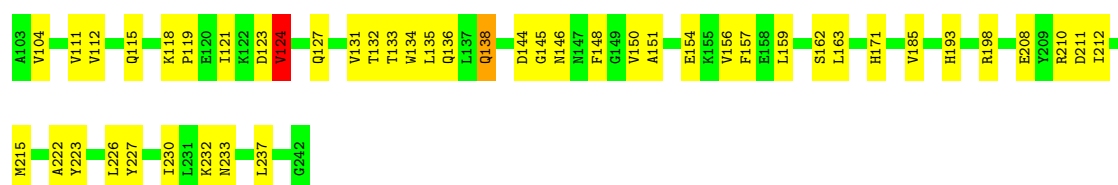
- Molecule 2: 11S REGULATOR

Chain L:  73% 24% ..



- Molecule 2: 11S REGULATOR

Chain N:  67% 31% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.60Å 134.30Å 116.20Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.4 (10.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.249 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11361	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	1.17	1/482 (0.2%)	1.36	5/650 (0.8%)
1	C	1.16	1/482 (0.2%)	1.47	6/650 (0.9%)
1	E	1.11	0/482	1.36	5/650 (0.8%)
1	G	1.05	0/482	1.36	6/650 (0.9%)
1	I	0.99	0/482	1.38	8/650 (1.2%)
1	K	1.01	0/482	1.35	5/650 (0.8%)
1	M	1.14	1/482 (0.2%)	1.36	4/650 (0.6%)
2	B	1.30	1/1167 (0.1%)	1.21	5/1572 (0.3%)
2	D	1.31	2/1167 (0.2%)	1.21	6/1572 (0.4%)
2	F	1.23	4/1167 (0.3%)	1.20	2/1572 (0.1%)
2	H	1.22	2/1167 (0.2%)	1.18	2/1572 (0.1%)
2	J	1.27	3/1167 (0.3%)	1.19	5/1572 (0.3%)
2	L	1.21	2/1167 (0.2%)	1.17	3/1572 (0.2%)
2	N	1.32	2/1167 (0.2%)	1.19	2/1572 (0.1%)
All	All	1.22	19/11543 (0.2%)	1.25	64/15554 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	225	VAL	CA-CB	-5.77	1.47	1.54
2	D	225	VAL	CA-CB	-5.71	1.47	1.54
2	J	111	VAL	CA-CB	-5.69	1.46	1.54
1	A	12	ALA	CA-CB	-5.61	1.44	1.53
2	J	194	VAL	CA-CB	-5.43	1.47	1.53
2	B	185	VAL	CA-CB	-5.33	1.47	1.54
1	M	42	ALA	CA-CB	-5.32	1.44	1.53
2	N	185	VAL	CA-CB	-5.32	1.47	1.54
2	L	207	ALA	CA-CB	-5.28	1.44	1.53
2	L	142	ILE	CA-C	-5.22	1.47	1.52
2	N	230	ILE	CA-CB	-5.12	1.47	1.54
2	F	222	ALA	CA-CB	-5.11	1.45	1.53
1	C	42	ALA	CA-CB	-5.09	1.45	1.53
2	F	212	ILE	CA-CB	-5.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	104	VAL	CA-CB	-5.05	1.48	1.54
2	J	142	ILE	CA-C	-5.04	1.47	1.52
2	H	207	ALA	CA-CB	-5.03	1.45	1.53
2	F	150	VAL	CA-CB	-5.01	1.48	1.54
2	F	207	ALA	CA-CB	-5.00	1.45	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	ASN	N-CA-C	-10.37	101.12	113.88
1	K	46	GLU	CA-C-N	9.57	129.67	119.05
1	K	46	GLU	C-N-CA	9.57	129.67	119.05
1	E	46	GLU	CA-C-N	9.53	129.63	119.05
1	E	46	GLU	C-N-CA	9.53	129.63	119.05
1	A	46	GLU	CA-C-N	9.35	129.43	119.05
1	A	46	GLU	C-N-CA	9.35	129.43	119.05
1	E	56	ASN	N-CA-C	-9.04	102.39	113.50
1	G	46	GLU	CA-C-N	8.97	129.01	119.05
1	G	46	GLU	C-N-CA	8.97	129.01	119.05
1	M	46	GLU	CA-C-N	8.97	129.00	119.05
1	M	46	GLU	C-N-CA	8.97	129.00	119.05
1	I	46	GLU	CA-C-N	8.96	129.00	119.05
1	I	46	GLU	C-N-CA	8.96	129.00	119.05
1	C	46	GLU	CA-C-N	8.94	128.97	119.05
1	C	46	GLU	C-N-CA	8.94	128.97	119.05
1	G	56	ASN	N-CA-C	-8.08	103.56	113.50
1	I	56	ASN	N-CA-C	-7.93	103.39	113.23
1	K	56	ASN	N-CA-C	-7.60	103.81	113.23
1	M	56	ASN	N-CA-C	-7.55	103.87	113.23
2	J	144	ASP	N-CA-C	7.37	119.31	111.28
2	D	124	VAL	CB-CA-C	-7.22	102.72	111.97
2	B	144	ASP	N-CA-C	7.17	119.17	111.36
1	C	7	GLN	CA-C-N	7.09	126.61	119.24
1	C	7	GLN	C-N-CA	7.09	126.61	119.24
2	F	144	ASP	N-CA-C	7.02	119.01	111.36
2	L	144	ASP	N-CA-C	6.97	118.95	111.36
1	I	7	GLN	CA-C-N	6.80	126.60	119.05
1	I	7	GLN	C-N-CA	6.80	126.60	119.05
2	L	124	VAL	CB-CA-C	-6.78	103.30	111.97
2	N	124	VAL	CB-CA-C	-6.67	103.43	111.97
1	I	55	SER	N-CA-C	-6.65	105.15	113.20
2	B	124	VAL	CB-CA-C	-6.51	103.64	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	GLU	N-CA-C	6.44	118.84	111.11
2	N	144	ASP	N-CA-C	6.36	118.30	111.36
2	H	124	VAL	CB-CA-C	-6.33	103.87	111.97
1	A	56	ASN	N-CA-C	-6.17	105.24	112.89
2	H	144	ASP	N-CA-C	5.97	117.86	111.36
2	J	124	VAL	CB-CA-C	-5.94	104.37	111.97
2	F	124	VAL	CB-CA-C	-5.91	104.41	111.97
2	J	144	ASP	CA-C-N	-5.88	116.88	121.82
2	J	144	ASP	C-N-CA	-5.88	116.88	121.82
1	M	31	SER	N-CA-C	5.83	123.21	110.80
1	I	25	THR	N-CA-C	5.80	117.68	111.36
1	A	55	SER	N-CA-C	-5.78	106.18	113.18
1	G	7	GLN	CA-C-N	5.63	125.30	119.05
1	G	7	GLN	C-N-CA	5.63	125.30	119.05
2	B	229	ILE	N-CA-C	5.60	116.38	110.72
1	K	26	GLU	N-CA-C	-5.57	105.36	111.82
2	D	144	ASP	N-CA-C	5.55	117.33	111.28
2	L	229	ILE	N-CA-C	5.40	116.17	110.72
2	D	167	LEU	N-CA-C	5.27	117.94	111.82
1	E	31	SER	N-CA-C	5.25	121.99	110.80
2	D	108	GLU	N-CA-C	5.25	117.00	111.28
1	I	31	SER	N-CA-C	5.25	121.98	110.80
1	G	31	SER	N-CA-C	5.24	121.97	110.80
1	K	31	SER	N-CA-C	5.24	121.97	110.80
1	E	26	GLU	N-CA-C	-5.21	105.68	111.36
2	D	230	ILE	N-CA-C	-5.13	105.54	110.72
1	A	26	GLU	N-CA-C	-5.08	105.93	111.82
2	J	185	VAL	CB-CA-C	-5.06	105.40	111.88
2	D	163	LEU	N-CA-C	-5.06	105.21	111.33
1	C	31	SER	N-CA-C	5.01	121.48	110.80
2	B	172	THR	N-CA-C	5.01	117.63	111.82

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	475	0	485	16	0
1	C	475	0	485	15	0
1	E	475	0	485	20	0
1	G	475	0	485	15	0
1	I	475	0	485	14	0
1	K	475	0	485	16	0
1	M	475	0	485	16	0
2	B	1148	0	1177	31	0
2	D	1148	0	1177	30	0
2	F	1148	0	1177	37	0
2	H	1148	0	1177	32	0
2	J	1148	0	1177	38	0
2	L	1148	0	1177	25	0
2	N	1148	0	1177	27	0
All	All	11361	0	11634	287	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 12.

All (287) 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:I:63:ILE:HB	2:J:198:ARG:NH2	1.73	1.03
1:E:63:ILE:HB	2:F:198:ARG:NH1	1.86	0.90
1:K:63:ILE:HB	2:L:198:ARG:NH2	1.91	0.86
1:M:63:ILE:HB	2:N:198:ARG:NH2	1.91	0.85
2:B:122:LYS:HD2	2:N:210:ARG:HH11	1.46	0.80
1:E:63:ILE:HB	2:F:198:ARG:HH12	1.45	0.78
1:I:63:ILE:HB	2:J:198:ARG:HH22	1.46	0.77
2:B:123:ASP:O	2:B:127:GLN:HG2	1.85	0.76
1:I:53:ASN:HB2	1:I:56:ASN:ND2	2.02	0.74
1:M:63:ILE:HB	2:N:198:ARG:HH22	1.53	0.73
2:L:156:VAL:HG21	2:L:237:LEU:HD21	1.71	0.71
2:F:111:VAL:O	2:F:115:GLN:HG2	1.90	0.71
1:K:63:ILE:HB	2:L:198:ARG:HH22	1.56	0.71
2:D:123:ASP:O	2:D:127:GLN:HG2	1.90	0.70
1:I:54:LEU:O	1:I:57:LEU:HB3	1.92	0.69
2:F:123:ASP:O	2:F:127:GLN:HG2	1.94	0.68
2:J:233:ASN:O	2:J:237:LEU:HG	1.94	0.67
2:L:123:ASP:O	2:L:127:GLN:HG2	1.94	0.67
2:D:156:VAL:HG21	2:D:237:LEU:HD21	1.77	0.67
2:N:156:VAL:HG21	2:N:237:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:156:VAL:HG21	2:J:237:LEU:HD21	1.78	0.66
2:N:123:ASP:O	2:N:127:GLN:HG2	1.96	0.65
2:B:156:VAL:HG21	2:B:237:LEU:HD21	1.78	0.65
2:B:210:ARG:HD2	2:D:171:HIS:CE1	2.32	0.64
2:J:123:ASP:O	2:J:127:GLN:HG2	1.96	0.64
1:E:48:ALA:O	2:F:109:LYS:NZ	2.32	0.63
1:M:54:LEU:O	1:M:57:LEU:HB3	1.98	0.63
2:D:210:ARG:HD2	2:F:171:HIS:NE2	2.15	0.62
1:C:54:LEU:O	1:C:57:LEU:HB3	2.00	0.62
2:F:156:VAL:HG21	2:F:237:LEU:HD21	1.81	0.62
2:H:233:ASN:O	2:H:237:LEU:HG	1.99	0.61
2:H:208:GLU:O	2:H:212:ILE:HG13	2.00	0.61
1:M:15:ASP:O	1:M:19:GLU:HG3	2.00	0.61
2:H:156:VAL:HG21	2:H:237:LEU:HD21	1.83	0.60
2:B:233:ASN:O	2:B:237:LEU:HG	2.02	0.60
2:B:141:ARG:HG3	2:N:232:LYS:O	2.02	0.59
2:H:123:ASP:O	2:H:127:GLN:HG2	2.01	0.59
2:N:111:VAL:O	2:N:115:GLN:HG2	2.03	0.59
2:B:136:GLN:HG2	2:B:157:PHE:CE1	2.38	0.59
2:D:233:ASN:O	2:D:237:LEU:HG	2.03	0.59
2:N:233:ASN:O	2:N:237:LEU:HG	2.04	0.58
2:L:233:ASN:O	2:L:237:LEU:HG	2.03	0.58
1:A:46:GLU:O	1:A:50:ASN:ND2	2.36	0.58
2:N:136:GLN:HG2	2:N:157:PHE:CE1	2.39	0.58
2:D:136:GLN:HG2	2:D:157:PHE:CE1	2.38	0.58
1:M:46:GLU:HG2	1:M:47:PRO:HD2	1.87	0.57
2:L:117:LEU:HD22	2:L:212:ILE:HG23	1.85	0.57
2:H:111:VAL:O	2:H:115:GLN:HG2	2.04	0.57
1:C:46:GLU:HG2	1:C:47:PRO:HD2	1.87	0.56
2:B:215:MET:O	2:B:219:ILE:HG13	2.05	0.56
1:G:22:CYS:O	1:G:26:GLU:HG3	2.05	0.56
2:N:208:GLU:O	2:N:212:ILE:HG13	2.06	0.56
1:C:15:ASP:O	1:C:19:GLU:HG3	2.05	0.56
2:J:136:GLN:HG2	2:J:157:PHE:CE1	2.41	0.56
1:C:46:GLU:O	1:C:50:ASN:ND2	2.39	0.55
2:H:136:GLN:HG2	2:H:157:PHE:CE1	2.42	0.55
1:G:31:SER:C	1:G:34:PRO:HD2	2.32	0.55
2:J:208:GLU:O	2:J:212:ILE:HG13	2.06	0.55
2:B:132:THR:O	2:B:136:GLN:HG3	2.07	0.55
2:D:193:HIS:H	2:D:193:HIS:CD2	2.25	0.55
2:L:193:HIS:H	2:L:193:HIS:CD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:HG2	1:A:47:PRO:HD2	1.88	0.54
1:C:53:ASN:HB2	1:C:56:ASN:ND2	2.21	0.54
1:G:54:LEU:HD12	2:H:210:ARG:CZ	2.37	0.54
1:K:54:LEU:O	1:K:57:LEU:HB3	2.08	0.54
1:K:46:GLU:O	1:K:50:ASN:ND2	2.39	0.54
2:L:136:GLN:HG2	2:L:157:PHE:CE1	2.43	0.54
2:N:193:HIS:H	2:N:193:HIS:CD2	2.25	0.54
1:C:22:CYS:O	1:C:26:GLU:HG3	2.08	0.54
1:E:62:ASP:C	1:E:63:ILE:HG13	2.31	0.54
1:G:54:LEU:O	1:G:57:LEU:HB3	2.06	0.54
1:I:31:SER:C	1:I:34:PRO:HD2	2.33	0.54
2:F:136:GLN:HG2	2:F:157:PHE:CE1	2.43	0.54
2:J:199:GLN:O	2:J:203:GLU:HG2	2.08	0.54
1:E:46:GLU:O	1:E:50:ASN:ND2	2.41	0.53
2:F:108:GLU:O	2:F:112:VAL:HG13	2.09	0.53
1:K:35:LYS:O	1:K:39:GLU:HG3	2.09	0.53
1:E:54:LEU:O	1:E:57:LEU:HB3	2.09	0.53
1:G:15:ASP:O	1:G:19:GLU:HG3	2.08	0.53
1:A:35:LYS:O	1:A:39:GLU:HG3	2.09	0.53
2:F:215:MET:O	2:F:219:ILE:HG13	2.08	0.52
1:G:46:GLU:O	1:G:50:ASN:ND2	2.42	0.52
1:I:53:ASN:CB	1:I:56:ASN:ND2	2.72	0.52
2:J:193:HIS:CD2	2:J:193:HIS:H	2.25	0.52
2:H:210:ARG:HD2	2:J:171:HIS:NE2	2.24	0.52
2:J:132:THR:O	2:J:136:GLN:HG3	2.10	0.52
1:A:54:LEU:O	1:A:57:LEU:HB3	2.09	0.52
1:K:53:ASN:HB2	1:K:56:ASN:ND2	2.23	0.52
1:I:46:GLU:O	1:I:50:ASN:ND2	2.42	0.52
2:L:132:THR:O	2:L:136:GLN:HG3	2.10	0.52
2:N:148:PHE:O	2:N:151:ALA:HB3	2.09	0.52
1:A:48:ALA:HB1	2:B:113:LEU:HD21	1.92	0.52
1:M:7:GLN:HB3	1:M:9:GLU:OE1	2.10	0.52
2:N:132:THR:O	2:N:136:GLN:HG3	2.10	0.52
1:I:15:ASP:O	1:I:19:GLU:HG3	2.11	0.51
2:J:112:VAL:O	2:J:115:GLN:HB2	2.10	0.51
2:L:135:LEU:O	2:L:138:GLN:HB2	2.11	0.51
2:B:208:GLU:O	2:B:212:ILE:HG13	2.11	0.51
2:H:132:THR:O	2:H:136:GLN:HG3	2.11	0.51
1:C:7:GLN:HB3	1:C:9:GLU:OE1	2.11	0.51
2:H:215:MET:O	2:H:219:ILE:HG13	2.10	0.51
2:B:108:GLU:O	2:B:112:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:C	1:C:34:PRO:HD2	2.36	0.51
1:G:35:LYS:O	1:G:39:GLU:HG3	2.11	0.51
1:I:22:CYS:O	1:I:26:GLU:HG3	2.11	0.51
1:A:22:CYS:O	1:A:26:GLU:HG3	2.11	0.50
1:G:7:GLN:HB3	1:G:9:GLU:OE1	2.11	0.50
1:E:22:CYS:O	1:E:26:GLU:HG3	2.11	0.50
1:K:41:ASP:O	1:K:45:LYS:HG3	2.11	0.50
1:M:53:ASN:HB2	1:M:56:ASN:ND2	2.26	0.50
2:N:135:LEU:O	2:N:138:GLN:HB2	2.12	0.50
2:H:193:HIS:CD2	2:H:193:HIS:H	2.28	0.50
1:I:46:GLU:HG2	1:I:47:PRO:HD2	1.94	0.50
2:F:193:HIS:H	2:F:193:HIS:CD2	2.29	0.50
1:E:46:GLU:HG2	1:E:47:PRO:HD2	1.94	0.50
2:F:160:MET:HE2	2:F:230:ILE:HD11	1.94	0.50
2:H:117:LEU:HD22	2:H:212:ILE:HG23	1.93	0.50
1:K:46:GLU:HG2	1:K:47:PRO:HD2	1.94	0.49
1:M:22:CYS:O	1:M:26:GLU:HG3	2.13	0.49
2:D:215:MET:O	2:D:219:ILE:HG13	2.12	0.49
2:N:150:VAL:O	2:N:154:GLU:HG3	2.12	0.49
2:D:232:LYS:O	2:F:141:ARG:HG3	2.12	0.49
2:B:117:LEU:HD22	2:B:212:ILE:HG23	1.95	0.49
2:D:132:THR:O	2:D:136:GLN:HG3	2.13	0.48
2:D:136:GLN:HG2	2:D:157:PHE:HE1	1.77	0.48
2:F:208:GLU:O	2:F:212:ILE:HG13	2.14	0.48
2:F:233:ASN:O	2:F:237:LEU:HG	2.12	0.48
1:E:53:ASN:HB2	1:E:56:ASN:ND2	2.27	0.48
2:H:135:LEU:O	2:H:138:GLN:HB2	2.14	0.48
2:B:193:HIS:H	2:B:193:HIS:CD2	2.32	0.48
2:D:135:LEU:O	2:D:138:GLN:HB2	2.13	0.48
2:J:215:MET:O	2:J:219:ILE:HG13	2.14	0.48
1:E:15:ASP:O	1:E:19:GLU:HG3	2.14	0.48
2:B:160:MET:HE2	2:B:230:ILE:HD11	1.95	0.48
1:A:53:ASN:HB2	1:A:56:ASN:ND2	2.29	0.48
2:D:208:GLU:O	2:D:212:ILE:HG13	2.14	0.47
1:E:51:GLU:OE2	2:F:109:LYS:HE3	2.14	0.47
1:A:15:ASP:O	1:A:19:GLU:HG3	2.14	0.47
1:E:31:SER:C	1:E:34:PRO:HD2	2.39	0.47
2:F:132:THR:O	2:F:136:GLN:HG3	2.14	0.47
1:G:8:PRO:HG2	1:G:9:GLU:H	1.80	0.47
1:G:53:ASN:HB2	1:G:56:ASN:ND2	2.29	0.47
2:F:203:GLU:HG3	2:H:178:PHE:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:ASN:O	1:I:56:ASN:HB2	2.14	0.47
1:C:54:LEU:C	1:C:56:ASN:H	2.20	0.47
2:F:227:TYR:OH	1:G:6:VAL:HG11	2.14	0.47
2:H:108:GLU:O	2:H:112:VAL:HG13	2.15	0.47
2:H:135:LEU:HD23	2:H:157:PHE:HD1	1.80	0.47
2:N:121:ILE:O	2:N:124:VAL:HG23	2.15	0.47
2:F:148:PHE:O	2:F:151:ALA:HB3	2.15	0.47
2:N:211:ASP:O	2:N:215:MET:HG3	2.14	0.47
1:K:57:LEU:HA	2:L:109:LYS:HD2	1.97	0.47
2:B:111:VAL:O	2:B:115:GLN:HG2	2.15	0.46
2:B:210:ARG:HD2	2:D:171:HIS:HE1	1.77	0.46
1:G:46:GLU:HG2	1:G:47:PRO:HD2	1.98	0.46
1:I:41:ASP:O	1:I:45:LYS:HG3	2.16	0.46
2:B:136:GLN:HG2	2:B:157:PHE:HE1	1.80	0.46
2:D:148:PHE:O	2:D:151:ALA:HB3	2.15	0.46
2:J:136:GLN:HG2	2:J:157:PHE:HE1	1.80	0.46
2:J:108:GLU:O	2:J:112:VAL:HG13	2.16	0.46
1:A:33:PHE:HB2	1:A:34:PRO:HD3	1.98	0.46
2:J:227:TYR:OH	1:K:6:VAL:HG11	2.16	0.46
1:A:41:ASP:O	1:A:45:LYS:HG3	2.16	0.45
1:I:35:LYS:O	1:I:39:GLU:HG3	2.17	0.45
1:M:33:PHE:HB2	1:M:34:PRO:HD3	1.98	0.45
2:B:232:LYS:O	2:D:141:ARG:HG3	2.16	0.45
1:K:22:CYS:O	1:K:26:GLU:HG3	2.17	0.45
1:K:31:SER:C	1:K:34:PRO:HD2	2.42	0.45
2:N:124:VAL:HG13	2:N:223:TYR:CZ	2.51	0.45
2:B:199:GLN:O	2:B:203:GLU:HG2	2.16	0.45
2:D:111:VAL:O	2:D:115:GLN:HG2	2.15	0.45
2:D:156:VAL:HG12	2:D:160:MET:HE3	1.99	0.45
2:F:150:VAL:O	2:F:154:GLU:HG3	2.16	0.45
1:G:54:LEU:HD12	2:H:210:ARG:NH2	2.32	0.45
1:M:46:GLU:O	1:M:50:ASN:ND2	2.50	0.45
2:B:133:THR:O	2:B:134:TRP:C	2.60	0.45
2:N:163:LEU:HD23	2:N:163:LEU:HA	1.63	0.45
2:B:148:PHE:O	2:B:151:ALA:HB3	2.17	0.45
1:E:41:ASP:O	1:E:45:LYS:HG3	2.16	0.45
2:D:124:VAL:HG13	2:D:223:TYR:CZ	2.52	0.44
2:F:136:GLN:O	2:F:139:ILE:HG13	2.17	0.44
2:F:192:PRO:CA	2:F:198:ARG:HH21	2.29	0.44
1:K:7:GLN:HB3	1:K:9:GLU:OE1	2.17	0.44
1:K:54:LEU:HD23	1:K:54:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:156:VAL:HG12	2:L:160:MET:HE3	1.99	0.44
1:M:41:ASP:O	1:M:45:LYS:HG3	2.17	0.44
2:F:135:LEU:O	2:F:138:GLN:HB2	2.18	0.44
2:J:133:THR:O	2:J:134:TRP:C	2.60	0.44
2:L:133:THR:O	2:L:134:TRP:C	2.59	0.44
2:B:156:VAL:HG12	2:B:160:MET:HE3	2.00	0.44
1:A:18:ARG:NH2	2:B:137:LEU:O	2.50	0.44
2:B:160:MET:CE	2:B:230:ILE:HD11	2.47	0.44
2:F:156:VAL:HG12	2:F:160:MET:HE3	2.00	0.44
2:L:160:MET:HE2	2:L:230:ILE:HD11	1.99	0.44
2:D:227:TYR:OH	1:E:6:VAL:HG11	2.18	0.44
2:H:136:GLN:HG2	2:H:157:PHE:HE1	1.82	0.44
2:N:222:ALA:O	2:N:226:LEU:HB2	2.18	0.44
1:C:9:GLU:HG2	1:C:10:ALA:N	2.33	0.43
1:E:9:GLU:HG2	1:E:10:ALA:N	2.33	0.43
2:J:156:VAL:HG12	2:J:160:MET:HE3	2.01	0.43
2:L:124:VAL:HG13	2:L:223:TYR:CZ	2.53	0.43
2:H:121:ILE:O	2:H:124:VAL:HG23	2.19	0.43
2:H:203:GLU:HG3	2:J:178:PHE:CE2	2.54	0.43
1:I:46:GLU:HA	1:I:47:PRO:HD3	1.87	0.43
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.80	0.43
2:H:163:LEU:HA	2:H:163:LEU:HD23	1.71	0.43
2:B:189:ALA:O	2:B:192:PRO:HD3	2.18	0.43
1:M:46:GLU:HA	1:M:47:PRO:HD3	1.84	0.43
1:K:15:ASP:O	1:K:19:GLU:HG3	2.19	0.43
2:H:135:LEU:HD23	2:H:157:PHE:CD1	2.54	0.43
2:J:136:GLN:O	2:J:139:ILE:HG13	2.17	0.43
1:A:6:VAL:HG11	2:N:227:TYR:OH	2.19	0.43
2:J:111:VAL:O	2:J:115:GLN:HG2	2.19	0.43
2:D:213:ARG:HD3	2:F:126:GLU:OE2	2.19	0.42
2:H:160:MET:HE2	2:H:230:ILE:HD11	2.01	0.42
2:D:189:ALA:O	2:D:192:PRO:HD3	2.18	0.42
2:D:210:ARG:HD2	2:F:171:HIS:CE1	2.53	0.42
1:E:54:LEU:HD23	1:E:54:LEU:HA	1.78	0.42
2:F:163:LEU:HD23	2:F:163:LEU:HA	1.70	0.42
2:H:203:GLU:HG3	2:J:178:PHE:CD2	2.54	0.42
2:J:124:VAL:HG13	2:J:223:TYR:CZ	2.55	0.42
2:B:150:VAL:O	2:B:154:GLU:HG3	2.20	0.42
1:E:33:PHE:HB2	1:E:34:PRO:HD3	2.01	0.42
2:J:135:LEU:O	2:J:138:GLN:HB2	2.18	0.42
2:N:133:THR:O	2:N:134:TRP:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:145:GLY:O	2:N:146:ASN:HB3	2.19	0.42
2:H:211:ASP:O	2:H:215:MET:HG3	2.19	0.42
1:M:28:LEU:HD23	2:N:131:VAL:HG23	2.01	0.42
2:N:136:GLN:HG2	2:N:157:PHE:HE1	1.80	0.42
1:G:41:ASP:O	1:G:45:LYS:HG3	2.20	0.42
2:N:118:LYS:HB2	2:N:119:PRO:HD3	2.01	0.42
2:H:189:ALA:O	2:H:192:PRO:HD3	2.20	0.42
2:J:189:ALA:O	2:J:192:PRO:HD3	2.19	0.42
2:J:203:GLU:HG3	2:L:178:PHE:CD2	2.55	0.42
2:J:211:ASP:O	2:J:215:MET:HG3	2.20	0.42
1:C:61:LEU:HD12	1:C:61:LEU:HA	1.86	0.42
1:K:33:PHE:HB2	1:K:34:PRO:HD3	2.02	0.42
1:A:46:GLU:HA	1:A:47:PRO:HD3	1.88	0.42
2:F:192:PRO:HA	2:F:198:ARG:HH21	1.85	0.42
2:B:170:PHE:O	2:B:171:HIS:C	2.63	0.41
2:J:232:LYS:O	2:L:141:ARG:HG3	2.20	0.41
1:A:31:SER:C	1:A:34:PRO:HD2	2.46	0.41
2:D:150:VAL:O	2:D:154:GLU:HG3	2.20	0.41
2:F:124:VAL:HG13	2:F:223:TYR:CZ	2.55	0.41
1:C:35:LYS:O	1:C:39:GLU:HG3	2.20	0.41
1:E:48:ALA:HB1	2:F:113:LEU:HD21	2.02	0.41
2:H:160:MET:CE	2:H:230:ILE:HD11	2.50	0.41
2:H:222:ALA:O	2:H:226:LEU:HB2	2.21	0.41
2:J:108:GLU:O	2:J:109:LYS:C	2.62	0.41
2:L:208:GLU:O	2:L:212:ILE:HG13	2.21	0.41
1:M:61:LEU:CD1	2:N:104:VAL:HG11	2.50	0.41
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.82	0.41
2:H:203:GLU:OE1	2:J:118:LYS:NZ	2.53	0.41
2:L:160:MET:CE	2:L:230:ILE:HD11	2.51	0.41
2:B:135:LEU:O	2:B:138:GLN:HB2	2.21	0.41
1:E:57:LEU:CD1	2:F:109:LYS:HD2	2.50	0.41
2:F:210:ARG:NH2	2:H:118:LYS:HB3	2.36	0.41
2:L:148:PHE:O	2:L:151:ALA:HB3	2.20	0.41
1:C:57:LEU:HA	2:D:109:LYS:HD2	2.03	0.41
1:C:61:LEU:HD23	2:D:198:ARG:HG2	2.03	0.41
2:D:137:LEU:HD23	2:D:137:LEU:HA	1.88	0.41
1:E:46:GLU:HA	1:E:47:PRO:HD3	1.85	0.41
2:F:117:LEU:HD22	2:F:212:ILE:HG23	2.03	0.41
2:F:118:LYS:HG2	2:F:174:ILE:HD13	2.03	0.41
2:J:160:MET:HE2	2:J:230:ILE:HD11	2.03	0.41
2:J:234:PHE:O	2:J:235:GLU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:LEU:HD23	2:D:163:LEU:HA	1.63	0.41
2:H:232:LYS:O	2:J:141:ARG:HG3	2.21	0.41
2:L:155:LYS:O	2:L:155:LYS:HG3	2.20	0.41
1:M:54:LEU:HD23	1:M:54:LEU:HA	1.83	0.41
2:H:156:VAL:HG12	2:H:160:MET:HE3	2.03	0.41
2:J:121:ILE:O	2:J:124:VAL:HG23	2.21	0.41
2:J:137:LEU:HD23	2:J:137:LEU:HA	1.89	0.41
2:F:160:MET:CE	2:F:230:ILE:HD11	2.51	0.40
2:J:155:LYS:HG2	2:L:142:ILE:HD11	2.02	0.40
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.91	0.40
2:L:136:GLN:HG2	2:L:157:PHE:HE1	1.83	0.40
2:F:136:GLN:HG2	2:F:157:PHE:HE1	1.85	0.40
2:L:163:LEU:HD23	2:L:163:LEU:HA	1.74	0.40
2:L:234:PHE:O	2:L:235:GLU:C	2.65	0.40
1:M:31:SER:C	1:M:34:PRO:HD2	2.45	0.40
2:B:203:GLU:HG3	2:D:178:PHE:CD2	2.57	0.40
2:B:211:ASP:O	2:B:215:MET:HG3	2.21	0.40
2:D:155:LYS:O	2:D:155:LYS:HG3	2.21	0.40
1:G:9:GLU:HG2	1:G:10:ALA:N	2.36	0.40
2:J:110:ILE:O	2:J:111:VAL:C	2.65	0.40
2:J:222:ALA:O	2:J:226:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

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	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
1	C	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
1	E	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
1	G	58/60 (97%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
1	K	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
1	M	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
2	B	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
2	D	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
2	F	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
2	H	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
2	J	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
2	L	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
2	N	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
All	All	1372/1400 (98%)	1339 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	53/53 (100%)	50 (94%)	3 (6%)	18	49
1	C	53/53 (100%)	51 (96%)	2 (4%)	29	64
1	E	53/53 (100%)	51 (96%)	2 (4%)	29	64
1	G	53/53 (100%)	51 (96%)	2 (4%)	29	64
1	I	53/53 (100%)	50 (94%)	3 (6%)	18	49
1	K	53/53 (100%)	51 (96%)	2 (4%)	29	64
1	M	53/53 (100%)	51 (96%)	2 (4%)	29	64
2	B	126/126 (100%)	119 (94%)	7 (6%)	19	50
2	D	126/126 (100%)	120 (95%)	6 (5%)	23	56
2	F	126/126 (100%)	119 (94%)	7 (6%)	19	50
2	H	126/126 (100%)	119 (94%)	7 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	126/126 (100%)	119 (94%)	7 (6%)	19	50
2	L	126/126 (100%)	119 (94%)	7 (6%)	19	50
2	N	126/126 (100%)	120 (95%)	6 (5%)	23	56
All	All	1253/1253 (100%)	1190 (95%)	63 (5%)	22	54

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	28	LEU
1	A	31	SER
2	B	112	VAL
2	B	124	VAL
2	B	138	GLN
2	B	159	LEU
2	B	162	SER
2	B	171	HIS
2	B	199	GLN
1	C	28	LEU
1	C	31	SER
2	D	112	VAL
2	D	124	VAL
2	D	138	GLN
2	D	159	LEU
2	D	162	SER
2	D	171	HIS
1	E	28	LEU
1	E	31	SER
2	F	112	VAL
2	F	124	VAL
2	F	138	GLN
2	F	159	LEU
2	F	162	SER
2	F	171	HIS
2	F	199	GLN
1	G	28	LEU
1	G	31	SER
2	H	112	VAL
2	H	124	VAL
2	H	138	GLN
2	H	159	LEU

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Mol	Chain	Res	Type
2	H	162	SER
2	H	171	HIS
2	H	199	GLN
1	I	7	GLN
1	I	28	LEU
1	I	31	SER
2	J	112	VAL
2	J	124	VAL
2	J	138	GLN
2	J	159	LEU
2	J	162	SER
2	J	171	HIS
2	J	199	GLN
1	K	28	LEU
1	K	31	SER
2	L	112	VAL
2	L	124	VAL
2	L	138	GLN
2	L	159	LEU
2	L	162	SER
2	L	171	HIS
2	L	235	GLU
1	M	28	LEU
1	M	31	SER
2	N	112	VAL
2	N	124	VAL
2	N	138	GLN
2	N	159	LEU
2	N	162	SER
2	N	171	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	115	GLN
2	B	136	GLN
2	B	193	HIS
2	D	136	GLN
2	D	171	HIS
2	D	193	HIS
2	F	136	GLN
2	F	193	HIS

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Mol	Chain	Res	Type
2	F	202	HIS
2	H	115	GLN
2	H	136	GLN
2	H	193	HIS
1	I	56	ASN
2	J	115	GLN
2	J	136	GLN
2	J	193	HIS
2	L	115	GLN
2	L	136	GLN
2	L	193	HIS
2	L	202	HIS
1	M	7	GLN
1	M	56	ASN
2	N	136	GLN
2	N	193	HIS
2	N	202	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.