



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:32 PM UTC

PDB ID : 1DN0 / pdb_00001dn0
Title : STRUCTURE OF THE FAB FRAGMENT FROM A HUMAN IGM COLD AGGLUTININ
Authors : Cauerhff, A.; Braden, B.; Carvalho, J.G.; Leoni, J.; Polikarpov, I.; Goldbaum, F.
Deposited on : 1999-12-15
Resolution : 2.28 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

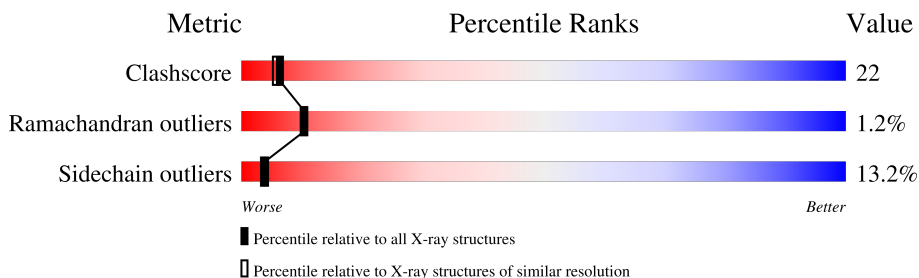
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)

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	215	53% 35% 11% .
1	C	215	61% 29% 9%
2	B	232	51% 30% 10% . 7%
2	D	232	56% 25% 9% . 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7208 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 IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1638	1023	275	335	5			
1	C	215	Total	C	N	O	S	0	0	0
			1638	1023	275	335	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	CYS	GLY	conflict	PIR A23746
A	89	CYS	GLY	conflict	PIR A23746
A	215	CYS	GLY	conflict	PIR A23746
C	23	CYS	GLY	conflict	PIR A23746
C	89	CYS	GLY	conflict	PIR A23746
C	215	CYS	GLY	conflict	PIR A23746

- Molecule 2 is a protein called IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1657	1052	279	321	5			
2	D	217	Total	C	N	O	S	0	0	0
			1661	1055	280	320	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	conflict	PIR B23746
B	200	ALA	GLN	conflict	PIR B23746
D	1	GLU	-	conflict	PIR B23746
D	200	ALA	GLN	conflict	PIR B23746

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	156	Total 156	O 156	0	0
3	C	149	Total 149	O 149	0	0
3	D	146	Total 146	O 146	0	0

3 Residue-property plots [i](#)

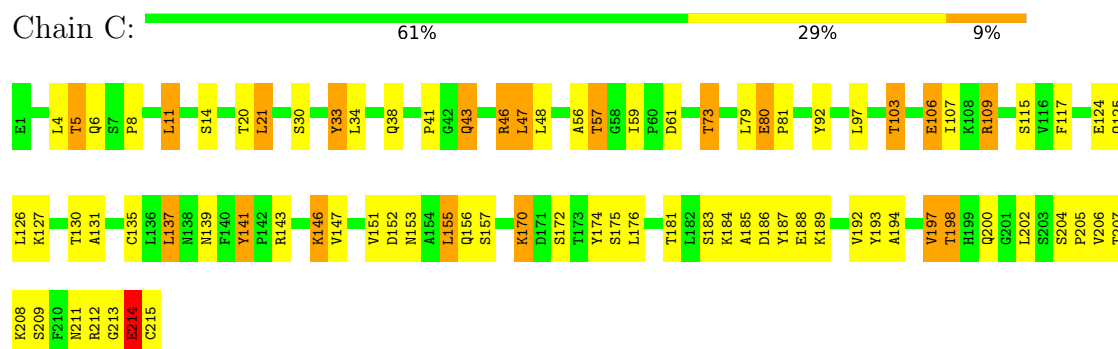
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

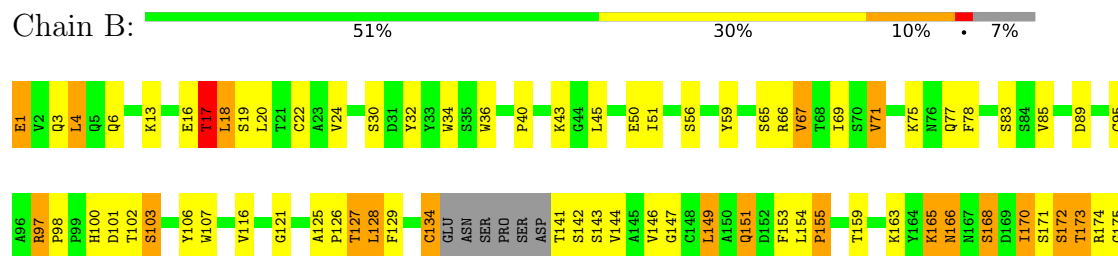
• Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)

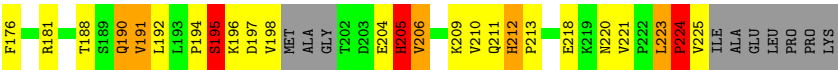


• Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)



• Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)





● Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.88Å 110.88Å 170.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.28	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.28)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7208	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	1.32	4/1673 (0.2%)	1.50	27/2273 (1.2%)
1	C	1.31	2/1673 (0.1%)	1.58	20/2273 (0.9%)
2	B	1.22	1/1703 (0.1%)	1.50	36/2325 (1.5%)
2	D	1.30	5/1708 (0.3%)	1.52	31/2332 (1.3%)
All	All	1.29	12/6757 (0.2%)	1.53	114/9203 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	67	VAL	CA-CB	-7.55	1.45	1.54
2	D	85	VAL	CA-CB	7.26	1.61	1.54
2	B	69	ILE	CA-CB	-6.85	1.46	1.54
1	A	197	VAL	CA-CB	6.75	1.62	1.54
2	D	199	MET	SD-CE	6.15	1.95	1.79
2	D	102	THR	CA-CB	6.11	1.63	1.53
2	D	97	ARG	CA-C	5.76	1.58	1.52
1	A	59	ILE	C-O	-5.72	1.17	1.24
1	A	154	ALA	CA-CB	-5.52	1.46	1.53
1	C	207	THR	CA-CB	5.38	1.60	1.53
1	C	57	THR	CB-CG2	-5.05	1.35	1.52
1	A	89	CYS	CA-C	5.04	1.58	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	ILE	N-CA-C	-8.53	96.23	108.17
1	C	57	THR	CB-CA-C	-8.43	97.19	109.84
1	C	107	ILE	CB-CA-C	-8.25	100.42	111.15
1	A	62	ARG	N-CA-C	-8.23	102.34	112.38
1	A	80	GLU	N-CA-C	-8.18	97.82	110.58
2	D	193	LEU	CA-C-N	-8.05	111.47	119.76
2	D	193	LEU	C-N-CA	-8.05	111.47	119.76
1	C	204	SER	CA-C-N	-8.05	111.49	119.78
1	C	204	SER	C-N-CA	-8.05	111.49	119.78
2	D	67	VAL	N-CA-C	7.93	120.53	108.71
1	C	46	ARG	NE-CZ-NH2	-7.92	112.07	119.20
2	B	71	VAL	CB-CA-C	-7.82	98.67	110.55
2	B	221	VAL	CA-C-N	7.77	128.22	119.83
2	B	221	VAL	C-N-CA	7.77	128.22	119.83
2	D	202	THR	N-CA-C	-7.76	102.17	112.72
2	B	106	TYR	N-CA-C	-7.72	97.66	109.85
1	C	115	SER	N-CA-C	-7.55	96.91	109.07
1	A	115	SER	N-CA-C	-7.53	97.30	109.96
1	A	191	LYS	N-CA-C	7.53	123.19	113.18
1	A	27	GLN	N-CA-C	-7.53	97.28	108.79
1	A	77	SER	N-CA-C	7.38	121.54	112.54
1	A	30	SER	N-CA-C	7.28	120.79	110.23
2	D	107	TRP	N-CA-C	7.16	120.57	108.90
2	D	106	TYR	N-CA-C	-7.08	98.67	109.85
2	B	30	SER	N-CA-C	7.04	120.90	110.48
2	D	152	ASP	N-CA-C	7.04	121.11	111.54
2	D	205	HIS	N-CA-C	7.01	117.76	107.88
2	D	98	PRO	CA-C-N	6.98	126.23	118.97
2	D	98	PRO	C-N-CA	6.98	126.23	118.97
1	C	57	THR	N-CA-CB	6.94	120.24	109.48
1	A	184	LYS	N-CA-C	-6.92	103.81	111.36
1	C	46	ARG	CG-CD-NE	-6.90	96.81	112.00
2	B	212	HIS	CA-C-N	6.82	127.09	119.32
2	B	212	HIS	C-N-CA	6.82	127.09	119.32
1	A	139	ASN	N-CA-C	6.80	120.63	111.24
2	D	197	ASP	N-CA-C	6.74	118.70	111.36
2	B	176	PHE	N-CA-C	6.73	119.60	110.31
2	B	129	PHE	CA-C-N	6.60	126.36	119.76
2	B	129	PHE	C-N-CA	6.60	126.36	119.76
2	B	223	LEU	N-CA-C	-6.60	101.75	109.93
1	C	4	LEU	CA-C-N	-6.59	113.70	122.99
1	C	4	LEU	C-N-CA	-6.59	113.70	122.99
1	A	107	ILE	CB-CA-C	-6.46	102.75	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	SER	N-CA-C	-6.42	102.06	110.33
2	D	203	ASP	N-CA-C	6.36	118.76	108.34
1	A	46	ARG	NE-CZ-NH2	-6.35	113.48	119.20
1	A	100	GLY	N-CA-C	-6.34	102.90	112.60
1	A	129	GLY	N-CA-C	6.34	124.13	115.00
2	B	125	ALA	N-CA-C	-6.32	101.10	110.20
1	C	43	GLN	CB-CA-C	-6.31	99.53	110.45
2	D	133	SER	N-CA-C	6.31	119.82	111.75
1	A	181	THR	N-CA-C	6.30	119.05	108.02
1	C	139	ASN	N-CA-C	6.26	119.99	111.17
1	C	61	ASP	N-CA-C	6.24	120.61	113.19
2	D	167	ASN	N-CA-C	6.22	124.05	110.80
2	D	146	VAL	CA-C-N	-6.13	114.98	121.48
2	D	146	VAL	C-N-CA	-6.13	114.98	121.48
2	D	179	VAL	CB-CA-C	6.08	119.20	110.33
1	C	30	SER	N-CA-C	6.02	118.78	110.35
1	C	197	VAL	N-CA-C	5.99	116.93	108.36
2	D	95	CYS	N-CA-C	-5.94	100.51	109.95
2	D	198	VAL	CB-CA-C	-5.92	104.28	112.04
2	B	191	VAL	N-CA-C	-5.90	99.77	108.85
2	D	170	ILE	N-CA-C	-5.89	99.40	107.99
1	C	11	LEU	N-CA-C	-5.88	99.31	108.90
2	D	67	VAL	CB-CA-C	-5.84	102.74	110.98
2	D	179	VAL	N-CA-CB	-5.83	103.01	111.52
2	B	67	VAL	N-CA-C	5.82	117.38	108.71
1	A	106	GLU	N-CA-CB	-5.79	101.59	110.85
1	A	175	SER	N-CA-C	-5.76	100.30	109.23
1	A	46	ARG	CG-CD-NE	-5.75	99.35	112.00
2	B	224	PRO	CA-C-N	5.66	131.90	121.70
2	B	224	PRO	C-N-CA	5.66	131.90	121.70
2	B	128	LEU	N-CA-C	5.56	118.88	109.76
1	A	137	LEU	N-CA-C	-5.56	99.23	108.34
2	B	107	TRP	N-CA-C	5.52	117.40	108.34
1	A	143	ARG	N-CA-C	5.51	118.05	111.71
2	B	197	ASP	CA-C-N	5.50	131.60	121.70
2	B	197	ASP	C-N-CA	5.50	131.60	121.70
1	C	97	LEU	N-CA-C	-5.49	102.15	110.28
2	B	32	TYR	CA-C-N	-5.47	115.49	122.77
2	B	32	TYR	C-N-CA	-5.47	115.49	122.77
1	C	181	THR	N-CA-C	5.41	117.22	108.41
2	D	16	GLU	CA-C-N	-5.40	115.55	123.00
2	D	16	GLU	C-N-CA	-5.40	115.55	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	GLY	N-CA-C	5.38	125.92	113.18
1	A	43	GLN	CB-CA-C	-5.36	100.95	109.80
1	A	152	ASP	N-CA-C	-5.36	104.02	111.52
2	B	211	GLN	N-CA-C	-5.34	101.18	109.72
2	B	165	LYS	N-CA-C	-5.31	104.91	111.33
2	B	36	TRP	N-CA-C	-5.25	100.83	109.40
2	B	83	SER	N-CA-C	5.20	117.24	110.53
1	C	183	SER	N-CA-C	-5.20	102.78	110.48
2	D	57	THR	N-CA-C	5.20	118.20	110.14
2	B	127	THR	N-CA-C	-5.18	101.25	109.59
1	A	62	ARG	CG-CD-NE	-5.17	100.62	112.00
1	C	175	SER	N-CA-C	-5.17	101.22	109.23
1	A	52	ALA	N-CA-C	5.14	121.75	110.80
2	B	146	VAL	CA-C-N	-5.14	117.50	121.82
2	B	146	VAL	C-N-CA	-5.14	117.50	121.82
2	D	122	SER	N-CA-C	-5.13	101.52	109.72
2	D	111	GLY	N-CA-C	-5.12	104.80	112.89
2	B	147	GLY	N-CA-C	5.11	118.60	111.14
2	B	95	CYS	N-CA-C	-5.10	102.51	110.42
1	A	201	GLY	N-CA-C	-5.09	106.92	115.62
2	B	205	HIS	N-CA-C	5.08	115.03	107.88
1	A	19	ALA	CA-C-N	-5.07	115.62	122.77
1	A	19	ALA	C-N-CA	-5.07	115.62	122.77
2	B	151	GLN	N-CA-C	5.06	117.11	109.41
2	D	225	VAL	N-CA-C	5.06	125.17	111.00
2	D	174	ARG	N-CA-C	-5.06	100.02	110.80
2	D	223	LEU	CA-C-N	5.04	125.12	119.87
2	D	223	LEU	C-N-CA	5.04	125.12	119.87
2	B	17	THR	N-CA-C	5.03	117.10	108.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	33	TYR	Sidechain
1	C	141	TYR	Sidechain
1	C	33	TYR	Sidechain

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	1638	0	1587	79	0
1	C	1638	0	1587	72	0
2	B	1657	0	1601	74	0
2	D	1661	0	1607	72	0
3	A	163	0	0	12	0
3	B	156	0	0	2	1
3	C	149	0	0	9	0
3	D	146	0	0	6	0
All	All	7208	0	6382	284	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 22.

All (284) 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)
2:B:1:GLU:OE1	2:B:1:GLU:N	1.75	1.19
1:C:198:THR:HG22	3:C:2200:HOH:O	1.55	1.04
1:C:215:CYS:HB3	2:D:134:CYS:HB2	1.38	1.04
2:D:1:GLU:N	2:D:1:GLU:OE1	1.91	1.03
2:B:1:GLU:H3	2:B:1:GLU:CD	1.68	1.00
2:B:1:GLU:N	2:B:1:GLU:CD	2.17	0.98
2:D:181:ARG:HB3	2:D:181:ARG:HH11	1.32	0.94
1:A:184:LYS:O	1:A:188:GLU:HG3	1.72	0.87
2:D:181:ARG:HB3	2:D:181:ARG:NH1	1.90	0.87
2:D:181:ARG:HH11	2:D:181:ARG:CB	1.87	0.87
2:D:209:LYS:HG2	2:D:218:GLU:HG2	1.54	0.86
1:C:213:GLY:O	1:C:215:CYS:N	2.09	0.86
1:A:176:LEU:HD23	1:A:176:LEU:C	2.02	0.85
2:B:163:LYS:HD2	2:B:209:LYS:NZ	1.95	0.81
2:D:144:VAL:HG11	2:D:224:PRO:HG3	1.63	0.81
2:B:18:LEU:HD11	2:B:20:LEU:HG	1.63	0.80
2:D:18:LEU:HD22	2:D:116:VAL:HG11	1.65	0.79
1:A:198:THR:HG23	3:A:2131:HOH:O	1.83	0.78
2:B:97:ARG:HD3	2:B:98:PRO:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:HD13	1:C:206:VAL:HG23	1.67	0.76
1:A:167:GLN:HG3	1:A:174:TYR:CZ	2.21	0.75
2:D:1:GLU:N	2:D:1:GLU:CD	2.38	0.75
2:B:18:LEU:HD12	2:B:19:SER:N	2.01	0.74
2:B:181:ARG:HG2	3:B:2444:HOH:O	1.87	0.74
2:B:205:HIS:C	2:B:205:HIS:HD1	1.95	0.74
1:A:198:THR:HG21	3:A:2507:HOH:O	1.88	0.73
2:D:149:LEU:HD23	2:D:188:THR:HG22	1.69	0.73
2:B:17:THR:HG22	3:B:2138:HOH:O	1.89	0.72
2:B:166:ASN:OD1	2:B:168:SER:HB2	1.90	0.72
2:B:18:LEU:HD12	2:B:18:LEU:C	2.15	0.72
1:A:8:PRO:O	1:A:103:THR:HB	1.90	0.71
2:B:143:SER:HA	2:B:194:PRO:HA	1.72	0.71
1:C:8:PRO:O	1:C:103:THR:HB	1.91	0.71
2:B:34:TRP:CH2	2:B:97:ARG:HG3	2.26	0.70
2:B:205:HIS:C	2:B:205:HIS:ND1	2.48	0.70
1:C:215:CYS:HB3	2:D:134:CYS:CB	2.20	0.70
1:C:153:ASN:ND2	3:C:2599:HOH:O	2.15	0.70
2:D:103:SER:HB2	3:D:2351:HOH:O	1.92	0.70
2:B:18:LEU:HD22	2:B:116:VAL:HG11	1.74	0.69
2:B:149:LEU:HD23	2:B:188:THR:HG22	1.74	0.69
1:C:143:ARG:HD2	1:C:143:ARG:O	1.92	0.69
2:D:209:LYS:HG2	2:D:218:GLU:CG	2.21	0.69
1:A:20:THR:HG23	3:A:2491:HOH:O	1.94	0.68
2:D:63:LEU:O	2:D:65:SER:OG	2.10	0.68
1:C:20:THR:HG23	3:C:2452:HOH:O	1.92	0.67
1:A:215:CYS:SG	2:B:134:CYS:CB	2.84	0.66
1:A:61:ASP:HB2	3:A:2460:HOH:O	1.96	0.66
2:B:172:SER:O	2:B:191:VAL:HA	1.96	0.66
2:D:173:THR:HG22	3:D:2576:HOH:O	1.95	0.66
2:B:142:SER:HA	2:B:195:SER:HB2	1.78	0.66
2:D:34:TRP:O	2:D:50:GLU:HA	1.96	0.66
2:B:40:PRO:HB2	2:B:43:LYS:HG3	1.78	0.65
1:A:37:TYR:OH	1:A:90:GLN:NE2	2.29	0.65
1:A:156:GLN:HG3	1:A:159:ASN:HD21	1.61	0.65
1:C:146:LYS:HB3	1:C:198:THR:HG23	1.78	0.65
2:D:1:GLU:CD	2:D:1:GLU:H3	1.92	0.65
2:B:165:LYS:HG3	2:B:205:HIS:CE1	2.31	0.64
2:B:170:ILE:HD11	2:B:206:VAL:CG2	2.26	0.64
2:B:163:LYS:HD2	2:B:209:LYS:HZ2	1.62	0.64
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLU:CD	2:B:1:GLU:H1	2.05	0.63
2:B:205:HIS:CD2	2:B:220:ASN:HB3	2.33	0.63
2:B:16:GLU:O	2:B:85:VAL:HG22	1.99	0.62
2:D:18:LEU:HD12	2:D:19:SER:N	2.15	0.62
2:D:17:THR:HG22	3:D:2216:HOH:O	2.01	0.61
3:C:2600:HOH:O	2:D:174:ARG:HD2	2.00	0.61
1:C:192:VAL:HG22	1:C:211:ASN:OD1	2.00	0.61
2:D:34:TRP:CZ3	2:D:97:ARG:HB2	2.36	0.61
2:B:142:SER:CA	2:B:195:SER:HB2	2.31	0.61
2:B:224:PRO:O	2:B:225:VAL:HG12	2.02	0.60
1:C:33:TYR:HB3	1:C:92:TYR:CD1	2.37	0.60
1:A:114:PRO:HB3	1:A:140:PHE:HB3	1.83	0.60
1:C:188:GLU:O	1:C:212:ARG:NH2	2.35	0.60
2:D:67:VAL:HG22	2:D:82:LEU:CD1	2.32	0.60
2:B:100:HIS:HB2	2:B:103:SER:HB2	1.83	0.59
1:C:124:GLU:OE1	2:D:219:LYS:NZ	2.33	0.59
1:A:103:THR:HG21	3:A:2086:HOH:O	2.03	0.59
1:C:43:GLN:NE2	1:C:43:GLN:N	2.51	0.59
2:D:144:VAL:HG11	2:D:224:PRO:CG	2.33	0.58
1:C:41:PRO:O	1:C:43:GLN:NE2	2.37	0.58
1:C:170:LYS:NZ	1:C:170:LYS:HB3	2.18	0.58
1:C:198:THR:HB	1:C:205:PRO:HG3	1.84	0.58
2:D:97:ARG:HD3	2:D:98:PRO:O	2.03	0.58
2:D:216:ASN:C	2:D:217:LYS:HG2	2.28	0.58
1:A:18:ARG:HH21	1:A:77:SER:HB2	1.69	0.57
2:D:1:GLU:OE1	2:D:1:GLU:CA	2.53	0.57
2:B:174:ARG:HG3	2:B:190:GLN:O	2.05	0.57
1:A:159:ASN:N	1:A:159:ASN:OD1	2.37	0.56
2:D:198:VAL:HG23	2:D:199:MET:N	2.20	0.56
1:A:109:ARG:HD3	1:A:110:THR:O	2.03	0.56
1:A:176:LEU:C	1:A:176:LEU:CD2	2.76	0.56
2:D:18:LEU:HD12	2:D:18:LEU:C	2.30	0.56
1:A:167:GLN:HG3	1:A:174:TYR:OH	2.04	0.56
2:B:18:LEU:CD1	2:B:20:LEU:HG	2.36	0.56
1:A:21:LEU:HD23	1:A:21:LEU:N	2.21	0.56
1:C:5:THR:HG23	3:C:2169:HOH:O	2.06	0.56
1:A:55:ARG:NH1	3:A:2402:HOH:O	2.40	0.55
2:D:144:VAL:CG1	2:D:224:PRO:HG3	2.35	0.55
2:D:197:ASP:OD2	2:D:197:ASP:N	2.39	0.55
1:C:184:LYS:O	1:C:188:GLU:HG3	2.07	0.55
2:D:148:CYS:HB2	2:D:162:TRP:CH2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:TYR:CZ	2:D:170:ILE:HG12	2.42	0.55
2:B:212:HIS:CG	2:B:213:PRO:HD2	2.42	0.55
1:C:80:GLU:HG3	1:C:81:PRO:CD	2.36	0.55
1:C:143:ARG:HG2	1:C:143:ARG:NH1	2.21	0.55
2:B:165:LYS:HG3	2:B:205:HIS:HE1	1.72	0.55
2:D:128:LEU:HD21	2:D:210:VAL:HG11	1.89	0.55
1:A:113:ALA:HB1	1:A:202:LEU:CD2	2.37	0.54
2:B:34:TRP:HB3	2:B:78:PHE:CZ	2.43	0.54
2:B:97:ARG:CD	2:B:98:PRO:O	2.54	0.54
1:C:126:LEU:HD21	1:C:131:ALA:HB2	1.90	0.53
1:A:47:LEU:HD13	1:A:56:ALA:HB2	1.89	0.53
1:A:103:THR:CG2	3:A:2086:HOH:O	2.56	0.53
2:B:142:SER:C	2:B:195:SER:HB2	2.34	0.53
2:D:63:LEU:HD22	2:D:82:LEU:HD11	1.91	0.53
1:A:148:GLN:HG2	1:A:155:LEU:CD2	2.39	0.53
1:A:22:SER:HB3	3:A:2264:HOH:O	2.08	0.53
1:A:206:VAL:CG1	1:A:207:THR:N	2.70	0.53
2:B:170:ILE:HD11	2:B:206:VAL:HG21	1.90	0.53
1:A:215:CYS:HB2	3:A:2424:HOH:O	2.08	0.52
1:C:6:GLN:HB3	1:C:103:THR:HG22	1.90	0.52
1:C:38:GLN:HB2	1:C:48:LEU:HD11	1.91	0.52
2:D:34:TRP:HB3	2:D:78:PHE:CZ	2.44	0.52
2:D:159:THR:O	2:D:210:VAL:HA	2.09	0.52
1:A:189:LYS:O	1:A:190:HIS:CG	2.63	0.52
1:A:18:ARG:HD3	3:A:2004:HOH:O	2.10	0.52
1:A:215:CYS:SG	2:B:134:CYS:HB3	2.49	0.52
1:C:109:ARG:HD2	1:C:141:TYR:CG	2.45	0.52
2:D:144:VAL:HG13	3:D:2573:HOH:O	2.09	0.52
2:B:142:SER:HA	2:B:195:SER:CB	2.40	0.51
2:D:131:LEU:HD23	3:D:2597:HOH:O	2.09	0.51
1:A:139:ASN:HD21	2:B:174:ARG:NH2	2.09	0.51
1:C:11:LEU:HD12	1:C:21:LEU:HD22	1.92	0.51
1:C:106:GLU:HG3	1:C:174:TYR:OH	2.10	0.51
2:B:209:LYS:HE2	2:B:218:GLU:OE2	2.11	0.51
1:A:119:PHE:HE2	1:A:136:LEU:HD22	1.76	0.51
1:A:136:LEU:HD23	2:B:190:GLN:NE2	2.26	0.51
1:A:144:GLU:CD	1:A:144:GLU:H	2.19	0.51
1:A:148:GLN:HG2	1:A:155:LEU:HD23	1.94	0.50
2:D:164:TYR:CE1	2:D:170:ILE:HG12	2.47	0.50
1:A:141:TYR:CD2	1:A:142:PRO:HA	2.46	0.50
2:B:209:LYS:HG2	2:B:218:GLU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLN:CG	1:A:159:ASN:HD21	2.25	0.50
1:A:62:ARG:HD2	1:A:83:ASP:OD2	2.12	0.50
1:C:186:ASP:HA	1:C:189:LYS:HE2	1.93	0.50
2:B:163:LYS:HD2	2:B:209:LYS:HZ1	1.75	0.49
2:D:198:VAL:CG2	2:D:199:MET:N	2.74	0.49
1:A:87:TYR:O	1:A:102:GLY:HA2	2.12	0.49
1:A:150:LYS:HB2	1:A:194:ALA:HB3	1.93	0.49
2:B:126:PRO:HB3	2:B:153:PHE:HB3	1.94	0.49
2:D:34:TRP:HB3	2:D:78:PHE:CE1	2.47	0.49
1:A:40:LYS:HB2	1:A:43:GLN:HG3	1.94	0.49
2:D:63:LEU:HB3	2:D:67:VAL:CG2	2.43	0.49
1:A:1:GLU:HG3	1:A:98:THR:HG21	1.93	0.49
2:B:34:TRP:CZ3	2:B:97:ARG:HG3	2.48	0.49
2:B:34:TRP:O	2:B:50:GLU:HA	2.11	0.49
2:B:143:SER:HA	2:B:195:SER:H	1.77	0.49
1:A:137:LEU:HD22	1:A:197:VAL:HG21	1.95	0.48
1:A:161:GLN:OE1	2:B:181:ARG:HD3	2.13	0.48
2:B:154:LEU:HD12	2:B:155:PRO:HA	1.96	0.48
1:C:146:LYS:HE2	1:C:198:THR:CG2	2.43	0.48
2:D:38:ARG:HD3	2:D:48:ILE:HD11	1.94	0.48
2:D:66:ARG:HH22	2:D:89:ASP:CG	2.22	0.48
2:D:163:LYS:NZ	2:D:169:ASP:OD1	2.43	0.48
2:B:170:ILE:HD11	2:B:206:VAL:HG22	1.94	0.48
2:B:205:HIS:HA	2:B:223:LEU:HG	1.95	0.47
1:C:143:ARG:HD2	1:C:143:ARG:C	2.39	0.47
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.96	0.47
1:A:136:LEU:C	1:A:137:LEU:HD23	2.38	0.47
1:C:43:GLN:N	1:C:43:GLN:CD	2.71	0.47
1:C:146:LYS:HB3	1:C:146:LYS:HE2	1.74	0.47
1:C:146:LYS:NZ	1:C:198:THR:HG21	2.29	0.47
2:D:181:ARG:NH1	2:D:181:ARG:CB	2.60	0.47
1:A:37:TYR:HE2	1:A:90:GLN:HE21	1.63	0.47
2:B:3:GLN:C	2:B:4:LEU:HD23	2.39	0.47
2:B:170:ILE:CD1	2:B:206:VAL:HG21	2.45	0.47
1:A:119:PHE:CE2	1:A:136:LEU:HD22	2.50	0.47
2:B:13:LYS:HE3	2:B:121:GLY:O	2.15	0.47
1:C:213:GLY:C	1:C:215:CYS:H	2.16	0.47
2:D:17:THR:HB	2:D:83:SER:HA	1.95	0.47
2:B:75:LYS:HB2	2:B:77:GLN:HG3	1.97	0.46
2:B:1:GLU:OE1	2:B:1:GLU:CA	2.57	0.46
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ARG:HH22	2:B:89:ASP:CG	2.23	0.46
1:A:125:GLN:HG2	1:A:130:THR:O	2.16	0.46
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.56	0.46
2:D:34:TRP:CZ3	2:D:97:ARG:HG3	2.49	0.46
2:D:28:SER:HB2	3:D:2376:HOH:O	2.16	0.46
1:A:18:ARG:NH2	1:A:77:SER:HB2	2.30	0.46
2:B:18:LEU:C	2:B:18:LEU:CD1	2.88	0.46
2:B:34:TRP:CZ3	2:B:97:ARG:HB2	2.50	0.46
1:A:144:GLU:CD	1:A:144:GLU:N	2.74	0.46
2:D:34:TRP:CH2	2:D:97:ARG:HG3	2.51	0.46
2:D:34:TRP:CE3	2:D:97:ARG:HB2	2.50	0.45
1:A:6:GLN:HB3	1:A:103:THR:HG22	1.98	0.45
2:B:24:VAL:HG21	2:B:34:TRP:CH2	2.51	0.45
1:A:32:ASN:OD1	1:A:68:SER:HA	2.15	0.45
1:A:138:ASN:HB3	1:A:139:ASN:ND2	2.32	0.45
1:C:215:CYS:CB	2:D:134:CYS:SG	3.04	0.45
2:D:33:TYR:HB3	2:D:50:GLU:HB2	1.99	0.45
1:C:92:TYR:CE1	2:D:104:GLY:HA3	2.51	0.45
2:B:128:LEU:HD11	2:B:210:VAL:HG22	1.97	0.45
2:D:64:LYS:NZ	2:D:64:LYS:HB3	2.31	0.45
1:C:193:TYR:HE1	1:C:212:ARG:HG3	1.82	0.45
1:C:5:THR:CG2	3:C:2169:HOH:O	2.63	0.45
2:D:66:ARG:NH2	2:D:89:ASP:OD2	2.49	0.45
2:D:102:THR:O	2:D:103:SER:O	2.34	0.45
1:A:198:THR:CG2	3:A:2131:HOH:O	2.52	0.44
1:C:146:LYS:HB3	1:C:198:THR:CG2	2.45	0.44
2:D:216:ASN:O	2:D:217:LYS:HG2	2.17	0.44
2:B:212:HIS:HA	2:B:213:PRO:HD3	1.80	0.44
1:A:176:LEU:HD23	1:A:177:SER:N	2.32	0.44
1:C:109:ARG:HD2	1:C:141:TYR:CB	2.48	0.44
1:C:6:GLN:HB3	1:C:103:THR:CG2	2.47	0.44
1:C:215:CYS:CB	2:D:134:CYS:HG	2.27	0.44
1:A:107:ILE:HB	1:A:167:GLN:HE22	1.82	0.44
1:A:213:GLY:O	1:C:127:LYS:HG2	2.17	0.44
2:B:4:LEU:HD23	2:B:4:LEU:N	2.33	0.44
1:C:185:ALA:O	1:C:189:LYS:HG3	2.17	0.44
2:D:5:GLN:O	2:D:22:CYS:HA	2.18	0.44
1:A:61:ASP:OD1	1:A:61:ASP:C	2.61	0.43
1:A:168:ASP:HB3	1:A:171:ASP:OD1	2.18	0.43
1:C:48:LEU:CD2	1:C:59:ILE:HD12	2.48	0.43
1:C:146:LYS:CB	1:C:198:THR:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:SER:O	2:B:173:THR:N	2.51	0.43
1:C:176:LEU:HD23	1:C:176:LEU:C	2.43	0.43
1:A:84:PHE:CD2	1:A:105:VAL:HG12	2.53	0.43
1:A:117:PHE:CD1	1:A:117:PHE:N	2.87	0.43
1:A:194:ALA:HB2	1:A:209:SER:HB3	2.01	0.43
1:A:206:VAL:HG12	1:A:207:THR:N	2.32	0.43
1:C:213:GLY:C	1:C:215:CYS:N	2.77	0.43
2:D:18:LEU:HD11	2:D:20:LEU:HG	2.00	0.43
1:A:43:GLN:HB2	3:A:2008:HOH:O	2.19	0.43
1:C:103:THR:CG2	3:C:2170:HOH:O	2.67	0.43
2:B:166:ASN:OD1	2:B:166:ASN:C	2.62	0.43
1:C:155:LEU:HD22	1:C:156:GLN:O	2.18	0.43
2:D:102:THR:HG22	2:D:103:SER:H	1.84	0.43
2:D:128:LEU:HD21	2:D:210:VAL:CG1	2.49	0.43
1:A:185:ALA:O	1:A:188:GLU:HB2	2.19	0.43
1:C:46:ARG:HD3	3:C:2049:HOH:O	2.19	0.43
1:C:47:LEU:HD13	1:C:56:ALA:HB2	1.99	0.43
1:C:151:VAL:HB	1:C:156:GLN:NE2	2.34	0.43
1:A:199:HIS:O	1:A:202:LEU:HB2	2.18	0.42
2:B:59:TYR:CE2	2:B:67:VAL:HG12	2.54	0.42
1:C:137:LEU:HD22	1:C:197:VAL:HG21	2.02	0.42
1:C:33:TYR:HB3	1:C:92:TYR:CE1	2.54	0.42
2:D:61:PRO:C	2:D:63:LEU:H	2.27	0.42
1:C:125:GLN:HG2	1:C:130:THR:O	2.19	0.42
2:D:170:ILE:HD11	2:D:206:VAL:HG22	2.01	0.42
1:C:212:ARG:O	1:C:214:GLU:N	2.50	0.42
1:C:126:LEU:CD2	1:C:131:ALA:HB2	2.49	0.42
1:C:187:TYR:CE2	1:C:212:ARG:HD3	2.54	0.42
1:A:141:TYR:CG	1:A:142:PRO:HA	2.54	0.42
1:A:193:TYR:O	1:A:209:SER:HA	2.19	0.42
1:C:11:LEU:CD1	1:C:21:LEU:HD22	2.49	0.42
1:C:215:CYS:CB	2:D:134:CYS:HB2	2.29	0.42
1:C:109:ARG:HG2	1:C:172:SER:HB2	2.01	0.42
1:A:176:LEU:HD23	1:A:176:LEU:O	2.17	0.41
1:C:193:TYR:O	1:C:209:SER:HB2	2.20	0.41
1:C:117:PHE:O	1:C:135:CYS:HA	2.20	0.41
1:C:147:VAL:HG22	1:C:197:VAL:HG22	2.02	0.41
1:C:194:ALA:CB	1:C:209:SER:HB3	2.51	0.41
2:D:102:THR:CG2	2:D:103:SER:N	2.84	0.41
1:A:137:LEU:CD2	1:A:197:VAL:HG21	2.51	0.41
2:B:143:SER:CA	2:B:195:SER:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASP:OD1	2:B:102:THR:N	2.54	0.41
1:A:62:ARG:HE	1:A:62:ARG:HB3	1.62	0.41
1:A:95:SER:HA	1:A:96:PRO:HA	1.78	0.41
2:B:51:ILE:HA	2:B:56:SER:O	2.21	0.41
1:C:152:ASP:O	1:C:153:ASN:HB2	2.20	0.41
1:C:208:LYS:HD3	1:C:208:LYS:HA	1.92	0.41
2:D:221:VAL:HA	2:D:222:PRO:HD3	1.82	0.41
1:A:143:ARG:HB2	1:A:174:TYR:CE1	2.55	0.40
1:C:73:THR:CG2	3:C:2538:HOH:O	2.68	0.40
2:D:209:LYS:CG	2:D:218:GLU:HG2	2.36	0.40
1:A:11:LEU:HD12	1:A:21:LEU:HD22	2.03	0.40
1:A:114:PRO:HB3	1:A:140:PHE:CD2	2.56	0.40
1:C:211:ASN:HB2	1:C:214:GLU:OE2	2.21	0.40
2:D:163:LYS:HE3	2:D:167:ASN:OD1	2.22	0.40
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.76	0.40
1:A:148:GLN:CG	1:A:155:LEU:HD21	2.51	0.40
2:B:101:ASP:OD1	2:B:102:THR:HG23	2.21	0.40
1:A:62:ARG:HG2	1:A:63:PHE:CD1	2.57	0.40
2:B:212:HIS:CD2	2:B:213:PRO:HD2	2.56	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)
3:B:2132:HOH:O	3:B:2132:HOH:O[6_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	213/215 (99%)	203 (95%)	9 (4%)	1 (0%)	24 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	24	29
2	B	210/232 (90%)	194 (92%)	12 (6%)	4 (2%)	6	5
2	D	213/232 (92%)	198 (93%)	11 (5%)	4 (2%)	6	5
All	All	849/894 (95%)	794 (94%)	45 (5%)	10 (1%)	10	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	SER
1	C	214	GLU
2	D	64	LYS
2	D	103	SER
2	D	167	ASN
2	B	195	SER
2	D	174	ARG
2	B	224	PRO
1	A	185	ALA
2	B	196	LYS

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	185/185 (100%)	165 (89%)	20 (11%)	6	6
1	C	185/185 (100%)	165 (89%)	20 (11%)	6	6
2	B	187/200 (94%)	159 (85%)	28 (15%)	3	2
2	D	186/200 (93%)	156 (84%)	30 (16%)	2	2
All	All	743/770 (96%)	645 (87%)	98 (13%)	4	4

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	21	LEU
1	A	34	LEU
1	A	47	LEU
1	A	79	LEU
1	A	90	GLN
1	A	95	SER
1	A	103	THR
1	A	107	ILE
1	A	109	ARG
1	A	136	LEU
1	A	137	LEU
1	A	142	PRO
1	A	156	GLN
1	A	176	LEU
1	A	177	SER
1	A	182	LEU
1	A	191	LYS
1	A	198	THR
2	B	1	GLU
2	B	4	LEU
2	B	6	GLN
2	B	17	THR
2	B	18	LEU
2	B	45	LEU
2	B	65	SER
2	B	71	VAL
2	B	97	ARG
2	B	103	SER
2	B	127	THR
2	B	134	CYS
2	B	141	THR
2	B	144	VAL
2	B	149	LEU
2	B	151	GLN
2	B	155	PRO
2	B	159	THR
2	B	166	ASN
2	B	168	SER
2	B	173	THR
2	B	190	GLN
2	B	192	LEU

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Mol	Chain	Res	Type
2	B	195	SER
2	B	198	VAL
2	B	204	GLU
2	B	205	HIS
2	B	206	VAL
1	C	5	THR
1	C	14	SER
1	C	21	LEU
1	C	34	LEU
1	C	47	LEU
1	C	57	THR
1	C	73	THR
1	C	79	LEU
1	C	80	GLU
1	C	103	THR
1	C	106	GLU
1	C	109	ARG
1	C	137	LEU
1	C	146	LYS
1	C	155	LEU
1	C	157	SER
1	C	170	LYS
1	C	198	THR
1	C	200	GLN
1	C	214	GLU
2	D	1	GLU
2	D	14	PRO
2	D	17	THR
2	D	18	LEU
2	D	28	SER
2	D	43	LYS
2	D	56	SER
2	D	64	LYS
2	D	65	SER
2	D	85	VAL
2	D	97	ARG
2	D	102	THR
2	D	122	SER
2	D	134	CYS
2	D	149	LEU
2	D	171	SER
2	D	173	THR

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Mol	Chain	Res	Type
2	D	179	VAL
2	D	181	ARG
2	D	188	THR
2	D	195	SER
2	D	196	LYS
2	D	197	ASP
2	D	199	MET
2	D	202	THR
2	D	203	ASP
2	D	204	GLU
2	D	206	VAL
2	D	208	CYS
2	D	217	LYS

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	90	GLN
1	A	138	ASN
1	A	153	ASN
1	A	156	GLN
1	A	200	GLN
2	B	190	GLN
2	B	211	GLN
1	C	43	GLN
2	D	76	ASN
2	D	100	HIS
2	D	151	GLN
2	D	205	HIS
2	D	211	GLN
2	D	214	ASN
2	D	220	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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

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.