



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:06 AM UTC

PDB ID : 1F15 / pdb_00001f15
Title : CUCUMBER MOSAIC VIRUS (STRAIN FNY)
Authors : Smith, T.J.; Chase, E.; Schmidt, T.; Perry, K.
Deposited on : 2000-05-18
Resolution : 3.20 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

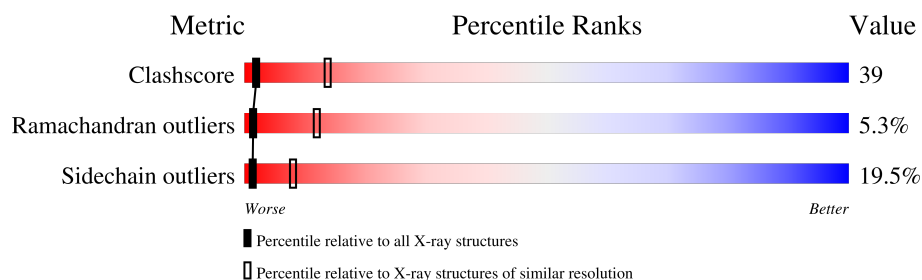
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	218	
1	B	218	
1	C	218	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4200 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 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1229	784	209	232	4			
1	B	190	Total	C	N	O	S	0	0	0
			1483	942	259	278	4			
1	C	191	Total	C	N	O	S	0	0	0
			1488	945	260	279	4			

There are 3 discrepancies between the modelled and reference sequences:

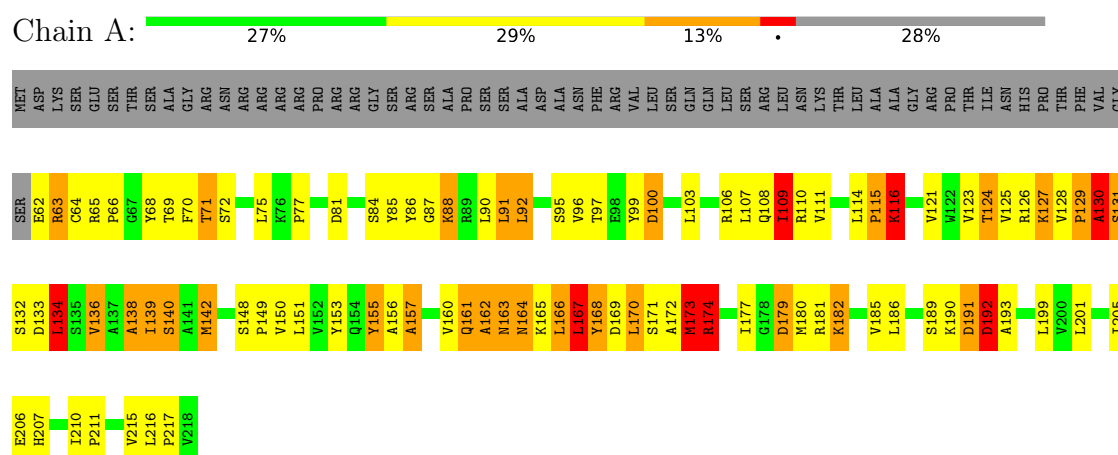
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	LEU	ILE	conflict	UNP P69466
B	107	LEU	ILE	conflict	UNP P69466
C	107	LEU	ILE	conflict	UNP P69466

3 Residue-property plots

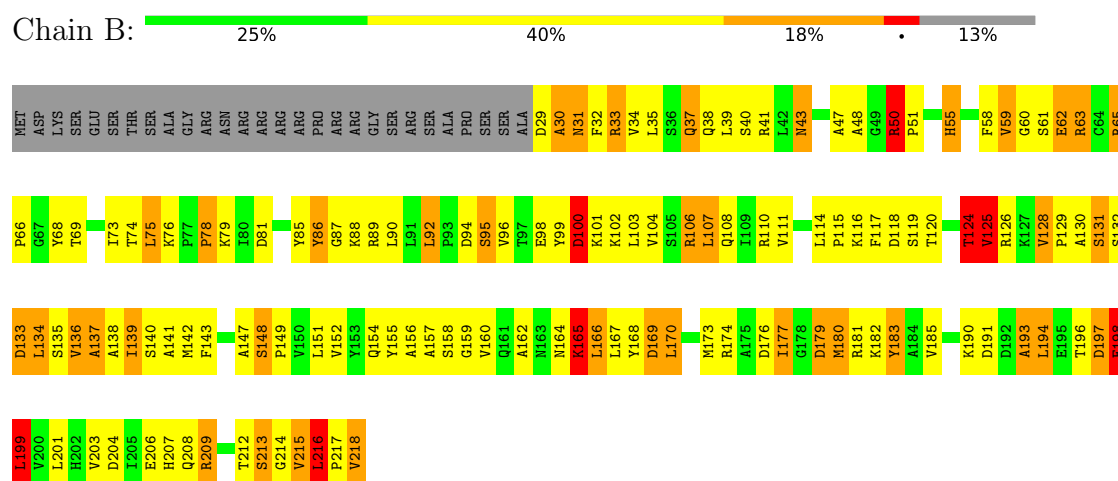
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

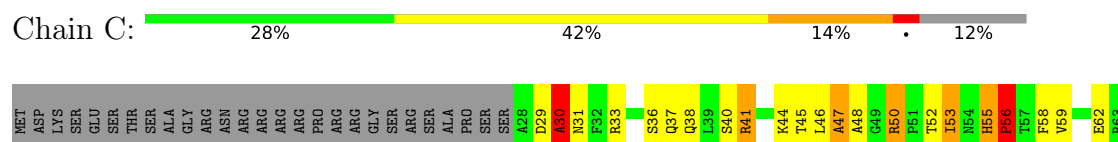
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4 ₂ 3 ₂	Depositor
Cell constants a, b, c, α , β , γ	336.00 Å 336.00 Å 336.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4200	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	5/1254 (0.4%)	1.58	27/1704 (1.6%)
1	B	1.02	3/1513 (0.2%)	1.61	39/2056 (1.9%)
1	C	0.96	1/1518 (0.1%)	1.58	33/2063 (1.6%)
All	All	1.03	9/4285 (0.2%)	1.59	99/5823 (1.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ALA	CA-CB	9.30	1.69	1.53
1	A	167	LEU	CA-C	9.07	1.63	1.53
1	A	168	TYR	N-CA	6.36	1.54	1.46
1	C	180	MET	SD-CE	-6.25	1.64	1.79
1	A	168	TYR	CA-C	6.05	1.60	1.52
1	B	125	VAL	CA-CB	-5.55	1.46	1.54
1	B	180	MET	SD-CE	-5.41	1.66	1.79
1	B	128	VAL	CA-CB	-5.38	1.49	1.54
1	A	142	MET	SD-CE	5.04	1.92	1.79

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	LEU	N-CA-C	14.31	126.65	108.19
1	C	55	HIS	CA-C-N	12.22	135.12	119.84
1	C	55	HIS	C-N-CA	12.22	135.12	119.84
1	B	198	GLU	N-CA-C	-12.21	84.78	110.80
1	A	155	TYR	N-CA-C	11.19	127.45	112.13
1	A	138	ALA	N-CA-C	-10.61	100.18	113.55
1	C	132	SER	N-CA-C	-9.89	101.42	113.19
1	B	92	LEU	CA-C-N	9.76	129.82	119.76
1	B	92	LEU	C-N-CA	9.76	129.82	119.76
1	C	172	ALA	N-CA-C	9.49	123.03	112.97
1	A	167	LEU	CA-C-N	9.29	139.29	121.54
1	A	167	LEU	C-N-CA	9.29	139.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	SER	CA-C-N	9.20	129.24	119.76
1	C	148	SER	C-N-CA	9.20	129.24	119.76
1	B	55	HIS	CA-C-N	8.70	130.72	119.84
1	B	55	HIS	C-N-CA	8.70	130.72	119.84
1	C	128	VAL	CA-C-N	8.55	130.53	119.84
1	C	128	VAL	C-N-CA	8.55	130.53	119.84
1	A	157	ALA	N-CA-C	-8.20	97.67	109.96
1	B	193	ALA	N-CA-C	-8.11	93.52	110.80
1	A	163	ASN	N-CA-C	7.96	122.54	109.24
1	A	130	ALA	N-CA-C	-7.89	94.00	110.80
1	B	148	SER	CA-C-N	7.43	127.41	119.76
1	B	148	SER	C-N-CA	7.43	127.41	119.76
1	B	62	GLU	N-CA-C	7.41	121.55	109.85
1	A	161	GLN	N-CA-C	-7.28	95.17	107.99
1	C	124	THR	CB-CA-C	-7.22	97.02	111.17
1	C	96	VAL	CB-CA-C	-7.20	103.31	111.80
1	B	30	ALA	N-CA-C	7.20	120.93	110.42
1	A	72	SER	N-CA-C	7.18	120.63	109.07
1	B	48	ALA	N-CA-C	7.17	120.35	110.24
1	C	77	PRO	N-CA-C	7.15	118.23	110.58
1	B	128	VAL	CA-C-N	7.08	127.48	119.83
1	B	128	VAL	C-N-CA	7.08	127.48	119.83
1	C	65	ARG	N-CA-C	-6.94	100.83	109.64
1	C	77	PRO	CA-C-N	6.88	126.81	120.21
1	C	77	PRO	C-N-CA	6.88	126.81	120.21
1	C	212	THR	N-CA-C	6.82	121.61	113.28
1	B	124	THR	CB-CA-C	-6.75	97.95	111.17
1	B	213	SER	N-CA-C	6.72	119.23	110.43
1	A	216	LEU	CA-C-N	6.61	126.99	119.92
1	A	216	LEU	C-N-CA	6.61	126.99	119.92
1	C	100	ASP	N-CA-C	6.60	120.59	112.54
1	B	173	MET	N-CA-C	6.55	120.26	112.93
1	B	165	LYS	N-CA-C	6.49	118.72	108.79
1	B	128	VAL	N-CA-C	6.33	114.42	108.15
1	A	92	LEU	CA-C-N	6.30	126.27	119.78
1	A	92	LEU	C-N-CA	6.30	126.27	119.78
1	A	109	ILE	CB-CA-C	-6.26	102.23	111.19
1	C	47	ALA	N-CA-C	-6.26	103.74	111.75
1	B	131	SER	N-CA-C	-6.26	104.21	112.34
1	C	64	CYS	N-CA-C	6.24	119.27	110.23
1	A	114	LEU	N-CA-C	-6.23	102.01	110.36
1	C	179	ASP	N-CA-C	6.22	118.87	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	N-CA-C	6.04	119.01	109.96
1	B	96	VAL	CB-CA-C	-5.97	104.10	111.92
1	C	116	LYS	N-CA-C	5.97	121.60	113.37
1	A	151	LEU	N-CA-C	-5.93	99.52	109.07
1	B	50	ARG	CA-C-N	5.84	126.03	120.31
1	B	50	ARG	C-N-CA	5.84	126.03	120.31
1	C	190	LYS	N-CA-C	5.83	121.88	110.56
1	A	168	TYR	CB-CA-C	-5.81	98.86	110.42
1	C	210	ILE	CA-C-N	5.81	125.82	119.90
1	C	210	ILE	C-N-CA	5.81	125.82	119.90
1	B	216	LEU	N-CA-C	-5.65	101.19	109.50
1	A	162	ALA	CA-C-N	-5.63	113.60	122.73
1	A	162	ALA	C-N-CA	-5.63	113.60	122.73
1	B	32	PHE	N-CA-C	-5.57	105.30	111.71
1	B	217	PRO	CA-C-N	5.56	131.71	121.70
1	B	217	PRO	C-N-CA	5.56	131.71	121.70
1	A	172	ALA	N-CA-C	5.55	119.91	113.20
1	C	69	THR	N-CA-C	-5.54	101.08	108.34
1	A	77	PRO	CA-C-N	5.50	126.71	119.84
1	A	77	PRO	C-N-CA	5.50	126.71	119.84
1	B	103	LEU	N-CA-C	5.47	118.17	109.96
1	A	115	PRO	N-CA-C	-5.47	102.60	111.14
1	C	138	ALA	N-CA-C	-5.46	104.72	111.33
1	C	109	ILE	N-CA-C	-5.46	100.59	108.89
1	A	173	MET	N-CA-C	-5.43	105.09	112.26
1	B	169	ASP	N-CA-C	5.41	117.46	108.20
1	C	108	GLN	N-CA-C	5.41	118.29	110.28
1	B	63	ARG	N-CA-C	-5.32	103.51	110.53
1	C	123	VAL	N-CA-C	5.27	117.45	108.86
1	C	175	ALA	N-CA-C	-5.26	101.37	109.52
1	C	62	GLU	N-CA-C	5.26	118.31	109.95
1	B	190	LYS	N-CA-C	5.25	119.69	113.12
1	B	76	LYS	CA-C-N	5.22	123.42	119.66
1	B	76	LYS	C-N-CA	5.22	123.42	119.66
1	A	100	ASP	N-CA-C	5.19	121.85	110.80
1	B	100	ASP	N-CA-C	5.17	121.81	110.80
1	B	51	PRO	N-CA-C	-5.13	103.77	111.57
1	C	56	PRO	N-CA-C	5.13	123.04	112.47
1	B	78	PRO	N-CA-C	-5.12	101.92	112.47
1	C	30	ALA	N-CA-C	5.11	121.68	110.80
1	B	60	GLY	CA-C-O	-5.09	117.19	122.28
1	B	157	ALA	CA-C-N	5.03	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ALA	C-N-CA	5.03	127.52	120.28
1	B	37	GLN	N-CA-C	-5.01	105.89	111.36
1	C	197	ASP	N-CA-C	5.01	121.47	110.80

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	1229	0	1254	99	0
1	B	1483	0	1513	135	0
1	C	1488	0	1518	119	0
All	All	4200	0	4285	329	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 39.

All (329) 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:130:ALA:HB3	1:A:133:ASP:HB3	1.23	1.10
1:A:64:CYS:SG	1:B:214:GLY:HA2	1.98	1.03
1:B:134:LEU:HD23	1:B:135:SER:H	1.31	0.96
1:A:69:THR:HG21	1:B:212:THR:HB	1.47	0.96
1:C:126:ARG:HD2	1:C:142:MET:HE2	1.48	0.95
1:C:107:LEU:HD22	1:C:180:MET:HE1	1.47	0.94
1:C:134:LEU:CD2	1:C:136:VAL:HG22	2.02	0.90
1:C:124:THR:HG23	1:C:149:PRO:O	1.72	0.89
1:C:126:ARG:HH22	1:C:147:ALA:HB3	1.40	0.87
1:C:126:ARG:NH2	1:C:147:ALA:HB3	1.90	0.86
1:B:120:THR:HG22	1:B:154:GLN:HG3	1.58	0.86
1:B:104:VAL:HG21	1:B:180:MET:SD	2.16	0.85
1:A:70:PHE:CZ	1:B:216:LEU:HD23	2.10	0.84
1:C:73:ILE:HD11	1:C:92:LEU:HD23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ARG:HB3	1:B:169:ASP:HA	1.62	0.81
1:A:64:CYS:HA	1:A:106:ARG:NH2	1.95	0.81
1:A:124:THR:HG23	1:A:149:PRO:O	1.81	0.80
1:C:134:LEU:HD21	1:C:136:VAL:HG22	1.63	0.80
1:B:73:ILE:HD11	1:B:92:LEU:HD23	1.64	0.79
1:A:70:PHE:CE2	1:B:216:LEU:HD23	2.18	0.79
1:A:64:CYS:HA	1:A:106:ARG:HH22	1.45	0.78
1:A:69:THR:HG22	1:B:213:SER:O	1.83	0.78
1:B:207:HIS:HD2	1:B:208:GLN:O	1.66	0.78
1:B:198:GLU:O	1:B:199:LEU:HB2	1.83	0.77
1:B:126:ARG:HD2	1:B:142:MET:HE2	1.68	0.76
1:A:130:ALA:HB3	1:A:133:ASP:CB	2.11	0.76
1:C:104:VAL:HG21	1:C:180:MET:SD	2.26	0.75
1:A:64:CYS:HB3	1:A:70:PHE:HE1	1.52	0.75
1:A:134:LEU:HD13	1:A:136:VAL:HG13	1.69	0.74
1:C:89:ARG:HD3	1:C:181:ARG:O	1.88	0.73
1:B:209:ARG:HH11	1:B:209:ARG:HB2	1.53	0.73
1:C:30:ALA:HA	1:C:33:ARG:HB3	1.69	0.73
1:A:96:VAL:HA	1:A:210:ILE:CD1	2.19	0.73
1:B:88:LYS:HD2	1:B:89:ARG:N	2.03	0.72
1:B:117:PHE:HB2	1:B:198:GLU:HB3	1.71	0.72
1:B:106:ARG:HD2	1:B:206:GLU:OE2	1.89	0.72
1:A:153:TYR:HA	1:A:161:GLN:HE22	1.53	0.72
1:B:134:LEU:HD23	1:B:135:SER:N	2.04	0.71
1:A:64:CYS:SG	1:B:214:GLY:CA	2.78	0.71
1:A:124:THR:HG22	1:A:125:VAL:H	1.56	0.71
1:C:108:GLN:HB2	1:C:167:LEU:HD23	1.73	0.71
1:A:97:THR:HG21	1:A:181:ARG:HH21	1.55	0.70
1:B:34:VAL:O	1:B:37:GLN:HG2	1.89	0.70
1:C:109:ILE:HD11	1:C:125:VAL:HG11	1.72	0.70
1:C:114:LEU:HD12	1:C:197:ASP:O	1.91	0.70
1:C:126:ARG:CD	1:C:142:MET:HE2	2.21	0.70
1:C:131:SER:C	1:C:133:ASP:H	2.00	0.69
1:C:90:LEU:HD22	1:C:203:VAL:HG11	1.74	0.69
1:A:179:ASP:HB3	1:A:182:LYS:HE2	1.74	0.69
1:B:194:LEU:HD11	1:B:199:LEU:HD13	1.75	0.68
1:B:138:ALA:HA	1:B:141:ALA:HB3	1.76	0.68
1:B:107:LEU:HD21	1:B:170:LEU:HD21	1.75	0.67
1:A:92:LEU:HD21	1:A:205:ILE:HD12	1.76	0.66
1:A:110:ARG:HA	1:A:164:ASN:O	1.95	0.65
1:B:126:ARG:NH1	1:B:142:MET:HG2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:HA	1:A:142:MET:HG3	1.78	0.65
1:C:52:THR:HG22	1:C:53:ILE:N	2.11	0.65
1:B:114:LEU:HB3	1:B:115:PRO:HD2	1.79	0.64
1:C:126:ARG:HD2	1:C:142:MET:CE	2.25	0.64
1:B:120:THR:CG2	1:B:154:GLN:HG3	2.27	0.64
1:B:29:ASP:HB2	1:C:31:ASN:ND2	2.11	0.64
1:B:111:VAL:O	1:B:164:ASN:HB2	1.98	0.64
1:C:124:THR:HG22	1:C:125:VAL:H	1.63	0.64
1:B:29:ASP:HB2	1:C:31:ASN:CG	2.22	0.64
1:A:192:ASP:O	1:A:193:ALA:HB3	1.98	0.63
1:C:134:LEU:HD22	1:C:136:VAL:HG22	1.78	0.63
1:B:29:ASP:CG	1:C:31:ASN:HA	2.24	0.62
1:B:117:PHE:CB	1:B:198:GLU:HB3	2.29	0.62
1:B:180:MET:HE3	1:B:180:MET:HA	1.81	0.62
1:A:161:GLN:C	1:A:163:ASN:H	2.07	0.62
1:B:126:ARG:CD	1:B:142:MET:HE2	2.30	0.62
1:C:125:VAL:HG23	1:C:168:TYR:HD2	1.64	0.62
1:B:126:ARG:NH2	1:B:147:ALA:HB3	2.15	0.61
1:C:124:THR:HG21	1:C:148:SER:OG	2.00	0.61
1:B:124:THR:HG23	1:B:149:PRO:O	2.01	0.61
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.65	0.61
1:B:207:HIS:CD2	1:B:208:GLN:O	2.52	0.61
1:B:209:ARG:HB2	1:B:209:ARG:NH1	2.16	0.61
1:B:117:PHE:HA	1:B:198:GLU:HB3	1.83	0.61
1:B:130:ALA:C	1:B:132:SER:N	2.59	0.60
1:A:64:CYS:HB3	1:A:70:PHE:CE1	2.33	0.60
1:B:170:LEU:HD22	1:B:183:TYR:HE2	1.66	0.60
1:C:88:LYS:HD3	1:C:89:ARG:N	2.17	0.60
1:A:136:VAL:O	1:A:139:ILE:HG12	2.01	0.60
1:B:118:ASP:HA	1:B:155:TYR:HB2	1.82	0.60
1:C:96:VAL:HG12	1:C:177:ILE:HD13	1.84	0.60
1:A:127:LYS:O	1:A:129:PRO:HD3	2.02	0.59
1:A:136:VAL:C	1:A:138:ALA:H	2.10	0.59
1:C:38:GLN:HA	1:C:41:ARG:NH1	2.18	0.59
1:A:64:CYS:HB2	1:A:206:GLU:OE2	2.02	0.59
1:B:114:LEU:HD21	1:C:144:ALA:HB2	1.84	0.59
1:C:55:HIS:HD2	1:C:58:PHE:O	1.86	0.59
1:C:47:ALA:O	1:C:50:ARG:HG3	2.03	0.58
1:A:179:ASP:O	1:A:182:LYS:HB2	2.03	0.58
1:B:33:ARG:HG3	1:B:33:ARG:NH1	2.18	0.58
1:B:114:LEU:CD2	1:C:144:ALA:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:PHE:CA	1:B:198:GLU:HB3	2.34	0.58
1:B:59:VAL:HG13	1:B:162:ALA:O	2.03	0.58
1:A:96:VAL:HA	1:A:210:ILE:HD12	1.86	0.58
1:A:75:LEU:HD21	1:A:86:TYR:HE2	1.69	0.57
1:A:161:GLN:O	1:A:163:ASN:N	2.37	0.57
1:C:71:THR:HG23	1:C:207:HIS:NE2	2.19	0.57
1:B:98:GLU:HG3	1:B:99:TYR:CD1	2.38	0.57
1:B:100:ASP:HA	1:B:177:ILE:HB	1.87	0.57
1:C:107:LEU:HD23	1:C:170:LEU:HD11	1.86	0.56
1:C:131:SER:C	1:C:133:ASP:N	2.61	0.56
1:C:78:PRO:HD2	1:C:86:TYR:CE1	2.40	0.56
1:C:153:TYR:OH	1:C:160:VAL:HG23	2.05	0.56
1:A:155:TYR:HD1	1:A:161:GLN:HB2	1.71	0.55
1:A:64:CYS:SG	1:B:215:VAL:N	2.80	0.55
1:C:75:LEU:HD13	1:C:86:TYR:OH	2.07	0.55
1:A:124:THR:HG21	1:A:148:SER:OG	2.07	0.54
1:A:161:GLN:HG2	1:A:163:ASN:H	1.72	0.54
1:B:130:ALA:C	1:B:132:SER:H	2.13	0.54
1:C:107:LEU:CD2	1:C:180:MET:HE1	2.30	0.54
1:B:88:LYS:HD2	1:B:89:ARG:H	1.72	0.54
1:C:87:GLY:HA2	1:C:185:VAL:O	2.08	0.54
1:B:120:THR:HG22	1:B:154:GLN:CG	2.33	0.54
1:A:92:LEU:HD12	1:A:177:ILE:HG23	1.90	0.53
1:A:185:VAL:O	1:A:186:LEU:HD23	2.08	0.53
1:A:92:LEU:HD13	1:A:96:VAL:HG11	1.90	0.53
1:B:134:LEU:HD22	1:B:137:ALA:HB3	1.91	0.53
1:C:151:LEU:HB2	1:C:166:LEU:HD12	1.91	0.53
1:C:52:THR:HG22	1:C:53:ILE:H	1.72	0.53
1:C:66:PRO:O	1:C:68:TYR:HD1	1.92	0.53
1:A:96:VAL:HG12	1:A:177:ILE:HG21	1.91	0.53
1:A:166:LEU:O	1:A:167:LEU:CD2	2.57	0.53
1:B:78:PRO:HD2	1:B:86:TYR:CE1	2.44	0.53
1:B:126:ARG:CZ	1:B:147:ALA:HB3	2.39	0.53
1:A:161:GLN:C	1:A:163:ASN:N	2.64	0.52
1:B:108:GLN:HB2	1:B:167:LEU:HD12	1.92	0.52
1:B:214:GLY:O	1:B:215:VAL:HG13	2.09	0.52
1:C:80:ILE:HB	1:C:194:LEU:HB3	1.91	0.52
1:A:192:ASP:O	1:A:193:ALA:CB	2.58	0.52
1:A:155:TYR:O	1:A:156:ALA:HB3	2.10	0.52
1:B:166:LEU:HD12	1:B:166:LEU:C	2.35	0.51
1:C:136:VAL:O	1:C:139:ILE:HB	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLY:HA2	1:C:154:GLN:OE1	2.10	0.51
1:C:82:ARG:HG3	1:C:82:ARG:HH11	1.76	0.51
1:B:47:ALA:O	1:B:50:ARG:HG3	2.11	0.51
1:B:78:PRO:HD2	1:B:86:TYR:CD1	2.45	0.51
1:B:183:TYR:N	1:B:183:TYR:CD1	2.79	0.51
1:C:180:MET:HE2	1:C:205:ILE:HD13	1.93	0.51
1:B:132:SER:O	1:B:134:LEU:N	2.43	0.51
1:C:88:LYS:HD3	1:C:88:LYS:C	2.34	0.50
1:A:63:ARG:HA	1:B:214:GLY:O	2.10	0.50
1:A:111:VAL:HG22	1:A:201:LEU:CD2	2.41	0.50
1:B:31:ASN:C	1:B:31:ASN:ND2	2.69	0.50
1:B:149:PRO:HB2	1:B:166:LEU:HD13	1.92	0.50
1:C:125:VAL:HA	1:C:184:ALA:O	2.11	0.50
1:C:59:VAL:HG22	1:C:162:ALA:O	2.12	0.50
1:B:73:ILE:HG22	1:B:75:LEU:HD23	1.94	0.50
1:C:80:ILE:CG2	1:C:189:SER:HB2	2.42	0.50
1:A:170:LEU:N	1:A:170:LEU:HD23	2.27	0.50
1:A:70:PHE:CE1	1:B:216:LEU:HA	2.47	0.50
1:B:30:ALA:HA	1:B:33:ARG:HH11	1.76	0.50
1:B:31:ASN:C	1:B:31:ASN:HD22	2.20	0.50
1:B:133:ASP:N	1:B:133:ASP:OD1	2.45	0.50
1:C:40:SER:O	1:C:44:LYS:HG3	2.11	0.50
1:C:139:ILE:HA	1:C:142:MET:SD	2.52	0.50
1:B:90:LEU:HD13	1:B:203:VAL:HG11	1.94	0.49
1:C:124:THR:HG22	1:C:125:VAL:N	2.25	0.49
1:B:30:ALA:HA	1:B:33:ARG:NH1	2.27	0.49
1:B:34:VAL:HA	1:B:37:GLN:NE2	2.27	0.49
1:C:100:ASP:HA	1:C:177:ILE:HB	1.94	0.49
1:B:85:TYR:CE1	1:B:139:ILE:HG13	2.46	0.49
1:C:134:LEU:HD13	1:C:138:ALA:HB2	1.94	0.49
1:A:185:VAL:C	1:A:186:LEU:HD23	2.37	0.49
1:A:164:ASN:N	1:A:164:ASN:ND2	2.61	0.49
1:A:99:TYR:CE2	1:A:211:PRO:CG	2.95	0.49
1:A:166:LEU:O	1:A:167:LEU:HD22	2.13	0.49
1:A:121:VAL:HG21	1:A:199:LEU:HD21	1.95	0.49
1:A:170:LEU:O	1:A:171:SER:C	2.54	0.49
1:B:61:SER:HB2	1:B:165:LYS:HE2	1.95	0.49
1:B:170:LEU:HD22	1:B:183:TYR:CE2	2.47	0.49
1:C:107:LEU:CD2	1:C:170:LEU:HD11	2.43	0.49
1:C:107:LEU:HD12	1:C:107:LEU:O	2.13	0.49
1:A:90:LEU:CD2	1:A:185:VAL:HG23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:O	1:A:193:ALA:N	2.46	0.48
1:C:214:GLY:O	1:C:215:VAL:HG23	2.12	0.48
1:A:157:ALA:HB3	1:A:160:VAL:CG2	2.44	0.48
1:B:124:THR:HG22	1:B:125:VAL:H	1.78	0.48
1:C:55:HIS:N	1:C:56:PRO:CD	2.77	0.48
1:C:140:SER:HA	1:C:143:PHE:CD1	2.49	0.48
1:A:62:GLU:HA	1:A:63:ARG:NH2	2.29	0.48
1:B:164:ASN:OD1	1:B:165:LYS:HG2	2.14	0.48
1:C:38:GLN:HA	1:C:41:ARG:HH11	1.77	0.48
1:A:106:ARG:HA	1:A:169:ASP:HA	1.96	0.48
1:C:55:HIS:N	1:C:56:PRO:HD2	2.27	0.48
1:A:106:ARG:HG2	1:A:206:GLU:OE1	2.14	0.48
1:A:128:VAL:HG13	1:A:128:VAL:O	2.14	0.48
1:C:46:LEU:C	1:C:48:ALA:N	2.69	0.48
1:A:71:THR:HG21	1:A:92:LEU:HD22	1.96	0.47
1:C:210:ILE:HG23	1:C:211:PRO:HD2	1.95	0.47
1:C:128:VAL:HG12	1:C:128:VAL:O	2.14	0.47
1:B:55:HIS:HD2	1:B:58:PHE:O	1.98	0.47
1:B:183:TYR:N	1:B:183:TYR:HD1	2.11	0.47
1:C:134:LEU:HD21	1:C:136:VAL:CG2	2.40	0.47
1:B:43:ASN:HD21	1:C:45:THR:HG21	1.80	0.47
1:B:129:PRO:C	1:B:131:SER:H	2.21	0.47
1:B:29:ASP:OD2	1:C:31:ASN:HA	2.15	0.47
1:B:85:TYR:CZ	1:B:139:ILE:HG13	2.50	0.47
1:C:216:LEU:HB3	1:C:217:PRO:HD2	1.96	0.47
1:A:71:THR:CG2	1:A:92:LEU:HD22	2.44	0.47
1:B:87:GLY:HA2	1:B:185:VAL:O	2.15	0.47
1:B:140:SER:HA	1:B:143:PHE:HD1	1.79	0.47
1:C:134:LEU:HD23	1:C:135:SER:N	2.30	0.47
1:C:210:ILE:CG2	1:C:211:PRO:HD2	2.44	0.47
1:A:81:ASP:HA	1:A:193:ALA:HB1	1.96	0.47
1:B:126:ARG:HH21	1:B:148:SER:HB2	1.80	0.47
1:B:106:ARG:NE	1:B:167:LEU:HD21	2.30	0.46
1:C:89:ARG:O	1:C:91:LEU:HG	2.15	0.46
1:C:166:LEU:HD23	1:C:166:LEU:C	2.41	0.46
1:A:65:ARG:HB3	1:A:66:PRO:HD2	1.97	0.46
1:B:169:ASP:C	1:B:169:ASP:OD1	2.58	0.46
1:C:82:ARG:HG3	1:C:82:ARG:NH1	2.31	0.46
1:C:93:PRO:O	1:C:96:VAL:HG23	2.15	0.46
1:A:68:TYR:CD2	1:A:207:HIS:C	2.94	0.46
1:B:138:ALA:HA	1:B:141:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD13	1:A:109:ILE:H	1.81	0.46
1:C:65:ARG:HD2	1:C:106:ARG:NH1	2.30	0.46
1:C:86:TYR:O	1:C:186:LEU:HA	2.16	0.46
1:C:104:VAL:HG11	1:C:180:MET:SD	2.56	0.46
1:C:207:HIS:O	1:C:208:GLN:C	2.58	0.46
1:A:124:THR:HG22	1:A:125:VAL:N	2.26	0.46
1:A:123:VAL:O	1:A:150:VAL:HG23	2.15	0.45
1:A:215:VAL:HG22	1:B:63:ARG:HA	1.98	0.45
1:C:59:VAL:HG13	1:C:162:ALA:O	2.17	0.45
1:B:151:LEU:HG	1:B:152:VAL:N	2.32	0.45
1:C:114:LEU:O	1:C:115:PRO:C	2.59	0.45
1:B:69:THR:HG23	1:B:209:ARG:NH1	2.32	0.45
1:C:130:ALA:O	1:C:132:SER:N	2.48	0.45
1:C:80:ILE:HD12	1:C:194:LEU:HD23	1.98	0.45
1:C:125:VAL:HG12	1:C:185:VAL:HA	1.98	0.45
1:A:124:THR:HG21	1:A:148:SER:HG	1.80	0.45
1:B:98:GLU:C	1:B:100:ASP:H	2.25	0.45
1:B:196:THR:O	1:B:197:ASP:HB2	2.16	0.45
1:C:30:ALA:N	1:C:33:ARG:HB2	2.32	0.45
1:C:128:VAL:HA	1:C:129:PRO:HD2	1.71	0.45
1:C:52:THR:CG2	1:C:53:ILE:N	2.80	0.44
1:B:136:VAL:H	1:B:139:ILE:HG12	1.81	0.44
1:B:90:LEU:N	1:B:90:LEU:HD23	2.31	0.44
1:C:83:GLY:HA2	1:C:189:SER:O	2.17	0.44
1:A:87:GLY:HA2	1:A:185:VAL:O	2.18	0.44
1:A:165:LYS:HE2	1:B:218:VAL:OXT	2.17	0.44
1:C:68:TYR:CE2	1:C:105:SER:HB3	2.52	0.44
1:C:99:TYR:HB3	1:C:102:LYS:HD3	2.00	0.44
1:A:115:PRO:O	1:A:116:LYS:CB	2.66	0.44
1:A:164:ASN:N	1:A:164:ASN:HD22	2.15	0.44
1:B:117:PHE:HB2	1:B:198:GLU:CB	2.46	0.44
1:C:80:ILE:HG21	1:C:189:SER:HB2	1.99	0.44
1:C:130:ALA:C	1:C:132:SER:H	2.25	0.44
1:B:102:LYS:O	1:B:176:ASP:HB2	2.17	0.44
1:A:217:PRO:HB2	1:B:110:ARG:HE	1.82	0.44
1:B:140:SER:HA	1:B:143:PHE:CD1	2.53	0.44
1:A:139:ILE:O	1:A:142:MET:HB2	2.18	0.44
1:C:108:GLN:HB2	1:C:167:LEU:CD2	2.45	0.44
1:C:33:ARG:O	1:C:37:GLN:HG2	2.18	0.43
1:A:91:LEU:H	1:A:91:LEU:HD12	1.83	0.43
1:A:136:VAL:HG22	1:A:138:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HG21	1:B:148:SER:HB2	2.00	0.43
1:C:58:PHE:CE2	1:C:160:VAL:CG2	3.01	0.43
1:C:165:LYS:HE3	1:C:165:LYS:HB2	1.63	0.43
1:C:117:PHE:HA	1:C:198:GLU:HB3	2.00	0.43
1:B:168:TYR:CD1	1:B:168:TYR:C	2.95	0.43
1:C:30:ALA:HA	1:C:33:ARG:CB	2.42	0.43
1:C:93:PRO:O	1:C:97:THR:HG23	2.19	0.43
1:C:96:VAL:C	1:C:98:GLU:N	2.75	0.43
1:A:108:GLN:OE1	1:A:110:ARG:HD3	2.19	0.43
1:C:107:LEU:HD22	1:C:180:MET:CE	2.33	0.43
1:B:34:VAL:O	1:B:35:LEU:C	2.62	0.43
1:B:34:VAL:HA	1:B:37:GLN:HG2	2.01	0.43
1:B:38:GLN:HE22	1:B:41:ARG:HH11	1.65	0.43
1:B:107:LEU:N	1:B:107:LEU:HD23	2.34	0.43
1:C:125:VAL:HG23	1:C:168:TYR:CD2	2.51	0.43
1:A:126:ARG:HH12	1:A:142:MET:HA	1.84	0.43
1:C:78:PRO:O	1:C:79:LYS:C	2.61	0.43
1:A:191:ASP:O	1:A:192:ASP:C	2.61	0.42
1:B:39:LEU:HA	1:B:39:LEU:HD23	1.53	0.42
1:B:65:ARG:O	1:B:68:TYR:HB2	2.19	0.42
1:B:155:TYR:CE1	1:B:156:ALA:O	2.72	0.42
1:B:181:ARG:HD2	1:B:181:ARG:N	2.34	0.42
1:C:44:LYS:O	1:C:47:ALA:HB3	2.19	0.42
1:A:139:ILE:HA	1:A:142:MET:CG	2.45	0.42
1:B:33:ARG:HH11	1:B:33:ARG:CG	2.29	0.42
1:A:110:ARG:HH11	1:A:110:ARG:HD2	1.68	0.42
1:B:134:LEU:CD2	1:B:135:SER:N	2.78	0.42
1:A:126:ARG:HH11	1:A:142:MET:HE2	1.84	0.42
1:B:34:VAL:O	1:B:37:GLN:N	2.53	0.42
1:C:66:PRO:C	1:C:68:TYR:H	2.27	0.42
1:C:153:TYR:HE1	1:C:164:ASN:HB3	1.85	0.42
1:A:64:CYS:SG	1:B:214:GLY:C	3.02	0.42
1:A:99:TYR:CE2	1:A:211:PRO:HG2	2.54	0.42
1:A:138:ALA:C	1:A:140:SER:N	2.78	0.42
1:C:138:ALA:O	1:C:141:ALA:HB3	2.19	0.42
1:A:165:LYS:HE2	1:B:218:VAL:C	2.44	0.42
1:B:179:ASP:HA	1:B:182:LYS:HE3	2.02	0.42
1:C:77:PRO:HB3	1:C:86:TYR:CZ	2.54	0.42
1:A:110:ARG:NH1	1:B:218:VAL:HG22	2.34	0.42
1:B:118:ASP:O	1:B:118:ASP:CG	2.61	0.42
1:C:107:LEU:HD23	1:C:170:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASP:O	1:B:95:SER:C	2.63	0.42
1:A:189:SER:OG	1:A:190:LYS:N	2.52	0.41
1:A:166:LEU:O	1:A:167:LEU:HD23	2.20	0.41
1:B:40:SER:O	1:B:41:ARG:C	2.63	0.41
1:B:68:TYR:N	1:B:68:TYR:CD1	2.89	0.41
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.73	0.41
1:A:126:ARG:HH12	1:A:142:MET:CA	2.33	0.41
1:C:55:HIS:HA	1:C:56:PRO:HD2	1.88	0.41
1:C:168:TYR:C	1:C:168:TYR:CD1	2.96	0.41
1:A:110:ARG:HD2	1:B:218:VAL:O	2.21	0.41
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.85	0.41
1:B:29:ASP:O	1:B:33:ARG:HG2	2.21	0.41
1:B:116:LYS:HD3	1:B:197:ASP:O	2.20	0.41
1:A:84:SER:C	1:A:85:TYR:CD1	2.99	0.41
1:A:173:MET:O	1:A:174:ARG:C	2.64	0.41
1:B:129:PRO:C	1:B:131:SER:N	2.78	0.41
1:B:89:ARG:NH2	1:B:128:VAL:O	2.47	0.41
1:A:107:LEU:HD22	1:A:180:MET:HE1	2.02	0.40
1:A:136:VAL:C	1:A:138:ALA:N	2.76	0.40
1:A:191:ASP:HB2	1:A:192:ASP:H	1.74	0.40
1:C:106:ARG:HH11	1:C:206:GLU:CD	2.29	0.40
1:B:88:LYS:HD2	1:B:88:LYS:C	2.45	0.40
1:B:181:ARG:N	1:B:181:ARG:CD	2.85	0.40
1:C:65:ARG:O	1:C:68:TYR:HB2	2.21	0.40
1:C:70:PHE:CD1	1:C:70:PHE:C	2.99	0.40
1:C:116:LYS:H	1:C:116:LYS:HG2	1.60	0.40
1:B:33:ARG:HG2	1:B:33:ARG:H	1.47	0.40
1:C:129:PRO:O	1:C:130:ALA:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/218 (71%)	116 (75%)	27 (17%)	12 (8%)	1	5
1	B	188/218 (86%)	151 (80%)	29 (15%)	8 (4%)	2	16
1	C	189/218 (87%)	149 (79%)	32 (17%)	8 (4%)	2	16
All	All	532/654 (81%)	416 (78%)	88 (16%)	28 (5%)	1	12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ALA
1	A	162	ALA
1	B	133	ASP
1	B	193	ALA
1	C	30	ALA
1	C	56	PRO
1	C	131	SER
1	A	100	ASP
1	A	134	LEU
1	A	168	TYR
1	A	174	ARG
1	A	192	ASP
1	B	194	LEU
1	B	198	GLU
1	C	174	ARG
1	C	213	SER
1	A	131	SER
1	B	134	LEU
1	A	88	LYS
1	A	116	LYS
1	B	197	ASP
1	C	130	ALA
1	B	137	ALA
1	B	199	LEU
1	C	136	VAL
1	A	129	PRO
1	C	129	PRO
1	A	136	VAL

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	137/188 (73%)	113 (82%)	24 (18%)	2	10
1	B	165/188 (88%)	125 (76%)	40 (24%)	1	4
1	C	165/188 (88%)	138 (84%)	27 (16%)	2	12
All	All	467/564 (83%)	376 (80%)	91 (20%)	1	8

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	71	THR
1	A	88	LYS
1	A	91	LEU
1	A	95	SER
1	A	109	ILE
1	A	116	LYS
1	A	124	THR
1	A	127	LYS
1	A	131	SER
1	A	132	SER
1	A	134	LEU
1	A	139	ILE
1	A	140	SER
1	A	164	ASN
1	A	166	LEU
1	A	167	LEU
1	A	170	LEU
1	A	173	MET
1	A	174	ARG
1	A	179	ASP
1	A	182	LYS
1	A	191	ASP
1	A	192	ASP
1	B	31	ASN
1	B	33	ARG
1	B	43	ASN
1	B	50	ARG
1	B	59	VAL
1	B	62	GLU
1	B	65	ARG

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Mol	Chain	Res	Type
1	B	66	PRO
1	B	74	THR
1	B	75	LEU
1	B	79	LYS
1	B	81	ASP
1	B	86	TYR
1	B	95	SER
1	B	100	ASP
1	B	101	LYS
1	B	106	ARG
1	B	107	LEU
1	B	119	SER
1	B	124	THR
1	B	125	VAL
1	B	136	VAL
1	B	139	ILE
1	B	158	SER
1	B	160	VAL
1	B	165	LYS
1	B	166	LEU
1	B	170	LEU
1	B	174	ARG
1	B	177	ILE
1	B	179	ASP
1	B	183	TYR
1	B	191	ASP
1	B	199	LEU
1	B	201	LEU
1	B	204	ASP
1	B	209	ARG
1	B	215	VAL
1	B	216	LEU
1	B	218	VAL
1	C	29	ASP
1	C	36	SER
1	C	41	ARG
1	C	50	ARG
1	C	53	ILE
1	C	65	ARG
1	C	82	ARG
1	C	88	LYS
1	C	91	LEU

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Mol	Chain	Res	Type
1	C	95	SER
1	C	96	VAL
1	C	98	GLU
1	C	101	LYS
1	C	104	VAL
1	C	115	PRO
1	C	116	LYS
1	C	123	VAL
1	C	124	THR
1	C	127	LYS
1	C	131	SER
1	C	134	LEU
1	C	160	VAL
1	C	166	LEU
1	C	167	LEU
1	C	191	ASP
1	C	199	LEU
1	C	204	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	154	GLN
1	A	163	ASN
1	A	164	ASN
1	B	31	ASN
1	B	38	GLN
1	B	55	HIS
1	B	202	HIS
1	B	207	HIS
1	C	55	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.