



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:50 pm GMT

PDB ID : 1F15
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

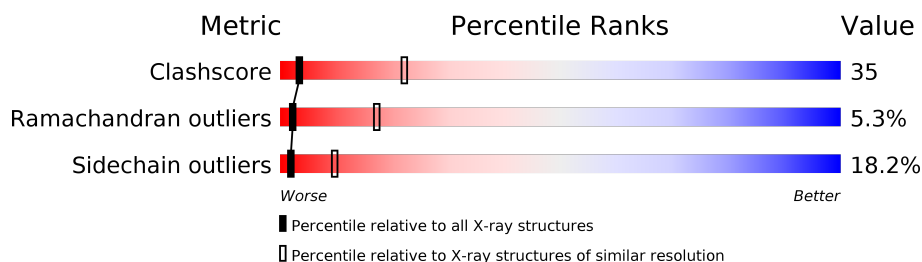
1 Overall quality at a glance

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	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

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:

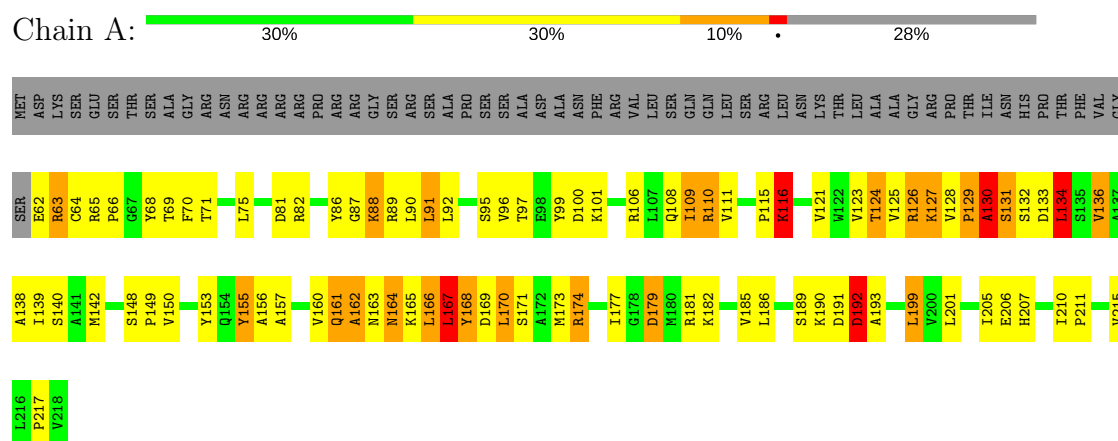
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	LEU	ILE	CONFLICT	UNP P69466
B	107	LEU	ILE	CONFLICT	UNP P69466
C	107	LEU	ILE	CONFLICT	UNP P69466

3 Residue-property plots

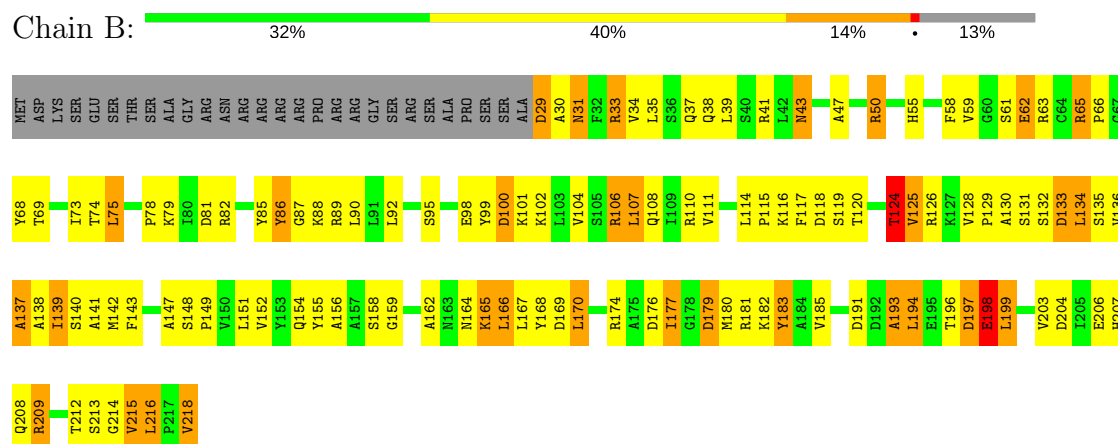
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

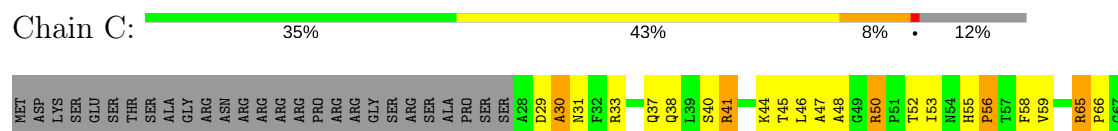
• Molecule 1: COAT PROTEIN

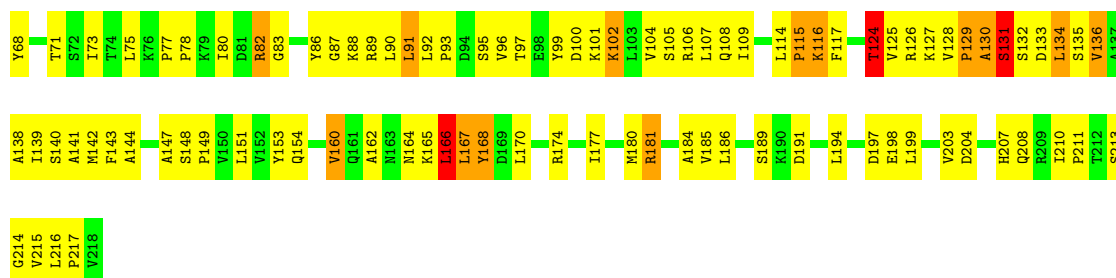


• Molecule 1: COAT PROTEIN



• 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 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	336.00Å 336.00Å 336.00Å 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

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	0.92	1/1254 (0.1%)	1.15	9/1704 (0.5%)
1	B	0.81	1/1513 (0.1%)	1.12	3/2056 (0.1%)
1	C	0.75	0/1518	1.09	2/2063 (0.1%)
All	All	0.83	2/4285 (0.0%)	1.11	14/5823 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ALA	CA-CB	7.97	1.69	1.52
1	B	198	GLU	CG-CD	5.01	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	GLU	N-CA-C	-9.71	84.78	111.00
1	C	166	LEU	CA-CB-CG	7.28	132.05	115.30
1	A	167	LEU	C-N-CA	7.04	139.29	121.70
1	B	193	ALA	N-CA-C	-6.47	93.52	111.00
1	A	130	ALA	N-CA-C	-6.30	94.00	111.00
1	A	126	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	167	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	155	TYR	N-CA-C	6.09	127.45	111.00
1	A	161	GLN	N-CA-C	-5.86	95.17	111.00
1	A	167	LEU	N-CA-C	5.80	126.65	111.00
1	A	168	TYR	CB-CA-C	-5.77	98.86	110.40
1	C	124	THR	CB-CA-C	-5.40	97.02	111.60
1	A	110	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	B	124	THR	CB-CA-C	-5.06	97.95	111.60

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	90	0
1	B	1483	0	1513	124	0
1	C	1488	0	1518	109	0
All	All	4200	0	4285	301	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 35.

All (301) 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: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
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:B:207:HIS:HD2	1:B:208:GLN:O	1.66	0.78
1:A:69:THR:HG22	1:B:213:SER:O	1.83	0.78
1:B:198:GLU:O	1:B:199:LEU:HB2	1.83	0.77
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:PHE:HB2	1:B:198:GLU:HB3	1.71	0.72
1:B:88:LYS:HD2	1:B:89:ARG:N	2.03	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:124:THR:HG22	1:A:125:VAL:H	1.56	0.71
1:A:64:CYS:SG	1:B:214:GLY:CA	2.78	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:114:LEU:HD12	1:C:197:ASP:O	1.91	0.70
1:C:109:ILE:HD11	1:C:125:VAL:HG11	1.72	0.70
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:C:126:ARG:HD2	1:C:142:MET:CE	2.25	0.67
1:C:107:LEU:HD22	1:C:180:MET:HE1	1.76	0.66
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
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:B:120:THR:CG2	1:B:154:GLN:HG3	2.27	0.64
1:B:111:VAL:O	1:B:164:ASN:HB2	1.98	0.64
1:B:29:ASP:HB2	1:C:31:ASN:ND2	2.11	0.64
1:C:124:THR:HG22	1:C:125:VAL:H	1.63	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:C:131:SER:C	1:C:133:ASP:H	2.00	0.62
1:B:117:PHE:CB	1:B:198:GLU:HB3	2.29	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:HIS:CD2	1:B:208:GLN:O	2.52	0.61
1:B:209:ARG:NH1	1:B:209:ARG:HB2	2.16	0.61
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.65	0.61
1:B:117:PHE:HA	1:B:198:GLU:HB3	1.83	0.61
1:C:126:ARG:HD2	1:C:142:MET:HE1	1.82	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:29:ASP:HB2	1:C:31:ASN:CG	2.22	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: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:114:LEU:CD2	1:C:144:ALA:HB2	2.33	0.58
1:B:33:ARG:NH1	1:B:33:ARG:HG3	2.18	0.58
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:B:29:ASP:CG	1:C:31:ASN:HA	2.24	0.58
1:A:161:GLN:O	1:A:163:ASN:N	2.37	0.57
1:A:75:LEU:HD21	1:A:86:TYR:HE2	1.69	0.57
1:C:71:THR:HG23	1:C:207:HIS:NE2	2.19	0.57
1:A:161:GLN:C	1:A:163:ASN:H	2.07	0.57
1:B:100:ASP:HA	1:B:177:ILE:HB	1.87	0.57
1:B:98:GLU:HG3	1:B:99:TYR:CD1	2.38	0.57
1:C:107:LEU:HD22	1:C:180:MET:CE	2.33	0.56
1:C:107:LEU:HD23	1:C:170:LEU:HD11	1.86	0.56
1:B:130:ALA:C	1:B:132:SER:N	2.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:C	1:A:138:ALA:H	2.10	0.54
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: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:131:SER:C	1:C:133:ASP:N	2.61	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:166:LEU:O	1:A:167:LEU:CD2	2.57	0.53
1:A:96:VAL:HG12	1:A:177:ILE:HG21	1.91	0.53
1:B:126:ARG:CZ	1:B:147:ALA:HB3	2.39	0.53
1:B:78:PRO:HD2	1:B:86:TYR:CE1	2.44	0.53
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:C:136:VAL:O	1:C:139:ILE:HB	2.09	0.51
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:183:TYR:CD1	1:B:183:TYR:N	2.79	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:132:SER:O	1:B:134:LEU:N	2.43	0.51
1:A:111:VAL:HG22	1:A:201:LEU:CD2	2.41	0.50
1:A:63:ARG:HA	1:B:214:GLY:O	2.10	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:A:161:GLN:C	1:A:163:ASN:N	2.64	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:133:ASP:OD1	1:B:133:ASP:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ALA:HA	1:B:33:ARG:HH11	1.76	0.50
1:C:139:ILE:HA	1:C:142:MET:SD	2.52	0.50
1:C:40:SER:O	1:C:44:LYS:HG3	2.11	0.50
1:B:130:ALA:C	1:B:132:SER:H	2.13	0.49
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:164:ASN:N	1:A:164:ASN:ND2	2.61	0.49
1:A:166:LEU:O	1:A:167:LEU:HD22	2.13	0.49
1:A:99:TYR:CE2	1:A:211:PRO:CG	2.95	0.49
1:A:121:VAL:HG21	1:A:199:LEU:HD21	1.95	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:O	1:C:107:LEU:HD12	2.13	0.49
1:A:191:ASP:O	1:A:193:ALA:N	2.46	0.48
1:A:90:LEU:CD2	1:A:185:VAL:HG23	2.43	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:140:SER:HA	1:C:143:PHE:CD1	2.49	0.48
1:C:55:HIS:N	1:C:56:PRO:CD	2.77	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:O	1:A:128:VAL:HG13	2.14	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:HD1	1:B:183:TYR:N	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:C:216:LEU:HB3	1:C:217:PRO:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TYR:CZ	1:B:139:ILE:HG13	2.50	0.47
1:C:180:MET:HE2	1:C:180:MET:HB3	1.69	0.47
1:B:29:ASP:OD2	1:C:31:ASN:HA	2.15	0.47
1:A:71:THR:CG2	1:A:92:LEU:HD22	2.44	0.47
1:B:140:SER:HA	1:B:143:PHE:HD1	1.79	0.47
1:B:87:GLY:HA2	1:B:185:VAL:O	2.15	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:166:LEU:C	1:B:166:LEU:HD12	2.35	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:A:65:ARG:HB3	1:A:66:PRO:HD2	1.97	0.46
1:C:82:ARG:NH1	1:C:82:ARG:HG3	2.31	0.46
1:C:93:PRO:O	1:C:96:VAL:HG23	2.15	0.46
1:B:138:ALA:HA	1:B:141:ALA:CB	2.46	0.46
1:C:46:LEU:C	1:C:48:ALA:N	2.69	0.46
1:C:88:LYS:C	1:C:88:LYS:HD3	2.34	0.46
1:A:109:ILE:HD13	1:A:109:ILE:H	1.81	0.46
1:A:124:THR:HG21	1:A:148:SER:HG	1.79	0.46
1:C:104:VAL:HG11	1:C:180:MET:SD	2.56	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:B:31:ASN:C	1:B:31:ASN:ND2	2.69	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:B:31:ASN:C	1:B:31:ASN:HD22	2.20	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:125:VAL:HG12	1:C:185:VAL:HA	1.98	0.45
1:C:80:ILE:HD12	1:C:194:LEU:HD23	1.98	0.45
1:B:196:THR:O	1:B:197:ASP:HB2	2.16	0.45
1:C:128:VAL:HA	1:C:129:PRO:HD2	1.71	0.45
1:C:30:ALA:N	1:C:33:ARG:HB2	2.32	0.45
1:A:185:VAL:C	1:A:186:LEU:HD23	2.37	0.44
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:LEU:O	1:A:171:SER:C	2.54	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:99:TYR:HB3	1:C:102:LYS:HD3	2.00	0.44
1:C:68:TYR:CE2	1:C:105:SER:HB3	2.52	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: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:B:129:PRO:C	1:B:131:SER:H	2.21	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:136:VAL:HG22	1:A:138:ALA:HB2	2.00	0.43
1:A:91:LEU:H	1:A:91:LEU:HD12	1.83	0.43
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:HB2	1:C:165:LYS:HE3	1.63	0.43
1:B:38:GLN:HA	1:B:38:GLN:NE2	2.33	0.43
1:C:117:PHE:HA	1:C:198:GLU:HB3	2.00	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:A:108:GLN:OE1	1:A:110:ARG:HD3	2.19	0.43
1:B:107:LEU:N	1:B:107:LEU:HD23	2.34	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: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:A:189:SER:OG	1:A:190:LYS:N	2.52	0.43
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HD2	1:A:110:ARG:HH11	1.68	0.42
1:B:134:LEU:CD2	1:B:135:SER:N	2.78	0.42
1:B:34:VAL:O	1:B:37:GLN:N	2.53	0.42
1:C:153:TYR:HE1	1:C:164:ASN:HB3	1.85	0.42
1:A:99:TYR:CE2	1:A:211:PRO:HG2	2.54	0.42
1:C:138:ALA:O	1:C:141:ALA:HB3	2.19	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:C:107:LEU:HD23	1:C:170:LEU:CD1	2.50	0.42
1:C:166:LEU:C	1:C:166:LEU:HD23	2.41	0.42
1:B:169:ASP:C	1:B:169:ASP:OD1	2.58	0.41
1:A:166:LEU:O	1:A:167:LEU:HD23	2.20	0.41
1:B:114:LEU:HA	1:B:114:LEU:HD23	1.73	0.41
1:B:68:TYR:N	1:B:68:TYR:CD1	2.89	0.41
1:A:126:ARG:HH12	1:A:142:MET:CA	2.33	0.41
1:A:68:TYR:CD2	1:A:207:HIS:C	2.94	0.41
1:B:61:SER:OG	1:B:62:GLU:N	2.51	0.41
1:C:55:HIS:HA	1:C:56:PRO:HD2	1.88	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:116:LYS:HD3	1:B:197:ASP:O	2.20	0.41
1:B:29:ASP:O	1:B:33:ARG:HG2	2.21	0.41
1:C:207:HIS:O	1:C:208:GLN:C	2.58	0.41
1:B:89:ARG:NH2	1:B:128:VAL:O	2.47	0.41
1:A:191:ASP:HB2	1:A:192:ASP:H	1.74	0.40
1:B:181:ARG:CD	1:B:181:ARG:N	2.85	0.40
1:C:114:LEU:O	1:C:115:PRO:C	2.59	0.40
1:C:116:LYS:HG2	1:C:116:LYS:H	1.60	0.40
1:C:65:ARG:O	1:C:68:TYR:HB2	2.21	0.40
1:B:33:ARG:H	1:B:33:ARG:HG2	1.47	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	155/218 (71%)	116 (75%)	27 (17%)	12 (8%)	1	7
1	B	188/218 (86%)	151 (80%)	29 (15%)	8 (4%)	3	23
1	C	189/218 (87%)	149 (79%)	32 (17%)	8 (4%)	3	23
All	All	532/654 (81%)	416 (78%)	88 (16%)	28 (5%)	2	17

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	11
1	B	165/188 (88%)	127 (77%)	38 (23%)	1	4
1	C	165/188 (88%)	142 (86%)	23 (14%)	4	19
All	All	467/564 (83%)	382 (82%)	85 (18%)	2	10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	82	ARG
1	A	88	LYS
1	A	89	ARG
1	A	91	LEU
1	A	95	SER
1	A	101	LYS
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	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	192	ASP
1	A	199	LEU
1	B	29	ASP
1	B	31	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	33	ARG
1	B	43	ASN
1	B	50	ARG
1	B	62	GLU
1	B	65	ARG
1	B	66	PRO
1	B	74	THR
1	B	75	LEU
1	B	79	LYS
1	B	81	ASP
1	B	82	ARG
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	139	ILE
1	B	158	SER
1	B	165	LYS
1	B	166	LEU
1	B	168	TYR
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	204	ASP
1	B	209	ARG
1	B	215	VAL
1	B	216	LEU
1	B	218	VAL
1	C	29	ASP
1	C	41	ARG
1	C	50	ARG
1	C	65	ARG
1	C	82	ARG
1	C	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	95	SER
1	C	101	LYS
1	C	102	LYS
1	C	115	PRO
1	C	116	LYS
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	168	TYR
1	C	181	ARG
1	C	191	ASP
1	C	199	LEU
1	C	204	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	A	202	HIS
1	B	31	ASN
1	B	37	GLN
1	B	38	GLN
1	B	55	HIS
1	B	207	HIS
1	C	31	ASN
1	C	54	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.