



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:12 PM UTC

PDB ID : 3VBU / pdb_00003vbu
Title : Crystal structure of empty human Enterovirus 71 particle
Authors : Wang, X.; Peng, W.; Ren, J.; Hu, Z.; Xu, J.; Lou, Z.; Li, X.; Yin, W.; Shen, X.; Porta, C.; Walter, T.S.; Evans, G.; Axford, D.; Owen, R.; Rowlands, D.J.; Wang, J.; Stuart, D.I.; Fry, E.E.; Rao, Z.
Deposited on : 2012-01-02
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

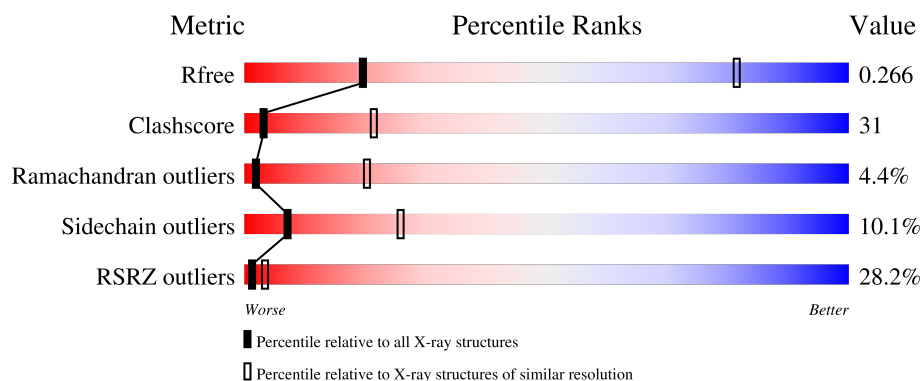
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	19% 39% 45% 12% ••
2	B	237	38% 41% 49% 8% •
3	C	239	27% 51% 38% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5397 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 Genome Polyprotein, capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1724	1107	290	316	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MET	CYS	SEE REMARK 999	UNP B2ZUN0

- Molecule 2 is a protein called Genome Polyprotein, capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1834	1179	301	346	8			

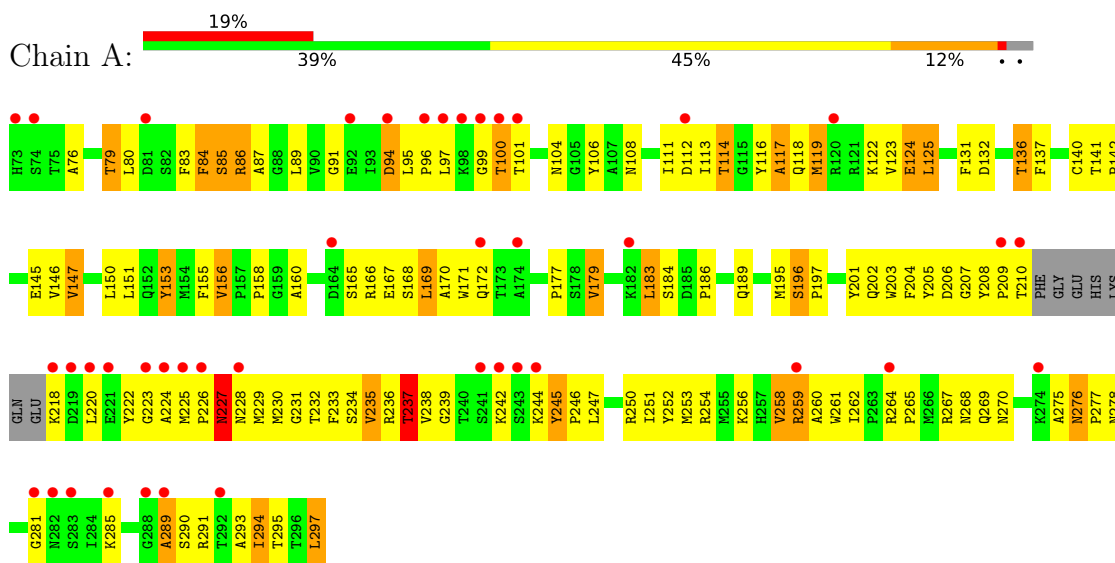
- Molecule 3 is a protein called Genome Polyprotein, capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	239	Total	C	N	O	S	0	0	0
			1839	1182	306	340	11			

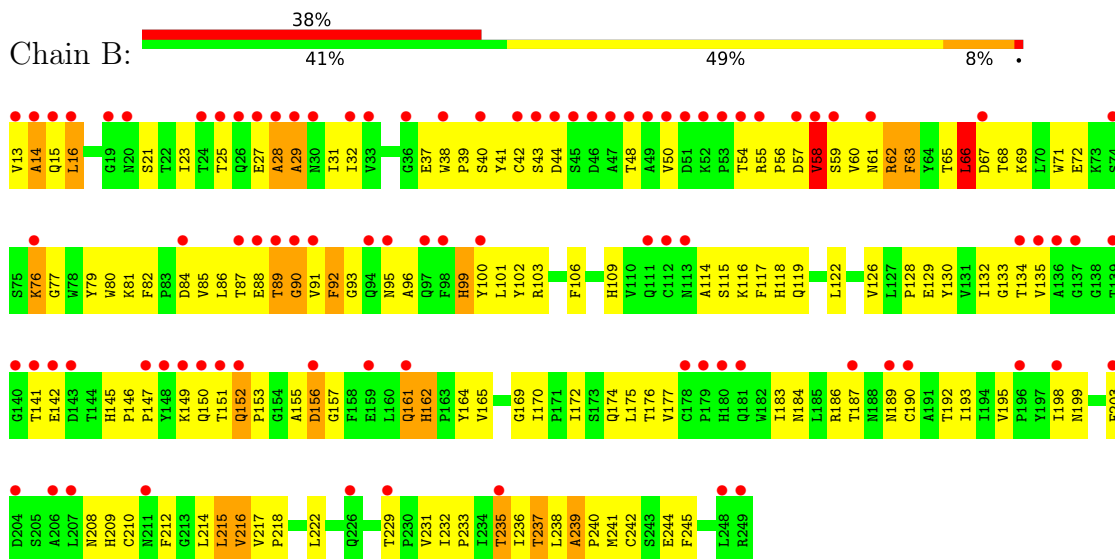
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

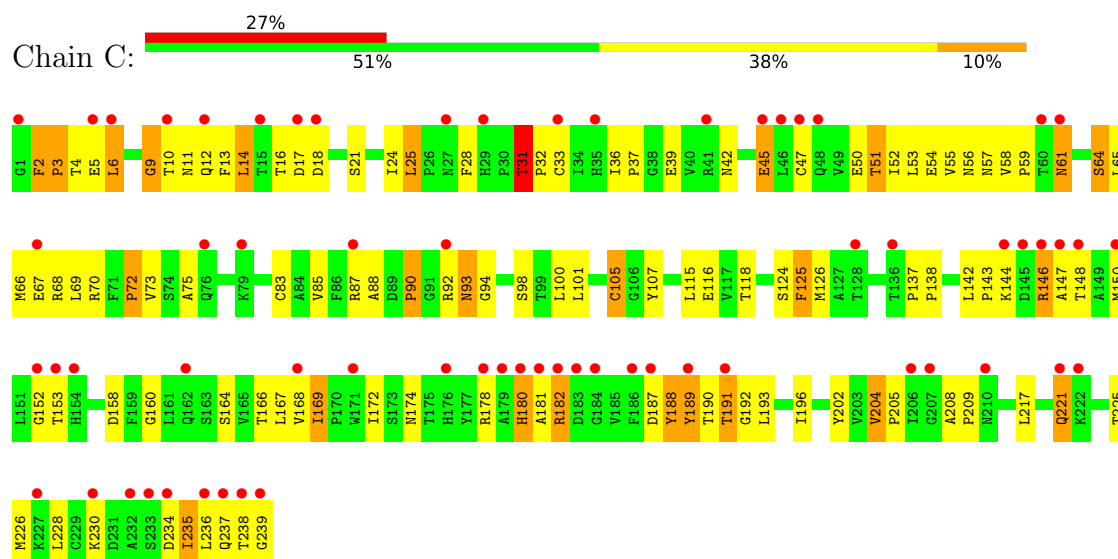
• Molecule 1: Genome Polyprotein, capsid protein VP1



• Molecule 2: Genome Polyprotein, capsid protein VP0



• Molecule 3: Genome Polyprotein, capsid protein VP3



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 ₂	Depositor
Cell constants a, b, c, α , β , γ	355.90Å 355.90Å 355.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 4.00 49.84 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.84-4.00) 98.7 (49.84-4.00)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.272 , 0.278 0.283 , 0.266	Depositor DCC
R_{free} test set	657 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	92.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 97.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.32	EDS
Total number of atoms	5397	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/1776	1.21	16/2419 (0.7%)
2	B	0.73	0/1889	1.20	25/2592 (1.0%)
3	C	0.63	0/1891	1.12	14/2586 (0.5%)
All	All	0.67	0/5556	1.18	55/7597 (0.7%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	THR	N-CA-C	-9.07	102.34	113.41
2	B	92	PHE	N-CA-C	-8.34	103.29	113.97
3	C	9	GLY	N-CA-C	-8.29	104.62	114.48
1	A	201	TYR	N-CA-C	-8.10	97.82	109.96
1	A	84	PHE	N-CA-C	7.88	123.20	113.50
2	B	63	PHE	N-CA-C	7.83	120.81	108.67
2	B	152	GLN	CA-C-N	7.70	129.46	119.84
2	B	152	GLN	C-N-CA	7.70	129.46	119.84
2	B	239	ALA	CA-C-N	7.18	126.94	119.76
2	B	239	ALA	C-N-CA	7.18	126.94	119.76
3	C	64	SER	N-CA-C	-7.17	102.97	114.09
3	C	94	GLY	CA-C-N	7.17	127.49	119.32
3	C	94	GLY	C-N-CA	7.17	127.49	119.32
1	A	153	TYR	N-CA-C	-7.04	97.76	109.24
2	B	229	THR	CA-C-N	7.03	127.18	119.87
2	B	229	THR	C-N-CA	7.03	127.18	119.87
1	A	237	THR	N-CA-C	-7.02	100.61	110.50
2	B	161	GLN	N-CA-C	-6.86	105.44	113.88
2	B	106	PHE	N-CA-C	6.60	119.48	108.13
2	B	66	LEU	N-CA-C	6.59	119.79	110.50
2	B	141	THR	N-CA-C	6.48	120.19	112.93
3	C	31	THR	CA-C-N	6.41	127.86	119.84
3	C	31	THR	C-N-CA	6.41	127.86	119.84
2	B	44	ASP	N-CA-C	6.28	118.93	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	169	ILE	CA-C-N	6.26	127.67	119.84
3	C	169	ILE	C-N-CA	6.26	127.67	119.84
2	B	195	VAL	N-CA-C	6.21	114.66	107.89
2	B	89	THR	N-CA-C	6.07	119.47	110.48
3	C	192	GLY	N-CA-C	-5.99	103.34	112.51
3	C	2	PHE	CA-C-N	5.91	126.11	119.90
3	C	2	PHE	C-N-CA	5.91	126.11	119.90
1	A	275	ALA	N-CA-C	5.82	118.50	111.40
2	B	156	ASP	N-CA-C	-5.82	106.22	113.38
1	A	276	ASN	N-CA-C	5.78	119.28	110.50
1	A	125	LEU	N-CA-C	-5.75	104.98	112.23
2	B	212	PHE	N-CA-C	5.70	115.63	108.45
2	B	93	GLY	N-CA-C	-5.69	106.69	115.73
3	C	45	GLU	N-CA-C	-5.67	105.01	111.14
3	C	3	PRO	N-CA-C	5.65	119.33	110.80
3	C	28	PHE	N-CA-C	5.64	118.76	110.30
1	A	119	MET	N-CA-C	5.59	117.82	111.11
2	B	15	GLN	N-CA-C	5.53	118.26	109.24
1	A	258	VAL	N-CA-C	5.45	116.43	108.58
2	B	118	HIS	N-CA-C	-5.41	102.04	110.42
1	A	132	ASP	N-CA-C	-5.38	101.80	110.14
1	A	285	LYS	N-CA-C	5.35	117.70	110.31
2	B	100	TYR	N-CA-C	5.34	118.26	111.69
1	A	160	ALA	CA-C-N	5.34	126.51	119.84
1	A	160	ALA	C-N-CA	5.34	126.51	119.84
1	A	247	LEU	N-CA-C	5.27	118.15	109.72
1	A	99	GLY	N-CA-C	5.26	118.38	110.18
2	B	84	ASP	N-CA-C	5.24	117.67	111.33
2	B	162	HIS	CA-C-N	5.10	125.38	119.47
2	B	162	HIS	C-N-CA	5.10	125.38	119.47
2	B	43	SER	N-CA-C	5.04	117.03	110.43

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	1724	0	1688	126	0
2	B	1834	0	1774	132	0
3	C	1839	0	1814	127	0
All	All	5397	0	5276	332	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 31.

All (332) 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:281:GLY:HA3	2:B:135:VAL:HG13	1.14	1.09
2:B:164:TYR:HA	3:C:66:MET:HE3	1.38	1.05
1:A:156:VAL:HG22	1:A:232:THR:HB	1.42	0.99
1:A:229:MET:HE2	1:A:231:GLY:H	1.26	0.97
2:B:134:THR:HG23	2:B:146:PRO:HG3	1.47	0.96
2:B:87:THR:HG22	2:B:96:ALA:HB1	1.51	0.92
2:B:55:ARG:HG2	2:B:244:GLU:HG2	1.56	0.87
1:A:76:ALA:O	1:A:79:THR:HG23	1.73	0.86
1:A:197:PRO:HA	3:C:31:THR:HG21	1.57	0.85
3:C:9:GLY:O	3:C:12:GLN:HG2	1.78	0.83
2:B:59:SER:O	2:B:62:ARG:HG2	1.78	0.83
2:B:172:ILE:HG21	3:C:66:MET:HE1	1.59	0.83
2:B:99:HIS:CD2	2:B:245:PHE:HB3	2.16	0.81
1:A:281:GLY:HA3	2:B:135:VAL:CG1	2.07	0.80
1:A:281:GLY:CA	2:B:135:VAL:HG13	2.04	0.79
2:B:56:PRO:HB3	2:B:60:VAL:HG21	1.63	0.78
2:B:164:TYR:CA	3:C:66:MET:HE3	2.14	0.78
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.82	0.78
1:A:294:ILE:HD12	3:C:56:ASN:HA	1.67	0.77
2:B:103:ARG:HG2	2:B:244:GLU:HB2	1.67	0.76
2:B:16:LEU:HD21	2:B:25:THR:CG2	2.16	0.76
2:B:95:ASN:O	2:B:99:HIS:HB2	1.85	0.76
1:A:229:MET:HE3	1:A:230:MET:H	1.50	0.76
1:A:117:ALA:HB1	3:C:236:LEU:HB3	1.67	0.74
2:B:134:THR:HG22	2:B:150:GLN:HE22	1.53	0.74
2:B:198:ILE:HG12	3:C:37:PRO:HG2	1.67	0.74
3:C:105:CYS:HA	3:C:226:MET:HE1	1.68	0.73
2:B:87:THR:HG22	2:B:96:ALA:CB	2.18	0.73
3:C:188:TYR:O	3:C:189:TYR:HD2	1.72	0.73
3:C:142:LEU:HD23	3:C:143:PRO:O	1.91	0.70
1:A:229:MET:HE2	1:A:231:GLY:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LEU:HD23	2:B:218:PRO:HA	1.72	0.70
3:C:180:HIS:CD2	3:C:181:ALA:H	2.09	0.70
3:C:158:ASP:C	3:C:160:GLY:H	1.99	0.69
3:C:92:ARG:HD3	3:C:188:TYR:HD2	1.58	0.68
3:C:10:THR:HG22	3:C:11:ASN:ND2	2.09	0.68
3:C:6:LEU:HD13	3:C:10:THR:HG21	1.74	0.68
3:C:92:ARG:HH22	3:C:191:THR:CG2	2.06	0.68
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.75	0.68
3:C:178:ARG:HH12	3:C:187:ASP:HB3	1.59	0.67
2:B:54:THR:O	2:B:56:PRO:HD3	1.95	0.67
1:A:80:LEU:HD21	1:A:260:ALA:HB3	1.75	0.66
3:C:42:ASN:O	3:C:45:GLU:HG3	1.95	0.66
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.78	0.66
2:B:119:GLN:NE2	3:C:209:PRO:HB2	2.11	0.65
1:A:270:ASN:HA	3:C:235:ILE:HG23	1.78	0.65
2:B:23:ILE:HG21	2:B:237:THR:HG21	1.79	0.65
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.32	0.64
2:B:21:SER:HB2	2:B:63:PHE:HB2	1.79	0.64
1:A:254:ARG:NH2	1:A:256:LYS:HD3	2.13	0.64
1:A:267:ARG:HD2	2:B:169:GLY:O	1.97	0.64
2:B:132:ILE:O	2:B:146:PRO:HG2	1.98	0.63
2:B:31:ILE:HG22	2:B:192:THR:HB	1.80	0.63
3:C:6:LEU:CD1	3:C:10:THR:HG21	2.28	0.63
1:A:165:SER:HB2	1:A:167:GLU:OE2	1.99	0.62
3:C:188:TYR:O	3:C:189:TYR:CD2	2.52	0.62
1:A:294:ILE:HD12	3:C:56:ASN:CA	2.29	0.62
1:A:153:TYR:HD1	1:A:235:VAL:HG13	1.65	0.62
1:A:156:VAL:HG23	1:A:156:VAL:O	2.00	0.62
2:B:172:ILE:CG2	3:C:66:MET:HE1	2.29	0.61
2:B:79:TYR:CB	2:B:215:LEU:HD12	2.30	0.61
1:A:94:ASP:C	1:A:96:PRO:HD3	2.24	0.61
1:A:206:ASP:OD1	2:B:81:LYS:HD2	2.01	0.61
3:C:2:PHE:CD1	3:C:3:PRO:HD2	2.35	0.61
1:A:150:LEU:O	1:A:151:LEU:HD23	2.01	0.61
2:B:48:THR:HG22	2:B:48:THR:O	2.00	0.61
1:A:294:ILE:HD11	3:C:55:VAL:HG12	1.82	0.61
1:A:104:ASN:O	1:A:166:ARG:HD2	2.01	0.60
2:B:69:LYS:HE3	2:B:156:ASP:O	2.02	0.60
2:B:32:ILE:HB	2:B:193:ILE:HG12	1.83	0.60
3:C:118:THR:HG23	3:C:166:THR:OG1	2.01	0.60
3:C:167:LEU:HD12	3:C:168:VAL:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:HB	1:A:142:PRO:HD2	1.84	0.59
3:C:180:HIS:CG	3:C:181:ALA:H	2.19	0.59
1:A:226:PRO:HG2	1:A:227:ASN:OD1	2.02	0.59
2:B:79:TYR:HB3	2:B:215:LEU:HD12	1.85	0.58
1:A:136:THR:HG23	1:A:189:GLN:HG3	1.85	0.58
1:A:156:VAL:O	1:A:156:VAL:CG2	2.50	0.58
2:B:56:PRO:HB3	2:B:60:VAL:CG2	2.30	0.58
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.69	0.58
3:C:90:PRO:CG	3:C:115:LEU:HD11	2.34	0.58
3:C:92:ARG:HH22	3:C:191:THR:HG21	1.68	0.58
3:C:4:THR:HG22	3:C:5:GLU:H	1.68	0.58
2:B:153:PRO:HB2	2:B:157:GLY:O	2.04	0.57
2:B:27:GLU:O	2:B:28:ALA:HB2	2.03	0.57
1:A:207:GLY:HA3	2:B:208:ASN:O	2.04	0.57
2:B:164:TYR:HA	3:C:66:MET:CE	2.24	0.57
1:A:156:VAL:CG2	1:A:232:THR:HB	2.25	0.56
2:B:231:VAL:O	2:B:232:ILE:HD13	2.05	0.56
2:B:149:LYS:H	2:B:149:LYS:HD2	1.70	0.56
2:B:184:ASN:HB3	2:B:187:THR:OG1	2.05	0.56
1:A:259:ARG:HG2	3:C:39:GLU:OE1	2.06	0.56
2:B:198:ILE:HG12	3:C:37:PRO:CG	2.35	0.56
2:B:177:VAL:HG22	2:B:177:VAL:O	2.04	0.56
1:A:277:PRO:HG2	2:B:133:GLY:HA3	1.88	0.56
2:B:149:LYS:HD2	2:B:149:LYS:N	2.20	0.56
3:C:6:LEU:HD13	3:C:10:THR:CG2	2.36	0.56
1:A:291:ARG:HD2	1:A:293:ALA:O	2.05	0.56
2:B:79:TYR:HA	2:B:214:LEU:O	2.06	0.56
3:C:92:ARG:NH2	3:C:191:THR:CG2	2.68	0.55
1:A:114:THR:HG23	3:C:237:GLN:HG2	1.89	0.55
1:A:202:GLN:HG2	1:A:225:MET:HE2	1.89	0.55
1:A:290:SER:OG	3:C:68:ARG:NH2	2.39	0.55
2:B:174:GLN:HA	3:C:51:THR:HG22	1.89	0.55
3:C:4:THR:HG22	3:C:5:GLU:N	2.21	0.55
3:C:167:LEU:HD12	3:C:168:VAL:H	1.71	0.55
1:A:117:ALA:HB1	3:C:236:LEU:HD23	1.89	0.55
2:B:92:PHE:CE1	2:B:245:PHE:HZ	2.25	0.55
2:B:172:ILE:C	2:B:174:GLN:H	2.14	0.54
1:A:295:THR:HA	3:C:85:VAL:HG12	1.89	0.54
3:C:146:ARG:O	3:C:146:ARG:HG2	2.06	0.54
2:B:164:TYR:HD1	3:C:66:MET:HE2	1.70	0.54
1:A:229:MET:HE3	1:A:230:MET:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ALA:HB1	3:C:172:ILE:HG21	1.89	0.54
2:B:41:TYR:CD1	2:B:55:ARG:HD3	2.43	0.54
3:C:105:CYS:CA	3:C:226:MET:HE1	2.37	0.54
1:A:202:GLN:HG2	1:A:225:MET:HG2	1.89	0.53
2:B:130:TYR:HE1	2:B:215:LEU:CD1	2.20	0.53
1:A:113:ILE:HG22	1:A:253:MET:HE1	1.89	0.53
1:A:208:TYR:CE1	1:A:222:TYR:HB2	2.44	0.53
2:B:71:TRP:CE2	2:B:222:LEU:HB2	2.44	0.53
3:C:105:CYS:SG	3:C:226:MET:HE1	2.48	0.53
1:A:224:ALA:O	1:A:226:PRO:HD3	2.09	0.53
2:B:82:PHE:O	2:B:210:CYS:HA	2.09	0.53
1:A:111:ILE:HD11	1:A:233:PHE:CE2	2.44	0.52
1:A:276:ASN:OD1	1:A:278:ASN:HB2	2.10	0.52
2:B:236:ILE:N	2:B:236:ILE:HD12	2.24	0.52
3:C:174:ASN:OD1	3:C:174:ASN:O	2.27	0.52
2:B:122:LEU:HB2	2:B:183:ILE:HB	1.92	0.52
3:C:83:CYS:HB3	3:C:196:ILE:HG22	1.90	0.52
1:A:84:PHE:O	1:A:85:SER:O	2.28	0.52
1:A:276:ASN:CB	1:A:277:PRO:HD2	2.40	0.52
2:B:134:THR:HG23	2:B:146:PRO:CG	2.29	0.52
3:C:90:PRO:HD2	3:C:188:TYR:OH	2.09	0.52
3:C:115:LEU:HB2	3:C:169:ILE:HB	1.92	0.52
1:A:155:PHE:O	1:A:177:PRO:HD2	2.10	0.52
1:A:245:TYR:CD1	1:A:245:TYR:N	2.78	0.52
1:A:254:ARG:NH1	3:C:18:ASP:HA	2.25	0.52
3:C:150:MET:O	3:C:150:MET:SD	2.67	0.51
1:A:140:CYS:HA	1:A:183:LEU:HD21	1.92	0.51
2:B:114:ALA:HB2	2:B:232:ILE:HD12	1.92	0.51
3:C:178:ARG:HH12	3:C:187:ASP:CB	2.23	0.51
1:A:104:ASN:HA	1:A:242:LYS:NZ	2.25	0.51
1:A:222:TYR:CE1	2:B:151:THR:HG23	2.45	0.51
3:C:178:ARG:NH1	3:C:187:ASP:HB3	2.25	0.51
2:B:119:GLN:HB3	3:C:124:SER:HA	1.92	0.50
1:A:220:LEU:HD23	2:B:145:HIS:HD2	1.77	0.50
2:B:16:LEU:HD21	2:B:25:THR:HG22	1.92	0.50
1:A:229:MET:CE	1:A:231:GLY:H	2.11	0.50
2:B:86:LEU:C	2:B:88:GLU:H	2.19	0.50
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.12	0.50
1:A:153:TYR:CD1	1:A:235:VAL:HG13	2.46	0.50
2:B:184:ASN:OD1	2:B:186:ARG:HG2	2.12	0.50
3:C:188:TYR:O	3:C:189:TYR:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HB	1:A:203:TRP:NE1	2.26	0.50
2:B:80:TRP:HZ3	2:B:216:VAL:CG1	2.25	0.50
3:C:61:ASN:ND2	3:C:64:SER:OG	2.44	0.49
1:A:123:VAL:C	1:A:125:LEU:H	2.21	0.49
2:B:161:GLN:O	2:B:162:HIS:HD2	1.95	0.49
3:C:105:CYS:HA	3:C:226:MET:CE	2.42	0.49
2:B:103:ARG:HD2	2:B:203:PHE:CE2	2.48	0.49
1:A:245:TYR:HB3	1:A:246:PRO:HD2	1.95	0.49
2:B:165:VAL:HA	2:B:170:ILE:O	2.12	0.49
1:A:123:VAL:HB	1:A:203:TRP:HE1	1.77	0.49
1:A:277:PRO:O	1:A:278:ASN:C	2.56	0.49
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.48	0.49
1:A:250:ARG:HG3	1:A:250:ARG:NH2	2.27	0.48
2:B:56:PRO:HB3	2:B:60:VAL:CB	2.44	0.48
2:B:116:LYS:HD3	3:C:125:PHE:CE1	2.48	0.48
3:C:66:MET:CE	3:C:69:LEU:HD11	2.42	0.48
1:A:168:SER:C	1:A:170:ALA:H	2.22	0.48
2:B:130:TYR:HE1	2:B:215:LEU:HD11	1.78	0.48
2:B:65:THR:OG1	2:B:237:THR:HG23	2.13	0.48
3:C:54:GLU:HG2	3:C:69:LEU:HD23	1.96	0.48
3:C:182:ARG:HH21	3:C:182:ARG:HG3	1.77	0.48
1:A:83:PHE:O	1:A:86:ARG:NH2	2.47	0.48
1:A:112:ASP:CG	1:A:114:THR:HG22	2.39	0.48
2:B:38:TRP:O	2:B:40:SER:N	2.46	0.48
2:B:41:TYR:CE1	2:B:55:ARG:HD3	2.49	0.48
3:C:236:LEU:N	3:C:236:LEU:HD12	2.29	0.47
2:B:86:LEU:C	2:B:88:GLU:N	2.72	0.47
1:A:116:TYR:CE2	1:A:118:GLN:HG3	2.48	0.47
2:B:28:ALA:O	2:B:29:ALA:O	2.33	0.47
2:B:99:HIS:HD2	2:B:245:PHE:HB3	1.70	0.47
2:B:241:MET:O	2:B:242:CYS:C	2.57	0.47
3:C:51:THR:HG21	3:C:100:LEU:HB2	1.95	0.47
3:C:144:LYS:HD3	3:C:148:THR:HG21	1.97	0.47
2:B:109:HIS:CE1	2:B:190:CYS:HB2	2.49	0.47
2:B:85:VAL:HG23	2:B:155:ALA:HA	1.96	0.47
3:C:182:ARG:HG3	3:C:182:ARG:NH2	2.29	0.47
2:B:71:TRP:HD1	2:B:72:GLU:N	2.13	0.47
3:C:105:CYS:SG	3:C:226:MET:CE	3.02	0.47
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.96	0.46
1:A:205:TYR:O	1:A:223:GLY:HA2	2.15	0.46
1:A:137:PHE:N	1:A:137:PHE:CD2	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:N	1:A:96:PRO:HD3	2.29	0.46
1:A:104:ASN:HB2	1:A:106:TYR:CD1	2.50	0.46
1:A:238:VAL:CG1	1:A:239:GLY:N	2.78	0.46
2:B:164:TYR:HD1	3:C:66:MET:CE	2.28	0.46
2:B:56:PRO:HG2	2:B:245:PHE:CD2	2.51	0.46
2:B:57:ASP:O	2:B:58:VAL:C	2.58	0.46
3:C:51:THR:HG21	3:C:100:LEU:CB	2.46	0.46
3:C:56:ASN:O	3:C:59:PRO:HD2	2.15	0.46
3:C:152:GLY:O	3:C:153:THR:C	2.57	0.46
2:B:103:ARG:HG3	2:B:103:ARG:HH11	1.80	0.46
1:A:220:LEU:HA	2:B:145:HIS:CD2	2.50	0.46
2:B:172:ILE:C	2:B:174:GLN:N	2.72	0.46
3:C:90:PRO:HG2	3:C:115:LEU:HD11	1.98	0.46
2:B:66:LEU:HD23	2:B:66:LEU:N	2.31	0.46
3:C:67:GLU:HG2	3:C:70:ARG:NH1	2.31	0.46
3:C:187:ASP:O	3:C:188:TYR:O	2.34	0.46
2:B:77:GLY:HA2	2:B:218:PRO:HD3	1.98	0.45
2:B:119:GLN:HB3	3:C:124:SER:CA	2.46	0.45
1:A:136:THR:HG21	3:C:13:PHE:CD2	2.52	0.45
3:C:75:ALA:HA	3:C:202:TYR:HB3	1.97	0.45
1:A:293:ALA:C	1:A:295:THR:H	2.24	0.45
1:A:179:VAL:HG22	1:A:179:VAL:O	2.15	0.45
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.52	0.45
1:A:85:SER:O	1:A:86:ARG:HB2	2.17	0.45
1:A:254:ARG:HH21	1:A:256:LYS:HB3	1.82	0.45
2:B:37:GLU:OE2	3:C:37:PRO:HA	2.16	0.45
3:C:24:ILE:HG23	3:C:25:LEU:HD22	1.99	0.45
2:B:13:VAL:O	2:B:14:ALA:HB2	2.17	0.45
2:B:13:VAL:HG22	2:B:14:ALA:N	2.32	0.45
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.46	0.45
3:C:92:ARG:HD3	3:C:188:TYR:CD2	2.45	0.45
1:A:104:ASN:HB2	1:A:106:TYR:CE1	2.51	0.45
3:C:126:MET:HE2	3:C:205:PRO:HG3	1.98	0.45
1:A:117:ALA:CB	3:C:236:LEU:HD23	2.45	0.45
2:B:129:GLU:OE2	2:B:209:HIS:NE2	2.50	0.45
1:A:226:PRO:HG2	1:A:227:ASN:H	1.82	0.44
1:A:195:MET:O	1:A:196:SER:C	2.60	0.44
1:A:291:ARG:O	3:C:58:VAL:HG12	2.17	0.44
2:B:116:LYS:HB3	3:C:125:PHE:CD1	2.52	0.44
2:B:119:GLN:HB3	3:C:124:SER:N	2.32	0.44
1:A:114:THR:HG21	3:C:237:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:SER:C	1:A:167:GLU:H	2.25	0.44
2:B:79:TYR:HB2	2:B:215:LEU:HD12	1.98	0.44
2:B:161:GLN:O	2:B:162:HIS:CD2	2.71	0.44
3:C:31:THR:HA	3:C:32:PRO:HD3	1.85	0.44
3:C:54:GLU:HG3	3:C:98:SER:CB	2.48	0.44
3:C:66:MET:HE2	3:C:69:LEU:HD11	1.98	0.44
3:C:65:LEU:O	3:C:68:ARG:HG3	2.17	0.44
1:A:195:MET:O	1:A:196:SER:O	2.35	0.44
1:A:244:LYS:HB2	1:A:245:TYR:CE1	2.53	0.44
2:B:82:PHE:O	2:B:210:CYS:CA	2.66	0.44
2:B:176:THR:OG1	3:C:50:GLU:O	2.22	0.44
3:C:56:ASN:O	3:C:56:ASN:CG	2.59	0.44
1:A:87:ALA:HB1	1:A:252:TYR:HB3	1.99	0.44
1:A:291:ARG:HG3	3:C:58:VAL:HG12	2.00	0.44
2:B:151:THR:HG22	2:B:152:GLN:NE2	2.32	0.44
1:A:136:THR:HG21	3:C:13:PHE:CE2	2.52	0.44
2:B:28:ALA:C	2:B:29:ALA:O	2.60	0.44
2:B:238:LEU:HD12	2:B:238:LEU:C	2.43	0.44
1:A:113:ILE:HG22	1:A:253:MET:SD	2.58	0.44
1:A:140:CYS:HB2	1:A:145:GLU:O	2.18	0.44
2:B:101:LEU:HB3	2:B:203:PHE:HD1	1.83	0.44
1:A:116:TYR:O	1:A:117:ALA:C	2.61	0.43
1:A:197:PRO:CG	1:A:227:ASN:HB3	2.48	0.43
1:A:270:ASN:HA	3:C:235:ILE:CG2	2.46	0.43
1:A:297:LEU:HD12	1:A:297:LEU:H	1.83	0.43
2:B:57:ASP:O	2:B:58:VAL:O	2.36	0.43
1:A:89:LEU:HD11	1:A:91:GLY:O	2.18	0.43
3:C:56:ASN:O	3:C:68:ARG:HA	2.19	0.43
3:C:193:LEU:HA	3:C:193:LEU:HD23	1.80	0.43
3:C:204:VAL:HG22	3:C:208:ALA:HB3	2.00	0.43
2:B:71:TRP:HD1	2:B:72:GLU:H	1.65	0.43
1:A:131:PHE:HB3	1:A:258:VAL:HG22	2.01	0.43
1:A:168:SER:C	1:A:170:ALA:N	2.76	0.43
1:A:169:LEU:HD12	1:A:169:LEU:N	2.34	0.43
3:C:180:HIS:CG	3:C:181:ALA:N	2.87	0.43
2:B:130:TYR:C	2:B:130:TYR:CD2	2.96	0.43
1:A:276:ASN:HB2	1:A:277:PRO:CD	2.48	0.43
1:A:218:LYS:NZ	1:A:220:LEU:HD23	2.34	0.43
2:B:91:VAL:HG22	2:B:91:VAL:O	2.19	0.43
2:B:115:SER:C	2:B:117:PHE:H	2.25	0.43
1:A:158:PRO:HB3	1:A:229:MET:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:SER:CB	2:B:63:PHE:HB2	2.46	0.42
2:B:174:GLN:O	2:B:177:VAL:HG12	2.18	0.42
2:B:128:PRO:O	2:B:129:GLU:C	2.59	0.42
3:C:47:CYS:HB3	3:C:101:LEU:CD1	2.49	0.42
3:C:158:ASP:C	3:C:160:GLY:N	2.64	0.42
3:C:147:ALA:O	3:C:150:MET:HB3	2.19	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.35	0.42
3:C:178:ARG:HD3	3:C:180:HIS:HB3	2.01	0.42
1:A:209:PRO:O	1:A:210:THR:C	2.63	0.42
2:B:239:ALA:HA	2:B:240:PRO:HD3	1.80	0.42
3:C:54:GLU:OE2	3:C:68:ARG:NH1	2.49	0.42
3:C:138:PRO:HB3	3:C:190:THR:HA	2.01	0.42
2:B:117:PHE:CE2	3:C:126:MET:HG3	2.54	0.42
2:B:184:ASN:HB3	2:B:187:THR:HG1	1.85	0.42
2:B:232:ILE:HA	2:B:233:PRO:HD2	1.90	0.42
3:C:93:ASN:N	3:C:93:ASN:HD22	2.16	0.42
1:A:123:VAL:HG23	1:A:124:GLU:N	2.34	0.42
1:A:147:VAL:HG11	1:A:245:TYR:CD2	2.55	0.42
2:B:27:GLU:O	2:B:28:ALA:CB	2.67	0.42
2:B:122:LEU:CD2	2:B:218:PRO:HA	2.45	0.42
3:C:52:ILE:HA	3:C:217:LEU:HD23	2.02	0.42
3:C:158:ASP:OD1	3:C:160:GLY:CA	2.68	0.42
1:A:226:PRO:C	1:A:228:ASN:H	2.28	0.41
2:B:235:THR:C	2:B:236:ILE:HD12	2.45	0.41
2:B:13:VAL:N	2:B:27:GLU:HG3	2.35	0.41
3:C:172:ILE:O	3:C:172:ILE:HD12	2.20	0.41
3:C:238:THR:O	3:C:239:GLY:O	2.39	0.41
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.84	0.41
1:A:277:PRO:HG2	2:B:133:GLY:CA	2.51	0.41
2:B:61:ASN:OD1	2:B:240:PRO:HB2	2.20	0.41
2:B:89:THR:HG22	2:B:90:GLY:N	2.35	0.41
3:C:188:TYR:O	3:C:189:TYR:CB	2.68	0.41
2:B:189:ASN:CG	2:B:190:CYS:N	2.78	0.41
1:A:104:ASN:HA	1:A:242:LYS:HZ1	1.85	0.41
1:A:108:ASN:ND2	1:A:234:SER:OG	2.54	0.41
1:A:113:ILE:O	1:A:119:MET:HG2	2.21	0.41
1:A:122:LYS:HG2	3:C:107:TYR:CE1	2.56	0.41
1:A:289:ALA:HB3	3:C:93:ASN:HB3	2.02	0.41
2:B:76:LYS:HZ2	2:B:76:LYS:HB3	1.85	0.41
3:C:16:THR:O	3:C:17:ASP:C	2.64	0.41
1:A:268:ASN:ND2	1:A:269:GLN:HE21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:VAL:HA	2:B:218:PRO:HD3	1.88	0.41
3:C:54:GLU:OE2	3:C:68:ARG:HD3	2.21	0.41
1:A:204:PHE:CE1	1:A:264:ARG:HD3	2.56	0.40
3:C:178:ARG:NH1	3:C:187:ASP:CB	2.84	0.40
1:A:166:ARG:HH21	1:A:237:THR:HG23	1.85	0.40
2:B:68:THR:OG1	2:B:235:THR:HG23	2.20	0.40
2:B:86:LEU:HD23	2:B:89:THR:HB	2.03	0.40
2:B:199:ASN:OD1	2:B:209:HIS:CE1	2.75	0.40
1:A:97:LEU:HD11	1:A:246:PRO:HD3	2.03	0.40
2:B:132:ILE:HG21	2:B:150:GLN:HE21	1.86	0.40
1:A:89:LEU:HD12	1:A:251:ILE:O	2.22	0.40
1:A:171:TRP:CE2	1:A:236:ARG:HD2	2.57	0.40
2:B:68:THR:HG21	2:B:233:PRO:HB2	2.04	0.40
2:B:175:LEU:C	2:B:177:VAL:H	2.29	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	214/225 (95%)	188 (88%)	15 (7%)	11 (5%)	1	18
2	B	235/237 (99%)	196 (83%)	31 (13%)	8 (3%)	3	24
3	C	237/239 (99%)	202 (85%)	24 (10%)	11 (5%)	2	20
All	All	686/701 (98%)	586 (85%)	70 (10%)	30 (4%)	2	20

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
2	B	28	ALA
2	B	29	ALA

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Mol	Chain	Res	Type
2	B	58	VAL
3	C	93	ASN
3	C	188	TYR
1	A	86	ARG
1	A	196	SER
1	A	227	ASN
2	B	14	ALA
2	B	90	GLY
3	C	180	HIS
3	C	182	ARG
3	C	189	TYR
1	A	124	GLU
1	A	289	ALA
2	B	39	PRO
3	C	221	GLN
1	A	117	ALA
1	A	169	LEU
3	C	72	PRO
3	C	137	PRO
2	B	67	ASP
3	C	57	ASN
3	C	105	CYS
3	C	191	THR
1	A	186	PRO
1	A	294	ILE
2	B	147	PRO
1	A	262	ILE

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	187/193 (97%)	167 (89%)	20 (11%)	6	24
2	B	201/201 (100%)	186 (92%)	15 (8%)	12	36
3	C	199/199 (100%)	175 (88%)	24 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	587/593 (99%)	528 (90%)	59 (10%)	7 26

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	114	THR
1	A	136	THR
1	A	146	VAL
1	A	147	VAL
1	A	156	VAL
1	A	172	GLN
1	A	179	VAL
1	A	183	LEU
1	A	184	SER
1	A	227	ASN
1	A	235	VAL
1	A	237	THR
1	A	245	TYR
1	A	259	ARG
1	A	265	PRO
1	A	297	LEU
2	B	16	LEU
2	B	42	CYS
2	B	50	VAL
2	B	58	VAL
2	B	62	ARG
2	B	66	LEU
2	B	76	LYS
2	B	99	HIS
2	B	102	TYR
2	B	126	VAL
2	B	142	GLU
2	B	215	LEU
2	B	216	VAL
2	B	235	THR
2	B	237	THR
3	C	6	LEU
3	C	14	LEU

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Mol	Chain	Res	Type
3	C	21	SER
3	C	25	LEU
3	C	31	THR
3	C	33	CYS
3	C	51	THR
3	C	53	LEU
3	C	61	ASN
3	C	72	PRO
3	C	73	VAL
3	C	87	ARG
3	C	90	PRO
3	C	116	GLU
3	C	125	PHE
3	C	146	ARG
3	C	164	SER
3	C	204	VAL
3	C	221	GLN
3	C	225	THR
3	C	228	LEU
3	C	230	LYS
3	C	234	ASP
3	C	235	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	152	GLN
1	A	228	ASN
1	A	268	ASN
1	A	278	ASN
2	B	99	HIS
2	B	111	GLN
2	B	113	ASN
2	B	119	GLN
2	B	145	HIS
2	B	150	GLN
2	B	152	GLN
2	B	162	HIS
2	B	208	ASN
3	C	48	GLN
3	C	61	ASN

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Mol	Chain	Res	Type
3	C	93	ASN
3	C	154	HIS
3	C	162	GLN
3	C	174	ASN
3	C	180	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	218/225 (96%)	1.45	42 (19%)	3 6	79, 97, 150, 207	0
2	B	237/237 (100%)	1.99	90 (37%)	1 2	81, 111, 194, 237	0
3	C	239/239 (100%)	1.56	64 (26%)	1 3	80, 99, 180, 232	0
All	All	694/701 (99%)	1.67	196 (28%)	1 3	79, 100, 180, 237	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	239	GLY	10.0
2	B	44	ASP	9.1
2	B	45	SER	8.7
1	A	221	GLU	8.4
2	B	46	ASP	8.0
1	A	73	HIS	7.7
2	B	28	ALA	7.5
1	A	210	THR	7.4
2	B	58	VAL	7.2
1	A	219	ASP	7.1
1	A	220	LEU	7.1
3	C	1	GLY	7.0
3	C	238	THR	6.7
3	C	183	ASP	6.7
3	C	180	HIS	6.4
2	B	27	GLU	6.3
1	A	218	LYS	6.2
3	C	5	GLU	6.1
2	B	57	ASP	5.9
3	C	181	ALA	5.8
2	B	149	LYS	5.8
3	C	182	ARG	5.7
2	B	15	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	24	THR	5.5
2	B	161	GLN	5.4
2	B	142	GLU	5.4
2	B	43	SER	5.3
2	B	47	ALA	5.3
2	B	137	GLY	5.3
1	A	283	SER	5.2
1	A	100	THR	5.1
2	B	249	ARG	5.1
3	C	189	TYR	5.0
2	B	53	PRO	5.0
3	C	179	ALA	5.0
2	B	148	TYR	5.0
2	B	26	GLN	4.8
2	B	14	ALA	4.6
2	B	30	ASN	4.6
1	A	223	GLY	4.5
2	B	16	LEU	4.5
2	B	48	THR	4.4
2	B	134	THR	4.3
2	B	51	ASP	4.2
2	B	229	THR	4.2
2	B	143	ASP	4.2
2	B	29	ALA	4.2
3	C	237	GLN	4.2
2	B	139	THR	4.1
3	C	234	ASP	4.1
1	A	241	SER	4.1
2	B	91	VAL	4.0
2	B	150	GLN	4.0
3	C	29	HIS	4.0
2	B	59	SER	3.9
2	B	20	ASN	3.9
2	B	94	GLN	3.9
1	A	259	ARG	3.9
1	A	101	THR	3.8
3	C	60	THR	3.8
2	B	67	ASP	3.8
1	A	282	ASN	3.8
1	A	98	LYS	3.8
3	C	87	ARG	3.8
2	B	248	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	274	LYS	3.7
2	B	36	GLY	3.7
2	B	90	GLY	3.7
2	B	226	GLN	3.6
2	B	141	THR	3.6
3	C	230	LYS	3.6
3	C	18	ASP	3.6
2	B	189	ASN	3.6
1	A	94	ASP	3.5
1	A	224	ALA	3.5
1	A	244	LYS	3.5
2	B	97	GLN	3.5
3	C	232	ALA	3.5
2	B	187	THR	3.5
2	B	49	ALA	3.4
3	C	144	LYS	3.4
2	B	206	ALA	3.4
3	C	191	THR	3.4
1	A	242	LYS	3.3
2	B	87	THR	3.3
3	C	41	ARG	3.3
2	B	74	SER	3.3
1	A	112	ASP	3.2
1	A	285	LYS	3.2
3	C	76	GLN	3.2
2	B	33	VAL	3.2
2	B	111	GLN	3.2
2	B	55	ARG	3.2
3	C	48	GLN	3.2
3	C	178	ARG	3.2
3	C	145	ASP	3.1
3	C	45	GLU	3.1
2	B	25	THR	3.1
2	B	50	VAL	3.1
3	C	33	CYS	3.1
2	B	207	LEU	3.1
2	B	159	GLU	3.1
3	C	128	THR	3.0
2	B	178	CYS	3.0
3	C	79	LYS	3.0
2	B	76	LYS	3.0
2	B	136	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	2.9
3	C	153	THR	2.9
3	C	146	ARG	2.9
3	C	186	PHE	2.8
3	C	27	ASN	2.8
2	B	88	GLU	2.8
1	A	225	MET	2.8
2	B	52	LYS	2.8
3	C	92	ARG	2.8
3	C	61	ASN	2.8
1	A	292	THR	2.8
1	A	97	LEU	2.7
1	A	174	ALA	2.7
1	A	182	LYS	2.7
2	B	38	TRP	2.7
2	B	113	ASN	2.7
2	B	140	GLY	2.6
2	B	13	VAL	2.6
3	C	171	TRP	2.6
3	C	221	GLN	2.6
2	B	95	ASN	2.6
2	B	147	PRO	2.6
2	B	98	PHE	2.5
1	A	164	ASP	2.5
3	C	147	ALA	2.5
2	B	54	THR	2.5
1	A	243	SER	2.5
2	B	190	CYS	2.5
1	A	209	PRO	2.5
3	C	227	LYS	2.5
3	C	184	GLY	2.5
1	A	289	ALA	2.5
3	C	148	THR	2.5
2	B	211	ASN	2.5
2	B	89	THR	2.4
1	A	226	PRO	2.4
1	A	92	GLU	2.4
3	C	67	GLU	2.4
3	C	152	GLY	2.4
2	B	100	TYR	2.4
3	C	176	HIS	2.4
1	A	264	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	10	THR	2.4
3	C	233	SER	2.4
1	A	288	GLY	2.4
2	B	204	ASP	2.4
2	B	19	GLY	2.4
3	C	17	ASP	2.4
2	B	179	PRO	2.3
2	B	152	GLN	2.3
1	A	281	GLY	2.3
1	A	96	PRO	2.3
2	B	156	ASP	2.3
3	C	47	CYS	2.3
1	A	228	ASN	2.3
3	C	15	THR	2.3
2	B	40	SER	2.3
2	B	135	VAL	2.3
3	C	210	ASN	2.3
2	B	180	HIS	2.3
3	C	6	LEU	2.3
3	C	154	HIS	2.3
2	B	61	ASN	2.2
1	A	74	SER	2.2
3	C	150	MET	2.2
3	C	35	HIS	2.2
2	B	84	ASP	2.2
2	B	32	ILE	2.2
3	C	12	GLN	2.2
2	B	151	THR	2.2
2	B	203	PHE	2.2
3	C	206	ILE	2.2
3	C	187	ASP	2.2
2	B	198	ILE	2.2
3	C	162	GLN	2.2
1	A	120	ARG	2.2
2	B	42	CYS	2.1
2	B	196	PRO	2.1
3	C	236	LEU	2.1
1	A	81	ASP	2.1
2	B	181	GLN	2.1
2	B	112	CYS	2.1
3	C	222	LYS	2.1
3	C	168	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	207	GLY	2.1
2	B	235	THR	2.1
3	C	136	THR	2.0
1	A	172	GLN	2.0
3	C	46	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.