



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:28 PM UTC

PDB ID : 3VBR / pdb_00003vbr
Title : Crystal structure of formaldehyde treated empty human Enterovirus 71 particle (room temperature)
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 : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

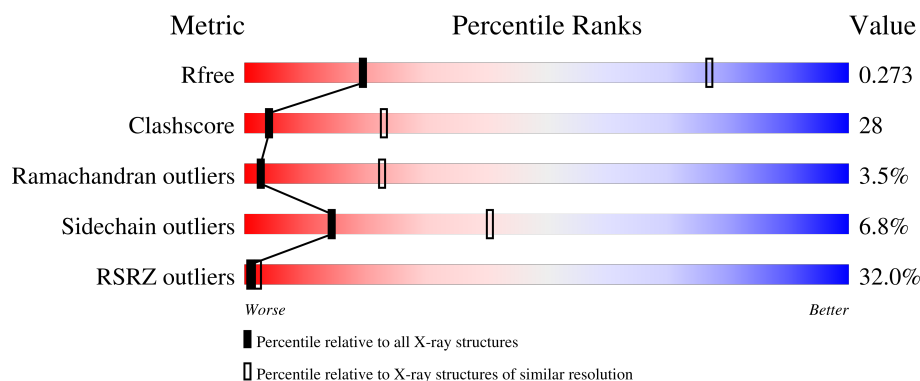
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	
2	B	237	
3	C	239	

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			

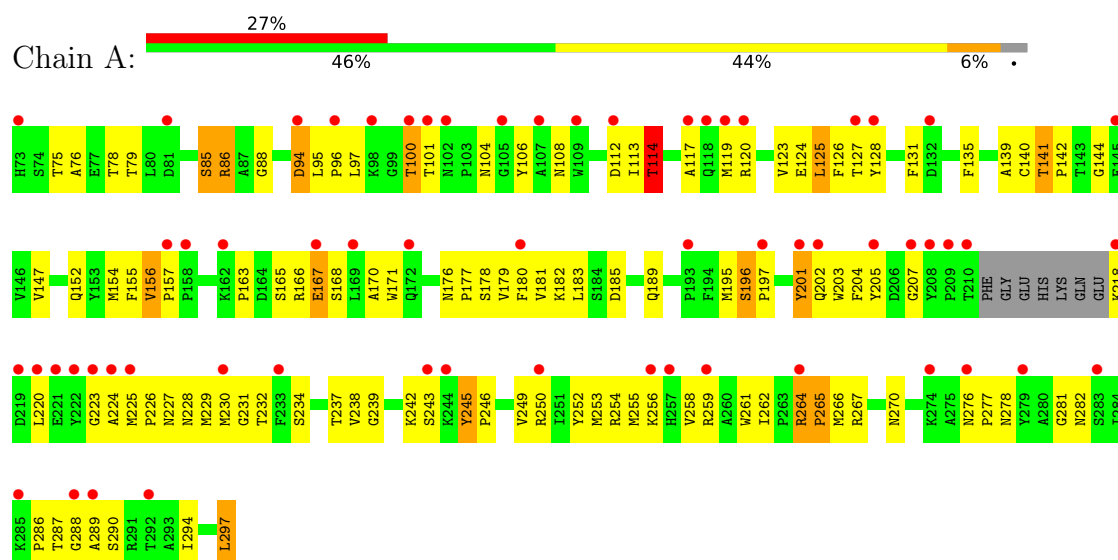
- Molecule 3 is a protein called Genome Polyprotein, capsid protein VP3.

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

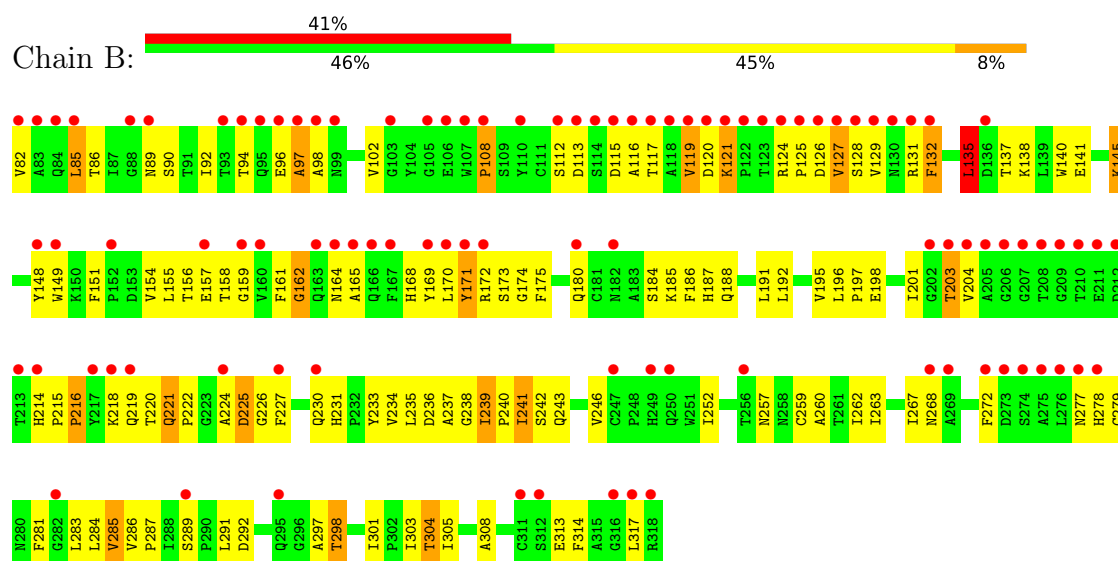
3 Residue-property plots

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.

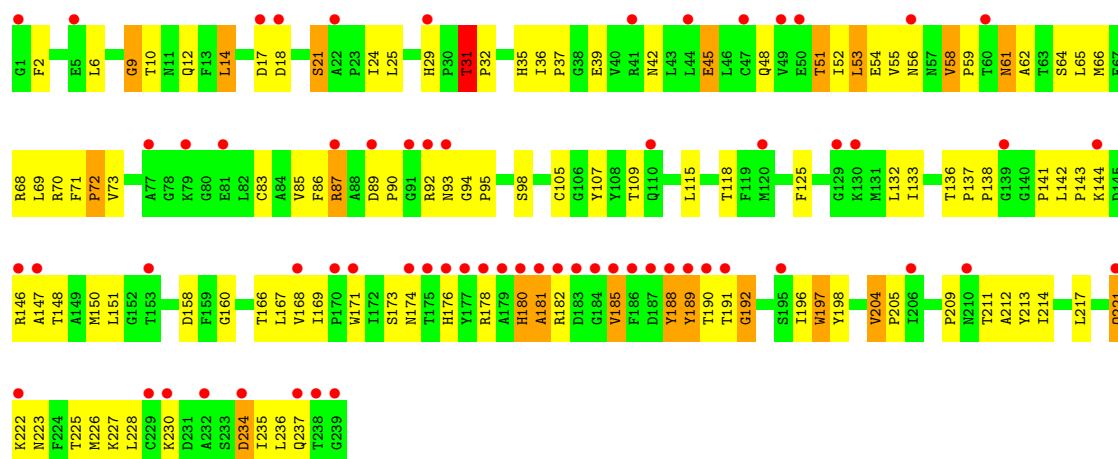
• Molecule 1: Genome Polyprotein, capsid protein VP1



• 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	354.90Å 354.90Å 354.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 3.80 49.70 – 3.80	Depositor EDS
% Data completeness (in resolution range)	90.3 (49.70-3.80) 90.2 (49.70-3.80)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.284 0.256 , 0.273	Depositor DCC
R_{free} test set	683 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 113.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.39	EDS
Total number of atoms	5397	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% 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 (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	0.55	0/1776	1.09	13/2419 (0.5%)
2	B	0.62	0/1889	1.08	18/2592 (0.7%)
3	C	0.60	0/1891	1.08	15/2586 (0.6%)
All	All	0.59	0/5556	1.08	46/7597 (0.6%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	192	GLY	N-CA-C	-7.48	103.33	111.93
3	C	94	GLY	CA-C-N	7.05	128.65	119.84
3	C	94	GLY	C-N-CA	7.05	128.65	119.84
3	C	45	GLU	N-CA-C	-6.98	103.61	111.14
3	C	9	GLY	N-CA-C	-6.96	104.98	115.00
3	C	31	THR	CA-C-N	6.76	126.80	119.90
3	C	31	THR	C-N-CA	6.76	126.80	119.90
1	A	125	LEU	N-CA-C	-6.30	105.42	113.23
3	C	234	ASP	N-CA-C	-6.29	105.74	113.41
1	A	264	ARG	N-CA-C	6.15	115.38	108.25
1	A	201	TYR	N-CA-C	-6.09	101.27	110.28
2	B	225	ASP	N-CA-C	-6.09	105.68	113.23
2	B	175	PHE	N-CA-C	6.00	119.26	109.06
1	A	225	MET	CA-C-N	5.96	125.51	119.19
1	A	225	MET	C-N-CA	5.96	125.51	119.19
2	B	298	THR	CA-C-N	5.93	126.44	120.04
2	B	298	THR	C-N-CA	5.93	126.44	120.04
2	B	132	PHE	N-CA-C	5.89	117.89	108.41
1	A	119	MET	N-CA-C	5.88	118.20	111.02
2	B	241	ILE	N-CA-C	-5.88	103.56	111.44
3	C	29	HIS	CA-C-N	5.81	125.74	119.76
3	C	29	HIS	C-N-CA	5.81	125.74	119.76
2	B	162	GLY	N-CA-C	-5.80	107.14	114.16
2	B	221	GLN	CA-C-N	5.79	127.07	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	GLN	C-N-CA	5.79	127.07	119.84
1	A	282	ASN	N-CA-C	-5.67	105.39	112.93
1	A	141	THR	N-CA-C	-5.63	102.82	110.36
3	C	169	ILE	CA-C-N	5.54	126.76	119.84
3	C	169	ILE	C-N-CA	5.54	126.76	119.84
2	B	161	PHE	N-CA-C	-5.49	104.82	112.45
2	B	169	TYR	N-CA-C	5.49	117.34	111.36
1	A	114	THR	N-CA-C	-5.47	106.56	113.18
1	A	100	THR	N-CA-C	-5.46	105.74	112.90
2	B	289	SER	N-CA-C	-5.45	100.05	109.15
3	C	185	VAL	N-CA-C	5.41	115.88	107.28
3	C	2	PHE	CA-C-N	5.38	125.64	119.83
3	C	2	PHE	C-N-CA	5.38	125.64	119.83
2	B	308	ALA	CA-C-N	5.34	125.50	119.90
2	B	308	ALA	C-N-CA	5.34	125.50	119.90
2	B	135	LEU	N-CA-C	5.32	117.58	110.35
1	A	258	VAL	N-CA-C	5.32	116.95	108.87
1	A	288	GLY	N-CA-C	5.27	118.80	111.10
1	A	147	VAL	N-CA-C	5.25	113.50	109.19
2	B	113	ASP	N-CA-C	5.18	117.83	111.82
2	B	262	ILE	N-CA-C	5.12	115.64	108.17
2	B	192	LEU	N-CA-C	-5.03	101.51	109.96

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	110	0
2	B	1834	0	1774	120	0
3	C	1839	0	1814	110	0
All	All	5397	0	5276	296	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 28.

All (296) 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:229:MET:HE2	1:A:231:GLY:H	1.13	1.11
1:A:281:GLY:HA3	2:B:204:VAL:HG13	1.35	1.03
3:C:105:CYS:HA	3:C:226:MET:HE1	1.41	1.02
2:B:124:ARG:HG2	2:B:313:GLU:HG2	1.48	0.93
2:B:233:TYR:HA	3:C:66:MET:HE3	1.49	0.91
1:A:104:ASN:O	1:A:166:ARG:HD2	1.75	0.85
1:A:229:MET:HE2	1:A:231:GLY:N	1.94	0.80
1:A:281:GLY:CA	2:B:204:VAL:HG13	2.10	0.80
2:B:85:LEU:HD21	2:B:94:THR:CG2	2.12	0.80
3:C:6:LEU:HD13	3:C:10:THR:HG21	1.65	0.78
2:B:243:GLN:HA	3:C:51:THR:HG22	1.66	0.77
3:C:144:LYS:HD3	3:C:148:THR:HG21	1.63	0.77
1:A:156:VAL:HG22	1:A:232:THR:HB	1.66	0.77
3:C:9:GLY:O	3:C:12:GLN:HG2	1.86	0.76
1:A:197:PRO:HA	3:C:31:THR:HG21	1.69	0.74
2:B:241:ILE:HG21	3:C:66:MET:HE1	1.67	0.74
2:B:252:ILE:HA	2:B:257:ASN:HD21	1.51	0.74
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.69	0.74
2:B:138:LYS:HE3	2:B:225:ASP:O	1.87	0.73
3:C:42:ASN:O	3:C:45:GLU:HG3	1.88	0.73
2:B:188:GLN:NE2	3:C:209:PRO:HB2	2.04	0.72
2:B:128:SER:O	2:B:131:ARG:HG2	1.89	0.72
2:B:233:TYR:CA	3:C:66:MET:HE3	2.21	0.71
1:A:297:LEU:HD12	1:A:297:LEU:H	1.56	0.71
3:C:167:LEU:HD12	3:C:168:VAL:H	1.55	0.71
2:B:90:SER:HB2	2:B:132:PHE:HB2	1.72	0.71
2:B:240:PRO:HG3	2:B:243:GLN:NE2	2.07	0.70
3:C:188:TYR:O	3:C:189:TYR:HD2	1.74	0.70
2:B:85:LEU:HD21	2:B:94:THR:HG22	1.72	0.70
3:C:105:CYS:HA	3:C:226:MET:CE	2.19	0.69
3:C:105:CYS:CA	3:C:226:MET:HE1	2.20	0.68
1:A:226:PRO:C	1:A:228:ASN:H	2.02	0.68
3:C:235:ILE:C	3:C:236:LEU:HD12	2.19	0.67
3:C:188:TYR:O	3:C:189:TYR:CD2	2.48	0.66
1:A:76:ALA:O	1:A:79:THR:HG23	1.95	0.66
3:C:73:VAL:HA	3:C:198:TYR:OH	1.95	0.66
3:C:142:LEU:HD23	3:C:143:PRO:O	1.95	0.66
1:A:141:THR:HB	1:A:142:PRO:HD2	1.78	0.65
1:A:75:THR:HG22	3:C:225:THR:HG22	1.77	0.65
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HD11	3:C:55:VAL:HG12	1.80	0.63
1:A:117:ALA:HB1	3:C:236:LEU:HD23	1.80	0.63
1:A:152:GLN:HG3	1:A:180:PHE:CE2	2.34	0.63
3:C:190:THR:O	3:C:192:GLY:N	2.33	0.62
1:A:112:ASP:CG	1:A:114:THR:HG22	2.25	0.62
2:B:82:VAL:N	2:B:96:GLU:HG3	2.14	0.62
2:B:267:ILE:HG12	3:C:37:PRO:HG2	1.82	0.61
2:B:191:LEU:HD23	2:B:287:PRO:HA	1.83	0.61
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.83	0.61
1:A:229:MET:HE3	1:A:230:MET:H	1.66	0.61
3:C:180:HIS:CD2	3:C:181:ALA:H	2.18	0.61
3:C:138:PRO:HB3	3:C:190:THR:HA	1.83	0.61
3:C:167:LEU:HD12	3:C:168:VAL:N	2.16	0.61
2:B:187:HIS:CD2	2:B:301:ILE:HD11	2.36	0.60
2:B:85:LEU:HD23	2:B:85:LEU:H	1.67	0.60
3:C:54:GLU:HG2	3:C:69:LEU:HD23	1.82	0.60
1:A:254:ARG:NH2	1:A:256:LYS:HD3	2.16	0.60
2:B:204:VAL:HG22	2:B:231:HIS:HE1	1.67	0.60
3:C:204:VAL:HG22	3:C:205:PRO:HD2	1.82	0.59
3:C:65:LEU:O	3:C:68:ARG:HG3	2.03	0.59
2:B:268:ASN:OD1	2:B:278:HIS:HE1	1.85	0.58
3:C:133:ILE:HG12	3:C:196:ILE:HG12	1.85	0.58
1:A:267:ARG:HD2	2:B:238:GLY:O	2.02	0.58
1:A:254:ARG:NH1	3:C:18:ASP:HA	2.18	0.58
2:B:164:ASN:O	2:B:168:HIS:HB2	2.04	0.58
1:A:97:LEU:HD11	1:A:246:PRO:HD3	1.86	0.58
1:A:125:LEU:HD23	1:A:126:PHE:CE2	2.39	0.58
1:A:229:MET:CE	1:A:231:GLY:H	2.02	0.58
2:B:203:THR:HG23	2:B:219:GLN:HE22	1.68	0.57
3:C:58:VAL:H	3:C:59:PRO:HD2	1.68	0.57
3:C:185:VAL:O	3:C:185:VAL:HG23	2.04	0.57
3:C:66:MET:HE2	3:C:66:MET:HA	1.87	0.57
1:A:270:ASN:HA	3:C:235:ILE:HG23	1.86	0.57
2:B:117:THR:CG2	2:B:120:ASP:HB3	2.35	0.57
1:A:254:ARG:HH21	1:A:256:LYS:HD3	1.68	0.56
1:A:154:MET:HE2	1:A:176:ASN:HB2	1.86	0.56
2:B:85:LEU:HD23	2:B:85:LEU:N	2.20	0.56
2:B:148:TYR:HB3	2:B:284:LEU:HD12	1.86	0.56
1:A:294:ILE:HD12	3:C:56:ASN:HA	1.87	0.56
1:A:104:ASN:HA	1:A:242:LYS:NZ	2.21	0.56
3:C:180:HIS:CG	3:C:181:ALA:H	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PRO:HB3	2:B:129:VAL:HG21	1.88	0.55
1:A:229:MET:CE	1:A:230:MET:H	2.20	0.55
2:B:148:TYR:CB	2:B:284:LEU:HD12	2.37	0.55
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.39	0.55
2:B:185:LYS:HD3	3:C:125:PHE:CE1	2.41	0.55
2:B:135:LEU:HD23	2:B:135:LEU:N	2.21	0.55
2:B:184:SER:C	2:B:186:PHE:H	2.13	0.54
2:B:156:THR:HG22	2:B:165:ALA:HB1	1.90	0.54
1:A:94:ASP:C	1:A:96:PRO:HD3	2.31	0.54
1:A:123:VAL:C	1:A:125:LEU:H	2.16	0.54
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.42	0.54
1:A:281:GLY:HA3	2:B:204:VAL:CG1	2.24	0.54
3:C:144:LYS:CD	3:C:148:THR:HG21	2.34	0.54
1:A:290:SER:OG	3:C:68:ARG:NH2	2.41	0.54
1:A:112:ASP:OD2	1:A:114:THR:HG22	2.08	0.54
2:B:168:HIS:CD2	2:B:314:PHE:HB3	2.43	0.54
2:B:235:LEU:O	2:B:236:ASP:C	2.51	0.53
3:C:227:LYS:O	3:C:228:LEU:HB2	2.07	0.53
1:A:156:VAL:HG23	1:A:156:VAL:O	2.08	0.53
1:A:156:VAL:O	1:A:156:VAL:CG2	2.56	0.53
1:A:253:MET:HE3	1:A:255:MET:HG3	1.91	0.53
2:B:203:THR:CG2	2:B:219:GLN:HE22	2.22	0.53
3:C:56:ASN:O	3:C:68:ARG:HA	2.09	0.52
2:B:154:VAL:HG23	2:B:224:ALA:HA	1.91	0.52
1:A:237:THR:HG21	1:A:243:SER:HB2	1.92	0.52
3:C:221:GLN:HB3	3:C:223:ASN:OD1	2.09	0.52
1:A:262:ILE:HG21	2:B:197:PRO:HG2	1.92	0.52
2:B:137:THR:HG23	2:B:303:ILE:O	2.10	0.52
3:C:52:ILE:HA	3:C:217:LEU:HD23	1.91	0.52
2:B:126:ASP:O	2:B:127:VAL:O	2.28	0.51
3:C:71:PHE:HE1	3:C:214:ILE:HD12	1.75	0.51
1:A:127:THR:HG23	1:A:264:ARG:NH2	2.25	0.51
1:A:117:ALA:CB	3:C:236:LEU:HD23	2.40	0.51
1:A:154:MET:HE2	1:A:176:ASN:CB	2.39	0.51
1:A:205:TYR:O	1:A:223:GLY:HA2	2.10	0.51
2:B:137:THR:OG1	2:B:304:THR:HG23	2.09	0.51
2:B:222:PRO:HB3	2:B:227:PHE:HB2	1.90	0.51
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.39	0.51
1:A:265:PRO:HB2	2:B:239:ILE:HB	1.92	0.51
1:A:238:VAL:HG12	1:A:239:GLY:N	2.24	0.51
2:B:140:TRP:CE2	2:B:291:LEU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:TRP:HD1	2:B:141:GLU:N	2.09	0.51
1:A:165:SER:HB2	1:A:167:GLU:OE2	2.11	0.50
2:B:145:LYS:HZ2	2:B:145:LYS:HB3	1.76	0.50
1:A:224:ALA:O	1:A:226:PRO:HD3	2.11	0.50
2:B:117:THR:HG21	2:B:120:ASP:HB3	1.93	0.50
2:B:156:THR:HG22	2:B:165:ALA:CB	2.42	0.50
2:B:241:ILE:C	2:B:243:GLN:H	2.20	0.50
1:A:181:VAL:HG23	1:A:185:ASP:HB2	1.92	0.50
1:A:195:MET:O	1:A:196:SER:C	2.55	0.50
3:C:142:LEU:HD23	3:C:142:LEU:C	2.37	0.50
1:A:226:PRO:O	1:A:228:ASN:N	2.44	0.49
3:C:197:TRP:N	3:C:197:TRP:CD1	2.80	0.49
3:C:147:ALA:O	3:C:150:MET:HB3	2.11	0.49
1:A:152:GLN:HG3	1:A:180:PHE:CZ	2.47	0.49
3:C:171:TRP:HE1	3:C:173:SER:HB2	1.77	0.49
2:B:149:TRP:HZ3	2:B:285:VAL:CG1	2.25	0.49
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.94	0.49
2:B:172:ARG:HD2	2:B:272:PHE:CZ	2.48	0.49
2:B:119:VAL:O	2:B:121:LYS:HG2	2.13	0.49
2:B:145:LYS:HB3	2:B:145:LYS:NZ	2.27	0.49
3:C:109:THR:HB	3:C:228:LEU:CB	2.42	0.49
1:A:197:PRO:CA	3:C:31:THR:HG21	2.42	0.49
3:C:109:THR:HB	3:C:228:LEU:HB2	1.93	0.49
3:C:90:PRO:HD2	3:C:188:TYR:OH	2.13	0.49
3:C:174:ASN:OD1	3:C:174:ASN:O	2.31	0.48
3:C:70:ARG:HG2	3:C:213:TYR:CD2	2.48	0.48
1:A:104:ASN:HB2	1:A:106:TYR:CD1	2.48	0.48
2:B:155:LEU:HD23	2:B:158:THR:HB	1.96	0.48
2:B:230:GLN:O	2:B:231:HIS:CD2	2.67	0.48
3:C:66:MET:CE	3:C:69:LEU:HD11	2.44	0.48
1:A:195:MET:O	1:A:196:SER:O	2.31	0.48
3:C:132:LEU:HD23	3:C:132:LEU:C	2.39	0.48
3:C:66:MET:HE1	3:C:69:LEU:HD11	1.96	0.48
1:A:95:LEU:N	1:A:96:PRO:HD3	2.28	0.47
1:A:245:TYR:CD1	1:A:245:TYR:N	2.81	0.47
1:A:204:PHE:CE1	1:A:264:ARG:HD3	2.50	0.47
1:A:139:ALA:HB2	1:A:249:VAL:HG22	1.96	0.47
1:A:201:TYR:HA	1:A:228:ASN:HD21	1.79	0.47
3:C:90:PRO:CG	3:C:115:LEU:HD11	2.45	0.47
3:C:141:PRO:O	3:C:142:LEU:C	2.57	0.47
1:A:289:ALA:HB3	3:C:93:ASN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:HB3	1:A:168:SER:HB3	1.97	0.47
2:B:305:ILE:N	2:B:305:ILE:HD12	2.30	0.47
2:B:235:LEU:HD21	2:B:241:ILE:HG13	1.97	0.47
1:A:156:VAL:CG2	1:A:232:THR:HB	2.41	0.46
2:B:218:LYS:HD2	2:B:218:LYS:N	2.30	0.46
2:B:108:PRO:HB3	2:B:174:GLY:HA3	1.96	0.46
1:A:180:PHE:CD1	1:A:180:PHE:N	2.83	0.46
1:A:226:PRO:C	1:A:228:ASN:N	2.69	0.46
1:A:297:LEU:HD12	1:A:297:LEU:N	2.26	0.46
2:B:85:LEU:HD21	2:B:94:THR:HG21	1.95	0.46
3:C:176:HIS:HB2	3:C:189:TYR:CE2	2.50	0.46
1:A:201:TYR:HA	1:A:228:ASN:ND2	2.30	0.46
1:A:266:MET:HE1	3:C:107:TYR:HE2	1.81	0.46
1:A:189:GLN:HG2	3:C:21:SER:HB3	1.97	0.46
2:B:241:ILE:C	2:B:243:GLN:N	2.72	0.46
3:C:58:VAL:CG2	3:C:59:PRO:HD3	2.42	0.46
1:A:85:SER:O	1:A:86:ARG:O	2.34	0.46
1:A:97:LEU:HD21	1:A:245:TYR:C	2.41	0.46
1:A:104:ASN:HA	1:A:242:LYS:HZ2	1.81	0.46
1:A:108:ASN:ND2	1:A:234:SER:OG	2.49	0.46
2:B:151:PHE:O	2:B:279:CYS:HA	2.15	0.46
1:A:113:ILE:HB	1:A:253:MET:HE1	1.98	0.45
3:C:71:PHE:CE1	3:C:214:ILE:HB	2.51	0.45
1:A:177:PRO:HB2	3:C:24:ILE:HD11	1.98	0.45
1:A:181:VAL:CG2	1:A:185:ASP:HB2	2.47	0.45
1:A:276:ASN:OD1	1:A:278:ASN:HB2	2.16	0.45
2:B:222:PRO:HB2	2:B:226:GLY:O	2.16	0.45
3:C:93:ASN:N	3:C:93:ASN:HD22	2.13	0.45
1:A:218:LYS:CA	2:B:216:PRO:HA	2.47	0.45
1:A:238:VAL:CG1	1:A:239:GLY:N	2.78	0.45
2:B:233:TYR:HA	3:C:66:MET:CE	2.34	0.45
2:B:243:GLN:O	2:B:246:VAL:HG12	2.16	0.45
2:B:171:TYR:CE2	2:B:173:SER:HB3	2.52	0.45
2:B:220:THR:HG22	2:B:221:GLN:NE2	2.31	0.45
2:B:195:VAL:HG13	2:B:281:PHE:CD2	2.51	0.45
2:B:125:PRO:HB3	2:B:129:VAL:CG2	2.47	0.45
3:C:109:THR:HG21	3:C:228:LEU:HD12	1.99	0.44
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.81	0.44
1:A:266:MET:O	2:B:240:PRO:HD3	2.17	0.44
2:B:185:LYS:HB3	3:C:125:PHE:HD1	1.82	0.44
2:B:148:TYR:HA	2:B:283:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:LYS:HD2	2:B:218:LYS:H	1.82	0.44
1:A:220:LEU:HD23	2:B:214:HIS:HD2	1.82	0.44
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.85	0.44
2:B:117:THR:HG22	2:B:117:THR:O	2.18	0.44
2:B:140:TRP:NE1	2:B:291:LEU:HB2	2.32	0.44
3:C:158:ASP:C	3:C:160:GLY:H	2.26	0.44
3:C:188:TYR:O	3:C:189:TYR:HB3	2.16	0.44
1:A:123:VAL:HB	1:A:203:TRP:NE1	2.33	0.44
2:B:85:LEU:CD2	2:B:94:THR:HG22	2.44	0.44
2:B:185:LYS:HB3	3:C:125:PHE:CD1	2.53	0.44
2:B:115:ASP:CG	2:B:116:ALA:H	2.24	0.44
2:B:148:TYR:C	2:B:148:TYR:CD1	2.96	0.44
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.17	0.44
3:C:148:THR:HA	3:C:151:LEU:HD12	1.99	0.44
1:A:88:GLY:O	1:A:252:TYR:HA	2.18	0.44
1:A:286:PRO:O	1:A:287:THR:C	2.61	0.44
2:B:268:ASN:OD1	2:B:278:HIS:CE1	2.67	0.44
1:A:135:PHE:O	1:A:189:GLN:HA	2.18	0.43
1:A:281:GLY:N	2:B:204:VAL:HG13	2.33	0.43
1:A:140:CYS:SG	1:A:144:GLY:HA2	2.57	0.43
1:A:154:MET:HE3	1:A:178:SER:OG	2.18	0.43
2:B:96:GLU:O	2:B:97:ALA:HB2	2.17	0.43
2:B:188:GLN:HG3	2:B:292:ASP:HB3	2.00	0.43
1:A:120:ARG:HH11	3:C:237:GLN:HE22	1.65	0.43
1:A:135:PHE:CE1	1:A:253:MET:HB2	2.53	0.43
1:A:218:LYS:HA	2:B:216:PRO:HA	2.00	0.43
2:B:184:SER:C	2:B:186:PHE:N	2.72	0.43
2:B:234:VAL:HA	2:B:239:ILE:O	2.19	0.43
1:A:131:PHE:CD1	1:A:131:PHE:C	2.97	0.43
1:A:207:GLY:HA3	2:B:277:ASN:O	2.19	0.43
2:B:89:ASN:HD21	2:B:131:ARG:NH1	2.16	0.43
2:B:168:HIS:CE1	2:B:317:LEU:HD13	2.54	0.43
2:B:198:GLU:OE2	2:B:278:HIS:NE2	2.51	0.43
2:B:241:ILE:O	2:B:243:GLN:N	2.52	0.43
3:C:53:LEU:CD2	3:C:95:PRO:HB3	2.49	0.43
3:C:144:LYS:CG	3:C:148:THR:HG21	2.49	0.43
1:A:163:PRO:HG3	1:A:170:ALA:HB3	2.00	0.43
3:C:89:ASP:HA	3:C:188:TYR:CE1	2.54	0.43
3:C:211:THR:HG22	3:C:212:ALA:N	2.34	0.43
2:B:86:THR:HG23	2:B:90:SER:O	2.18	0.43
3:C:83:CYS:HB3	3:C:196:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PRO:HD2	1:A:176:ASN:OD1	2.19	0.42
3:C:118:THR:HG23	3:C:166:THR:OG1	2.19	0.42
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.53	0.42
1:A:128:TYR:HD1	1:A:202:GLN:HB3	1.84	0.42
2:B:92:ILE:O	2:B:92:ILE:HG13	2.19	0.42
2:B:140:TRP:CD1	2:B:141:GLU:N	2.87	0.42
2:B:222:PRO:HB2	2:B:226:GLY:C	2.45	0.42
3:C:180:HIS:O	3:C:181:ALA:C	2.62	0.42
1:A:117:ALA:HB1	3:C:236:LEU:HB3	2.01	0.42
1:A:266:MET:O	1:A:267:ARG:C	2.62	0.42
3:C:58:VAL:H	3:C:59:PRO:CD	2.32	0.42
3:C:54:GLU:HG3	3:C:98:SER:CB	2.49	0.42
3:C:85:VAL:HG22	3:C:86:PHE:N	2.34	0.42
3:C:92:ARG:HD3	3:C:188:TYR:CD2	2.55	0.42
2:B:156:THR:HA	2:B:162:GLY:HA2	2.00	0.42
2:B:170:LEU:HB3	2:B:272:PHE:HB3	2.01	0.42
2:B:172:ARG:HD3	2:B:313:GLU:OE2	2.20	0.42
3:C:71:PHE:CE1	3:C:214:ILE:HD12	2.53	0.42
2:B:148:TYR:HB3	2:B:284:LEU:CD1	2.49	0.42
3:C:61:ASN:ND2	3:C:64:SER:OG	2.53	0.42
3:C:188:TYR:O	3:C:189:TYR:CB	2.67	0.41
2:B:241:ILE:CG2	3:C:66:MET:HE1	2.44	0.41
3:C:87:ARG:HG3	3:C:89:ASP:OD2	2.20	0.41
2:B:121:LYS:HG2	2:B:121:LYS:H	1.57	0.41
2:B:171:TYR:CD1	2:B:171:TYR:C	2.96	0.41
1:A:259:ARG:HG2	3:C:39:GLU:OE1	2.21	0.41
3:C:53:LEU:HD21	3:C:95:PRO:CB	2.51	0.41
1:A:114:THR:HG23	3:C:237:GLN:HG2	2.01	0.41
2:B:252:ILE:HD11	2:B:260:ALA:HB3	2.01	0.41
2:B:215:PRO:HA	2:B:216:PRO:HD3	1.94	0.41
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.56	0.41
1:A:286:PRO:HA	2:B:233:TYR:HE2	1.86	0.41
2:B:246:VAL:O	2:B:246:VAL:HG22	2.21	0.41
2:B:297:ALA:O	2:B:298:THR:C	2.63	0.41
3:C:180:HIS:CG	3:C:181:ALA:N	2.88	0.41
2:B:155:LEU:C	2:B:157:GLU:N	2.79	0.41
3:C:90:PRO:CD	3:C:188:TYR:OH	2.68	0.41
1:A:155:PHE:O	1:A:177:PRO:HD2	2.20	0.40
2:B:102:VAL:HA	2:B:263:ILE:HB	2.03	0.40
2:B:259:CYS:O	2:B:259:CYS:SG	2.79	0.40
2:B:283:LEU:HD12	2:B:284:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:GLN:OE1	3:C:222:LYS:HA	2.21	0.40
1:A:104:ASN:HB2	1:A:106:TYR:CE1	2.55	0.40
2:B:155:LEU:C	2:B:157:GLU:H	2.29	0.40
2:B:196:LEU:HD12	2:B:196:LEU:C	2.45	0.40
2:B:201:ILE:HG21	2:B:219:GLN:HE21	1.86	0.40
3:C:31:THR:HA	3:C:32:PRO:HD3	1.89	0.40
1:A:181:VAL:HG22	1:A:182:LYS:O	2.22	0.40
2:B:108:PRO:CB	2:B:174:GLY:HA3	2.52	0.40
3:C:35:HIS:O	3:C:36:ILE:HD13	2.20	0.40
3:C:90:PRO:HG2	3:C:115:LEU:HD11	2.02	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%)	185 (86%)	24 (11%)	5 (2%)	5	30
2	B	235/237 (99%)	196 (83%)	30 (13%)	9 (4%)	2	21
3	C	237/239 (99%)	207 (87%)	20 (8%)	10 (4%)	2	19
All	All	686/701 (98%)	588 (86%)	74 (11%)	24 (4%)	3	23

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
2	B	127	VAL
2	B	159	GLY
3	C	180	HIS
3	C	188	TYR
1	A	85	SER
1	A	86	ARG

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Mol	Chain	Res	Type
1	A	124	GLU
2	B	97	ALA
2	B	237	ALA
3	C	62	ALA
3	C	182	ARG
3	C	189	TYR
3	C	191	THR
1	A	227	ASN
2	B	98	ALA
2	B	216	PRO
3	C	72	PRO
2	B	108	PRO
2	B	242	SER
3	C	181	ALA
2	B	112	SER
3	C	58	VAL
3	C	137	PRO

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%)	175 (94%)	12 (6%)	16	42
2	B	201/201 (100%)	190 (94%)	11 (6%)	19	45
3	C	199/199 (100%)	182 (92%)	17 (8%)	10	33
All	All	587/593 (99%)	547 (93%)	40 (7%)	14	40

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	114	THR

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Mol	Chain	Res	Type
1	A	156	VAL
1	A	167	GLU
1	A	179	VAL
1	A	183	LEU
1	A	245	TYR
1	A	265	PRO
1	A	297	LEU
2	B	85	LEU
2	B	119	VAL
2	B	121	LYS
2	B	135	LEU
2	B	145	LYS
2	B	171	TYR
2	B	180	GLN
2	B	203	THR
2	B	239	ILE
2	B	285	VAL
2	B	304	THR
3	C	14	LEU
3	C	21	SER
3	C	25	LEU
3	C	31	THR
3	C	51	THR
3	C	53	LEU
3	C	61	ASN
3	C	72	PRO
3	C	87	ARG
3	C	136	THR
3	C	146	ARG
3	C	178	ARG
3	C	197	TRP
3	C	204	VAL
3	C	221	GLN
3	C	230	LYS
3	C	234	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	189	GLN
1	A	202	GLN

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Mol	Chain	Res	Type
1	A	228	ASN
2	B	168	HIS
2	B	188	GLN
2	B	214	HIS
2	B	219	GLN
2	B	257	ASN
2	B	258	ASN
2	B	277	ASN
3	C	11	ASN
3	C	48	GLN
3	C	61	ASN
3	C	93	ASN
3	C	162	GLN
3	C	174	ASN
3	C	176	HIS
3	C	221	GLN
3	C	237	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	1.49	61 (27%)	1 2	70, 97, 150, 190	0
2	B	237/237 (100%)	2.22	98 (41%)	0 1	72, 118, 199, 202	0
3	C	239/239 (100%)	1.53	63 (26%)	1 3	72, 98, 188, 202	0
All	All	694/701 (99%)	1.75	222 (31%)	1 2	70, 102, 189, 202	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	115	ASP	10.4
2	B	212	ASP	9.6
3	C	186	PHE	8.8
2	B	96	GLU	8.7
2	B	206	GLY	7.8
2	B	211	GLU	7.4
2	B	122	PRO	7.0
2	B	120	ASP	6.8
3	C	189	TYR	6.8
2	B	123	THR	6.7
2	B	93	THR	6.4
2	B	116	ALA	6.3
1	A	218	LYS	6.3
2	B	217	TYR	6.1
3	C	239	GLY	6.0
1	A	274	LYS	6.0
1	A	224	ALA	5.8
2	B	317	LEU	5.8
2	B	166	GLN	5.7
2	B	208	THR	5.5
2	B	169	TYR	5.4
2	B	117	THR	5.2
3	C	182	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	220	LEU	5.2
2	B	127	VAL	5.1
3	C	91	GLY	4.9
2	B	210	THR	4.9
3	C	177	TYR	4.9
2	B	85	LEU	4.8
3	C	176	HIS	4.8
1	A	219	ASP	4.8
2	B	105	GLY	4.8
2	B	219	GLN	4.8
2	B	82	VAL	4.8
2	B	180	GLN	4.7
3	C	187	ASP	4.7
2	B	89	ASN	4.7
3	C	5	GLU	4.7
2	B	160	VAL	4.7
2	B	113	ASP	4.6
3	C	238	THR	4.6
2	B	88	GLY	4.6
2	B	83	ALA	4.5
2	B	273	ASP	4.5
2	B	318	ARG	4.5
1	A	73	HIS	4.5
2	B	97	ALA	4.5
3	C	183	ASP	4.4
2	B	84	GLN	4.4
2	B	272	PHE	4.4
3	C	60	THR	4.4
2	B	94	THR	4.3
1	A	221	GLU	4.2
3	C	237	GLN	4.1
2	B	118	ALA	4.1
1	A	202	GLN	4.0
2	B	203	THR	3.9
2	B	316	GLY	3.9
2	B	124	ARG	3.9
1	A	102	ASN	3.8
2	B	274	SER	3.8
3	C	232	ALA	3.8
2	B	167	PHE	3.7
2	B	204	VAL	3.7
1	A	225	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	285	LYS	3.7
2	B	126	ASP	3.6
1	A	101	THR	3.6
3	C	184	GLY	3.6
2	B	130	ASN	3.6
2	B	295	GLN	3.6
2	B	121	LYS	3.6
2	B	213	THR	3.6
2	B	230	GLN	3.6
3	C	210	ASN	3.5
3	C	178	ARG	3.5
3	C	180	HIS	3.5
3	C	185	VAL	3.5
2	B	128	SER	3.5
3	C	234	ASP	3.4
3	C	29	HIS	3.4
3	C	18	ASP	3.4
3	C	175	THR	3.4
1	A	205	TYR	3.3
3	C	92	ARG	3.3
2	B	107	TRP	3.3
2	B	114	SER	3.2
1	A	208	TYR	3.2
2	B	119	VAL	3.2
3	C	56	ASN	3.2
1	A	117	ALA	3.2
1	A	283	SER	3.2
3	C	144	LYS	3.2
2	B	214	HIS	3.2
3	C	191	THR	3.1
3	C	171	TRP	3.1
1	A	276	ASN	3.1
3	C	206	ILE	3.1
3	C	47	CYS	3.1
2	B	148	TYR	3.1
2	B	149	TRP	3.1
2	B	224	ALA	3.1
2	B	275	ALA	3.1
2	B	103	GLY	3.1
2	B	202	GLY	3.1
2	B	98	ALA	3.0
2	B	250	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	165	ALA	3.0
3	C	77	ALA	3.0
3	C	168	VAL	3.0
3	C	179	ALA	3.0
2	B	99	ASN	3.0
2	B	110	TYR	2.9
3	C	229	CYS	2.9
2	B	106	GLU	2.9
2	B	170	LEU	2.9
2	B	247	CYS	2.9
2	B	112	SER	2.8
3	C	49	VAL	2.8
2	B	163	GLN	2.8
2	B	108	PRO	2.8
2	B	256	THR	2.8
3	C	195	SER	2.8
2	B	95	GLN	2.8
2	B	289	SER	2.8
2	B	282	GLY	2.8
1	A	107	ALA	2.8
3	C	230	LYS	2.8
1	A	197	PRO	2.8
2	B	157	GLU	2.8
3	C	81	GLU	2.7
3	C	139	GLY	2.7
3	C	87	ARG	2.7
1	A	158	PRO	2.7
2	B	164	ASN	2.7
3	C	1	GLY	2.7
2	B	209	GLY	2.6
1	A	222	TYR	2.6
1	A	279	TYR	2.6
3	C	50	GLU	2.6
1	A	243	SER	2.6
1	A	105	GLY	2.6
3	C	129	GLY	2.6
2	B	277	ASN	2.6
3	C	222	LYS	2.6
2	B	278	HIS	2.6
2	B	205	ALA	2.6
3	C	181	ALA	2.5
1	A	120	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	172	ARG	2.5
1	A	193	PRO	2.5
1	A	288	GLY	2.5
1	A	100	THR	2.5
2	B	171	TYR	2.5
1	A	98	LYS	2.5
1	A	230	MET	2.5
1	A	172	GLN	2.5
2	B	131	ARG	2.5
3	C	146	ARG	2.5
2	B	182	ASN	2.5
1	A	169	LEU	2.5
3	C	174	ASN	2.4
1	A	109	TRP	2.4
3	C	89	ASP	2.4
1	A	259	ARG	2.4
1	A	96	PRO	2.4
2	B	268	ASN	2.4
2	B	218	LYS	2.4
1	A	201	TYR	2.3
1	A	233	PHE	2.3
1	A	128	TYR	2.3
1	A	292	THR	2.3
3	C	110	GLN	2.3
3	C	147	ALA	2.3
1	A	132	ASP	2.3
1	A	207	GLY	2.3
1	A	256	LYS	2.3
1	A	289	ALA	2.3
3	C	22	ALA	2.3
2	B	159	GLY	2.3
2	B	227	PHE	2.2
1	A	223	GLY	2.2
2	B	269	ALA	2.2
3	C	130	LYS	2.2
1	A	250	ARG	2.2
2	B	276	LEU	2.2
1	A	210	THR	2.2
1	A	244	LYS	2.2
2	B	312	SER	2.2
3	C	221	GLN	2.2
3	C	41	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	112	ASP	2.2
1	A	118	GLN	2.2
1	A	180	PHE	2.2
1	A	209	PRO	2.2
3	C	170	PRO	2.2
3	C	79	LYS	2.2
1	A	257	HIS	2.1
3	C	17	ASP	2.1
2	B	125	PRO	2.1
1	A	94	ASP	2.1
2	B	311	CYS	2.1
3	C	188	TYR	2.1
3	C	120	MET	2.1
1	A	162	LYS	2.1
2	B	152	PRO	2.1
1	A	119	MET	2.1
1	A	264	ARG	2.1
2	B	132	PHE	2.1
1	A	81	ASP	2.1
2	B	136	ASP	2.1
1	A	145	GLU	2.1
1	A	167	GLU	2.1
3	C	153	THR	2.1
3	C	93	ASN	2.1
3	C	190	THR	2.0
1	A	127	THR	2.0
3	C	44	LEU	2.0
2	B	129	VAL	2.0
2	B	207	GLY	2.0
1	A	157	PRO	2.0
2	B	249	HIS	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.