



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 AM UTC

PDB ID : 3VBO / pdb_00003vbo
Title : Crystal structure of formaldehyde treated empty human Enterovirus 71 particle (cryo at 100K)
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 : 2.88 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

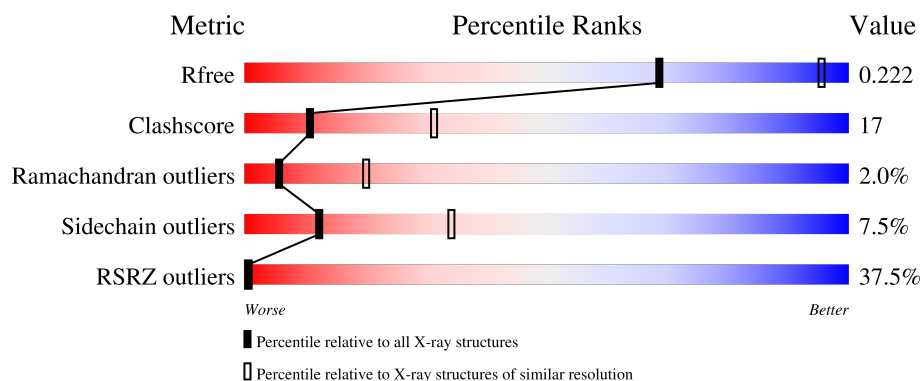
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	297	
2	B	237	
3	C	239	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5466 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 VP2.

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			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		

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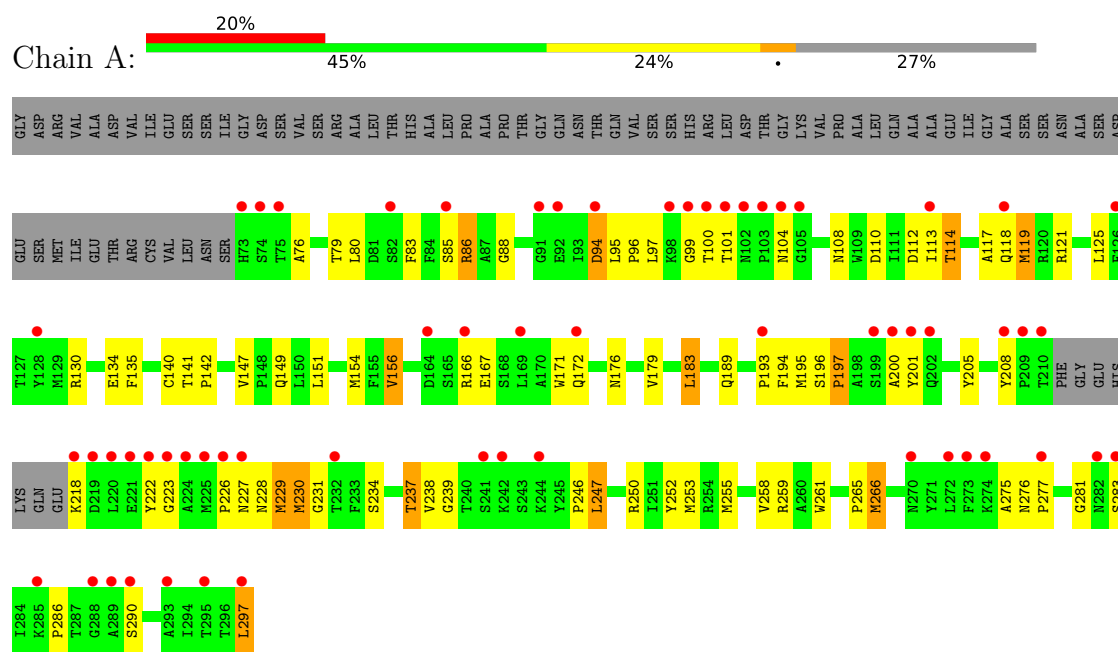
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	23	Total	O	0	0
			23	23		
5	C	25	Total	O	0	0
			25	25		

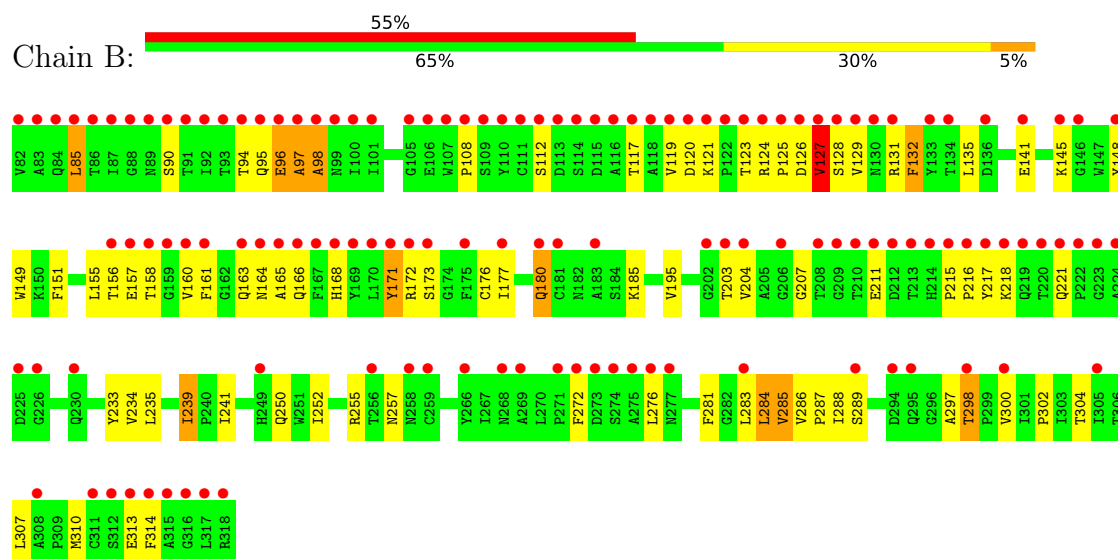
3 Residue-property plots

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.

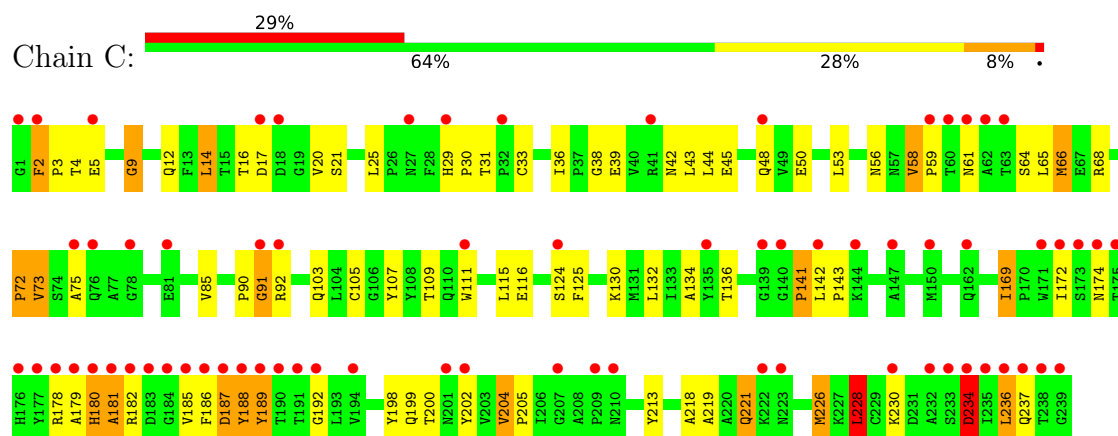
• Molecule 1: Genome Polyprotein, capsid protein VP1



• Molecule 2: Genome Polyprotein, capsid protein VP2



● Molecule 3: Genome Polyprotein, capsid protein VP3



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	353.10Å 353.10Å 353.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 2.88 49.94 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.94-2.88) 99.4 (49.94-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.38	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.236 0.220 , 0.222	Depositor DCC
R_{free} test set	1667 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	5466	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.21% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.63	1/1776 (0.1%)	1.14	15/2419 (0.6%)
2	B	0.59	0/1889	1.15	18/2592 (0.7%)
3	C	0.69	2/1891 (0.1%)	1.11	12/2586 (0.5%)
All	All	0.64	3/5556 (0.1%)	1.13	45/7597 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	MET	SD-CE	5.89	1.94	1.79
3	C	66	MET	SD-CE	-5.02	1.67	1.79
3	C	226	MET	SD-CE	-5.01	1.67	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	CA-C-N	9.72	129.65	120.03
1	A	95	LEU	C-N-CA	9.72	129.65	120.03
2	B	221	GLN	CA-C-N	9.64	131.89	119.84
2	B	221	GLN	C-N-CA	9.64	131.89	119.84
3	C	192	GLY	N-CA-C	-8.95	100.47	112.82
3	C	9	GLY	N-CA-C	-8.12	104.14	114.37
1	A	125	LEU	N-CA-C	-7.30	103.84	112.89
2	B	289	SER	CA-C-N	7.09	127.13	119.89
2	B	289	SER	C-N-CA	7.09	127.13	119.89
2	B	158	THR	N-CA-C	6.93	119.42	108.67
2	B	298	THR	CA-C-N	6.86	127.01	119.87
2	B	298	THR	C-N-CA	6.86	127.01	119.87
2	B	161	PHE	N-CA-C	-6.78	103.13	111.40
2	B	112	SER	N-CA-C	6.75	120.01	110.50
3	C	234	ASP	N-CA-C	-6.55	105.45	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	169	ILE	N-CA-C	-6.42	101.72	107.56
1	A	201	TYR	N-CA-C	-6.33	102.00	110.55
2	B	132	PHE	N-CA-C	6.31	118.45	108.67
1	A	196	SER	N-CA-C	6.22	116.76	109.60
1	A	275	ALA	N-CA-C	6.00	120.60	113.28
1	A	258	VAL	N-CA-C	5.84	117.16	109.21
2	B	176	CYS	N-CA-C	-5.81	99.06	108.52
1	A	237	THR	N-CA-C	-5.76	101.95	110.48
2	B	157	GLU	N-CA-C	-5.68	106.49	113.41
1	A	119	MET	N-CA-C	5.65	117.11	111.07
2	B	163	GLN	N-CA-C	-5.57	104.90	110.97
1	A	99	GLY	N-CA-C	5.53	118.45	111.09
1	A	197	PRO	N-CA-C	-5.53	106.80	114.27
3	C	2	PHE	CA-C-N	5.50	125.77	119.83
3	C	2	PHE	C-N-CA	5.50	125.77	119.83
2	B	239	ILE	CA-C-N	5.36	126.20	119.98
2	B	239	ILE	C-N-CA	5.36	126.20	119.98
1	A	247	LEU	N-CA-C	5.33	117.97	109.81
3	C	38	GLY	N-CA-C	5.33	123.32	114.48
3	C	91	GLY	N-CA-C	5.28	120.55	114.16
3	C	187	ASP	N-CA-C	5.26	118.22	110.59
1	A	147	VAL	CA-C-N	5.25	126.41	119.84
1	A	147	VAL	C-N-CA	5.25	126.41	119.84
3	C	134	ALA	N-CA-C	5.24	118.00	109.24
2	B	288	ILE	N-CA-C	-5.24	107.30	111.81
2	B	289	SER	N-CA-C	-5.18	99.21	109.10
2	B	302	PRO	N-CA-C	5.15	118.65	110.21
1	A	110	ASP	N-CA-C	-5.14	102.67	110.28
3	C	199	GLN	N-CA-C	-5.12	104.66	112.04
3	C	73	VAL	N-CA-C	-5.03	101.01	108.45

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	69	0
2	B	1834	0	1774	62	0
3	C	1839	0	1814	79	0
4	A	1	0	0	0	0
5	A	20	0	0	1	0
5	B	23	0	0	2	0
5	C	25	0	0	1	0
All	All	5466	0	5276	177	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 17.

All (177) 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)
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.37	1.03
1:A:281:GLY:HA3	2:B:204:VAL:HG13	1.45	0.98
2:B:233:TYR:HA	3:C:66:MET:HE3	1.48	0.95
1:A:229:MET:HE2	1:A:231:GLY:H	1.39	0.85
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.08	0.83
2:B:233:TYR:CA	3:C:66:MET:HE3	2.07	0.82
2:B:250:GLN:HG3	5:B:419:HOH:O	1.80	0.81
2:B:218:LYS:HD2	2:B:218:LYS:H	1.45	0.79
1:A:140:CYS:HA	1:A:183:LEU:HD21	1.64	0.78
1:A:154:MET:HE2	1:A:176:ASN:HB2	1.66	0.77
3:C:178:ARG:HH12	3:C:187:ASP:HB3	1.50	0.76
3:C:14:LEU:HD22	3:C:16:THR:H	1.50	0.76
1:A:297:LEU:HD12	1:A:297:LEU:H	1.51	0.75
1:A:130:ARG:NH2	3:C:31:THR:O	2.21	0.74
1:A:281:GLY:CA	2:B:204:VAL:HG13	2.16	0.74
2:B:241:ILE:HG21	3:C:66:MET:HE1	1.71	0.73
3:C:178:ARG:HH12	3:C:187:ASP:CB	2.02	0.72
3:C:105:CYS:HA	3:C:226:MET:CE	2.20	0.72
1:A:104:ASN:O	1:A:166:ARG:HD2	1.90	0.72
2:B:233:TYR:HA	3:C:66:MET:CE	2.21	0.70
2:B:85:LEU:HD21	2:B:94:THR:HG22	1.75	0.69
2:B:124:ARG:HG2	2:B:313:GLU:HG2	1.75	0.67
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.27	0.67
3:C:105:CYS:HA	3:C:226:MET:HE2	1.77	0.66
1:A:114:THR:HG23	3:C:237:GLN:HG2	1.77	0.66
3:C:92:ARG:HD3	3:C:188:TYR:HD2	1.59	0.66
2:B:204:VAL:HG12	2:B:207:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:CE	1:A:255:MET:HE3	2.25	0.65
1:A:119:MET:HE3	1:A:255:MET:HE3	1.78	0.64
1:A:141:THR:HB	1:A:142:PRO:HD2	1.79	0.64
1:A:114:THR:HG21	3:C:237:GLN:HE21	1.63	0.64
2:B:85:LEU:HD21	2:B:94:THR:CG2	2.27	0.64
2:B:218:LYS:HD2	2:B:218:LYS:N	2.12	0.63
2:B:195:VAL:HG13	2:B:281:PHE:CD2	2.33	0.63
3:C:91:GLY:HA3	3:C:111:TRP:CZ2	2.34	0.63
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.80	0.62
2:B:125:PRO:HB3	2:B:129:VAL:HG21	1.81	0.62
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.34	0.62
1:A:197:PRO:HA	3:C:31:THR:HG21	1.80	0.62
3:C:180:HIS:HE1	3:C:185:VAL:HG13	1.64	0.61
1:A:281:GLY:HA3	2:B:204:VAL:CG1	2.26	0.61
1:A:226:PRO:C	1:A:228:ASN:H	2.09	0.60
1:A:121:ARG:CZ	1:A:266:MET:HE3	2.31	0.60
3:C:188:TYR:O	3:C:189:TYR:HB3	2.02	0.60
1:A:112:ASP:OD1	1:A:114:THR:HG22	2.02	0.59
1:A:208:TYR:CE1	1:A:222:TYR:HB2	2.39	0.58
1:A:117:ALA:HB1	3:C:236:LEU:HB3	1.86	0.58
2:B:203:THR:HG23	2:B:215:PRO:HG3	1.85	0.58
3:C:132:LEU:C	3:C:132:LEU:HD23	2.30	0.57
3:C:105:CYS:HA	3:C:226:MET:HE1	1.87	0.57
3:C:65:LEU:O	3:C:68:ARG:HG3	2.05	0.57
2:B:148:TYR:HB3	2:B:284:LEU:CD1	2.35	0.56
1:A:134:GLU:HG3	3:C:21:SER:OG	2.06	0.56
2:B:128:SER:O	2:B:131:ARG:HG2	2.05	0.56
3:C:9:GLY:O	3:C:12:GLN:HG2	2.05	0.56
1:A:266:MET:HE1	3:C:107:TYR:HE2	1.71	0.56
2:B:108:PRO:HG2	2:B:310:MET:HE2	1.88	0.56
2:B:180:GLN:HB3	5:B:415:HOH:O	2.07	0.55
2:B:123:THR:O	2:B:125:PRO:HD3	2.07	0.55
3:C:180:HIS:CD2	3:C:181:ALA:H	2.25	0.55
3:C:73:VAL:HA	3:C:198:TYR:OH	2.07	0.55
3:C:130:LYS:HB2	3:C:200:THR:HG23	1.87	0.55
2:B:149:TRP:HZ3	2:B:285:VAL:HG13	1.71	0.54
1:A:205:TYR:O	1:A:223:GLY:HA2	2.08	0.54
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.73	0.54
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.08	0.54
3:C:178:ARG:HG2	3:C:179:ALA:N	2.23	0.53
1:A:238:VAL:HG12	1:A:239:GLY:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:TYR:HA	2:B:283:LEU:O	2.09	0.53
3:C:115:LEU:HB2	3:C:169:ILE:HB	1.90	0.53
3:C:204:VAL:HG22	3:C:205:PRO:HD2	1.91	0.53
2:B:155:LEU:HD21	2:B:307:LEU:HD11	1.90	0.53
2:B:241:ILE:CG2	3:C:66:MET:HE1	2.37	0.53
3:C:44:LEU:O	3:C:48:GLN:HG3	2.09	0.53
3:C:174:ASN:O	3:C:174:ASN:OD1	2.27	0.52
2:B:126:ASP:O	2:B:127:VAL:C	2.51	0.52
1:A:290:SER:OG	3:C:68:ARG:NH2	2.42	0.52
3:C:85:VAL:HG21	3:C:142:LEU:HD12	1.91	0.52
2:B:156:THR:HG22	2:B:165:ALA:HB1	1.93	0.51
3:C:109:THR:HB	3:C:228:LEU:HB3	1.91	0.51
1:A:151:LEU:HD11	1:A:183:LEU:HD12	1.91	0.51
5:A:401:HOH:O	3:C:31:THR:HG23	2.09	0.51
2:B:171:TYR:CE2	2:B:173:SER:HB3	2.47	0.50
3:C:58:VAL:CG2	3:C:59:PRO:CD	2.86	0.50
3:C:178:ARG:HD3	3:C:180:HIS:HB3	1.93	0.50
1:A:229:MET:HE2	1:A:231:GLY:N	2.17	0.50
2:B:117:THR:CG2	2:B:120:ASP:HB3	2.42	0.50
1:A:194:PHE:CZ	1:A:200:ALA:HA	2.47	0.49
1:A:229:MET:HA	1:A:229:MET:HE3	1.94	0.49
2:B:96:GLU:O	2:B:97:ALA:HB2	2.12	0.49
1:A:112:ASP:OD2	1:A:114:THR:HB	2.12	0.49
2:B:235:LEU:HD21	2:B:241:ILE:HG13	1.94	0.48
3:C:92:ARG:HD2	3:C:187:ASP:OD1	2.11	0.48
1:A:149:GLN:HG2	1:A:247:LEU:HD11	1.94	0.48
3:C:180:HIS:CG	3:C:181:ALA:H	2.32	0.48
1:A:76:ALA:O	1:A:79:THR:HG23	2.13	0.47
3:C:234:ASP:O	3:C:236:LEU:HD12	2.14	0.47
1:A:86:ARG:HG2	3:C:16:THR:HG22	1.96	0.47
3:C:2:PHE:CD1	3:C:3:PRO:HD2	2.49	0.47
1:A:218:LYS:N	2:B:217:TYR:H	2.12	0.47
3:C:50:GLU:HA	3:C:219:ALA:HB2	1.96	0.47
3:C:142:LEU:HD23	3:C:143:PRO:O	2.14	0.47
2:B:168:HIS:CD2	2:B:314:PHE:HB3	2.49	0.47
3:C:188:TYR:O	3:C:189:TYR:HD2	1.98	0.47
1:A:226:PRO:O	1:A:228:ASN:N	2.44	0.46
2:B:151:PHE:CE2	2:B:307:LEU:HD22	2.51	0.46
1:A:94:ASP:C	1:A:96:PRO:HD3	2.41	0.46
1:A:156:VAL:HG22	1:A:156:VAL:O	2.14	0.46
2:B:185:LYS:HD3	3:C:125:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:LYS:H	2:B:121:LYS:HG2	1.56	0.45
2:B:252:ILE:HA	2:B:257:ASN:HD21	1.82	0.45
2:B:185:LYS:HD3	3:C:125:PHE:CE1	2.52	0.45
1:A:114:THR:HG23	1:A:114:THR:O	2.15	0.45
2:B:172:ARG:HD2	2:B:272:PHE:CZ	2.52	0.45
1:A:135:PHE:O	1:A:189:GLN:HA	2.17	0.45
1:A:226:PRO:C	1:A:228:ASN:N	2.75	0.45
3:C:72:PRO:HB3	3:C:213:TYR:CE2	2.51	0.45
2:B:155:LEU:HD11	2:B:307:LEU:CD1	2.46	0.44
3:C:109:THR:HB	3:C:228:LEU:CB	2.48	0.44
1:A:193:PRO:HG2	1:A:195:MET:SD	2.57	0.44
2:B:141:GLU:HG2	2:B:300:VAL:HG12	2.00	0.44
2:B:203:THR:HG23	2:B:215:PRO:CG	2.48	0.44
3:C:188:TYR:O	3:C:189:TYR:CB	2.66	0.44
1:A:238:VAL:CG1	1:A:239:GLY:N	2.81	0.43
2:B:168:HIS:CG	2:B:314:PHE:HB3	2.53	0.43
1:A:229:MET:CE	1:A:230:MET:H	2.32	0.43
1:A:286:PRO:HB2	3:C:68:ARG:NH1	2.33	0.43
2:B:90:SER:HB2	2:B:132:PHE:HB2	2.01	0.43
2:B:297:ALA:O	2:B:298:THR:C	2.61	0.43
2:B:97:ALA:C	2:B:98:ALA:O	2.60	0.43
2:B:203:THR:HG23	2:B:215:PRO:CD	2.48	0.43
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.54	0.43
1:A:208:TYR:HE1	1:A:222:TYR:HB2	1.83	0.43
1:A:281:GLY:N	2:B:204:VAL:HG13	2.32	0.43
1:A:83:PHE:CD1	3:C:43:LEU:HD11	2.54	0.43
3:C:91:GLY:HA3	3:C:111:TRP:HZ2	1.80	0.43
1:A:97:LEU:HD11	1:A:246:PRO:HD3	2.01	0.43
3:C:105:CYS:CA	3:C:226:MET:HE1	2.47	0.42
1:A:114:THR:CG2	3:C:237:GLN:HG2	2.47	0.42
1:A:265:PRO:HB2	2:B:239:ILE:HB	2.00	0.42
1:A:297:LEU:H	1:A:297:LEU:CD1	2.18	0.42
3:C:4:THR:HG22	3:C:5:GLU:N	2.33	0.42
3:C:50:GLU:HA	3:C:218:ALA:O	2.18	0.42
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.53	0.42
3:C:61:ASN:ND2	3:C:64:SER:OG	2.52	0.42
2:B:95:GLN:O	2:B:96:GLU:C	2.62	0.42
1:A:218:LYS:N	2:B:217:TYR:N	2.66	0.42
3:C:75:ALA:HA	3:C:202:TYR:HB3	2.01	0.42
1:A:266:MET:HE2	3:C:103:GLN:HB3	2.01	0.42
2:B:172:ARG:HD3	2:B:313:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:PRO:HA	2:B:216:PRO:HD3	1.80	0.42
3:C:141:PRO:O	3:C:142:LEU:C	2.63	0.42
1:A:108:ASN:ND2	1:A:234:SER:OG	2.52	0.41
1:A:259:ARG:NH1	3:C:39:GLU:OE1	2.53	0.41
3:C:221:GLN:HG3	5:C:308:HOH:O	2.19	0.41
3:C:29:HIS:HA	3:C:30:PRO:HD2	1.86	0.41
3:C:105:CYS:SG	3:C:226:MET:CE	3.08	0.41
1:A:113:ILE:HG22	1:A:253:MET:HE1	2.01	0.41
1:A:154:MET:HE2	1:A:176:ASN:CB	2.45	0.41
1:A:156:VAL:O	1:A:156:VAL:CG2	2.67	0.41
2:B:148:TYR:HB3	2:B:284:LEU:HD12	2.03	0.41
2:B:164:ASN:O	2:B:168:HIS:HB2	2.20	0.41
2:B:177:ILE:HG21	2:B:283:LEU:HD22	2.03	0.41
2:B:234:VAL:HA	2:B:239:ILE:O	2.21	0.41
3:C:14:LEU:HB3	3:C:17:ASP:HB2	2.03	0.41
3:C:58:VAL:H	3:C:59:PRO:HD2	1.85	0.41
1:A:117:ALA:HB1	3:C:236:LEU:HD23	2.03	0.41
3:C:42:ASN:O	3:C:45:GLU:HG3	2.21	0.41
1:A:88:GLY:O	1:A:252:TYR:HA	2.21	0.41
2:B:233:TYR:N	3:C:66:MET:HE3	2.34	0.41
1:A:266:MET:HE3	1:A:266:MET:HB3	1.81	0.41
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.89	0.41
2:B:166:GLN:HG2	2:B:276:LEU:HD21	2.03	0.40
1:A:108:ASN:HD22	1:A:108:ASN:HA	1.67	0.40
1:A:118:GLN:H	1:A:118:GLN:HG2	1.54	0.40
2:B:255:ARG:NH2	3:C:124:SER:O	2.55	0.40
3:C:188:TYR:O	3:C:189:TYR:CD2	2.75	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	214/297 (72%)	201 (94%)	10 (5%)	3 (1%)	9	28
2	B	235/237 (99%)	221 (94%)	10 (4%)	4 (2%)	7	23
3	C	237/239 (99%)	216 (91%)	14 (6%)	7 (3%)	3	12
All	All	686/773 (89%)	638 (93%)	34 (5%)	14 (2%)	6	20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	GLU
2	B	127	VAL
3	C	180	HIS
3	C	188	TYR
1	A	227	ASN
2	B	97	ALA
2	B	98	ALA
3	C	181	ALA
3	C	189	TYR
1	A	85	SER
1	A	86	ARG
3	C	58	VAL
3	C	182	ARG
3	C	228	LEU

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	187/251 (74%)	173 (92%)	14 (8%)	12	34
2	B	201/201 (100%)	189 (94%)	12 (6%)	17	44
3	C	199/199 (100%)	181 (91%)	18 (9%)	9	26
All	All	587/651 (90%)	543 (92%)	44 (8%)	12	34

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	114	THR
1	A	156	VAL
1	A	167	GLU
1	A	172	GLN
1	A	179	VAL
1	A	183	LEU
1	A	229	MET
1	A	266	MET
1	A	283	SER
1	A	297	LEU
2	B	85	LEU
2	B	119	VAL
2	B	127	VAL
2	B	135	LEU
2	B	145	LYS
2	B	160	VAL
2	B	171	TYR
2	B	180	GLN
2	B	211	GLU
2	B	284	LEU
2	B	285	VAL
2	B	304	THR
3	C	14	LEU
3	C	20	VAL
3	C	25	LEU
3	C	33	CYS
3	C	53	LEU
3	C	72	PRO
3	C	90	PRO
3	C	116	GLU
3	C	136	THR
3	C	141	PRO
3	C	172	ILE
3	C	186	PHE
3	C	204	VAL
3	C	221	GLN
3	C	228	LEU
3	C	230	LYS
3	C	234	ASP

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Mol	Chain	Res	Type
3	C	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	108	ASN
1	A	228	ASN
2	B	95	GLN
2	B	182	ASN
2	B	214	HIS
2	B	277	ASN
3	C	11	ASN
3	C	61	ASN
3	C	93	ASN
3	C	162	GLN
3	C	174	ASN
3	C	176	HIS
3	C	180	HIS
3	C	210	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	218/297 (73%)	1.76	60 (27%)  	32, 50, 103, 161	0
2	B	237/237 (100%)	2.86	130 (54%)  	34, 64, 147, 190	0
3	C	239/239 (100%)	1.99	70 (29%)  	33, 52, 133, 186	0
All	All	694/773 (89%)	2.22	260 (37%)  	32, 54, 133, 190	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	239	GLY	13.7
2	B	114	SER	11.9
1	A	73	HIS	11.5
2	B	112	SER	11.4
3	C	182	ARG	10.9
2	B	120	ASP	10.6
3	C	180	HIS	10.3
3	C	176	HIS	10.2
1	A	220	LEU	10.1
2	B	127	VAL	10.0
3	C	183	ASP	9.8
2	B	118	ALA	9.7
2	B	96	GLU	9.4
1	A	210	THR	9.4
2	B	82	VAL	9.3
1	A	218	LYS	9.1
2	B	113	ASP	9.1
3	C	179	ALA	8.9
2	B	117	THR	8.8
2	B	115	ASP	8.8
3	C	238	THR	8.6
3	C	181	ALA	8.5
2	B	126	ASP	8.4

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Mol	Chain	Res	Type	RSRZ
3	C	189	TYR	8.4
1	A	219	ASP	8.4
3	C	177	TYR	8.4
2	B	83	ALA	8.3
2	B	128	SER	8.3
2	B	97	ALA	8.2
2	B	217	TYR	8.1
2	B	121	LYS	8.1
2	B	84	GLN	7.9
3	C	178	ARG	7.6
2	B	317	LEU	7.4
2	B	122	PRO	7.4
2	B	116	ALA	7.4
1	A	221	GLU	7.3
3	C	187	ASP	7.3
2	B	119	VAL	7.2
1	A	224	ALA	7.2
3	C	184	GLY	6.9
2	B	95	GLN	6.7
3	C	1	GLY	6.4
2	B	166	GLN	6.2
3	C	186	PHE	6.1
2	B	211	GLU	6.1
1	A	225	MET	6.1
3	C	234	ASP	6.0
2	B	212	ASP	6.0
2	B	318	ARG	6.0
2	B	136	ASP	5.8
2	B	110	TYR	5.8
2	B	167	PHE	5.7
2	B	206	GLY	5.5
2	B	130	ASN	5.4
2	B	208	THR	5.3
2	B	218	LYS	5.2
2	B	111	CYS	5.1
1	A	100	THR	5.1
2	B	99	ASN	5.1
3	C	233	SER	5.0
2	B	258	ASN	5.0
2	B	131	ARG	5.0
2	B	98	ALA	4.9
3	C	140	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	209	PRO	4.8
3	C	232	ALA	4.8
2	B	312	SER	4.8
2	B	107	TRP	4.8
3	C	76	GLN	4.8
2	B	225	ASP	4.7
2	B	89	ASN	4.7
2	B	164	ASN	4.6
2	B	94	THR	4.6
2	B	273	ASP	4.6
2	B	220	THR	4.6
2	B	214	HIS	4.5
2	B	276	LEU	4.5
2	B	93	THR	4.4
2	B	88	GLY	4.4
2	B	295	GLN	4.4
1	A	103	PRO	4.4
2	B	230	GLN	4.3
3	C	191	THR	4.3
2	B	163	GLN	4.3
2	B	169	TYR	4.3
2	B	124	ARG	4.3
1	A	98	LYS	4.3
2	B	165	ALA	4.3
2	B	159	GLY	4.3
1	A	200	ALA	4.2
2	B	274	SER	4.2
1	A	101	THR	4.2
2	B	272	PHE	4.2
2	B	210	THR	4.1
3	C	175	THR	4.1
2	B	145	LYS	4.1
2	B	219	GLN	4.1
2	B	157	GLU	4.0
2	B	125	PRO	4.0
2	B	203	THR	4.0
2	B	160	VAL	3.9
1	A	282	ASN	3.9
2	B	259	CYS	3.9
3	C	139	GLY	3.9
2	B	216	PRO	3.9
3	C	190	THR	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	18	ASP	3.8
1	A	227	ASN	3.8
2	B	275	ALA	3.8
2	B	209	GLY	3.8
2	B	215	PRO	3.8
2	B	90	SER	3.8
1	A	164	ASP	3.8
3	C	207	GLY	3.7
3	C	60	THR	3.7
2	B	277	ASN	3.7
3	C	222	LYS	3.7
1	A	293	ALA	3.7
1	A	102	ASN	3.7
1	A	223	GLY	3.7
2	B	316	GLY	3.7
1	A	74	SER	3.7
2	B	180	GLN	3.6
2	B	311	CYS	3.6
3	C	61	ASN	3.6
2	B	156	THR	3.6
2	B	268	ASN	3.5
3	C	237	GLN	3.5
3	C	172	ILE	3.5
1	A	202	GLN	3.5
3	C	188	TYR	3.5
1	A	226	PRO	3.5
1	A	169	LEU	3.4
3	C	29	HIS	3.4
2	B	161	PHE	3.4
1	A	199	SER	3.4
2	B	129	VAL	3.3
2	B	171	TYR	3.3
1	A	274	LYS	3.2
2	B	123	THR	3.2
3	C	171	TRP	3.2
3	C	144	LYS	3.2
2	B	269	ALA	3.2
1	A	75	THR	3.2
2	B	85	LEU	3.1
1	A	283	SER	3.1
2	B	221	GLN	3.1
3	C	162	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	147	ALA	3.1
3	C	63	THR	3.1
3	C	27	ASN	3.0
3	C	174	ASN	3.0
2	B	313	GLU	3.0
2	B	289	SER	3.0
3	C	48	GLN	3.0
3	C	41	ARG	3.0
2	B	315	ALA	3.0
2	B	204	VAL	3.0
1	A	105	GLY	2.9
1	A	85	SER	2.9
1	A	295	THR	2.9
2	B	223	GLY	2.8
1	A	241	SER	2.8
2	B	298	THR	2.8
3	C	202	TYR	2.8
2	B	172	ARG	2.7
3	C	75	ALA	2.7
3	C	59	PRO	2.7
2	B	183	ALA	2.7
2	B	226	GLY	2.7
2	B	109	SER	2.7
1	A	166	ARG	2.7
3	C	210	ASN	2.6
2	B	300	VAL	2.6
2	B	92	ILE	2.6
3	C	5	GLU	2.6
3	C	124	SER	2.6
3	C	92	ARG	2.6
3	C	236	LEU	2.6
1	A	273	PHE	2.6
1	A	277	PRO	2.5
1	A	270	ASN	2.5
1	A	285	LYS	2.5
1	A	118	GLN	2.5
3	C	17	ASP	2.5
1	A	126	PHE	2.5
1	A	244	LYS	2.5
1	A	99	GLY	2.5
2	B	224	ALA	2.5
2	B	308	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	62	ALA	2.5
3	C	2	PHE	2.4
3	C	150	MET	2.4
2	B	100	ILE	2.4
2	B	134	THR	2.4
2	B	249	HIS	2.4
1	A	272	LEU	2.4
3	C	142	LEU	2.4
2	B	222	PRO	2.4
1	A	113	ILE	2.4
2	B	314	PHE	2.3
1	A	193	PRO	2.3
2	B	108	PRO	2.3
2	B	141	GLU	2.3
2	B	86	THR	2.3
2	B	105	GLY	2.3
3	C	192	GLY	2.3
1	A	172	GLN	2.3
2	B	168	HIS	2.3
3	C	173	SER	2.3
3	C	185	VAL	2.3
1	A	91	GLY	2.3
2	B	170	LEU	2.3
3	C	230	LYS	2.3
3	C	194	VAL	2.3
2	B	202	GLY	2.3
2	B	175	PHE	2.2
2	B	173	SER	2.2
3	C	78	GLY	2.2
2	B	283	LEU	2.2
2	B	294	ASP	2.2
1	A	128	TYR	2.2
1	A	297	LEU	2.2
3	C	223	ASN	2.2
2	B	87	ILE	2.2
2	B	181	CYS	2.2
2	B	148	TYR	2.2
3	C	81	GLU	2.2
1	A	94	ASP	2.2
1	A	232	THR	2.2
1	A	242	LYS	2.2
2	B	266	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLU	2.2
2	B	133	TYR	2.1
1	A	290	SER	2.1
1	A	104	ASN	2.1
2	B	271	PRO	2.1
3	C	209	PRO	2.1
2	B	91	THR	2.1
2	B	158	THR	2.1
1	A	201	TYR	2.1
3	C	135	TYR	2.1
2	B	305	ILE	2.1
3	C	201	ASN	2.1
2	B	213	THR	2.1
2	B	256	THR	2.1
2	B	177	ILE	2.1
1	A	288	GLY	2.1
2	B	146	GLY	2.1
3	C	91	GLY	2.1
1	A	289	ALA	2.1
3	C	111	TRP	2.1
3	C	32	PRO	2.0
2	B	101	ILE	2.0
3	C	235	ILE	2.0
1	A	82	SER	2.0
2	B	106	GLU	2.0
1	A	208	TYR	2.0
1	A	222	TYR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	A	301	1/1	0.57	0.23	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.