



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:08 PM UTC

PDB ID : 3NAP / pdb_00003nap
Title : Structure of Triatoma Virus (TrV)
Authors : Squires, G.; Pous, J.
Deposited on : 2010-06-02
Resolution : 2.50 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

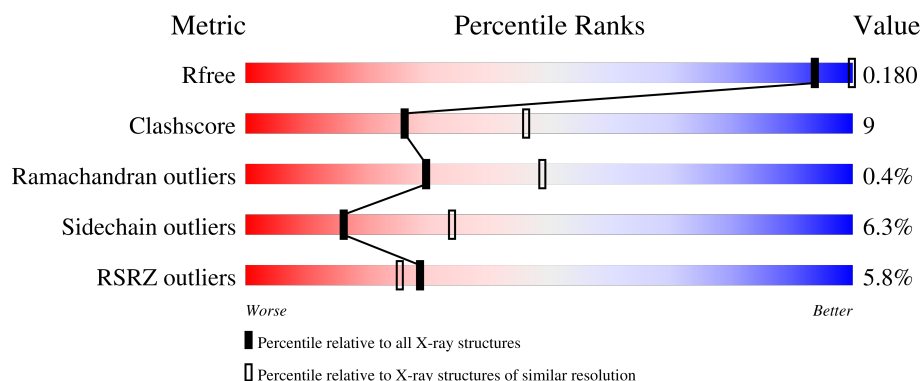
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	271	8% 75% 19% • •
2	B	255	5% 73% 19% • • •
3	C	285	3% 76% 16% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6749 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2047	1311	336	392	8			

- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	0	0
			1953	1254	325	369	5			

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	276	Total	C	N	O	S	0	0	0
			2196	1421	356	415	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	54	MET	VAL	conflict	UNP Q9QEY5

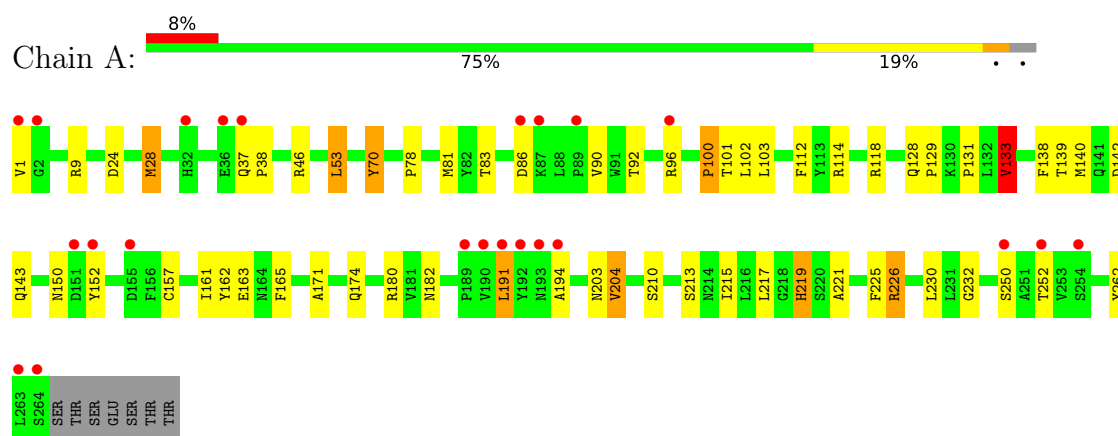
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	180	Total	O	0	0
			180	180		
4	C	217	Total	O	0	0
			217	217		

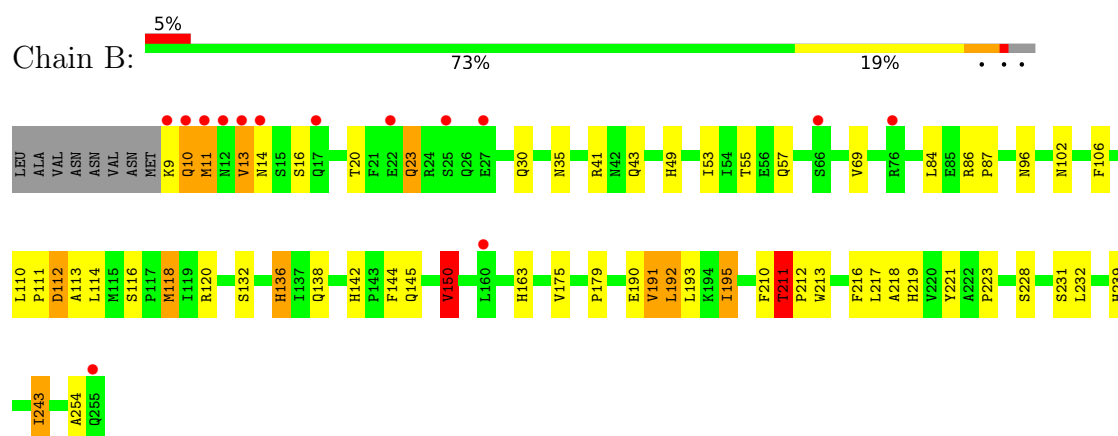
3 Residue-property plots [i](#)

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.

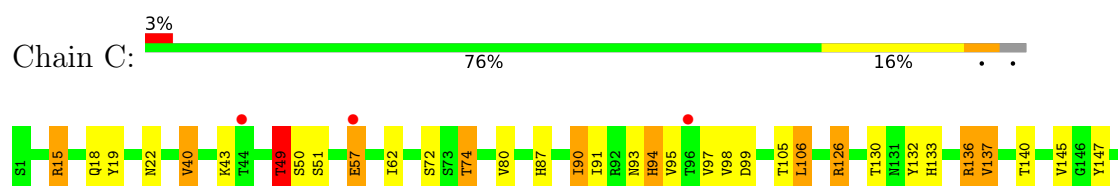
• Molecule 1: Capsid protein

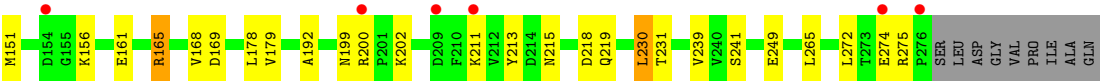


• Molecule 2: Capsid protein



• Molecule 3: Capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	343.66Å 360.46Å 341.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (30.00-2.50) 92.2 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.173 0.180 , 0.180	Depositor DCC
R_{free} test set	13284 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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	0.66	1/2098 (0.0%)	1.10	10/2856 (0.4%)
2	B	0.71	1/2002 (0.0%)	1.17	20/2729 (0.7%)
3	C	0.60	0/2259	1.11	14/3095 (0.5%)
All	All	0.66	2/6359 (0.0%)	1.13	44/8680 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	118	MET	SD-CE	-6.93	1.62	1.79
1	A	140	MET	SD-CE	6.70	1.96	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	VAL	CB-CA-C	-9.45	95.94	110.50
2	B	211	THR	N-CA-C	8.51	128.61	109.81
2	B	150	VAL	CB-CA-C	-8.12	98.61	110.63
2	B	211	THR	CA-C-N	8.10	128.57	119.83
2	B	211	THR	C-N-CA	8.10	128.57	119.83
3	C	50	SER	N-CA-C	-7.09	103.79	113.30
2	B	132	SER	N-CA-C	-7.03	101.06	110.55
3	C	230	LEU	N-CA-C	-7.03	104.84	113.41
3	C	49	THR	CB-CA-C	-6.98	95.48	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	PRO	N-CA-C	-6.88	100.43	111.03
2	B	210	PHE	CA-C-N	6.26	137.07	121.80
2	B	210	PHE	C-N-CA	6.26	137.07	121.80
2	B	11	MET	N-CA-C	-6.05	105.73	112.57
2	B	210	PHE	O-C-N	5.99	130.62	122.48
2	B	212	PRO	N-CA-C	-5.80	102.11	111.03
2	B	136	HIS	CA-C-N	-5.77	116.04	123.19
2	B	136	HIS	C-N-CA	-5.77	116.04	123.19
3	C	147	TYR	N-CA-C	5.76	119.56	112.54
3	C	105	THR	N-CA-C	-5.61	103.29	110.53
3	C	231	THR	CA-C-N	-5.60	114.48	120.03
3	C	231	THR	C-N-CA	-5.60	114.48	120.03
3	C	91	ILE	N-CA-C	5.54	117.16	109.29
1	A	204	VAL	N-CA-CB	-5.46	102.50	111.45
1	A	112	PHE	N-CA-C	5.42	117.65	109.41
1	A	157	CYS	N-CA-C	5.42	118.91	111.54
2	B	195	ILE	N-CA-CB	-5.35	106.70	112.37
2	B	69	VAL	N-CA-C	5.34	118.94	112.80
3	C	192	ALA	N-CA-C	5.33	118.04	110.10
3	C	168	VAL	N-CA-C	5.30	115.73	107.99
2	B	223	PRO	N-CA-C	5.29	119.52	111.11
1	A	86	ASP	N-CA-C	5.28	117.68	110.24
3	C	239	VAL	N-CA-C	5.26	118.69	113.53
1	A	100	PRO	N-CA-C	5.26	119.44	111.19
1	A	70	TYR	CA-C-N	5.24	126.39	119.84
1	A	70	TYR	C-N-CA	5.24	126.39	119.84
2	B	10	GLN	N-CA-C	-5.19	107.24	113.21
3	C	94	HIS	N-CA-C	-5.17	102.03	110.20
1	A	139	THR	N-CA-C	5.10	120.13	112.94
1	A	90	VAL	N-CA-C	5.09	115.30	110.42
3	C	137	VAL	N-CA-CB	-5.07	103.93	112.44
2	B	221	TYR	N-CA-C	-5.05	105.96	112.68
2	B	175	VAL	N-CA-C	-5.04	106.24	111.58
3	C	72	SER	N-CA-C	5.03	115.68	108.74
2	B	243	ILE	N-CA-C	5.02	115.58	109.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	70	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	132	TYR	Sidechain

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	2047	0	2010	43	0
2	B	1953	0	1933	41	0
3	C	2196	0	2165	40	0
4	A	156	0	0	5	0
4	B	180	0	0	3	0
4	C	217	0	0	8	0
All	All	6749	0	6108	116	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 9.

All (116) 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:163:GLU:HG2	1:A:171:ALA:HA	1.45	0.99
2:B:138:GLN:HG2	2:B:190:GLU:HG3	1.43	0.97
3:C:215:ASN:HB3	4:C:546:HOH:O	1.75	0.86
1:A:118:ARG:HE	1:A:174:GLN:HE21	1.22	0.83
3:C:130:THR:H	3:C:133:HIS:HD2	1.31	0.77
2:B:110:LEU:HD11	2:B:216:PHE:CE1	2.20	0.77
1:A:92:THR:HG23	4:A:310:HOH:O	1.86	0.76
2:B:111:PRO:HD3	2:B:213:TRP:CZ3	2.22	0.74
1:A:46:ARG:NH2	1:A:46:ARG:HG2	2.03	0.73
1:A:96:ARG:HD3	4:A:645:HOH:O	1.89	0.71
1:A:191:LEU:HD12	1:A:191:LEU:N	2.06	0.71
1:A:9:ARG:HD3	4:A:290:HOH:O	1.91	0.71
3:C:94:HIS:HD2	3:C:99:ASP:OD1	1.76	0.69
1:A:81:MET:HE2	3:C:275:ARG:HA	1.76	0.68
1:A:101:THR:OG1	1:A:219:HIS:HE1	1.77	0.67
2:B:110:LEU:HD11	2:B:216:PHE:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HH21	1:A:174:GLN:HE22	1.42	0.67
3:C:133:HIS:HE1	3:C:241:SER:O	1.80	0.65
3:C:130:THR:H	3:C:133:HIS:CD2	2.17	0.62
1:A:138:PHE:HE2	1:A:143:GLN:HG3	1.65	0.61
1:A:180:ARG:HE	1:A:203:ASN:HD21	1.47	0.61
3:C:15:ARG:HD3	3:C:18:GLN:OE1	2.01	0.61
3:C:140:THR:HG22	3:C:165:ARG:HB2	1.82	0.61
2:B:11:MET:HE2	2:B:55:THR:HB	1.84	0.60
2:B:23:GLN:NE2	2:B:23:GLN:HA	2.15	0.60
2:B:102:ASN:OD1	2:B:219:HIS:HD2	1.85	0.60
1:A:46:ARG:HG2	1:A:46:ARG:HH21	1.65	0.60
3:C:80:VAL:HG21	3:C:151:MET:HG2	1.83	0.60
2:B:163:HIS:ND1	4:B:556:HOH:O	2.27	0.59
3:C:49:THR:HG22	3:C:51:SER:H	1.68	0.59
1:A:138:PHE:CE2	1:A:143:GLN:HG3	2.38	0.58
1:A:219:HIS:HD2	4:A:356:HOH:O	1.86	0.58
2:B:23:GLN:HA	2:B:23:GLN:HE21	1.67	0.58
3:C:19:TYR:HA	3:C:22:ASN:HD22	1.68	0.57
1:A:191:LEU:HD12	1:A:191:LEU:H	1.70	0.56
3:C:49:THR:HG21	3:C:51:SER:HB2	1.87	0.55
2:B:120:ARG:NH2	2:B:254:ALA:O	2.38	0.55
1:A:114:ARG:NH2	3:C:40:VAL:HG13	2.21	0.55
1:A:118:ARG:HH21	1:A:174:GLN:NE2	2.05	0.55
2:B:49:HIS:CD2	2:B:53:ILE:HG21	2.42	0.55
1:A:128:GLN:HB3	1:A:129:PRO:HD3	1.88	0.55
2:B:14:ASN:HB2	2:B:41:ARG:HG2	1.88	0.55
2:B:110:LEU:HD11	2:B:216:PHE:CD1	2.42	0.54
1:A:118:ARG:HE	1:A:174:GLN:NE2	1.99	0.53
1:A:53:LEU:HD22	1:A:102:LEU:HD13	1.89	0.53
2:B:23:GLN:HE21	2:B:23:GLN:CA	2.21	0.53
1:A:78:PRO:HD3	1:A:100:PRO:HD3	1.92	0.52
2:B:86:ARG:HH11	2:B:118:MET:HE2	1.74	0.52
2:B:84:LEU:HB2	2:B:243:ILE:HD13	1.92	0.52
3:C:49:THR:CG2	3:C:51:SER:H	2.23	0.52
3:C:57:GLU:O	3:C:57:GLU:HG3	2.10	0.52
1:A:37:GLN:HB3	1:A:38:PRO:HD3	1.93	0.51
2:B:111:PRO:O	2:B:113:ALA:N	2.43	0.51
1:A:78:PRO:CD	1:A:100:PRO:HD3	2.40	0.50
3:C:19:TYR:HA	3:C:22:ASN:ND2	2.27	0.50
1:A:180:ARG:HE	1:A:203:ASN:ND2	2.10	0.49
2:B:10:GLN:H	2:B:10:GLN:CD	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:HIS:H	2:B:145:GLN:NE2	2.10	0.49
2:B:142:HIS:H	2:B:145:GLN:HE21	1.62	0.48
3:C:126:ARG:HH11	3:C:249:GLU:CD	2.22	0.48
1:A:161:ILE:C	1:A:161:ILE:HD12	2.39	0.47
1:A:92:THR:HG21	3:C:275:ARG:HE	1.79	0.47
2:B:13:VAL:HG11	2:B:16:SER:HB2	1.95	0.47
3:C:275:ARG:NH1	4:C:619:HOH:O	2.47	0.47
1:A:250:SER:O	1:A:252:THR:HG23	2.14	0.47
2:B:20:THR:HA	2:B:35:ASN:O	2.15	0.47
1:A:96:ARG:HH11	1:A:96:ARG:HG3	1.79	0.47
3:C:98:VAL:HG12	3:C:98:VAL:O	2.14	0.47
1:A:191:LEU:N	1:A:191:LEU:CD1	2.74	0.46
1:A:150:ASN:HD21	1:A:152:TYR:HB2	1.80	0.46
2:B:86:ARG:HH11	2:B:118:MET:CE	2.28	0.46
1:A:225:PHE:O	1:A:226:ARG:HG2	2.16	0.46
1:A:226:ARG:HD3	4:A:391:HOH:O	2.15	0.46
1:A:133:VAL:HG13	1:A:210:SER:HB3	1.98	0.46
3:C:202:LYS:NZ	4:C:423:HOH:O	2.44	0.46
1:A:24:ASP:HA	3:C:179:VAL:HB	1.97	0.45
3:C:178:LEU:C	3:C:178:LEU:HD12	2.40	0.45
1:A:28:MET:HB3	1:A:28:MET:HE3	1.69	0.45
2:B:10:GLN:CD	2:B:10:GLN:N	2.75	0.45
2:B:96:ASN:HB3	2:B:231:SER:HB3	1.96	0.45
3:C:87:HIS:HD2	4:C:293:HOH:O	1.98	0.45
2:B:106:PHE:CD1	2:B:106:PHE:C	2.94	0.45
3:C:199:ASN:O	3:C:200:ARG:C	2.60	0.45
2:B:9:LYS:C	2:B:11:MET:H	2.24	0.45
3:C:74:THR:CG2	4:C:550:HOH:O	2.64	0.45
2:B:114:LEU:N	2:B:114:LEU:HD12	2.33	0.44
1:A:221:ALA:HB1	1:A:225:PHE:HB3	1.99	0.44
2:B:111:PRO:O	2:B:112:ASP:C	2.61	0.44
3:C:219:GLN:NE2	3:C:219:GLN:H	2.15	0.44
1:A:133:VAL:HG22	1:A:165:PHE:CE1	2.53	0.44
2:B:116:SER:O	2:B:120:ARG:HG3	2.18	0.44
3:C:93:ASN:ND2	4:C:348:HOH:O	2.51	0.44
3:C:74:THR:HG22	4:C:550:HOH:O	2.18	0.43
3:C:94:HIS:CD2	3:C:99:ASP:OD1	2.65	0.43
2:B:142:HIS:HD2	2:B:144:PHE:H	1.67	0.43
2:B:14:ASN:ND2	2:B:43:GLN:H	2.17	0.43
2:B:150:VAL:O	2:B:218:ALA:HA	2.19	0.43
2:B:41:ARG:NH2	4:B:314:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LEU:HD12	3:C:178:LEU:O	2.18	0.42
1:A:182:ASN:ND2	3:C:43:LYS:HE2	2.35	0.42
2:B:23:GLN:NE2	2:B:23:GLN:CA	2.80	0.42
1:A:215:ILE:HD12	1:A:217:LEU:HD21	2.01	0.42
1:A:230:LEU:HD23	3:C:62:ILE:HG13	2.01	0.42
2:B:191:VAL:C	2:B:192:LEU:HD23	2.45	0.41
2:B:35:ASN:ND2	4:B:337:HOH:O	2.49	0.41
1:A:83:THR:HB	3:C:275:ARG:HB3	2.02	0.41
2:B:136:HIS:ND1	2:B:190:GLU:OE1	2.44	0.41
2:B:145:GLN:HE22	2:B:232:LEU:HD21	1.85	0.41
3:C:136:ARG:HG3	3:C:169:ASP:HA	2.03	0.41
2:B:87:PRO:HA	2:B:239:HIS:HB3	2.03	0.41
3:C:230:LEU:HA	3:C:230:LEU:HD23	1.86	0.41
3:C:90:ILE:HA	3:C:90:ILE:HD12	1.68	0.40
3:C:211:LYS:HD3	4:C:590:HOH:O	2.19	0.40
1:A:232:GLY:HA2	3:C:106:LEU:HG	2.02	0.40
3:C:213:TYR:CZ	3:C:218:ASP:HB2	2.56	0.40
2:B:86:ARG:NH1	2:B:118:MET:HE2	2.36	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	262/271 (97%)	251 (96%)	10 (4%)	1 (0%)	30	49
2	B	245/255 (96%)	235 (96%)	8 (3%)	2 (1%)	16	31
3	C	274/285 (96%)	267 (97%)	7 (3%)	0	100	100
All	All	781/811 (96%)	753 (96%)	25 (3%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	112	ASP
1	A	194	ALA
2	B	211	THR

5.3.2 Protein sidechains [i](#)

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	224/231 (97%)	211 (94%)	13 (6%)	18	38
2	B	224/231 (97%)	212 (95%)	12 (5%)	20	41
3	C	251/258 (97%)	232 (92%)	19 (8%)	12	26
All	All	699/720 (97%)	655 (94%)	44 (6%)	16	34

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

Mol	Chain	Res	Type
1	A	1	VAL
1	A	28	MET
1	A	53	LEU
1	A	103	LEU
1	A	131	PRO
1	A	133	VAL
1	A	142	ASP
1	A	191	LEU
1	A	204	VAL
1	A	213	SER
1	A	219	HIS
1	A	226	ARG
1	A	262	TYR
2	B	13	VAL
2	B	23	GLN
2	B	30	GLN
2	B	57	GLN
2	B	150	VAL
2	B	191	VAL
2	B	192	LEU

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Mol	Chain	Res	Type
2	B	193	LEU
2	B	195	ILE
2	B	211	THR
2	B	217	LEU
2	B	228	SER
3	C	15	ARG
3	C	40	VAL
3	C	49	THR
3	C	57	GLU
3	C	74	THR
3	C	90	ILE
3	C	95	VAL
3	C	97	VAL
3	C	106	LEU
3	C	126	ARG
3	C	136	ARG
3	C	137	VAL
3	C	145	VAL
3	C	156	LYS
3	C	161	GLU
3	C	165	ARG
3	C	265	LEU
3	C	272	LEU
3	C	274	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	141	GLN
1	A	150	ASN
1	A	160	ASN
1	A	174	GLN
1	A	196	ASN
1	A	203	ASN
1	A	219	HIS
2	B	14	ASN
2	B	23	GLN
2	B	30	GLN
2	B	42	ASN
2	B	49	HIS
2	B	142	HIS

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Mol	Chain	Res	Type
2	B	145	GLN
2	B	203	GLN
2	B	219	HIS
2	B	255	GLN
3	C	22	ASN
3	C	87	HIS
3	C	94	HIS
3	C	133	HIS
3	C	215	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](#)

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	264/271 (97%)	0.72	23 (8%) 16 14	12, 19, 52, 104	0
2	B	247/255 (96%)	0.52	14 (5%) 29 26	10, 18, 41, 100	0
3	C	276/285 (96%)	0.39	9 (3%) 49 45	10, 17, 38, 61	0
All	All	787/811 (97%)	0.54	46 (5%) 29 25	10, 18, 46, 104	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	SER	11.4
2	B	12	ASN	8.7
2	B	10	GLN	7.8
1	A	192	TYR	7.6
1	A	193	ASN	7.4
1	A	250	SER	6.3
1	A	191	LEU	5.7
1	A	152	TYR	5.6
1	A	151	ASP	5.3
2	B	11	MET	4.7
1	A	1	VAL	4.5
1	A	155	ASP	4.2
2	B	13	VAL	3.8
2	B	14	ASN	3.7
3	C	276	PRO	3.7
1	A	190	VAL	3.6
2	B	9	LYS	3.6
3	C	44	THR	3.3
1	A	194	ALA	2.9
1	A	36	GLU	2.8
2	B	22	GLU	2.8
3	C	274	GLU	2.8
1	A	87	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	255	GLN	2.7
2	B	76	ARG	2.7
1	A	86	ASP	2.6
1	A	96	ARG	2.6
1	A	189	PRO	2.5
3	C	57	GLU	2.5
3	C	209	ASP	2.5
3	C	200	ARG	2.5
1	A	252	THR	2.5
3	C	211	LYS	2.4
2	B	66	SER	2.4
1	A	32	HIS	2.3
1	A	2	GLY	2.3
1	A	89	PRO	2.3
1	A	37	GLN	2.2
2	B	17	GLN	2.2
3	C	96	THR	2.2
2	B	160	LEU	2.1
1	A	263	LEU	2.1
2	B	27	GLU	2.1
1	A	254	SER	2.1
3	C	154	ASP	2.1
2	B	25	SER	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.