



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:29 AM UTC

PDB ID : 5MNT / pdb_00005mnt
Title : Bacteriophage Qbeta maturation protein
Authors : Rumnieks, J.; Tars, K.
Deposited on : 2016-12-13
Resolution : 3.32 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

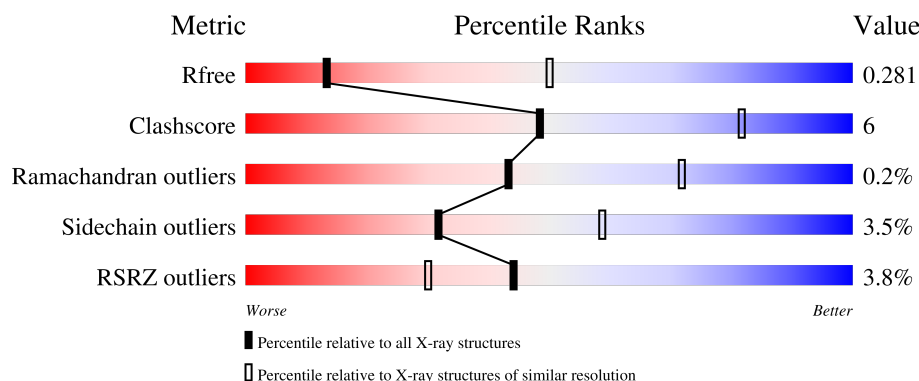
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	421	5% 84% 15% .
1	B	421	4% 80% 19% .
1	C	421	2% 85% 15% .
1	D	421	3% 86% 13% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13774 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 A2 maturation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3444	2213	616	612	3			
1	B	421	Total	C	N	O	S	0	0	0
			3448	2215	617	613	3			
1	C	420	Total	C	N	O	S	0	0	0
			3444	2213	616	612	3			
1	D	419	Total	C	N	O	S	0	0	0
			3438	2210	615	610	3			

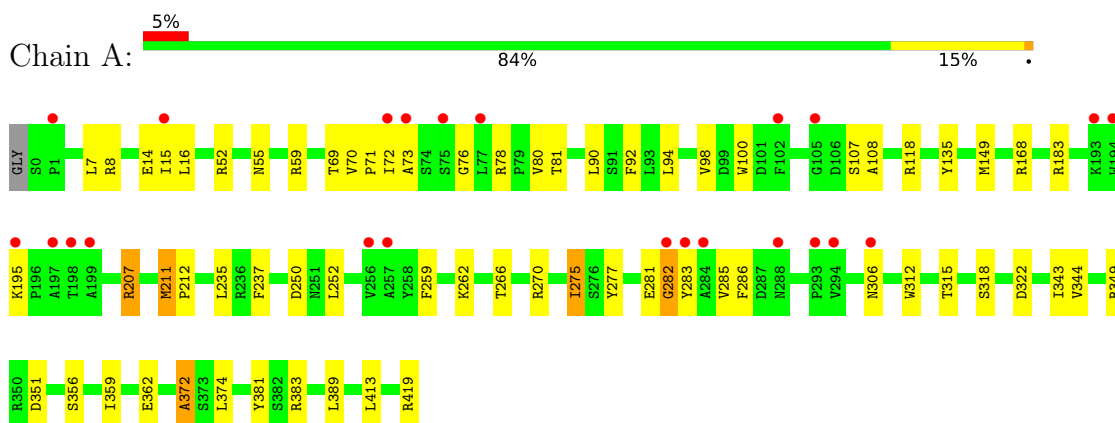
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8LTE2
A	0	SER	-	expression tag	UNP Q8LTE2
B	-1	GLY	-	expression tag	UNP Q8LTE2
B	0	SER	-	expression tag	UNP Q8LTE2
C	-1	GLY	-	expression tag	UNP Q8LTE2
C	0	SER	-	expression tag	UNP Q8LTE2
D	-1	GLY	-	expression tag	UNP Q8LTE2
D	0	SER	-	expression tag	UNP Q8LTE2

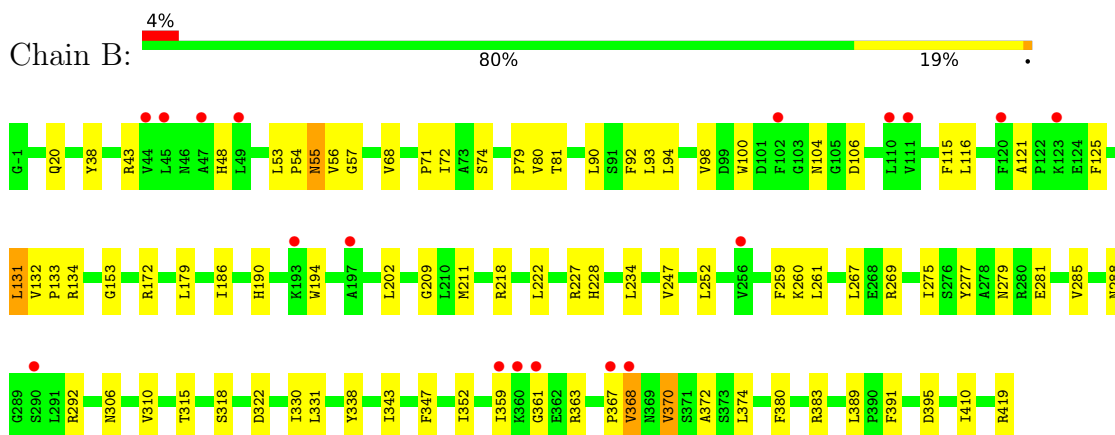
3 Residue-property plots

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.

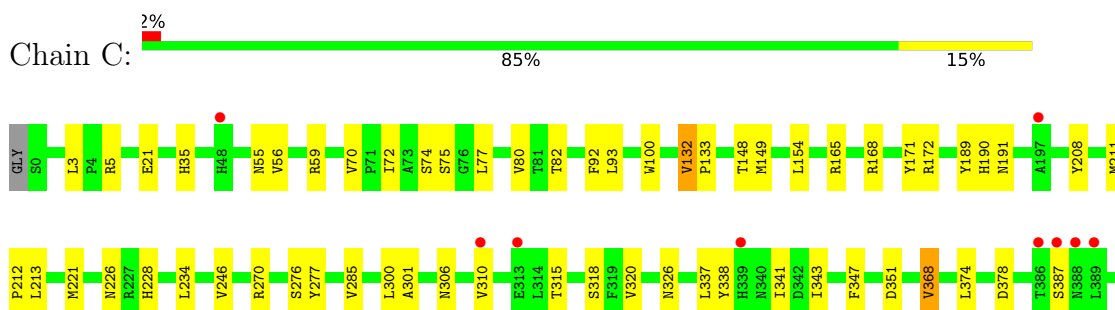
• Molecule 1: A2 maturation protein



• Molecule 1: A2 maturation protein

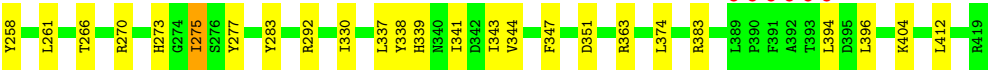
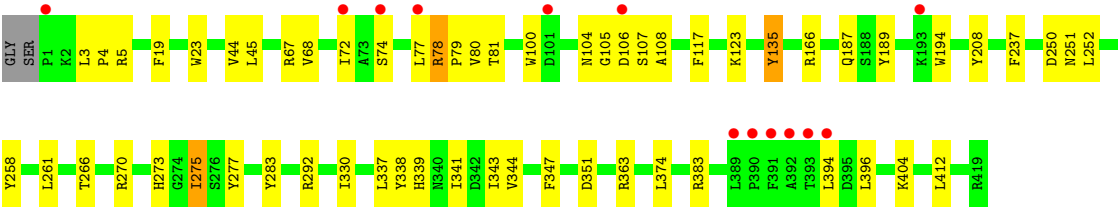
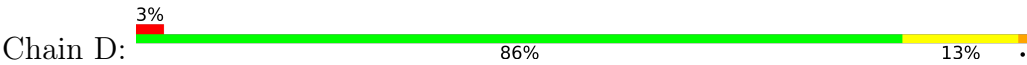


• Molecule 1: A2 maturation protein





● Molecule 1: A2 maturation protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.79Å 232.51Å 353.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	176.74 – 3.32 176.74 – 3.32	Depositor EDS
% Data completeness (in resolution range)	97.0 (176.74-3.32) 97.0 (176.74-3.32)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.228 , 0.279 0.235 , 0.281	Depositor DCC
R_{free} test set	3335 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13774	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	0.65	0/3538	0.94	7/4799 (0.1%)
1	B	0.65	0/3542	0.93	3/4804 (0.1%)
1	C	0.63	0/3538	0.92	3/4799 (0.1%)
1	D	0.62	0/3532	0.89	3/4790 (0.1%)
All	All	0.64	0/14150	0.92	16/19192 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ILE	N-CA-C	6.78	113.46	106.21
1	C	3	LEU	CA-C-N	6.57	126.95	119.92
1	C	3	LEU	C-N-CA	6.57	126.95	119.92
1	B	306	ASN	CA-C-N	6.22	125.63	118.85
1	B	306	ASN	C-N-CA	6.22	125.63	118.85
1	A	282	GLY	N-CA-C	6.20	120.14	112.64
1	D	105	GLY	N-CA-C	6.19	121.35	113.24
1	A	283	TYR	N-CA-C	6.12	118.03	111.36
1	A	72	ILE	N-CA-C	5.78	118.71	113.10
1	B	104	ASN	N-CA-C	5.54	119.08	111.54
1	A	306	ASN	CA-C-N	5.42	124.88	119.24
1	A	306	ASN	C-N-CA	5.42	124.88	119.24
1	C	132	VAL	N-CA-CB	5.38	113.89	110.50
1	A	372	ALA	N-CA-C	5.35	117.32	109.24
1	D	3	LEU	CA-C-N	5.02	126.11	119.84
1	D	3	LEU	C-N-CA	5.02	126.11	119.84

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	3444	0	3386	32	0
1	B	3448	0	3389	52	0
1	C	3444	0	3386	35	0
1	D	3438	0	3381	35	0
All	All	13774	0	13542	151	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 6.

All (151) 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:B:56:VAL:HG12	1:B:57:GLY:O	1.77	0.85
1:B:90:LEU:HG	1:B:121:ALA:HB2	1.65	0.79
1:D:81:THR:O	1:D:383:ARG:NH1	2.22	0.73
1:A:237:PHE:HB2	1:A:275:ILE:HG22	1.71	0.72
1:D:106:ASP:OD2	1:D:363:ARG:NH1	2.24	0.70
1:B:80:VAL:HG21	1:B:347:PHE:HB3	1.74	0.69
1:B:98:VAL:HG11	1:B:259:PHE:CZ	2.27	0.69
1:B:132:VAL:HG13	1:B:133:PRO:HD3	1.75	0.69
1:B:277:TYR:CZ	1:B:343:ILE:HD11	2.30	0.67
1:B:261:LEU:HD23	1:B:361:GLY:HA3	1.77	0.66
1:B:363:ARG:HG2	1:B:367:PRO:CG	2.27	0.64
1:A:100:TRP:CZ2	1:A:108:ALA:HB3	2.34	0.62
1:A:207:ARG:HD3	1:A:312:TRP:CD2	2.34	0.62
1:A:237:PHE:HB2	1:A:275:ILE:CG2	2.31	0.61
1:B:38:TYR:CD1	1:B:55:ASN:HB3	2.37	0.60
1:B:368:VAL:HG13	1:B:370:VAL:HG13	1.83	0.59
1:B:228:HIS:ND1	1:B:338:TYR:OH	2.35	0.59
1:C:189:TYR:CZ	1:C:213:LEU:HD23	2.38	0.58
1:C:75:SER:HB3	1:C:337:LEU:HD13	1.87	0.57
1:C:80:VAL:HG11	1:C:347:PHE:HB3	1.87	0.56
1:B:277:TYR:CZ	1:B:343:ILE:CD1	2.89	0.56
1:C:100:TRP:CD1	1:C:368:VAL:CG2	2.88	0.56
1:A:7:LEU:HD21	1:A:70:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HD3	1:A:312:TRP:CE2	2.40	0.55
1:B:275:ILE:CG2	1:B:343:ILE:HD12	2.36	0.55
1:C:228:HIS:ND1	1:C:338:TYR:OH	2.33	0.55
1:D:72:ILE:HG22	1:D:77:LEU:O	2.07	0.55
1:A:315:THR:HG22	1:A:318:SER:HB3	1.89	0.54
1:B:363:ARG:HG2	1:B:367:PRO:HG3	1.88	0.54
1:C:100:TRP:CD1	1:C:368:VAL:HG22	2.43	0.54
1:D:72:ILE:HG12	1:D:283:TYR:HB2	1.88	0.54
1:A:359:ILE:HD12	1:A:372:ALA:HB3	1.88	0.53
1:B:153:GLY:HA2	1:B:227:ARG:HD2	1.91	0.53
1:B:94:LEU:HD11	1:B:372:ALA:HB1	1.90	0.53
1:B:100:TRP:CZ3	1:B:106:ASP:HB3	2.44	0.53
1:A:98:VAL:HG11	1:A:259:PHE:CZ	2.43	0.53
1:C:168:ARG:HH12	1:C:172:ARG:NH2	2.08	0.52
1:B:267:LEU:HD13	1:B:352:ILE:HG23	1.91	0.52
1:B:132:VAL:HG13	1:B:133:PRO:CD	2.39	0.52
1:C:149:MET:HE1	1:C:234:LEU:HD11	1.91	0.52
1:A:275:ILE:HD11	1:A:343:ILE:CD1	2.41	0.51
1:D:80:VAL:HG11	1:D:347:PHE:CD2	2.45	0.51
1:B:72:ILE:HG23	1:B:79:PRO:HD3	1.93	0.51
1:B:292:ARG:HD3	1:B:330:ILE:HG12	1.93	0.51
1:B:359:ILE:CD1	1:B:372:ALA:HB3	2.41	0.50
1:C:92:PHE:HB3	1:C:374:LEU:HD11	1.93	0.50
1:D:292:ARG:NE	1:D:330:ILE:HD11	2.26	0.50
1:A:235:LEU:HB3	1:A:277:TYR:HB2	1.94	0.50
1:A:252:LEU:HD12	1:A:252:LEU:O	2.12	0.50
1:B:92:PHE:HB3	1:B:374:LEU:HD11	1.94	0.50
1:B:359:ILE:HD13	1:B:372:ALA:HB3	1.93	0.50
1:C:315:THR:HG22	1:C:318:SER:HB3	1.94	0.49
1:D:100:TRP:CZ2	1:D:108:ALA:HB3	2.47	0.49
1:C:171:TYR:CD1	1:C:320:VAL:HG21	2.46	0.49
1:D:338:TYR:HA	1:D:341:ILE:HD11	1.94	0.49
1:D:45:LEU:CD2	1:D:106:ASP:HB2	2.42	0.49
1:D:5:ARG:HG3	1:D:67:ARG:HG2	1.95	0.49
1:D:72:ILE:CG1	1:D:283:TYR:HB2	2.43	0.49
1:A:207:ARG:NH1	1:D:208:TYR:OH	2.46	0.49
1:D:277:TYR:CE1	1:D:343:ILE:HG13	2.47	0.48
1:A:59:ARG:HG3	1:A:118:ARG:HH21	1.78	0.48
1:D:270:ARG:HB3	1:D:351:ASP:OD1	2.13	0.48
1:B:194:TRP:NE1	1:C:306:ASN:OD1	2.46	0.48
1:C:270:ARG:HB3	1:C:351:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLN:OE1	1:D:194:TRP:HB3	2.13	0.48
1:C:300:LEU:HD11	1:C:326:ASN:HB3	1.96	0.48
1:C:168:ARG:HD3	1:C:413:LEU:HD11	1.95	0.48
1:B:43:ARG:HB3	1:B:48:HIS:CD2	2.50	0.47
1:C:59:ARG:HH12	1:C:378:ASP:CG	2.23	0.47
1:B:81:THR:O	1:B:383:ARG:NH1	2.48	0.47
1:B:179:LEU:HD23	1:B:202:LEU:HD23	1.96	0.47
1:C:35:HIS:CD2	1:C:93:LEU:HD11	2.50	0.47
1:D:74:SER:HB3	1:D:337:LEU:HD11	1.97	0.47
1:B:115:PHE:CE2	1:B:252:LEU:HD13	2.50	0.47
1:C:189:TYR:CE2	1:C:213:LEU:HD23	2.50	0.47
1:A:207:ARG:CD	1:A:312:TRP:CE2	2.98	0.46
1:C:72:ILE:HG21	1:C:77:LEU:HD22	1.96	0.46
1:A:211:MET:N	1:A:212:PRO:HD2	2.31	0.46
1:B:125:PHE:HB3	1:B:269:ARG:NH1	2.31	0.46
1:A:94:LEU:HD11	1:A:372:ALA:HB1	1.97	0.46
1:B:190:HIS:HB3	1:B:194:TRP:CZ3	2.50	0.45
1:B:352:ILE:HD12	1:B:380:PHE:HB3	1.98	0.45
1:A:81:THR:O	1:A:383:ARG:NH1	2.49	0.45
1:B:363:ARG:CG	1:B:367:PRO:HG3	2.45	0.45
1:C:59:ARG:NH1	1:C:378:ASP:OD2	2.49	0.45
1:A:16:LEU:HD11	1:A:285:VAL:HG13	1.98	0.45
1:D:80:VAL:HG22	1:D:383:ARG:HH11	1.82	0.45
1:C:132:VAL:CG1	1:C:133:PRO:HD3	2.46	0.45
1:A:168:ARG:HE	1:A:413:LEU:HD11	1.81	0.45
1:B:100:TRP:CH2	1:B:106:ASP:HB3	2.52	0.44
1:D:80:VAL:HG11	1:D:347:PHE:HB3	1.97	0.44
1:D:80:VAL:HG13	1:D:80:VAL:O	2.17	0.44
1:A:349:ARG:HD2	1:A:381:TYR:CE2	2.53	0.44
1:B:93:LEU:HD23	1:B:116:LEU:HB3	2.00	0.44
1:B:275:ILE:HG23	1:B:343:ILE:HG23	1.99	0.44
1:B:315:THR:HB	1:B:318:SER:HB3	1.99	0.44
1:B:252:LEU:O	1:B:252:LEU:HD12	2.17	0.44
1:A:92:PHE:HB3	1:A:374:LEU:HD11	2.00	0.43
1:A:69:THR:O	1:A:78:ARG:NH1	2.51	0.43
1:B:71:PRO:HG2	1:B:288:ASN:OD1	2.18	0.43
1:B:322:ASP:OD1	1:B:419:ARG:NH2	2.52	0.43
1:D:237:PHE:HB2	1:D:275:ILE:HG13	2.00	0.43
1:A:282:GLY:O	1:A:286:PHE:HB2	2.19	0.43
1:C:59:ARG:NH1	1:C:378:ASP:OD1	2.49	0.43
1:D:78:ARG:CB	1:D:79:PRO:CD	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:OD1	1:A:419:ARG:NH2	2.52	0.43
1:B:259:PHE:HB3	1:B:363:ARG:HD2	2.01	0.43
1:A:8:ARG:N	1:A:16:LEU:O	2.52	0.42
1:D:19:PHE:HD2	1:D:23:TRP:CZ3	2.38	0.42
1:D:78:ARG:HB3	1:D:79:PRO:CD	2.49	0.42
1:C:74:SER:OG	1:C:337:LEU:HD21	2.19	0.42
1:C:221:MET:HE2	1:C:301:ALA:HB2	2.01	0.42
1:B:53:LEU:HB3	1:B:54:PRO:HD2	2.01	0.42
1:B:218:ARG:O	1:B:222:LEU:HD22	2.20	0.42
1:D:394:LEU:HD23	1:D:396:LEU:HD21	2.02	0.42
1:A:73:ALA:O	1:A:76:GLY:N	2.53	0.42
1:C:100:TRP:CG	1:C:368:VAL:CG2	3.02	0.42
1:D:339:HIS:CG	1:D:404:LYS:HE3	2.54	0.42
1:C:132:VAL:HG13	1:C:133:PRO:HD3	2.02	0.42
1:B:131:LEU:O	1:B:134:ARG:N	2.52	0.42
1:D:166:ARG:HD2	1:D:189:TYR:OH	2.19	0.42
1:C:277:TYR:CZ	1:C:343:ILE:HD11	2.55	0.42
1:C:59:ARG:NH1	1:C:378:ASP:CG	2.78	0.42
1:C:77:LEU:HD11	1:C:276:SER:HB3	2.01	0.42
1:B:186:ILE:HD12	1:B:209:GLY:HA3	2.02	0.41
1:D:250:ASP:OD1	1:D:251:ASN:N	2.52	0.41
1:A:183:ARG:HD3	1:A:195:LYS:HE3	2.03	0.41
1:B:279:ASN:OD1	1:B:279:ASN:C	2.63	0.41
1:C:190:HIS:O	1:C:191:ASN:C	2.63	0.41
1:C:285:VAL:O	1:C:285:VAL:HG12	2.21	0.41
1:B:115:PHE:HE2	1:B:252:LEU:HD13	1.84	0.41
1:D:135:TYR:OH	1:D:273:HIS:ND1	2.52	0.41
1:A:90:LEU:O	1:A:118:ARG:HA	2.21	0.41
1:B:285:VAL:HG12	1:B:285:VAL:O	2.21	0.41
1:D:44:VAL:HG21	1:D:258:TYR:CD2	2.55	0.41
1:D:45:LEU:HD21	1:D:106:ASP:HB2	2.02	0.41
1:D:252:LEU:HB2	1:D:261:LEU:HB2	2.03	0.41
1:D:80:VAL:HG22	1:D:383:ARG:NH1	2.35	0.41
1:D:117:PHE:HB2	1:D:252:LEU:HD11	2.02	0.41
1:C:211:MET:HB3	1:C:212:PRO:HD3	2.02	0.41
1:D:252:LEU:N	1:D:252:LEU:HD22	2.36	0.41
1:A:250:ASP:HB3	1:A:262:LYS:HG3	2.03	0.40
1:D:78:ARG:HB3	1:D:79:PRO:HD2	2.03	0.40
1:A:270:ARG:HB3	1:A:351:ASP:OD1	2.21	0.40
1:C:341:ILE:HB	1:C:397:ASP:HA	2.04	0.40
1:B:331:LEU:HD13	1:B:410:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASN:OD1	1:B:281:GLU:N	2.52	0.40
1:C:5:ARG:NH2	1:C:21:GLU:OE1	2.54	0.40
1:A:275:ILE:HD12	1:A:389:LEU:CD2	2.52	0.40
1:B:211:MET:HE1	1:C:208:TYR:CD2	2.55	0.40
1:B:389:LEU:HD23	1:B:391:PHE:CZ	2.57	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	418/421 (99%)	395 (94%)	23 (6%)	0	100	100
1	B	419/421 (100%)	402 (96%)	17 (4%)	0	100	100
1	C	418/421 (99%)	401 (96%)	15 (4%)	2 (0%)	24	56
1	D	417/421 (99%)	403 (97%)	12 (3%)	2 (0%)	24	56
All	All	1672/1684 (99%)	1601 (96%)	67 (4%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	104	ASN
1	C	56	VAL
1	D	4	PRO
1	C	310	VAL

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	366/366 (100%)	350 (96%)	16 (4%)	25	54
1	B	366/366 (100%)	353 (96%)	13 (4%)	31	58
1	C	366/366 (100%)	354 (97%)	12 (3%)	33	60
1	D	365/366 (100%)	355 (97%)	10 (3%)	39	63
All	All	1463/1464 (100%)	1412 (96%)	51 (4%)	32	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	52	ARG
1	A	55	ASN
1	A	71	PRO
1	A	80	VAL
1	A	107	SER
1	A	135	TYR
1	A	149	MET
1	A	207	ARG
1	A	211	MET
1	A	266	THR
1	A	275	ILE
1	A	281	GLU
1	A	344	VAL
1	A	356	SER
1	A	362	GLU
1	B	20	GLN
1	B	55	ASN
1	B	68	VAL
1	B	74	SER
1	B	131	LEU
1	B	172	ARG
1	B	234	LEU
1	B	247	VAL
1	B	260	LYS
1	B	310	VAL
1	B	368	VAL
1	B	370	VAL
1	B	395	ASP
1	C	55	ASN

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Mol	Chain	Res	Type
1	C	70	VAL
1	C	82	THR
1	C	148	THR
1	C	154	LEU
1	C	165	ARG
1	C	226	ASN
1	C	246	VAL
1	C	368	VAL
1	C	387	SER
1	C	402	SER
1	C	409	SER
1	D	68	VAL
1	D	78	ARG
1	D	107	SER
1	D	123	LYS
1	D	135	TYR
1	D	266	THR
1	D	275	ILE
1	D	344	VAL
1	D	374	LEU
1	D	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	201	ASN
1	A	279	ASN
1	A	308	HIS
1	A	369	ASN
1	B	95	ASN
1	B	109	ASN
1	B	113	ASN
1	B	190	HIS
1	B	225	GLN
1	B	333	GLN
1	B	336	GLN
1	C	13	ASN
1	C	20	GLN
1	C	35	HIS
1	D	20	GLN
1	D	35	HIS

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Mol	Chain	Res	Type
1	D	143	ASN
1	D	225	GLN
1	D	232	GLN
1	D	333	GLN
1	D	388	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	420/421 (99%)	0.16	23 (5%) 30 21	58, 87, 147, 171	0
1	B	421/421 (100%)	0.19	18 (4%) 40 26	58, 91, 161, 196	0
1	C	420/421 (99%)	0.06	10 (2%) 59 40	63, 87, 112, 145	0
1	D	419/421 (99%)	0.25	13 (3%) 51 35	66, 101, 137, 182	0
All	All	1680/1684 (99%)	0.16	64 (3%) 44 30	58, 92, 143, 196	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ASN	5.8
1	D	77	LEU	5.4
1	A	77	LEU	4.9
1	D	392	ALA	4.5
1	D	391	PHE	4.2
1	B	49	LEU	4.2
1	A	198	THR	3.9
1	A	256	VAL	3.7
1	C	388	ASN	3.6
1	A	197	ALA	3.5
1	B	197	ALA	3.5
1	A	194	TRP	3.4
1	D	389	LEU	3.4
1	C	310	VAL	3.3
1	B	359	ILE	3.3
1	A	283	TYR	3.3
1	D	390	PRO	3.3
1	A	284	ALA	3.1
1	B	110	LEU	3.0
1	D	193	LYS	2.9
1	A	73	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	387	SER	2.8
1	A	199	ALA	2.7
1	D	1	PRO	2.7
1	A	15	ILE	2.7
1	B	193	LYS	2.6
1	A	105	GLY	2.6
1	B	368	VAL	2.6
1	D	74	SER	2.6
1	A	294	VAL	2.6
1	D	101	ASP	2.5
1	C	386	THR	2.5
1	D	72	ILE	2.5
1	B	102	PHE	2.5
1	A	72	ILE	2.4
1	A	288	ASN	2.4
1	B	45	LEU	2.3
1	A	193	LYS	2.3
1	D	393	THR	2.3
1	B	47	ALA	2.3
1	B	361	GLY	2.3
1	B	256	VAL	2.3
1	C	48	HIS	2.2
1	A	282	GLY	2.2
1	B	120	PHE	2.2
1	C	197	ALA	2.2
1	A	75	SER	2.2
1	D	394	LEU	2.2
1	A	195	LYS	2.1
1	A	102	PHE	2.1
1	B	111	VAL	2.1
1	B	290	SER	2.1
1	C	389	LEU	2.1
1	D	106	ASP	2.1
1	A	293	PRO	2.1
1	A	1	PRO	2.1
1	B	367	PRO	2.1
1	B	123	LYS	2.0
1	B	44	VAL	2.0
1	C	339	HIS	2.0
1	A	257	ALA	2.0
1	B	360	LYS	2.0
1	C	313	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	419	ARG	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.