



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:16 AM UTC

PDB ID : 2AMQ / pdb_00002amq
Title : Crystal Structure Of SARS_CoV Mpro in Complex with an Inhibitor N3
Authors : Yang, H.; Xue, X.; Yang, K.; Zhao, Q.; Bartlam, M.; Rao, Z.
Deposited on : 2005-08-10
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

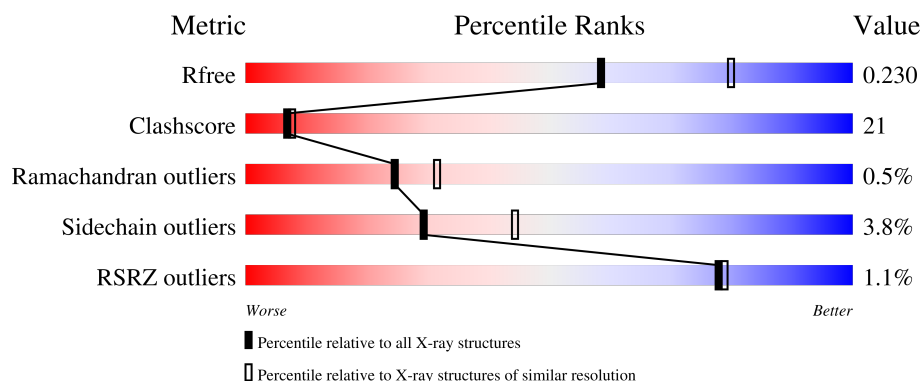
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	311	17% 69% 26% • •
1	B	311	62% 30% 5% •
2	C	6	33% 33% 33%
2	D	6	17% 33% 17% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	02J	C	1	-	X	-	-
2	02J	D	1	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5111 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2351	1489	401	439	22			
1	B	302	Total	C	N	O	S	0	0	0
			2336	1476	400	438	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	cloning artifact	UNP P59641
A	-3	PRO	-	cloning artifact	UNP P59641
A	-2	LEU	-	cloning artifact	UNP P59641
A	-1	GLY	-	cloning artifact	UNP P59641
A	0	SER	-	cloning artifact	UNP P59641
B	-4	GLY	-	cloning artifact	UNP P59641
B	-3	PRO	-	cloning artifact	UNP P59641
B	-2	LEU	-	cloning artifact	UNP P59641
B	-1	GLY	-	cloning artifact	UNP P59641
B	0	SER	-	cloning artifact	UNP P59641

- Molecule 2 is a protein called N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	D	6	Total	C	N	O	0	0	0
			49	35	6	8			

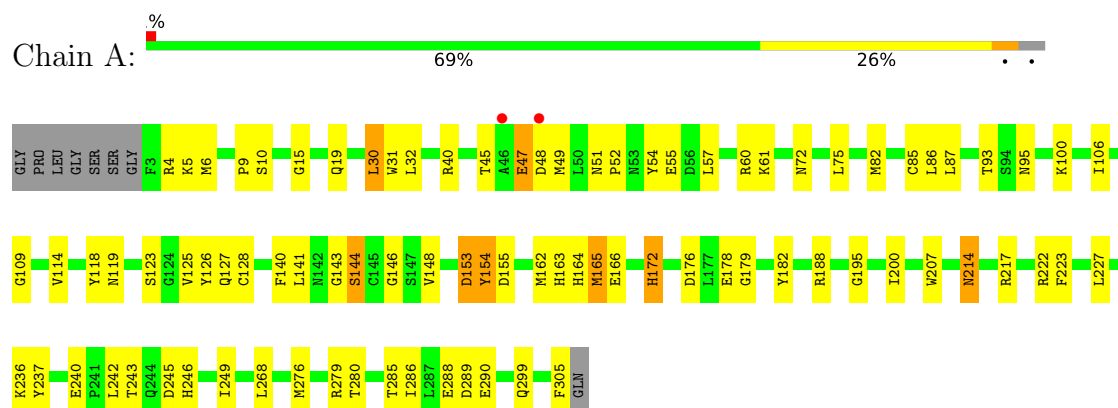
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total 170	O 170	0	0
3	B	150	Total 150	O 150	0	0
3	C	2	Total 2	O 2	0	0
3	D	4	Total 4	O 4	0	0

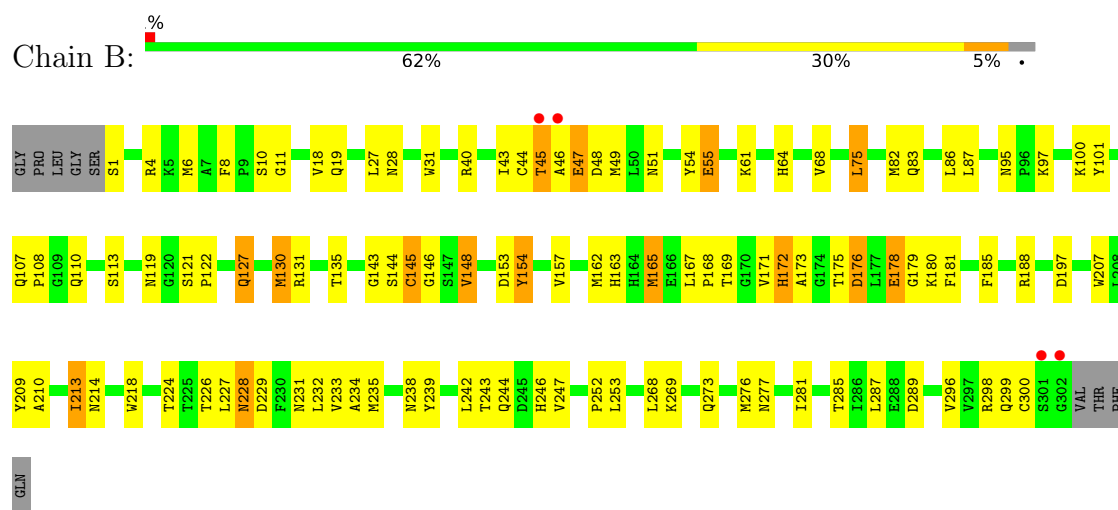
3 Residue-property plots

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.

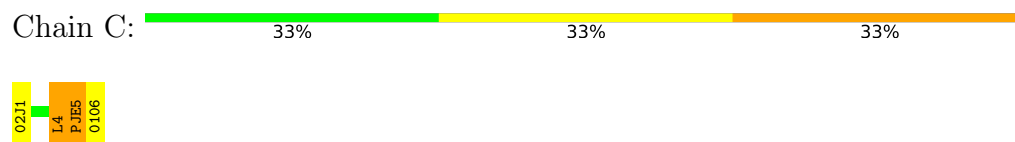
• Molecule 1: 3C-like proteinase



• Molecule 1: 3C-like proteinase

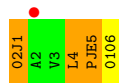


• Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE



- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE

Chain D: 17% 33% 17% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.06Å 95.70Å 67.59Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 95.0 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.230 0.194 , 0.230	Depositor DCC
R_{free} test set	1320 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5111	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: 02J, PJE, 010

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	0.60	3/2404 (0.1%)	1.00	12/3267 (0.4%)
1	B	0.63	3/2388 (0.1%)	1.02	12/3244 (0.4%)
2	C	0.45	0/19	0.73	0/25
2	D	0.32	0/19	0.87	0/25
All	All	0.61	6/4830 (0.1%)	1.01	24/6561 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	MET	SD-CE	-10.48	1.53	1.79
1	A	144	SER	N-CA	7.24	1.55	1.46
1	B	49	MET	C-O	-6.18	1.16	1.24
1	B	162	MET	C-N	-5.93	1.25	1.33
1	A	143	GLY	C-N	5.49	1.42	1.33
1	A	148	VAL	C-O	-5.04	1.19	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ASP	N-CA-C	-7.97	99.35	110.35
1	B	100	LYS	N-CA-C	-7.94	98.53	110.28
1	A	100	LYS	N-CA-C	-7.24	99.73	110.23
1	A	165	MET	N-CA-C	6.83	119.56	109.24
1	A	148	VAL	N-CA-C	6.76	118.53	108.46
1	B	130	MET	N-CA-C	-6.49	100.06	109.59
1	A	182	TYR	N-CA-C	-6.22	99.52	109.96
1	B	10	SER	N-CA-C	5.87	120.44	113.28
1	B	172	HIS	N-CA-C	5.81	119.02	109.72
1	B	146	GLY	N-CA-C	-5.75	107.85	114.69
1	B	148	VAL	N-CA-C	5.72	118.18	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	PHE	N-CA-C	5.70	118.15	109.95
1	B	176	ASP	N-CA-C	-5.64	101.61	110.36
1	B	226	THR	N-CA-C	-5.45	101.98	110.42
1	A	9	PRO	N-CA-C	-5.42	102.68	111.03
1	B	165	MET	N-CA-C	5.26	116.14	108.14
1	B	11	GLY	N-CA-C	5.21	118.94	112.64
1	A	195	GLY	N-CA-C	-5.20	104.55	112.51
1	B	178	GLU	N-CA-C	-5.20	106.62	113.17
1	A	217	ARG	N-CA-C	5.19	120.26	112.94
1	A	172	HIS	N-CA-C	5.17	117.67	109.50
1	A	10	SER	N-CA-C	5.11	119.50	113.16
1	B	218	TRP	N-CA-C	5.02	116.75	111.28
1	A	178	GLU	N-CA-C	-5.02	106.57	113.30

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	2351	0	2302	81	0
1	B	2336	0	2288	117	0
2	C	49	0	41	5	0
2	D	49	0	41	8	0
3	A	170	0	0	23	0
3	B	150	0	0	34	0
3	C	2	0	0	1	0
3	D	4	0	0	4	0
All	All	5111	0	4672	201	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 21.

All (201) 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:45:THR:HG21	1:B:47:GLU:OE1	1.45	1.15
1:A:6:MET:HE2	1:A:299:GLN:HG3	1.32	1.09
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.16	1.02
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.22	1.00
1:B:19:GLN:NE2	1:B:119:ASN:HD22	1.60	0.99
1:B:55:GLU:HB2	3:B:472:HOH:O	1.68	0.92
1:B:4:ARG:H	1:B:299:GLN:HE22	1.16	0.92
1:A:127:GLN:HB2	3:A:554:HOH:O	1.70	0.91
1:B:64:HIS:HE1	3:B:493:HOH:O	1.54	0.90
1:B:45:THR:CG2	1:B:47:GLU:OE1	2.22	0.88
1:B:135:THR:HG22	3:B:539:HOH:O	1.72	0.88
1:A:61:LYS:HE2	3:A:448:HOH:O	1.74	0.88
1:B:233:VAL:HG21	1:B:269:LYS:HE2	1.55	0.87
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.07	0.86
1:B:165:MET:HE2	1:B:181:PHE:CE2	2.09	0.86
1:B:231:ASN:HB3	1:B:235:MET:HE3	1.60	0.83
1:B:135:THR:HA	3:B:539:HOH:O	1.76	0.83
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.42	0.83
1:B:45:THR:HG23	1:B:46:ALA:N	1.93	0.82
1:B:51:ASN:HD22	1:B:188:ARG:HH12	1.28	0.81
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.11	0.81
1:A:5:LYS:HE2	1:A:127:GLN:HB3	1.63	0.80
1:B:19:GLN:HE21	1:B:119:ASN:HD22	1.25	0.80
1:B:224:THR:HG22	3:B:526:HOH:O	1.83	0.79
1:B:4:ARG:H	1:B:299:GLN:NE2	1.79	0.78
2:D:6:O10:C1	3:D:101:HOH:O	2.32	0.78
1:A:51:ASN:ND2	1:A:188:ARG:HE	1.82	0.77
1:B:68:VAL:HG23	1:B:75:LEU:HB2	1.68	0.75
1:A:5:LYS:HD3	3:A:547:HOH:O	1.86	0.75
1:B:165:MET:HE2	1:B:181:PHE:CZ	2.21	0.75
1:B:51:ASN:HD22	1:B:188:ARG:NH1	1.86	0.73
1:B:168:PRO:HG3	2:D:1:O2J:C	2.19	0.72
1:B:47:GLU:H	1:B:47:GLU:CD	1.97	0.72
1:A:165:MET:HG2	2:C:4:LEU:HD12	1.70	0.72
1:B:168:PRO:HG3	2:D:1:O2J:O	1.89	0.72
1:B:231:ASN:HB3	1:B:235:MET:CE	2.20	0.72
1:A:236:LYS:N	3:A:488:HOH:O	2.23	0.71
1:A:153:ASP:O	1:A:154:TYR:HB2	1.90	0.70
1:B:45:THR:C	3:B:494:HOH:O	2.34	0.69
1:B:110:GLN:HG2	3:B:512:HOH:O	1.93	0.68
1:B:244:GLN:O	1:B:247:VAL:HG22	1.94	0.68
1:B:107:GLN:NE2	3:B:535:HOH:O	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:HG3	3:B:470:HOH:O	1.93	0.67
1:A:155:ASP:HA	3:A:446:HOH:O	1.95	0.66
1:A:279:ARG:HB3	3:A:473:HOH:O	1.96	0.65
1:B:45:THR:CG2	1:B:47:GLU:CD	2.70	0.65
1:A:40:ARG:HA	1:A:87:LEU:HG	1.79	0.64
1:A:222:ARG:HG2	1:A:222:ARG:O	1.97	0.63
1:A:243:THR:H	1:A:246:HIS:HD2	1.47	0.63
1:B:45:THR:HG23	1:B:47:GLU:H	1.63	0.63
1:A:15:GLY:HA2	3:A:544:HOH:O	1.97	0.63
1:A:305:PHE:HB3	3:A:446:HOH:O	1.98	0.63
1:A:6:MET:CE	1:A:299:GLN:HG3	2.20	0.62
1:B:131:ARG:HD3	1:B:197:ASP:OD1	2.00	0.61
1:A:86:LEU:HG	1:A:179:GLY:CA	2.31	0.61
1:A:286:ILE:C	1:A:286:ILE:HD12	2.25	0.61
1:A:19:GLN:NE2	1:A:119:ASN:HD22	1.98	0.60
2:D:6:O10:H1	3:D:101:HOH:O	1.96	0.60
1:B:276:MET:HE3	1:B:281:ILE:HG13	1.82	0.60
1:B:285:THR:HB	3:B:456:HOH:O	2.02	0.59
1:B:167:LEU:HD21	1:B:185:PHE:CE2	2.36	0.59
1:B:209:TYR:O	1:B:213:ILE:HG23	2.02	0.59
1:B:45:THR:CG2	1:B:46:ALA:N	2.66	0.58
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.86	0.57
1:B:213:ILE:CD1	1:B:300:CYS:HB3	2.35	0.56
1:A:243:THR:H	1:A:246:HIS:CD2	2.23	0.56
1:B:40:ARG:HA	1:B:87:LEU:HG	1.86	0.56
1:B:46:ALA:N	3:B:494:HOH:O	2.37	0.56
1:B:169:THR:CG2	1:B:171:VAL:HG22	2.36	0.56
1:A:242:LEU:HD12	3:A:570:HOH:O	2.04	0.56
1:A:127:GLN:CB	3:A:554:HOH:O	2.41	0.56
1:B:51:ASN:HA	1:B:188:ARG:NH1	2.20	0.56
1:B:4:ARG:N	1:B:299:GLN:HE22	1.95	0.56
1:B:44:CYS:HB3	1:B:48:ASP:HB2	1.88	0.55
1:A:6:MET:C	3:A:554:HOH:O	2.49	0.55
1:B:131:ARG:HH22	1:B:289:ASP:CG	2.15	0.55
1:A:5:LYS:HZ2	1:B:4:ARG:HH12	1.55	0.55
1:B:269:LYS:NZ	3:B:462:HOH:O	2.34	0.55
1:A:55:GLU:H	1:A:55:GLU:CD	2.15	0.54
1:A:222:ARG:NH1	1:A:222:ARG:CG	2.68	0.54
1:B:45:THR:HG23	1:B:47:GLU:CD	2.31	0.54
1:B:169:THR:HG23	1:B:171:VAL:HG22	1.88	0.54
1:B:244:GLN:NE2	1:B:247:VAL:CG2	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:OG1	1:A:47:GLU:OE1	2.25	0.54
1:A:141:LEU:HD23	1:B:1:SER:HB2	1.88	0.54
1:B:180:LYS:HE3	3:B:543:HOH:O	2.07	0.53
1:A:240:GLU:HG3	3:A:511:HOH:O	2.09	0.53
1:A:118:TYR:CE1	1:A:144:SER:HB3	2.44	0.53
1:B:1:SER:HB3	3:B:430:HOH:O	2.09	0.53
1:B:61:LYS:NZ	3:B:426:HOH:O	2.32	0.53
1:A:60:ARG:NH1	3:A:448:HOH:O	2.42	0.53
1:A:86:LEU:HG	1:A:179:GLY:HA2	1.89	0.53
1:B:252:PRO:HD2	3:B:528:HOH:O	2.10	0.52
1:A:214:ASN:OD1	1:A:214:ASN:C	2.52	0.52
1:B:19:GLN:HE21	1:B:119:ASN:ND2	2.01	0.52
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.45	0.51
1:A:82:MET:HE3	3:A:495:HOH:O	2.09	0.51
1:B:229:ASP:HB3	3:B:462:HOH:O	2.11	0.51
1:B:298:ARG:NH2	3:B:437:HOH:O	2.44	0.51
1:A:236:LYS:HG2	1:A:237:TYR:CE1	2.45	0.51
1:B:238:ASN:HB3	3:B:550:HOH:O	2.10	0.51
1:A:276:MET:HE2	1:A:279:ARG:O	2.11	0.51
1:B:244:GLN:HA	1:B:247:VAL:HG22	1.92	0.51
1:B:110:GLN:CG	3:B:512:HOH:O	2.55	0.51
1:B:47:GLU:CD	1:B:47:GLU:N	2.67	0.50
1:A:222:ARG:HG2	1:A:222:ARG:NH1	2.15	0.50
1:A:52:PRO:HG2	1:A:54:TYR:CE1	2.47	0.50
1:B:131:ARG:CD	1:B:197:ASP:OD1	2.59	0.50
1:B:8:PHE:HD1	1:B:113:SER:HG	1.58	0.49
1:B:244:GLN:NE2	1:B:247:VAL:HG21	2.27	0.49
3:A:423:HOH:O	1:B:1:SER:HA	2.13	0.49
1:B:153:ASP:O	1:B:154:TYR:HB2	2.11	0.49
1:B:213:ILE:HD11	1:B:300:CYS:HB3	1.93	0.49
1:A:75:LEU:HD21	1:A:93:THR:HB	1.93	0.49
1:B:108:PRO:HA	1:B:130:MET:CG	2.43	0.49
1:A:126:TYR:CD2	1:B:6:MET:HE2	2.48	0.49
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.48	0.48
1:B:28:ASN:ND2	1:B:144:SER:O	2.45	0.48
1:A:164:HIS:O	2:C:5:PJE:N	2.46	0.48
1:B:31:TRP:CE2	1:B:95:ASN:HB2	2.48	0.48
1:B:244:GLN:O	1:B:247:VAL:CG2	2.61	0.48
1:A:51:ASN:HD22	1:A:188:ARG:HE	1.56	0.48
1:B:6:MET:HE3	1:B:299:GLN:NE2	2.29	0.47
1:B:97:LYS:NZ	3:B:522:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:N	3:B:526:HOH:O	2.29	0.47
1:A:31:TRP:CE2	1:A:75:LEU:HD11	2.49	0.47
1:B:180:LYS:CE	3:B:543:HOH:O	2.63	0.47
1:B:287:LEU:HD12	3:B:428:HOH:O	2.14	0.47
1:A:146:GLY:O	1:A:162:MET:HE2	2.14	0.47
1:B:64:HIS:CE1	3:B:493:HOH:O	2.43	0.47
1:A:19:GLN:HE21	1:A:119:ASN:HD22	1.63	0.46
1:B:144:SER:O	1:B:145:CYS:C	2.56	0.46
1:B:165:MET:CE	1:B:181:PHE:CE2	2.92	0.46
2:D:6:010:C	3:D:101:HOH:O	2.63	0.46
1:B:298:ARG:NH2	3:B:434:HOH:O	2.29	0.46
1:A:126:TYR:HE1	1:A:128:CYS:HG	1.62	0.46
1:A:240:GLU:HG2	3:A:481:HOH:O	2.15	0.46
1:A:286:ILE:HD11	1:A:288:GLU:OE2	2.15	0.46
1:B:45:THR:HG23	1:B:46:ALA:H	1.77	0.46
1:B:83:GLN:HG2	1:B:178:GLU:O	2.15	0.46
2:D:4:LEU:HD12	2:D:4:LEU:HA	1.81	0.46
1:A:240:GLU:CG	3:A:511:HOH:O	2.64	0.45
1:B:269:LYS:CE	3:B:462:HOH:O	2.65	0.45
1:A:166:GLU:HB2	2:C:5:PJE:C29	2.47	0.45
1:B:143:GLY:HA2	2:D:5:PJE:O	2.16	0.45
1:A:114:VAL:O	1:A:125:VAL:HA	2.16	0.45
1:A:285:THR:OG1	3:A:528:HOH:O	2.21	0.45
2:C:5:PJE:C	3:C:101:HOH:O	2.65	0.45
1:B:244:GLN:C	1:B:247:VAL:HG22	2.42	0.45
1:A:236:LYS:HG2	1:A:237:TYR:CD1	2.52	0.45
1:A:155:ASP:C	1:A:155:ASP:OD1	2.60	0.45
1:B:40:ARG:CZ	1:B:54:TYR:CD1	3.00	0.45
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.52	0.44
2:D:6:010:C6	3:D:101:HOH:O	2.60	0.44
1:B:101:TYR:HA	1:B:157:VAL:O	2.18	0.44
1:B:243:THR:H	1:B:246:HIS:CD2	2.34	0.44
1:A:214:ASN:OD1	1:A:214:ASN:O	2.35	0.44
1:A:245:ASP:O	1:A:249:ILE:HG13	2.17	0.44
1:A:45:THR:O	1:A:49:MET:HE2	2.17	0.44
1:A:72:ASN:ND2	3:A:552:HOH:O	2.50	0.44
1:A:276:MET:CE	1:A:280:THR:HA	2.47	0.44
1:B:176:ASP:HB2	3:B:408:HOH:O	2.16	0.44
1:B:46:ALA:HB3	1:B:47:GLU:OE2	2.18	0.44
1:B:227:LEU:HD21	1:B:242:LEU:O	2.18	0.44
1:B:45:THR:CG2	1:B:47:GLU:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG22	3:B:414:HOH:O	2.17	0.43
1:B:175:THR:HG22	1:B:181:PHE:HA	2.00	0.43
1:B:228:ASN:O	1:B:232:LEU:HG	2.18	0.43
1:A:30:LEU:HD11	1:A:32:LEU:HD11	1.99	0.43
1:A:48:ASP:OD2	1:A:57:LEU:HD11	2.19	0.43
1:B:45:THR:HG23	1:B:47:GLU:OE2	2.19	0.43
1:B:213:ILE:HG13	1:B:214:ASN:N	2.32	0.43
1:A:286:ILE:HD12	1:A:286:ILE:O	2.18	0.43
1:B:234:ALA:O	1:B:239:TYR:HB2	2.18	0.43
1:B:68:VAL:HG23	1:B:75:LEU:CB	2.44	0.43
1:B:269:LYS:HE3	3:B:462:HOH:O	2.19	0.43
1:B:277:ASN:HA	3:B:549:HOH:O	2.18	0.43
1:A:127:GLN:HG2	3:A:413:HOH:O	2.18	0.42
1:A:240:GLU:CG	3:A:481:HOH:O	2.67	0.42
1:A:126:TYR:HE1	1:A:128:CYS:SG	2.43	0.42
1:B:269:LYS:O	1:B:273:GLN:HG3	2.19	0.42
1:B:207:TRP:O	1:B:210:ALA:HB3	2.19	0.42
1:B:253:LEU:HD21	1:B:296:VAL:HG12	2.02	0.42
1:A:40:ARG:HG2	1:A:85:CYS:O	2.20	0.42
1:A:49:MET:HE1	2:C:6:010:H2	2.02	0.42
1:B:121:SER:HA	1:B:122:PRO:HD3	1.82	0.42
1:A:141:LEU:O	1:A:144:SER:OG	2.34	0.42
1:B:27:LEU:C	1:B:27:LEU:HD12	2.44	0.42
1:B:86:LEU:HG	1:B:179:GLY:HA2	2.02	0.42
1:A:140:PHE:HB3	1:A:144:SER:OG	2.20	0.41
1:A:153:ASP:OD1	1:A:153:ASP:N	2.53	0.41
1:A:207:TRP:NE1	3:A:561:HOH:O	2.38	0.41
1:B:40:ARG:O	1:B:43:ILE:HG12	2.19	0.41
1:A:5:LYS:NZ	1:A:290:GLU:OE1	2.54	0.41
1:B:173:ALA:HB2	3:B:539:HOH:O	2.21	0.41
1:A:240:GLU:CB	3:A:481:HOH:O	2.68	0.40
1:B:18:VAL:HA	3:B:500:HOH:O	2.22	0.40
1:B:82:MET:HG2	3:B:527:HOH:O	2.21	0.40
1:B:108:PRO:HA	1:B:130:MET:HG3	2.02	0.40
1:B:113:SER:OG	1:B:127:GLN:NE2	2.55	0.40
1:A:30:LEU:CD1	1:A:32:LEU:HD11	2.51	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	301/311 (97%)	287 (95%)	13 (4%)	1 (0%)	36	46
1	B	300/311 (96%)	289 (96%)	9 (3%)	2 (1%)	18	23
2	C	3/6 (50%)	3 (100%)	0	0	100	100
2	D	3/6 (50%)	3 (100%)	0	0	100	100
All	All	607/634 (96%)	582 (96%)	22 (4%)	3 (0%)	24	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	CYS
1	A	154	TYR
1	B	154	TYR

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	261/266 (98%)	251 (96%)	10 (4%)	29	44
1	B	259/266 (97%)	251 (97%)	8 (3%)	35	52
2	C	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	D	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	524/536 (98%)	504 (96%)	20 (4%)	29	44

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	30	LEU
1	A	47	GLU
1	A	106	ILE
1	A	123	SER
1	A	153	ASP
1	A	214	ASN
1	A	227	LEU
1	A	268	LEU
1	A	289	ASP
1	B	45	THR
1	B	47	GLU
1	B	55	GLU
1	B	75	LEU
1	B	127	GLN
1	B	213	ILE
1	B	228	ASN
1	B	268	LEU
2	C	4	LEU
2	D	4	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	51	ASN
1	A	119	ASN
1	A	228	ASN
1	A	246	HIS
1	A	277	ASN
1	B	19	GLN
1	B	51	ASN
1	B	69	GLN
1	B	74	GLN
1	B	127	GLN
1	B	142	ASN
1	B	228	ASN
1	B	244	GLN
1	B	246	HIS
1	B	299	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PJE	D	5	2	11,13,14	2.04	1 (9%)	11,16,18	7.31	6 (54%)
2	02J	C	1	2	8,8,9	5.59	4 (50%)	9,10,12	7.90	6 (66%)
2	02J	D	1	2	8,8,9	7.31	4 (50%)	9,10,12	6.69	6 (66%)
2	PJE	C	5	2	11,13,14	2.15	2 (18%)	11,16,18	6.69	6 (54%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PJE	D	5	2	-	5/7/18/19	0/1/1/1
2	02J	C	1	2	-	0/1/2/4	0/1/1/1
2	02J	D	1	2	-	1/1/2/4	0/1/1/1
2	PJE	C	5	2	-	3/7/18/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	02J	CA-N	18.15	1.57	1.31
2	C	1	02J	C4-CA	14.47	1.68	1.41
2	D	1	02J	C4-CA	-9.05	1.25	1.41
2	C	5	PJE	C21-C20	6.17	1.56	1.33
2	D	5	PJE	C21-C20	6.17	1.56	1.33
2	C	1	02J	CA-N	-4.77	1.24	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	02J	C-CA	2.92	1.56	1.45
2	C	5	PJE	C21-C	2.87	1.52	1.44
2	D	1	02J	C-CA	2.60	1.55	1.45
2	D	1	02J	O1-N	2.24	1.46	1.42
2	C	1	02J	O1-N	2.13	1.46	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	PJE	CA-C20-C21	-17.26	98.01	124.42
2	C	1	02J	O1-N-CA	16.20	118.39	105.65
2	C	5	PJE	CA-C20-C21	-15.81	100.23	124.42
2	C	1	02J	C4-CA-N	-14.62	97.82	111.19
2	D	1	02J	C-CA-N	-13.41	94.94	118.78
2	C	5	PJE	C25-CA-C20	-10.90	94.32	110.99
2	D	5	PJE	C25-CA-C20	-10.52	94.90	110.99
2	D	5	PJE	C25-CA-N	9.24	130.67	110.48
2	D	1	02J	CA-C4-C5	8.91	116.13	105.23
2	D	1	02J	C4-CA-N	-8.75	103.20	111.19
2	C	5	PJE	C25-CA-N	7.89	127.72	110.48
2	D	5	PJE	O-C-C21	7.27	148.80	125.61
2	C	5	PJE	C20-CA-N	6.35	123.22	110.24
2	C	1	02J	O1-C5-C6	5.56	123.54	115.89
2	D	1	02J	O1-C5-C6	5.49	123.44	115.89
2	D	5	PJE	C20-CA-N	5.13	120.72	110.24
2	D	1	02J	C6-C5-C4	-4.73	125.89	134.05
2	C	1	02J	C6-C5-C4	-4.63	126.05	134.05
2	C	1	02J	C-CA-N	4.47	126.72	118.78
2	C	1	02J	C5-O1-N	-3.36	105.05	108.47
2	D	1	02J	C5-O1-N	-3.35	105.05	108.47
2	C	5	PJE	O8-C29-N6	-3.17	121.33	125.76
2	D	5	PJE	O8-C29-N6	-3.15	121.36	125.76
2	C	5	PJE	O-C-C21	2.61	133.93	125.61

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	02J	O-C-CA-C4
2	C	5	PJE	O-C-C21-C20
2	D	5	PJE	C26-C25-CA-N
2	D	5	PJE	O-C-C21-C20

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Mol	Chain	Res	Type	Atoms
2	D	5	PJE	CA-C20-C21-C
2	C	5	PJE	CA-C25-C26-C27
2	D	5	PJE	CA-C25-C26-C27
2	C	5	PJE	CA-C20-C21-C
2	D	5	PJE	CA-C25-C26-C29

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5	PJE	1	0
2	D	1	02J	2	0
2	C	5	PJE	3	0

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	303/311 (97%)	-0.20	2 (0%) 84 85	16, 29, 50, 68	0
1	B	302/311 (97%)	-0.16	4 (1%) 75 76	17, 30, 46, 64	0
2	C	3/6 (50%)	0.84	0 100 100	52, 52, 54, 59	0
2	D	3/6 (50%)	1.67	1 (33%) 1 1	49, 49, 50, 57	0
All	All	611/634 (96%)	-0.16	7 (1%) 78 79	16, 30, 51, 68	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	SER	3.1
1	A	46	ALA	2.8
1	B	45	THR	2.6
2	D	2	ALA	2.5
1	B	302	GLY	2.2
1	B	46	ALA	2.1
1	A	48	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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(Å ²)	Q<0.9
2	02J	C	1	8/9	0.66	0.21	65,68,69,70	0
2	02J	D	1	8/9	0.71	0.19	65,69,70,70	0
2	PJE	C	5	13/14	0.88	0.14	52,53,65,66	0
2	PJE	D	5	13/14	0.89	0.13	50,52,60,62	0

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.