



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:51 PM UTC

PDB ID : 1UK2 / pdb_00001uk2
Title : Crystal structure of SARS Coronavirus Main Proteinase (3CLpro) At pH8.0
Authors : Yang, H.; Yang, M.; Liu, Y.; Bartlam, M.; Ding, Y.; Lou, Z.; Sun, L.; Zhou, Z.; Ye, S.; Anand, K.; Pang, H.; Gao, G.F.; Hilgenfeld, R.; Rao, Z.
Deposited on : 2003-08-14
Resolution : 2.20 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

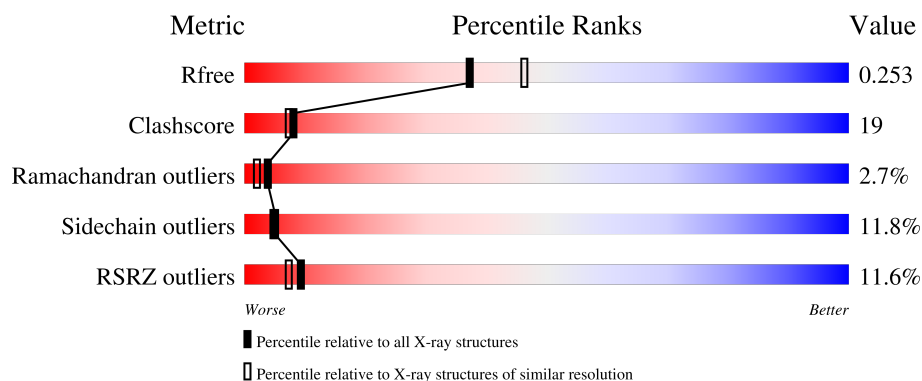
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	306	12% 62% 25% 10% ..
1	B	306	10% 59% 30% 7% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4752 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	302	Total	C	N	O	S	0	0	0
			2336	1476	400	438	22			
1	B	302	Total	C	N	O	S	0	0	0
			2336	1476	400	438	22			

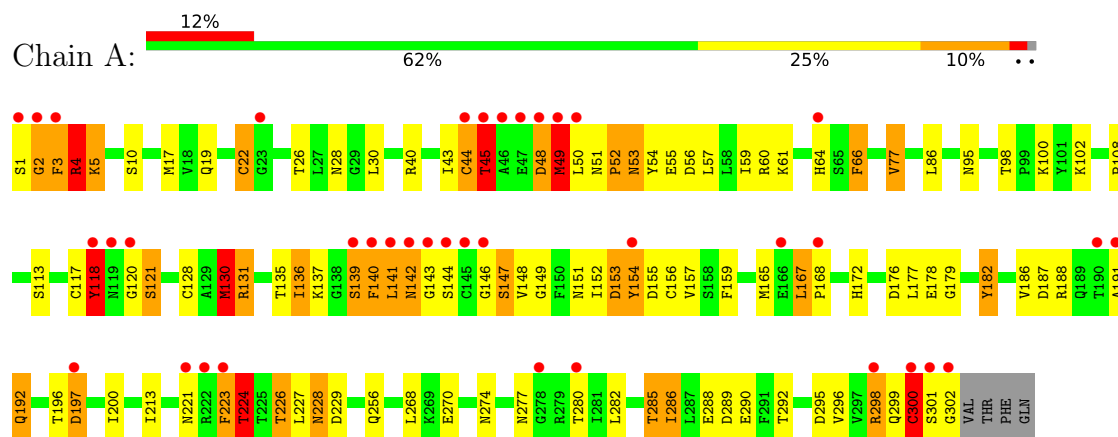
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	39	Total	O	0	0
			39	39		

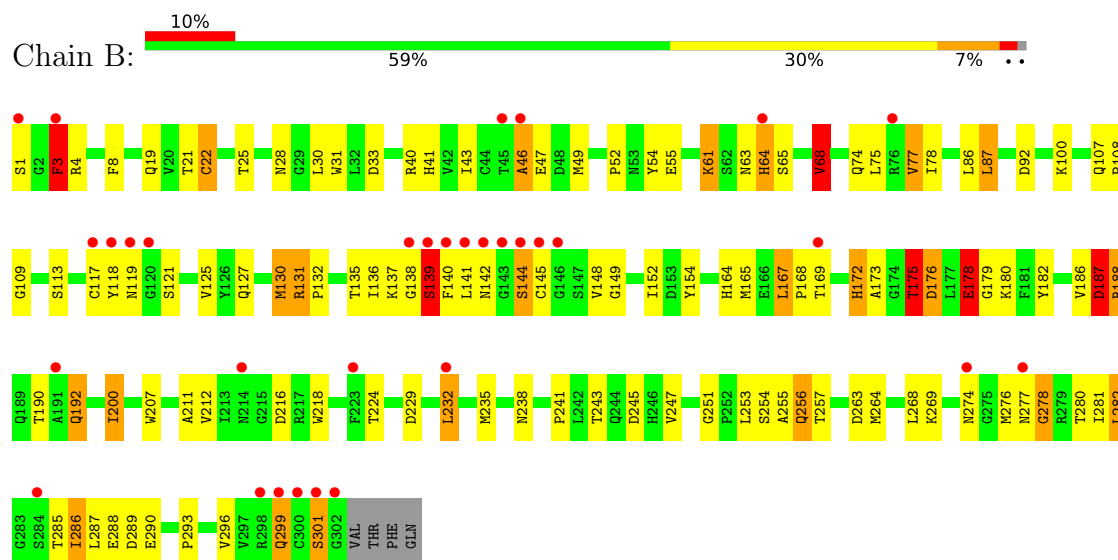
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.48Å 97.43Å 67.53Å 90.00° 101.70° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 93.8 (50.00-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.253 0.225 , 0.253	Depositor DCC
R_{free} test set	1551 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4752	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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	1.17	4/2388 (0.2%)	1.45	28/3244 (0.9%)
1	B	1.13	5/2388 (0.2%)	1.40	37/3244 (1.1%)
All	All	1.15	9/4776 (0.2%)	1.43	65/6488 (1.0%)

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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	PHE	CA-C	7.43	1.61	1.53
1	A	213	ILE	CA-CB	6.22	1.62	1.54
1	A	224	THR	CA-CB	5.85	1.63	1.53
1	A	17	MET	SD-CE	-5.84	1.65	1.79
1	B	264	MET	SD-CE	-5.62	1.65	1.79
1	B	212	VAL	CA-CB	5.39	1.60	1.54
1	B	130	MET	SD-CE	-5.26	1.66	1.79
1	B	125	VAL	CA-CB	5.19	1.62	1.54
1	B	68	VAL	CA-CB	5.19	1.60	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SER	N-CA-C	-12.75	91.61	110.48
1	A	52	PRO	N-CA-C	9.60	126.11	111.14
1	A	2	GLY	N-CA-C	8.97	121.63	110.96
1	A	5	LYS	N-CA-C	-8.41	96.39	109.76
1	B	178	GLU	N-CA-C	-8.34	102.66	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	LYS	N-CA-C	-8.26	98.25	110.23
1	B	144	SER	N-CA-C	8.09	121.60	108.41
1	A	146	GLY	N-CA-C	-8.09	103.51	115.72
1	B	100	LYS	N-CA-C	-7.83	98.22	109.96
1	B	190	THR	N-CA-C	-7.80	96.97	109.76
1	A	301	SER	N-CA-C	-7.79	94.20	110.80
1	B	3	PHE	N-CA-C	7.67	121.73	108.76
1	A	178	GLU	N-CA-C	-7.64	103.07	113.30
1	B	301	SER	N-CA-C	7.33	120.74	108.13
1	B	172	HIS	N-CA-C	7.11	121.62	110.17
1	B	52	PRO	N-CA-C	6.79	122.94	111.32
1	A	165	MET	N-CA-C	6.77	120.55	109.85
1	A	139	SER	CA-C-N	-6.75	112.82	122.94
1	A	139	SER	C-N-CA	-6.75	112.82	122.94
1	B	263	ASP	N-CA-C	-6.68	103.93	111.14
1	A	224	THR	N-CA-C	6.66	124.99	110.80
1	A	182	TYR	N-CA-C	-6.61	98.48	109.46
1	B	299	GLN	N-CA-C	6.58	119.00	111.11
1	A	44	CYS	CB-CA-C	-6.50	99.14	109.80
1	A	285	THR	N-CA-C	-6.42	105.08	113.17
1	B	61	LYS	N-CA-C	6.41	119.98	109.72
1	B	87	LEU	N-CA-C	-6.21	99.58	109.76
1	A	130	MET	N-CA-C	-6.18	99.94	109.76
1	A	140	PHE	N-CA-C	6.13	119.39	109.40
1	A	141	LEU	CA-CB-CG	6.07	137.54	116.30
1	A	66	PHE	N-CA-C	6.04	118.50	109.25
1	B	218	TRP	N-CA-C	6.00	118.61	111.71
1	B	224	THR	N-CA-C	-5.99	100.67	109.18
1	B	175	THR	N-CA-CB	-5.98	101.15	111.55
1	B	256	GLN	N-CA-C	-5.96	98.10	110.80
1	B	130	MET	N-CA-C	-5.93	101.07	109.96
1	B	241	PRO	N-CA-C	-5.85	101.91	111.68
1	B	188	ARG	N-CA-C	5.80	118.51	109.52
1	B	47	GLU	N-CA-C	-5.79	104.89	111.14
1	B	145	CYS	N-CA-CB	-5.74	101.53	109.97
1	B	182	TYR	N-CA-C	-5.74	99.17	108.52
1	B	139	SER	N-CA-C	5.73	118.49	108.52
1	B	144	SER	CA-C-N	5.69	128.96	120.87
1	B	144	SER	C-N-CA	5.69	128.96	120.87
1	A	57	LEU	N-CA-C	-5.65	105.12	111.28
1	B	148	VAL	N-CA-C	5.62	118.02	108.86
1	B	46	ALA	N-CA-C	-5.58	98.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	GLN	N-CA-C	5.57	119.00	110.20
1	B	285	THR	N-CA-C	-5.57	106.26	113.16
1	A	10	SER	N-CA-C	5.56	120.06	113.16
1	B	33	ASP	CB-CA-C	-5.48	110.23	116.54
1	B	176	ASP	N-CA-C	-5.48	101.87	110.36
1	B	280	THR	N-CA-C	5.48	118.50	109.85
1	A	142	ASN	N-CA-C	-5.36	100.92	109.23
1	B	144	SER	CA-C-O	5.25	125.92	120.30
1	B	121	SER	N-CA-C	5.23	116.99	109.04
1	B	192	GLN	N-CA-C	-5.22	101.36	109.24
1	B	54	TYR	N-CA-C	5.18	117.67	111.71
1	B	55	GLU	N-CA-C	-5.17	105.64	111.28
1	A	176	ASP	N-CA-C	-5.14	101.77	109.79
1	A	292	THR	N-CA-C	5.13	117.56	110.07
1	A	155	ASP	N-CA-C	-5.11	105.95	113.61
1	A	45	THR	N-CA-C	-5.09	103.76	110.43
1	A	121	SER	CA-C-N	5.08	125.88	119.98
1	A	121	SER	C-N-CA	5.08	125.88	119.98

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	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	2336	0	2289	110	0
1	B	2336	0	2289	96	0
2	A	41	0	0	5	0
2	B	39	0	0	1	0
All	All	4752	0	4578	180	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 19.

All (180) 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:226:THR:HG22	1:A:229:ASP:H	1.17	1.10
1:A:4:ARG:HH11	1:B:138:GLY:HA2	1.14	1.08
1:A:139:SER:HB2	1:B:4:ARG:H	1.23	1.03
1:A:139:SER:HB2	1:B:4:ARG:N	1.73	1.02
1:A:45:THR:HG23	1:A:48:ASP:H	1.31	0.93
1:A:22:CYS:SG	1:A:61:LYS:NZ	2.43	0.90
1:A:139:SER:CB	1:B:4:ARG:HB3	2.06	0.85
1:A:4:ARG:NH1	1:B:138:GLY:HA2	1.92	0.85
1:A:1:SER:HB3	2:A:331:HOH:O	1.76	0.84
1:A:2:GLY:O	1:A:282:LEU:HD22	1.77	0.84
1:A:152:ILE:HD12	1:A:157:VAL:HG22	1.59	0.83
1:B:229:ASP:OD2	1:B:269:LYS:NZ	2.11	0.82
1:A:4:ARG:HG3	1:B:138:GLY:HA2	1.62	0.81
1:A:4:ARG:HH11	1:B:138:GLY:CA	1.93	0.81
1:B:109:GLY:HA2	1:B:200:ILE:HD12	1.66	0.78
1:B:139:SER:HA	1:B:172:HIS:HE1	1.49	0.77
1:A:108:PRO:HA	1:A:130:MET:HG2	1.67	0.77
1:B:64:HIS:CD2	1:B:64:HIS:H	2.04	0.76
1:B:269:LYS:HD3	2:B:343:HOH:O	1.86	0.75
1:A:226:THR:CG2	1:A:229:ASP:H	1.98	0.75
1:B:140:PHE:C	1:B:142:ASN:H	1.94	0.75
1:B:68:VAL:CG2	1:B:75:LEU:HB2	2.18	0.73
1:A:4:ARG:NH1	1:B:138:GLY:CA	2.52	0.72
1:B:3:PHE:HB2	1:B:282:LEU:HG	1.71	0.72
1:A:137:LYS:NZ	1:A:197:ASP:OD1	2.23	0.72
1:A:118:TYR:HA	1:A:143:GLY:O	1.91	0.70
1:A:139:SER:HB3	1:B:4:ARG:HB3	1.73	0.70
1:A:186:VAL:H	1:A:192:GLN:HE22	1.40	0.70
1:B:164:HIS:CD2	1:B:175:THR:HB	2.26	0.69
1:A:139:SER:HB2	1:B:4:ARG:CB	2.23	0.69
1:B:164:HIS:NE2	1:B:175:THR:HB	2.07	0.68
1:A:139:SER:HB2	1:B:4:ARG:HB3	1.74	0.68
1:A:139:SER:C	1:A:140:PHE:HD1	2.02	0.68
1:A:118:TYR:CG	1:A:118:TYR:O	2.48	0.67
1:A:139:SER:O	1:A:140:PHE:HD1	1.79	0.66
1:A:224:THR:HG22	2:A:329:HOH:O	1.95	0.66
1:B:64:HIS:CD2	1:B:64:HIS:N	2.62	0.66
1:A:55:GLU:O	1:A:59:ILE:HG12	1.96	0.66
1:A:300:CYS:O	1:A:300:CYS:SG	2.54	0.66
1:A:224:THR:CG2	2:A:329:HOH:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:CYS:SG	1:A:61:LYS:CE	2.86	0.64
1:A:295:ASP:OD1	1:A:298:ARG:NH2	2.31	0.64
1:A:118:TYR:O	1:A:118:TYR:CD1	2.51	0.63
1:B:86:LEU:HG	1:B:179:GLY:HA2	1.80	0.63
1:B:135:THR:C	1:B:136:ILE:HD12	2.24	0.63
1:A:277:ASN:HD22	1:A:277:ASN:H	1.44	0.63
1:A:144:SER:O	1:A:147:SER:HB3	1.98	0.63
1:A:52:PRO:O	1:A:188:ARG:NH2	2.31	0.62
1:B:277:ASN:O	1:B:278:GLY:O	2.18	0.62
1:A:28:ASN:ND2	1:A:117:CYS:HB2	2.16	0.61
1:A:139:SER:HB2	1:B:4:ARG:CA	2.30	0.61
1:B:276:MET:HE3	1:B:281:ILE:HG13	1.82	0.60
1:A:4:ARG:NH1	1:B:138:GLY:N	2.49	0.60
1:A:4:ARG:HH12	1:B:137:LYS:C	2.08	0.60
1:A:226:THR:HG21	1:A:229:ASP:OD1	2.00	0.60
1:B:186:VAL:H	1:B:192:GLN:HE22	1.48	0.60
1:A:286:ILE:HD13	2:A:322:HOH:O	2.01	0.60
1:B:286:ILE:N	1:B:286:ILE:HD13	2.17	0.60
1:A:299:GLN:HB3	1:B:141:LEU:CD1	2.32	0.59
1:A:102:LYS:HE3	1:A:156:CYS:SG	2.43	0.59
1:B:175:THR:CG2	1:B:176:ASP:O	2.50	0.59
1:A:152:ILE:CD1	1:A:157:VAL:HG22	2.31	0.58
1:A:86:LEU:HG	1:A:179:GLY:HA2	1.85	0.58
1:A:135:THR:C	1:A:136:ILE:HD12	2.28	0.58
1:A:139:SER:O	1:A:140:PHE:CD1	2.56	0.58
1:B:22:CYS:SG	1:B:61:LYS:CE	2.92	0.58
1:A:53:ASN:HD22	1:A:53:ASN:C	2.10	0.57
1:A:277:ASN:HD22	1:A:277:ASN:N	1.97	0.57
1:B:43:ILE:HG22	1:B:61:LYS:HE2	1.86	0.57
1:A:226:THR:HG22	1:A:229:ASP:N	2.02	0.57
1:A:4:ARG:HH12	1:B:138:GLY:N	2.03	0.56
1:B:8:PHE:HB3	1:B:152:ILE:HD12	1.86	0.56
1:A:4:ARG:NH1	1:B:137:LYS:C	2.64	0.56
1:A:191:ALA:O	1:A:192:GLN:O	2.24	0.55
1:B:22:CYS:SG	1:B:61:LYS:HE2	2.47	0.55
1:B:132:PRO:HD3	1:B:200:ILE:HD11	1.88	0.55
1:B:277:ASN:O	1:B:278:GLY:C	2.49	0.55
1:B:68:VAL:HG23	1:B:75:LEU:HB2	1.89	0.54
1:A:22:CYS:SG	1:A:61:LYS:HE3	2.47	0.54
1:B:286:ILE:HD13	1:B:286:ILE:H	1.72	0.54
1:B:22:CYS:SG	1:B:61:LYS:NZ	2.78	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:THR:HG22	1:B:176:ASP:O	2.08	0.54
1:B:78:ILE:O	1:B:78:ILE:HG22	2.07	0.54
1:A:302:GLY:O	1:B:118:TYR:CZ	2.62	0.53
1:A:19:GLN:HB3	1:A:120:GLY:HA3	1.90	0.53
1:A:28:ASN:CG	1:A:117:CYS:HB2	2.34	0.53
1:A:130:MET:HE1	1:A:182:TYR:CD1	2.43	0.53
1:A:139:SER:CB	1:B:4:ARG:H	2.09	0.52
1:B:167:LEU:HD21	1:B:173:ALA:HB2	1.92	0.52
1:A:153:ASP:O	1:A:154:TYR:HB2	2.10	0.52
1:A:40:ARG:O	1:A:43:ILE:HG12	2.09	0.52
1:A:151:ASN:O	1:A:152:ILE:HD13	2.10	0.52
1:B:288:GLU:OE1	1:B:290:GLU:HB2	2.10	0.51
1:A:49:MET:HA	1:A:49:MET:HE2	1.91	0.51
1:A:48:ASP:O	1:A:50:LEU:N	2.43	0.51
1:B:139:SER:HA	1:B:172:HIS:CE1	2.37	0.51
1:B:255:ALA:C	1:B:256:GLN:O	2.49	0.51
1:A:140:PHE:O	1:B:1:SER:OG	2.23	0.51
1:B:119:ASN:H	1:B:144:SER:CB	2.24	0.51
1:B:178:GLU:HG2	1:B:180:LYS:NZ	2.26	0.51
1:B:136:ILE:HD12	1:B:136:ILE:N	2.26	0.50
1:B:164:HIS:HE2	1:B:175:THR:HB	1.74	0.50
1:B:86:LEU:HG	1:B:179:GLY:CA	2.41	0.50
1:A:139:SER:CB	1:B:4:ARG:CB	2.81	0.50
1:A:131:ARG:NH2	1:A:289:ASP:OD1	2.45	0.50
1:B:140:PHE:C	1:B:142:ASN:N	2.63	0.50
1:A:277:ASN:N	1:A:277:ASN:ND2	2.60	0.50
1:A:3:PHE:CZ	1:A:288:GLU:HG2	2.47	0.49
1:A:131:ARG:HH21	1:A:200:ILE:HG13	1.77	0.49
1:A:51:ASN:HD22	1:A:188:ARG:HE	1.59	0.49
1:B:131:ARG:HH22	1:B:289:ASP:CG	2.21	0.49
1:A:226:THR:CG2	1:A:229:ASP:OD1	2.60	0.49
1:A:3:PHE:N	1:B:139:SER:HB3	2.28	0.48
1:A:131:ARG:HH11	1:A:137:LYS:NZ	2.11	0.48
1:B:243:THR:OG1	1:B:245:ASP:OD1	2.29	0.48
1:A:139:SER:OG	1:B:299:GLN:NE2	2.47	0.47
1:A:2:GLY:HA3	1:B:139:SER:CB	2.44	0.47
1:B:63:ASN:O	1:B:77:VAL:CG1	2.63	0.47
1:A:44:CYS:SG	1:A:54:TYR:CE2	3.07	0.47
1:A:142:ASN:HB2	2:A:338:HOH:O	2.14	0.47
1:A:43:ILE:HG22	1:A:61:LYS:HE3	1.96	0.47
1:A:140:PHE:HB2	1:A:172:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASN:OD1	1:A:117:CYS:HB3	2.15	0.46
1:B:175:THR:HG23	1:B:176:ASP:O	2.15	0.46
1:A:270:GLU:HG3	1:A:274:ASN:OD1	2.16	0.46
1:B:68:VAL:HG22	1:B:75:LEU:HB2	1.96	0.46
1:B:276:MET:CE	1:B:281:ILE:HG13	2.46	0.46
1:B:132:PRO:HD3	1:B:200:ILE:CD1	2.45	0.46
1:A:118:TYR:CD1	1:A:118:TYR:C	2.93	0.45
1:B:136:ILE:HG22	1:B:138:GLY:H	1.82	0.45
1:A:28:ASN:OD1	1:A:120:GLY:N	2.48	0.45
1:A:44:CYS:SG	1:A:54:TYR:HE2	2.40	0.45
1:A:187:ASP:C	1:A:188:ARG:CG	2.89	0.45
1:B:251:GLY:O	1:B:254:SER:N	2.49	0.45
1:A:128:CYS:HA	1:A:290:GLU:OE1	2.17	0.45
1:A:139:SER:C	1:A:140:PHE:CD1	2.90	0.45
1:B:63:ASN:HB3	1:B:77:VAL:O	2.17	0.45
1:B:253:LEU:HD21	1:B:296:VAL:HG12	1.99	0.45
1:A:51:ASN:ND2	1:A:188:ARG:HH21	2.14	0.45
1:A:86:LEU:HG	1:A:179:GLY:CA	2.47	0.44
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.17	0.44
1:A:3:PHE:H	1:B:139:SER:HB3	1.81	0.44
1:B:19:GLN:O	1:B:68:VAL:HA	2.18	0.44
1:A:221:ASN:HB3	1:A:270:GLU:OE1	2.18	0.43
1:B:117:CYS:O	1:B:144:SER:HB3	2.17	0.43
1:B:127:GLN:HE21	1:B:127:GLN:HA	1.82	0.43
1:B:140:PHE:O	1:B:142:ASN:N	2.48	0.43
1:A:28:ASN:CG	1:A:117:CYS:CB	2.91	0.43
1:A:48:ASP:O	1:A:49:MET:C	2.61	0.43
1:A:66:PHE:HB2	1:A:77:VAL:HG11	2.01	0.43
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.31	0.43
1:A:221:ASN:C	1:A:223:PHE:H	2.26	0.43
1:A:131:ARG:HH11	1:A:137:LYS:HZ2	1.67	0.43
1:A:148:VAL:HG21	1:A:159:PHE:CD1	2.54	0.43
1:B:21:THR:HA	1:B:25:THR:O	2.20	0.42
1:B:31:TRP:CZ2	1:B:75:LEU:HD21	2.55	0.42
1:B:108:PRO:CD	1:B:130:MET:HE3	2.50	0.42
1:B:211:ALA:HA	1:B:282:LEU:HD13	2.01	0.42
1:A:4:ARG:HH11	1:A:4:ARG:HG3	1.85	0.42
1:A:113:SER:O	1:A:149:GLY:HA2	2.20	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD13	1.88	0.41
1:A:296:VAL:O	1:A:300:CYS:HB3	2.20	0.41
1:B:113:SER:O	1:B:149:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:VAL:N	1:B:192:GLN:HE22	2.17	0.41
1:A:2:GLY:HA3	1:B:139:SER:HB3	2.03	0.41
1:A:196:THR:O	1:A:197:ASP:C	2.62	0.41
1:B:108:PRO:N	1:B:130:MET:HE3	2.35	0.41
1:B:41:HIS:HE1	1:B:164:HIS:O	2.03	0.41
1:A:226:THR:CG2	1:A:228:ASN:HB3	2.51	0.41
1:B:107:GLN:C	1:B:130:MET:CE	2.94	0.41
1:B:167:LEU:O	1:B:169:THR:N	2.54	0.41
1:B:253:LEU:HD21	1:B:296:VAL:CG1	2.51	0.41
1:B:137:LYS:O	1:B:139:SER:N	2.54	0.41
1:B:232:LEU:HD12	1:B:232:LEU:O	2.20	0.40
1:B:167:LEU:CD2	1:B:173:ALA:HB2	2.51	0.40
1:B:207:TRP:CE2	1:B:288:GLU:HB3	2.56	0.40
1:A:60:ARG:HH11	1:A:60:ARG:HD3	1.77	0.40
1:B:40:ARG:NE	1:B:187:ASP:OD1	2.38	0.40
1:A:3:PHE:CE2	1:A:288:GLU:HG2	2.57	0.40
1:A:167:LEU:HB3	1:A:168:PRO:HD2	2.04	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	300/306 (98%)	271 (90%)	19 (6%)	10 (3%)	3	1
1	B	300/306 (98%)	275 (92%)	19 (6%)	6 (2%)	6	4
All	All	600/612 (98%)	546 (91%)	38 (6%)	16 (3%)	4	2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	GLN

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Mol	Chain	Res	Type
1	A	300	CYS
1	A	49	MET
1	A	141	LEU
1	A	197	ASP
1	A	224	THR
1	B	278	GLY
1	A	3	PHE
1	A	154	TYR
1	B	187	ASP
1	B	257	THR
1	B	46	ALA
1	A	4	ARG
1	A	118	TYR
1	B	154	TYR
1	B	168	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/263 (98%)	230 (89%)	29 (11%)	6	5
1	B	259/263 (98%)	227 (88%)	32 (12%)	4	4
All	All	518/526 (98%)	457 (88%)	61 (12%)	5	5

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	LYS
1	A	22	CYS
1	A	26	THR
1	A	30	LEU
1	A	45	THR
1	A	48	ASP
1	A	49	MET

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Mol	Chain	Res	Type
1	A	53	ASN
1	A	56	ASP
1	A	64	HIS
1	A	77	VAL
1	A	118	TYR
1	A	121	SER
1	A	130	MET
1	A	131	ARG
1	A	136	ILE
1	A	153	ASP
1	A	167	LEU
1	A	226	THR
1	A	227	LEU
1	A	228	ASN
1	A	256	GLN
1	A	268	LEU
1	A	280	THR
1	A	285	THR
1	A	286	ILE
1	A	298	ARG
1	A	300	CYS
1	B	3	PHE
1	B	22	CYS
1	B	28	ASN
1	B	30	LEU
1	B	49	MET
1	B	64	HIS
1	B	65	SER
1	B	68	VAL
1	B	77	VAL
1	B	87	LEU
1	B	92	ASP
1	B	131	ARG
1	B	139	SER
1	B	165	MET
1	B	167	LEU
1	B	175	THR
1	B	178	GLU
1	B	187	ASP
1	B	188	ARG
1	B	200	ILE
1	B	216	ASP

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Mol	Chain	Res	Type
1	B	232	LEU
1	B	235	MET
1	B	238	ASN
1	B	247	VAL
1	B	268	LEU
1	B	274	ASN
1	B	282	LEU
1	B	286	ILE
1	B	287	LEU
1	B	293	PRO
1	B	301	SER

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	53	ASN
1	A	134	HIS
1	A	163	HIS
1	A	192	GLN
1	A	277	ASN
1	A	299	GLN
1	B	64	HIS
1	B	69	GLN
1	B	127	GLN
1	B	134	HIS
1	B	163	HIS
1	B	172	HIS
1	B	192	GLN
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 ⓘ

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	302/306 (98%)	0.45	38 (12%) 8 6	12, 28, 65, 90	0
1	B	302/306 (98%)	0.54	32 (10%) 11 8	14, 32, 67, 91	0
All	All	604/612 (98%)	0.50	70 (11%) 9 7	12, 31, 67, 91	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PHE	7.0
1	A	141	LEU	7.0
1	A	46	ALA	6.4
1	B	141	LEU	5.7
1	A	3	PHE	5.1
1	A	50	LEU	4.9
1	A	45	THR	4.7
1	A	140	PHE	4.7
1	A	118	TYR	4.7
1	A	2	GLY	4.5
1	B	118	TYR	4.4
1	A	146	GLY	4.3
1	B	140	PHE	4.3
1	B	138	GLY	4.2
1	A	222	ARG	4.1
1	B	144	SER	4.1
1	A	49	MET	4.1
1	B	145	CYS	3.9
1	A	154	TYR	3.8
1	A	302	GLY	3.8
1	A	48	ASP	3.7
1	B	143	GLY	3.6
1	B	3	PHE	3.5
1	B	302	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	119	ASN	3.3
1	A	1	SER	3.3
1	A	145	CYS	3.2
1	A	300	CYS	3.1
1	B	119	ASN	3.1
1	A	47	GLU	3.1
1	A	278	GLY	3.1
1	A	191	ALA	3.1
1	A	168	PRO	3.1
1	A	139	SER	3.0
1	B	139	SER	3.0
1	B	142	ASN	3.0
1	B	214	ASN	3.0
1	B	300	CYS	3.0
1	A	144	SER	3.0
1	A	197	ASP	3.0
1	B	301	SER	2.9
1	B	46	ALA	2.8
1	A	190	THR	2.8
1	A	23	GLY	2.7
1	B	76	ARG	2.7
1	B	45	THR	2.6
1	B	146	GLY	2.6
1	A	142	ASN	2.5
1	B	277	ASN	2.5
1	B	298	ARG	2.5
1	A	221	ASN	2.5
1	A	120	GLY	2.5
1	B	1	SER	2.5
1	B	64	HIS	2.5
1	B	117	CYS	2.4
1	A	64	HIS	2.4
1	B	223	PHE	2.4
1	A	298	ARG	2.3
1	B	232	LEU	2.3
1	B	120	GLY	2.3
1	B	191	ALA	2.3
1	A	301	SER	2.3
1	A	44	CYS	2.3
1	A	143	GLY	2.2
1	A	166	GLU	2.2
1	B	299	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	280	THR	2.2
1	B	284	SER	2.2
1	B	169	THR	2.1
1	B	274	ASN	2.1

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.