Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2022 – 08:02 PM EDT

PDB ID	:	7T2V
Title	:	SARS CoV2 Mpro C145S mutant
Authors	:	Mathews, I.I.; Hameedi, M.A.; Wakatsuki, S.
Deposited on	:	2021-12-06
Resolution	:	2.47 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:

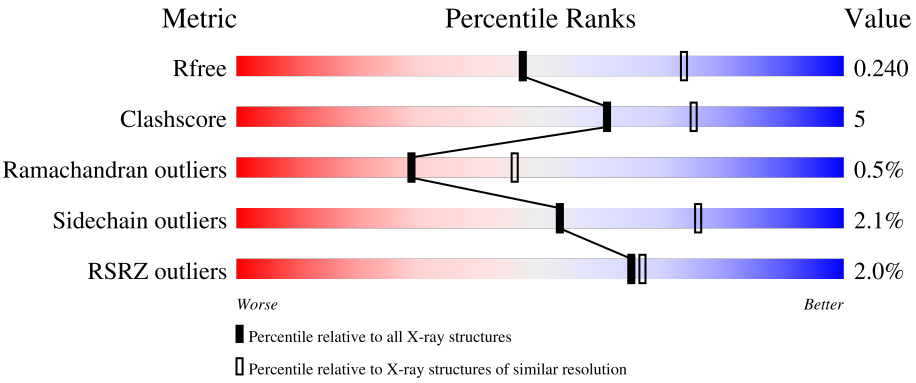
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	319	82% 14% .
1	B	319	4% 85% 11% .
1	C	319	4% 79% 16% . .
1	D	319	84% 11% . .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9471 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2361	1495	400	445	21			
1	B	305	Total	C	N	O	S	0	0	0
			2345	1487	395	442	21			
1	C	305	Total	C	N	O	S	0	0	0
			2354	1491	399	443	21			
1	D	306	Total	C	N	O	S	0	0	0
			2365	1498	401	445	21			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP P0DTD1
A	-11	HIS	-	expression tag	UNP P0DTD1
A	-10	HIS	-	expression tag	UNP P0DTD1
A	-9	HIS	-	expression tag	UNP P0DTD1
A	-8	HIS	-	expression tag	UNP P0DTD1
A	-7	HIS	-	expression tag	UNP P0DTD1
A	-6	HIS	-	expression tag	UNP P0DTD1
A	-5	GLU	-	expression tag	UNP P0DTD1
A	-4	ASN	-	expression tag	UNP P0DTD1
A	-3	LEU	-	expression tag	UNP P0DTD1
A	-2	TYR	-	expression tag	UNP P0DTD1
A	-1	PHE	-	expression tag	UNP P0DTD1
A	145	SER	CYS	engineered mutation	UNP P0DTD1
B	-12	MET	-	initiating methionine	UNP P0DTD1
B	-11	HIS	-	expression tag	UNP P0DTD1
B	-10	HIS	-	expression tag	UNP P0DTD1
B	-9	HIS	-	expression tag	UNP P0DTD1
B	-8	HIS	-	expression tag	UNP P0DTD1
B	-7	HIS	-	expression tag	UNP P0DTD1
B	-6	HIS	-	expression tag	UNP P0DTD1
B	-5	GLU	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASN	-	expression tag	UNP P0DTD1
B	-3	LEU	-	expression tag	UNP P0DTD1
B	-2	TYR	-	expression tag	UNP P0DTD1
B	-1	PHE	-	expression tag	UNP P0DTD1
B	145	SER	CYS	engineered mutation	UNP P0DTD1
C	-12	MET	-	initiating methionine	UNP P0DTD1
C	-11	HIS	-	expression tag	UNP P0DTD1
C	-10	HIS	-	expression tag	UNP P0DTD1
C	-9	HIS	-	expression tag	UNP P0DTD1
C	-8	HIS	-	expression tag	UNP P0DTD1
C	-7	HIS	-	expression tag	UNP P0DTD1
C	-6	HIS	-	expression tag	UNP P0DTD1
C	-5	GLU	-	expression tag	UNP P0DTD1
C	-4	ASN	-	expression tag	UNP P0DTD1
C	-3	LEU	-	expression tag	UNP P0DTD1
C	-2	TYR	-	expression tag	UNP P0DTD1
C	-1	PHE	-	expression tag	UNP P0DTD1
C	145	SER	CYS	engineered mutation	UNP P0DTD1
D	-12	MET	-	initiating methionine	UNP P0DTD1
D	-11	HIS	-	expression tag	UNP P0DTD1
D	-10	HIS	-	expression tag	UNP P0DTD1
D	-9	HIS	-	expression tag	UNP P0DTD1
D	-8	HIS	-	expression tag	UNP P0DTD1
D	-7	HIS	-	expression tag	UNP P0DTD1
D	-6	HIS	-	expression tag	UNP P0DTD1
D	-5	GLU	-	expression tag	UNP P0DTD1
D	-4	ASN	-	expression tag	UNP P0DTD1
D	-3	LEU	-	expression tag	UNP P0DTD1
D	-2	TYR	-	expression tag	UNP P0DTD1
D	-1	PHE	-	expression tag	UNP P0DTD1
D	145	SER	CYS	engineered mutation	UNP P0DTD1

- Molecule 2 is water.

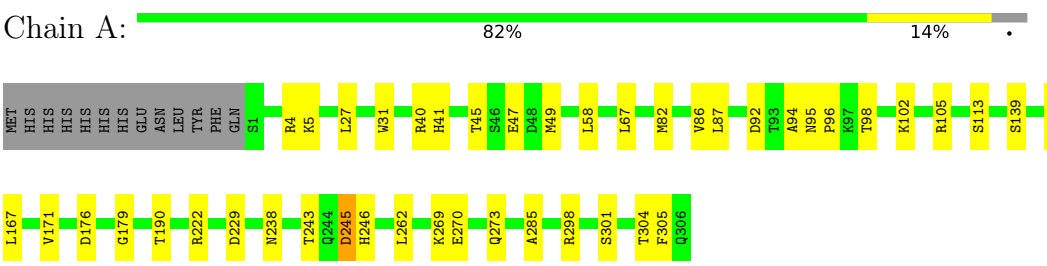
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	9	Total O 9 9	0	0
2	C	10	Total O 10 10	0	0
2	D	17	Total O 17 17	0	0

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.

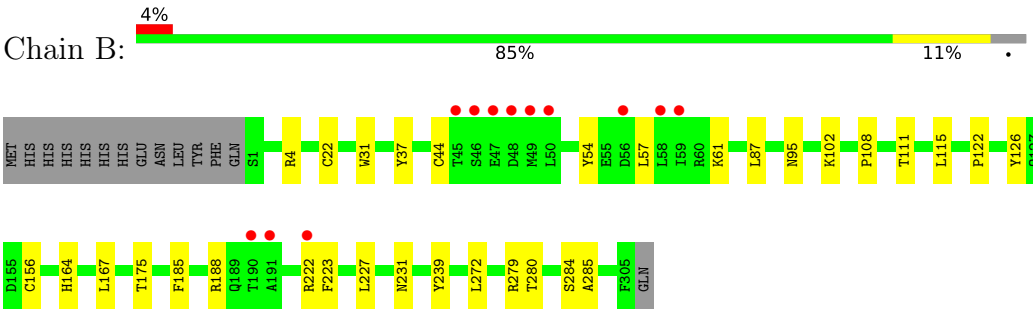
• Molecule 1: 3C-Like Protease

Chain A:



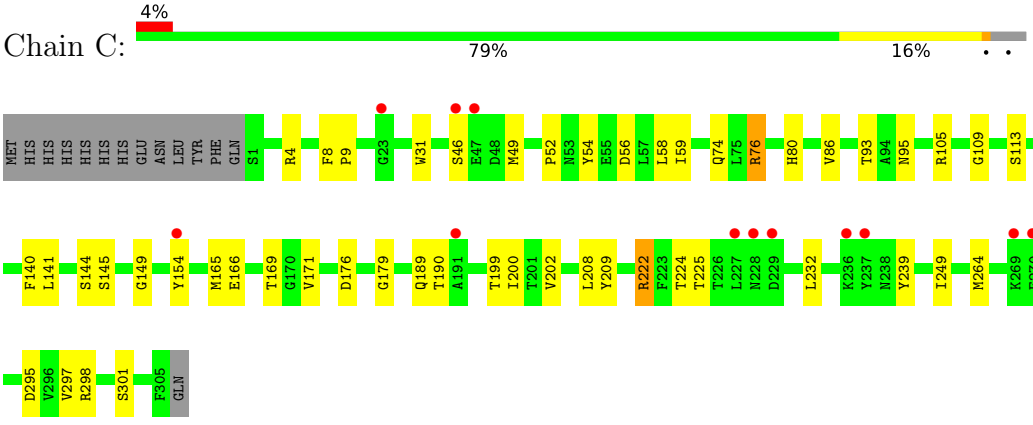
• Molecule 1: 3C-Like Protease

Chain B:



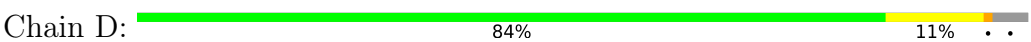
• Molecule 1: 3C-Like Protease

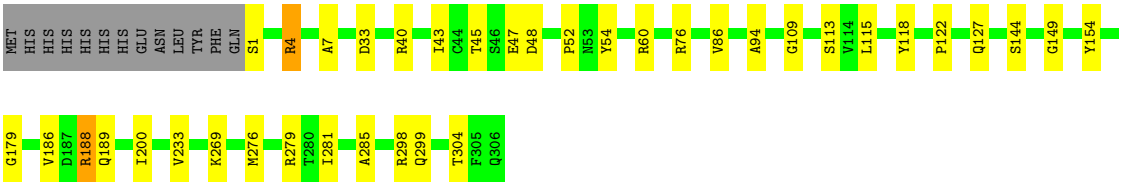
Chain C:



• Molecule 1: 3C-Like Protease

Chain D:




MET
HIS
HIS
HIS
HIS
HIS
HIS
GLU
ASN
LEU
TYR
PHE
GLN
S1
R4
A7
D33
R40
I43
C44
T45
S46
E47
D48
P52
N53
Y54
R60
R76
V86
A94
G109
S113
V114
L115
Y118
P122
Q127
S144
G149
Y154
G179
V186
D187
R188
Q189
I200
V233
K269
M276
R279
T280
I281
A285
R298
Q299
T304
F305
Q306

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.59Å 67.51Å 77.65Å 102.11° 89.30° 106.41°	Depositor
Resolution (Å)	38.05 – 2.47 38.05 – 2.47	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.05-2.47) 96.9 (38.05-2.47)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.196 , 0.237 0.202 , 0.240	Depositor DCC
R_{free} test set	2037 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9471	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.33	0/2414	0.62	0/3281
1	B	0.32	0/2398	0.59	0/3262
1	C	0.33	0/2407	0.61	0/3273
1	D	0.35	0/2418	0.63	0/3285
All	All	0.33	0/9637	0.61	0/13101

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	3
1	B	0	1
1	C	0	3
1	D	0	6
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	4	ARG	Sidechain
1	B	279	ARG	Sidechain
1	C	222	ARG	Sidechain
1	C	4	ARG	Sidechain
1	C	76	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	188	ARG	Sidechain
1	D	279	ARG	Sidechain
1	D	4	ARG	Sidechain
1	D	48	ASP	Peptide
1	D	60	ARG	Sidechain
1	D	76	ARG	Sidechain

5.2 Too-close contacts (i)

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	2361	0	2299	22	0
1	B	2345	0	2280	16	0
1	C	2354	0	2295	32	0
1	D	2365	0	2310	22	0
2	A	10	0	0	0	0
2	B	9	0	0	0	0
2	C	10	0	0	0	0
2	D	17	0	0	0	0
All	All	9471	0	9184	84	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 5.

All (84) 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:C:166:GLU:OE2	1:D:1:SER:HB3	1.85	0.76
1:A:269:LYS:O	1:A:273:GLN:HG3	1.96	0.65
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.79	0.65
1:D:113:SER:O	1:D:149:GLY:HA2	1.99	0.63
1:A:285:ALA:HB3	1:B:285:ALA:HB3	1.81	0.62
1:D:86:VAL:HG13	1:D:179:GLY:HA2	1.80	0.62
1:D:233:VAL:HG11	1:D:269:LYS:HG3	1.84	0.59
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.84	0.58
1:D:115:LEU:HD11	1:D:122:PRO:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:HD11	1:C:80:HIS:HD2	1.69	0.57
1:C:127:GLN:HE21	1:C:127:GLN:HA	1.70	0.56
1:A:40:ARG:HH11	1:A:82:MET:CE	2.19	0.54
1:B:44:CYS:SG	1:B:54:TYR:CE1	3.00	0.54
1:C:222:ARG:HG2	1:C:222:ARG:HH11	1.73	0.54
1:D:52:PRO:HG2	1:D:54:TYR:CE2	2.43	0.54
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.90	0.53
1:A:113:SER:O	1:A:149:GLY:HA2	2.09	0.53
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.90	0.52
1:A:41:HIS:HB2	1:A:49:MET:CE	2.41	0.51
1:D:4:ARG:O	1:D:299:GLN:NE2	2.41	0.51
1:B:22:CYS:SG	1:B:61:LYS:HE3	2.51	0.50
1:C:58:LEU:HD11	1:C:80:HIS:CD2	2.46	0.50
1:B:227:LEU:O	1:B:231:ASN:ND2	2.43	0.50
1:B:102:LYS:HE2	1:B:156:CYS:SG	2.52	0.50
1:C:8:PHE:HD2	1:C:113:SER:HG	1.59	0.50
1:D:186:VAL:HG23	1:D:188:ARG:HG2	1.94	0.50
1:C:295:ASP:OD1	1:C:298:ARG:NH1	2.45	0.49
1:C:140:PHE:HB3	1:C:144:SER:OG	2.12	0.49
1:C:127:GLN:HA	1:C:127:GLN:NE2	2.28	0.49
1:C:202:VAL:HG21	1:C:249:ILE:HD11	1.93	0.49
1:B:37:TYR:HA	1:B:87:LEU:O	2.12	0.49
1:D:109:GLY:HA2	1:D:200:ILE:HD13	1.95	0.49
1:B:102:LYS:HG2	1:B:156:CYS:SG	2.53	0.49
1:A:167:LEU:HD12	1:A:171:VAL:HG23	1.95	0.48
1:C:224:THR:HG22	1:C:225:THR:H	1.78	0.48
1:D:40:ARG:O	1:D:43:ILE:HG12	2.14	0.47
1:C:49:MET:O	1:C:49:MET:HG3	2.13	0.47
1:C:169:THR:HG23	1:C:171:VAL:HG22	1.95	0.47
1:B:167:LEU:HD11	1:B:185:PHE:CE1	2.50	0.47
1:C:56:ASP:O	1:C:59:ILE:HG22	2.15	0.47
1:A:245:ASP:N	1:A:245:ASP:OD1	2.47	0.47
1:D:45:THR:O	1:D:47:GLU:N	2.45	0.47
1:C:208:LEU:HB3	1:C:264:MET:HE1	1.98	0.46
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.49	0.46
1:C:285:ALA:HB3	1:D:285:ALA:HB3	1.97	0.46
1:C:74:GLN:HE21	1:C:76:ARG:NH1	2.14	0.46
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.16	0.45
1:D:7:ALA:HA	1:D:127:GLN:NE2	2.31	0.45
1:C:297:VAL:O	1:C:301:SER:OG	2.24	0.45
1:A:45:THR:HB	1:A:47:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:MET:CE	1:D:281:ILE:HG13	2.48	0.44
1:C:199:THR:HG21	1:C:239:TYR:CZ	2.52	0.44
1:D:52:PRO:HG2	1:D:54:TYR:CZ	2.53	0.44
1:C:113:SER:OG	1:C:127:GLN:NE2	2.47	0.44
1:C:189:GLN:O	1:C:190:THR:HG23	2.18	0.44
1:C:105:ARG:NH1	1:C:176:ASP:OD2	2.45	0.44
1:C:141:LEU:HD11	1:D:299:GLN:O	2.17	0.44
1:B:164:HIS:CD2	1:B:175:THR:HG23	2.53	0.44
1:C:209:TYR:CZ	1:C:264:MET:HG3	2.53	0.44
1:A:92:ASP:OD1	1:A:92:ASP:C	2.56	0.43
1:D:118:TYR:CE1	1:D:144:SER:HB3	2.52	0.43
1:C:31:TRP:CE2	1:C:95:ASN:HB2	2.53	0.43
1:C:118:TYR:CE1	1:C:144:SER:HB3	2.53	0.43
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.53	0.43
1:D:276:MET:HE1	1:D:281:ILE:HG13	1.99	0.43
1:B:280:THR:HA	1:B:284:SER:O	2.19	0.43
1:A:40:ARG:NH1	1:A:82:MET:CE	2.83	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.91	0.42
1:A:243:THR:O	1:A:246:HIS:N	2.49	0.42
1:A:105:ARG:NH1	1:A:176:ASP:OD2	2.49	0.42
1:B:126:TYR:HE2	1:B:128:CYS:HG	1.68	0.42
1:A:305:PHE:H	1:D:189:GLN:NE2	2.17	0.42
1:B:111:THR:HG22	1:B:129:ALA:HB2	2.01	0.42
1:D:33:ASP:O	1:D:94:ALA:HA	2.19	0.42
1:A:305:PHE:H	1:D:189:GLN:HE21	1.68	0.42
1:C:52:PRO:HG2	1:C:54:TYR:CE2	2.54	0.42
1:A:94:ALA:O	1:A:96:PRO:HD3	2.20	0.41
1:C:127:GLN:HE21	1:C:127:GLN:CA	2.31	0.41
1:C:113:SER:O	1:C:149:GLY:HA2	2.20	0.41
1:C:9:PRO:CG	1:D:122:PRO:HB2	2.51	0.41
1:A:102:LYS:HG2	1:A:156:CYS:SG	2.60	0.41
1:A:58:LEU:HD13	1:A:87:LEU:HD21	2.03	0.41
1:A:139:SER:HB2	1:B:4:ARG:HG2	2.03	0.41
1:A:31:TRP:O	1:A:95:ASN:ND2	2.44	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	304/319 (95%)	286 (94%)	17 (6%)	1 (0%)	41	59
1	B	303/319 (95%)	283 (93%)	18 (6%)	2 (1%)	22	36
1	C	303/319 (95%)	287 (95%)	14 (5%)	2 (1%)	22	36
1	D	304/319 (95%)	291 (96%)	12 (4%)	1 (0%)	41	59
All	All	1214/1276 (95%)	1147 (94%)	61 (5%)	6 (0%)	29	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	46	SER
1	A	238	ASN
1	B	223	PHE
1	D	154	TYR
1	B	154	TYR
1	C	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	261/276 (95%)	252 (97%)	9 (3%)	37	61
1	B	259/276 (94%)	254 (98%)	5 (2%)	57	78
1	C	261/276 (95%)	255 (98%)	6 (2%)	50	74
1	D	262/276 (95%)	260 (99%)	2 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1043/1104 (94%)	1021 (98%)	22 (2%)	53 76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	27	LEU
1	A	67	LEU
1	A	190	THR
1	A	229	ASP
1	A	245	ASP
1	A	270	GLU
1	A	301	SER
1	A	304	THR
1	B	57	LEU
1	B	108	PRO
1	B	128	CYS
1	B	188	ARG
1	B	222	ARG
1	C	93	THR
1	C	127	GLN
1	C	128	CYS
1	C	145	SER
1	C	165	MET
1	C	232	LEU
1	D	298	ARG
1	D	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	273	GLN
1	C	127	GLN
1	C	142	ASN
1	D	127	GLN
1	D	151	ASN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	306/319 (95%)	-0.16	0 100 100	27, 47, 77, 95	0
1	B	305/319 (95%)	0.02	12 (3%) 39 41	27, 51, 87, 147	0
1	C	305/319 (95%)	0.01	13 (4%) 35 37	29, 50, 93, 110	0
1	D	306/319 (95%)	-0.33	0 100 100	25, 39, 62, 102	0
All	All	1222/1276 (95%)	-0.12	25 (2%) 65 67	25, 46, 85, 147	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	LEU	9.7
1	B	49	MET	5.0
1	B	222	ARG	3.5
1	C	23	GLY	3.3
1	B	56	ASP	3.2
1	C	154	TYR	3.2
1	B	46	SER	3.1
1	C	191	ALA	3.1
1	B	59	ILE	2.9
1	C	229	ASP	2.9
1	C	237	TYR	2.8
1	C	228	ASN	2.6
1	B	45	THR	2.6
1	B	48	ASP	2.4
1	C	47	GLU	2.4
1	C	270	GLU	2.4
1	C	269	LYS	2.3
1	B	47	GLU	2.2
1	B	190	THR	2.2
1	C	46	SER	2.2
1	B	191	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	278	GLY	2.1
1	C	236	LYS	2.1
1	B	58	LEU	2.0
1	C	227	LEU	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 monosaccharides 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.