Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 06:11 PM JST

PDB ID	:	7E5X
Title	:	THE CRYSTAL STRUCTURE OF COVID-19 MAIN PROTEASE apo form at 2.2 angstrom
Authors	:	Liu, X.; Zhao, Y.; Yang, H.; Rao, Z.
Deposited on	:	2021-02-21
Resolution	:	2.19 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 (i) 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 (1)) were used in the production of this report:

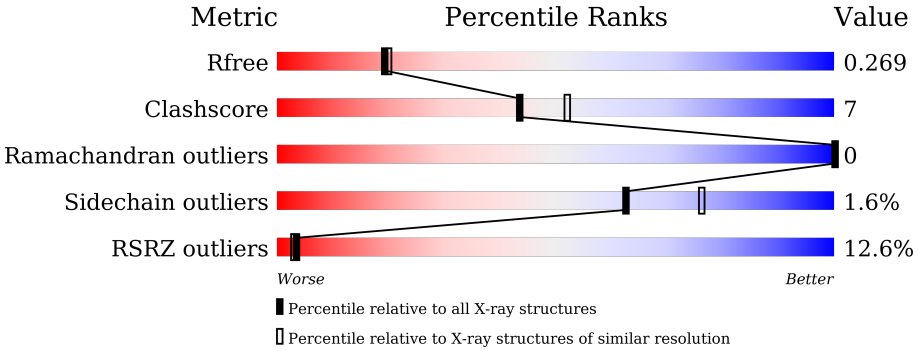
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	10% 81% 18%
1	B	306	12% 86% 14%
1	C	306	12% 82% 18% •
1	D	306	17% 88% 11% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9400 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
			Total	C	N	O	S			
1	A	306	2364	1496	401	445	22	0	0	0
1	B	306	2295	1449	395	430	21	0	0	0
1	C	306	2364	1496	401	445	22	0	0	0
1	D	306	2295	1449	395	430	21	0	0	0

- Molecule 2 is water.

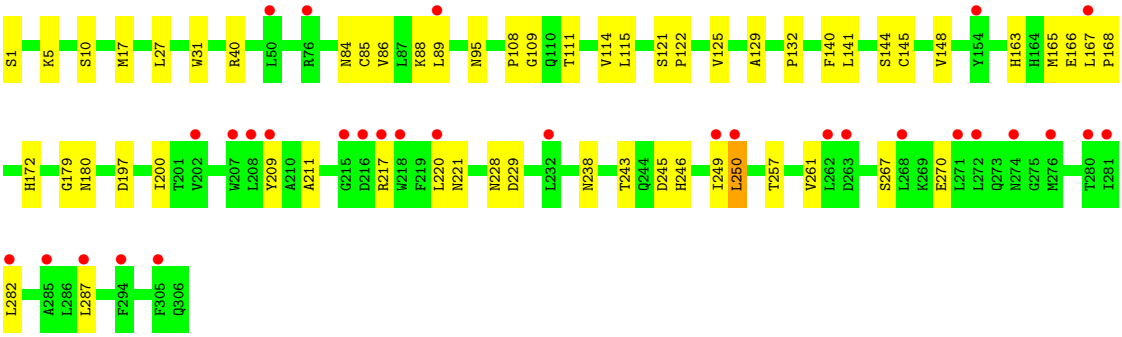
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	25	25	25	0	0
2	B	16	16	16	0	0
2	C	21	21	21	0	0
2	D	20	20	20	0	0

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.

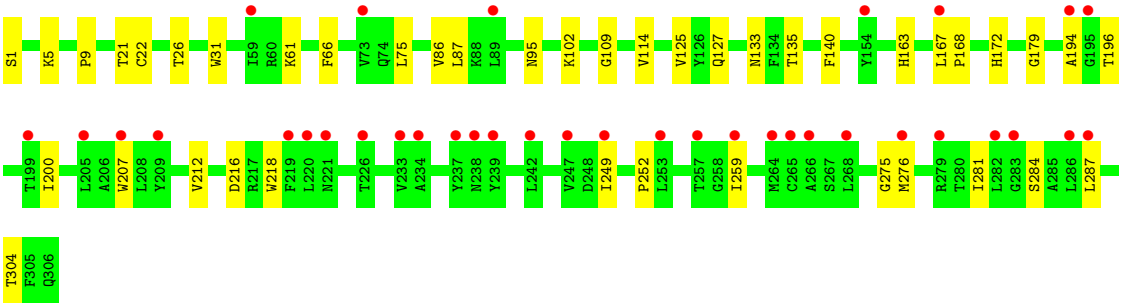
- Molecule 1: 3C-like proteinase

Chain A:



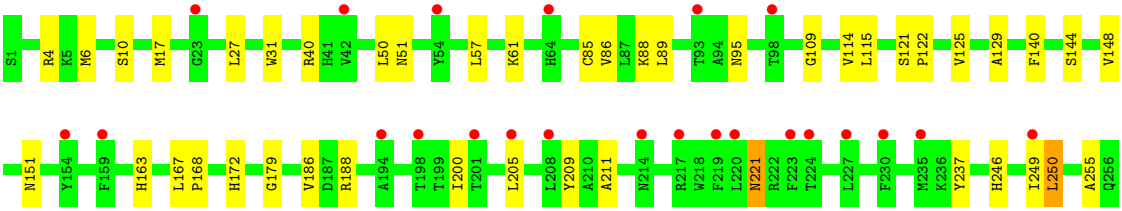
- Molecule 1: 3C-like proteinase

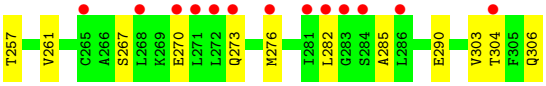
Chain B:



- Molecule 1: 3C-like proteinase

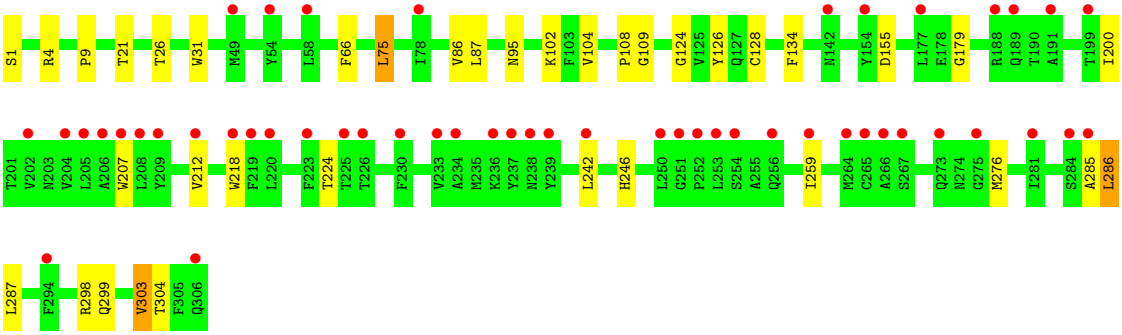
Chain C:





- Molecule 1: 3C-like proteinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.48Å 73.78Å 73.79Å 66.40° 90.01° 90.01°	Depositor
Resolution (Å)	46.33 – 2.19 46.28 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.33-2.19) 97.3 (46.28-2.19)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.266 0.238 , 0.269	Depositor DCC
R_{free} test set	3071 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l 0.023 for -h,l,k 0.487 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9400	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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 (i)

5.1 Standard geometry (i)

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	0.75	0/2417	0.92	0/3285
1	B	0.75	0/2346	0.92	0/3192
1	C	0.74	0/2417	0.91	0/3285
1	D	0.74	0/2346	0.91	0/3192
All	All	0.75	0/9526	0.91	0/12954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2364	0	2303	40	0
1	B	2295	0	2178	30	0
1	C	2364	0	2303	43	0
1	D	2295	0	2178	27	0
2	A	25	0	0	3	0
2	B	16	0	0	0	0
2	C	21	0	0	1	0
2	D	20	0	0	0	0
All	All	9400	0	8962	122	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 7.

All (122) 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:D:4:ARG:H	1:D:299:GLN:HE22	1.30	0.79
1:C:6:MET:HE1	1:D:124:GLY:HA3	1.70	0.73
1:A:238:ASN:HB2	2:A:404:HOH:O	1.90	0.69
1:A:228:ASN:N	2:A:401:HOH:O	2.22	0.67
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.77	0.66
1:A:197:ASP:HB3	2:A:405:HOH:O	1.95	0.65
1:D:86:VAL:HG13	1:D:179:GLY:HA2	1.78	0.65
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.79	0.64
1:C:89:LEU:HD22	1:C:89:LEU:N	2.15	0.61
1:A:84:ASN:ND2	1:A:180:ASN:OD1	2.35	0.60
1:A:89:LEU:HD12	1:A:89:LEU:N	2.18	0.59
1:D:66:PHE:CE1	1:D:87:LEU:HD21	2.38	0.59
1:C:209:TYR:HD1	1:C:257:THR:HG21	1.70	0.57
1:A:209:TYR:HD1	1:A:257:THR:HG21	1.70	0.57
1:B:66:PHE:CE1	1:B:87:LEU:HD21	2.40	0.56
1:C:237:TYR:OH	1:C:273:GLN:HA	2.03	0.56
1:B:212:VAL:HG11	1:B:259:ILE:CD1	2.36	0.56
1:C:285:ALA:HB3	1:D:285:ALA:HB3	1.89	0.55
1:C:211:ALA:HA	1:C:282:LEU:HG	1.89	0.55
1:A:165:MET:CE	1:C:303:VAL:HG21	2.37	0.55
1:B:21:THR:OG1	1:B:26:THR:HG22	2.07	0.54
1:A:267:SER:O	1:A:270:GLU:HG3	2.08	0.54
1:D:21:THR:OG1	1:D:26:THR:HG22	2.08	0.54
1:C:285:ALA:H	1:D:286:LEU:HD21	1.73	0.54
1:A:88:LYS:C	1:A:89:LEU:HD12	2.29	0.53
1:C:221:ASN:HD21	1:C:267:SER:HA	1.74	0.52
1:C:17:MET:HE1	1:C:148:VAL:HG22	1.90	0.52
1:A:145:CYS:SG	1:C:306:GLN:C	2.88	0.52
1:A:211:ALA:HA	1:A:282:LEU:HD13	1.90	0.52
1:C:6:MET:CE	1:D:124:GLY:HA3	2.40	0.52
1:A:221:ASN:HD21	1:A:267:SER:HA	1.75	0.51
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.46	0.51
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.92	0.51
1:D:31:TRP:CD2	1:D:95:ASN:HB2	2.46	0.50
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.47	0.50
1:C:31:TRP:CD2	1:C:95:ASN:HB2	2.47	0.50
1:A:108:PRO:HB3	1:A:132:PRO:HA	1.93	0.50
1:A:1:SER:O	1:A:1:SER:OG	2.23	0.50
1:B:218:TRP:HE1	1:B:281:ILE:HG13	1.77	0.50
1:C:285:ALA:N	1:D:286:LEU:HD21	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.48	0.49
1:B:31:TRP:CE2	1:B:75:LEU:HD21	2.48	0.49
1:C:4:ARG:HD3	1:D:126:TYR:CD2	2.48	0.48
1:A:166:GLU:OE2	1:B:1:SER:OG	2.22	0.48
1:C:129:ALA:N	1:C:290:GLU:OE1	2.44	0.48
1:C:121:SER:HB3	1:D:304:THR:HB	1.94	0.48
1:C:246:HIS:O	1:C:249:ILE:HG22	2.14	0.48
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.96	0.48
1:D:21:THR:HG23	1:D:26:THR:HG22	1.96	0.47
1:A:217:ARG:HB3	1:A:220:LEU:HD12	1.94	0.47
1:A:245:ASP:O	1:A:249:ILE:HG12	2.14	0.47
1:C:40:ARG:NE	1:C:85:CYS:HA	2.30	0.47
1:C:205:LEU:HB3	1:C:250:LEU:HD21	1.97	0.47
1:A:145:CYS:SG	1:C:306:GLN:OXT	2.73	0.47
1:C:250:LEU:HB3	1:C:261:VAL:HG22	1.96	0.47
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.80	0.46
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.97	0.46
1:B:135:THR:HG21	1:B:194:ALA:HB2	1.97	0.46
1:D:31:TRP:CE2	1:D:75:LEU:HD21	2.51	0.46
1:B:249:ILE:O	1:B:252:PRO:HD2	2.15	0.46
1:C:151:ASN:OD1	2:C:401:HOH:O	2.21	0.46
1:A:89:LEU:N	1:A:89:LEU:CD1	2.79	0.46
1:A:10:SER:HB2	1:A:115:LEU:HD13	1.98	0.46
1:B:133:ASN:HB3	1:B:196:THR:HB	1.97	0.46
1:C:267:SER:O	1:C:270:GLU:HG3	2.16	0.45
1:B:275:GLY:O	1:B:276:MET:HB2	2.16	0.45
1:D:102:LYS:HG2	1:D:104:VAL:HG13	1.99	0.45
1:A:250:LEU:HB3	1:A:261:VAL:HG22	1.99	0.45
1:B:86:VAL:HG23	1:B:179:GLY:HA2	1.97	0.45
1:D:287:LEU:HD12	1:D:287:LEU:H	1.82	0.45
1:A:111:THR:HG22	1:A:129:ALA:HB2	1.99	0.45
1:D:242:LEU:HD12	1:D:246:HIS:HB2	1.98	0.45
1:A:122:PRO:HB2	1:B:9:PRO:HG3	1.99	0.45
1:A:166:GLU:OE1	1:C:306:GLN:NE2	2.50	0.45
1:D:242:LEU:CD1	1:D:246:HIS:HB2	2.47	0.45
1:D:207:TRP:CZ3	1:D:287:LEU:HA	2.52	0.44
1:A:1:SER:HA	1:B:140:PHE:O	2.17	0.44
1:B:212:VAL:HG11	1:B:259:ILE:HD12	1.99	0.44
1:B:21:THR:HG23	1:B:26:THR:HG22	1.98	0.44
1:C:51:ASN:HD22	1:C:51:ASN:HA	1.61	0.44
1:C:282:LEU:HD23	1:C:282:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:SER:HB2	1:C:115:LEU:HD13	2.00	0.44
1:D:155:ASP:OD1	1:D:155:ASP:N	2.51	0.44
1:A:167:LEU:HB3	1:A:168:PRO:HD2	2.00	0.44
1:B:31:TRP:CZ2	1:B:75:LEU:HD21	2.53	0.44
1:D:218:TRP:CZ2	1:D:276:MET:HG2	2.52	0.43
1:A:121:SER:HB3	1:B:304:THR:HB	2.00	0.43
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.52	0.43
1:C:114:VAL:O	1:C:125:VAL:HA	2.18	0.43
1:C:186:VAL:HG21	1:C:188:ARG:NH2	2.33	0.43
1:B:22:CYS:SG	1:B:61:LYS:HE2	2.58	0.43
1:C:163:HIS:CE1	1:C:172:HIS:HB3	2.54	0.43
1:A:140:PHE:HB3	1:A:144:SER:OG	2.19	0.43
1:B:102:LYS:HE3	1:B:102:LYS:HB3	1.71	0.43
1:B:167:LEU:N	1:B:167:LEU:CD1	2.82	0.43
1:C:167:LEU:HB3	1:C:168:PRO:HD2	2.00	0.43
1:A:17:MET:HE1	1:A:148:VAL:HG22	2.00	0.42
1:A:114:VAL:O	1:A:125:VAL:HA	2.20	0.42
1:A:243:THR:HG22	1:A:246:HIS:CG	2.54	0.42
1:D:108:PRO:HG3	1:D:134:PHE:CE1	2.54	0.42
1:B:5:LYS:HG3	1:B:127:GLN:HB3	2.00	0.42
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.84	0.42
1:B:207:TRP:HZ3	1:B:287:LEU:HD23	1.84	0.42
1:C:89:LEU:N	1:C:89:LEU:CD2	2.83	0.42
1:A:122:PRO:HB2	1:B:9:PRO:CG	2.49	0.42
1:B:207:TRP:CZ3	1:B:287:LEU:HA	2.54	0.42
1:D:109:GLY:HA2	1:D:200:ILE:HD13	2.01	0.42
1:A:221:ASN:ND2	1:A:270:GLU:HG2	2.35	0.42
1:D:212:VAL:HG11	1:D:259:ILE:HD12	2.02	0.41
1:C:140:PHE:O	1:D:1:SER:N	2.47	0.41
1:B:109:GLY:HA2	1:B:200:ILE:HD13	2.01	0.41
1:C:122:PRO:HB2	1:D:9:PRO:HG3	2.02	0.41
1:C:163:HIS:HE1	1:C:172:HIS:HB3	1.85	0.41
1:C:255:ALA:HB1	1:C:304:THR:HG21	2.03	0.41
1:A:141:LEU:HD13	1:A:141:LEU:HA	1.92	0.41
1:A:40:ARG:NE	1:A:85:CYS:HA	2.36	0.40
1:C:140:PHE:HB3	1:C:144:SER:OG	2.20	0.40
1:C:50:LEU:HD13	1:C:50:LEU:HA	1.90	0.40
1:C:57:LEU:O	1:C:61:LYS:HG2	2.21	0.40
1:C:88:LYS:C	1:C:89:LEU:HD22	2.42	0.40
1:D:298:ARG:HB2	1:D:303:VAL:HG12	2.03	0.40
1:B:114:VAL:O	1:B:125:VAL:HA	2.22	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	304/306 (99%)	293 (96%)	11 (4%)	0	100	100
1	B	304/306 (99%)	293 (96%)	11 (4%)	0	100	100
1	C	304/306 (99%)	293 (96%)	11 (4%)	0	100	100
1	D	304/306 (99%)	295 (97%)	9 (3%)	0	100	100
All	All	1216/1224 (99%)	1174 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	262/263 (100%)	257 (98%)	5 (2%)	57	71
1	B	242/263 (92%)	240 (99%)	2 (1%)	81	90
1	C	262/263 (100%)	258 (98%)	4 (2%)	65	78
1	D	242/263 (92%)	237 (98%)	5 (2%)	53	67
All	All	1008/1052 (96%)	992 (98%)	16 (2%)	62	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	27	LEU
1	A	229	ASP
1	A	250	LEU
1	A	287	LEU
1	B	216	ASP
1	B	284	SER
1	C	27	LEU
1	C	221	ASN
1	C	250	LEU
1	C	276	MET
1	D	75	LEU
1	D	128	CYS
1	D	224	THR
1	D	286	LEU
1	D	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	273	GLN
1	C	51	ASN
1	C	164	HIS
1	C	221	ASN
1	D	163	HIS
1	D	299	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	306/306 (100%)	0.71	31 (10%)	7	6	39, 72, 129, 165	0
1	B	306/306 (100%)	0.81	36 (11%)	4	4	39, 78, 164, 184	0
1	C	306/306 (100%)	0.74	36 (11%)	4	4	40, 73, 132, 163	0
1	D	306/306 (100%)	0.92	51 (16%)	1	1	38, 79, 165, 196	0
All	All	1224/1224 (100%)	0.80	154 (12%)	3	3	38, 75, 153, 196	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	MET	8.9
1	D	253	LEU	8.4
1	A	262	LEU	8.3
1	D	225	THR	8.0
1	B	237	TYR	7.4
1	B	219	PHE	6.5
1	D	259	ILE	6.4
1	B	242	LEU	6.2
1	D	208	LEU	6.1
1	D	209	TYR	6.1
1	B	205	LEU	5.7
1	D	188	ARG	5.2
1	C	42	VAL	5.1
1	C	235	MET	5.1
1	C	281	ILE	5.0
1	B	239	TYR	5.0
1	A	287	LEU	5.0
1	D	189	GLN	4.8
1	D	256	GLN	4.8
1	D	233	VAL	4.8
1	C	265	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	272	LEU	4.7
1	D	207	TRP	4.7
1	D	251	GLY	4.6
1	A	268	LEU	4.6
1	D	223	PHE	4.6
1	D	54	TYR	4.4
1	D	265	CYS	4.4
1	B	249	ILE	4.3
1	B	259	ILE	4.3
1	D	252	PRO	4.2
1	A	305	PHE	4.1
1	C	249	ILE	4.1
1	D	284	SER	3.9
1	C	205	LEU	3.9
1	C	220	LEU	3.8
1	C	154	TYR	3.7
1	C	270	GLU	3.7
1	B	199	THR	3.7
1	A	271	LEU	3.7
1	C	286	LEU	3.7
1	B	265	CYS	3.6
1	A	208	LEU	3.6
1	C	23	GLY	3.6
1	D	234	ALA	3.6
1	D	236	LYS	3.5
1	B	283	GLY	3.5
1	B	209	TYR	3.5
1	B	282	LEU	3.5
1	D	205	LEU	3.5
1	B	233	VAL	3.5
1	B	287	LEU	3.5
1	D	267	SER	3.5
1	A	282	LEU	3.5
1	D	237	TYR	3.4
1	D	226	THR	3.4
1	B	264	MET	3.4
1	D	191	ALA	3.3
1	A	154	TYR	3.3
1	A	272	LEU	3.3
1	B	220	LEU	3.3
1	A	218	TRP	3.2
1	C	198	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	281	ILE	3.1
1	A	167	LEU	3.1
1	C	93	THR	3.0
1	C	273	GLN	3.0
1	C	223	PHE	3.0
1	D	238	ASN	3.0
1	D	206	ALA	3.0
1	D	220	LEU	3.0
1	A	280	THR	3.0
1	C	214	ASN	3.0
1	B	286	LEU	2.9
1	D	204	VAL	2.9
1	D	58	LEU	2.9
1	C	268	LEU	2.9
1	D	273	GLN	2.9
1	A	216	ASP	2.9
1	D	142	ASN	2.9
1	B	226	THR	2.8
1	A	249	ILE	2.8
1	C	98	THR	2.8
1	B	73	VAL	2.8
1	A	217	ARG	2.7
1	D	306	GLN	2.7
1	C	284	SER	2.7
1	B	207	TRP	2.7
1	A	263	ASP	2.7
1	D	254	SER	2.7
1	D	285	ALA	2.7
1	A	276	MET	2.7
1	D	239	TYR	2.6
1	B	266	ALA	2.6
1	B	238	ASN	2.6
1	C	217	ARG	2.6
1	C	230	PHE	2.6
1	A	220	LEU	2.6
1	B	268	LEU	2.6
1	C	227	LEU	2.6
1	D	250	LEU	2.6
1	A	207	TRP	2.5
1	B	167	LEU	2.5
1	C	282	LEU	2.5
1	D	242	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	304	THR	2.5
1	D	49	MET	2.5
1	D	230	PHE	2.5
1	A	89	LEU	2.4
1	C	64	HIS	2.4
1	B	234	ALA	2.4
1	D	219	PHE	2.4
1	B	221	ASN	2.4
1	B	253	LEU	2.4
1	D	177	LEU	2.4
1	A	215	GLY	2.4
1	C	201	THR	2.4
1	D	154	TYR	2.4
1	B	257	THR	2.4
1	A	50	LEU	2.4
1	A	274	ASN	2.3
1	D	202	VAL	2.3
1	C	194	ALA	2.3
1	C	224	THR	2.3
1	D	275	GLY	2.3
1	C	219	PHE	2.3
1	A	76	ARG	2.3
1	B	194	ALA	2.3
1	D	218	TRP	2.3
1	B	279	ARG	2.3
1	A	202	VAL	2.3
1	D	78	ILE	2.2
1	D	199	THR	2.2
1	B	154	TYR	2.2
1	D	294	PHE	2.2
1	B	59	ILE	2.2
1	C	283	GLY	2.2
1	A	250	LEU	2.2
1	A	294	PHE	2.1
1	C	271	LEU	2.1
1	D	212	VAL	2.1
1	A	209	TYR	2.1
1	D	264	MET	2.1
1	C	159	PHE	2.1
1	B	195	GLY	2.1
1	C	208	LEU	2.1
1	A	285	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	266	ALA	2.1
1	B	89	LEU	2.0
1	C	276	MET	2.0
1	B	247	VAL	2.0
1	C	54	TYR	2.0
1	D	281	ILE	2.0
1	A	232	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.