



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2022 – 12:19 PM JST

PDB ID : 7WKU
Title : Structure of PDCoV Mpro in complex with an inhibitor
Authors : Wang, F.H.; Yang, H.T.
Deposited on : 2022-01-11
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
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) : 2.28.1

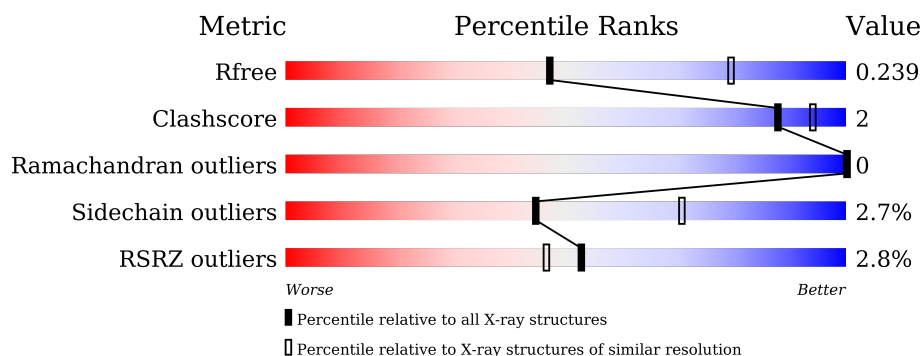
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.60 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.






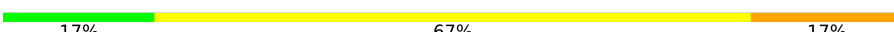
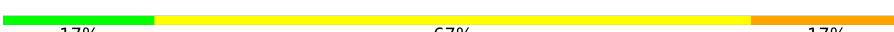

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	308	 93% 6% .
1	B	308	 90% 7% .
1	C	308	 94% . .
1	D	308	 92% 6% .
1	E	308	 84% 10% . 6%
1	F	308	 92% 5% .

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Mol	Chain	Length	Quality of chain
2	H	6	
2	I	6	
2	J	6	
2	K	6	
2	L	6	
2	M	6	

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	H	1	-	-	-	X
2	02J	I	1	-	-	-	X
2	02J	M	1	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14877 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 Peptidase C30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	2	0
			2412	1537	411	446	18			
1	B	299	Total	C	N	O	S	0	1	0
			2382	1519	406	441	16			
1	C	304	Total	C	N	O	S	0	0	0
			2371	1512	400	441	18			
1	D	302	Total	C	N	O	S	0	0	0
			2359	1505	400	436	18			
1	E	291	Total	C	N	O	S	0	0	0
			2276	1454	386	420	16			
1	F	298	Total	C	N	O	S	0	1	0
			2322	1478	394	434	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A166XB12
B	0	SER	-	expression tag	UNP A0A166XB12
C	0	SER	-	expression tag	UNP A0A166XB12
D	0	SER	-	expression tag	UNP A0A166XB12
E	0	SER	-	expression tag	UNP A0A166XB12
F	0	SER	-	expression tag	UNP A0A166XB12

- 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	H	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	I	6	Total	C	N	O	0	0	0
			49	35	6	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	K	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	L	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	M	6	Total	C	N	O	0	0	0
			49	35	6	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	152	Total	O	0	0
			152	152		
3	C	35	Total	O	0	0
			35	35		
3	D	31	Total	O	0	0
			31	31		
3	E	44	Total	O	0	0
			44	44		
3	F	47	Total	O	0	0
			47	47		
3	H	1	Total	O	0	0
			1	1		
3	I	1	Total	O	0	0
			1	1		
3	L	1	Total	O	0	0
			1	1		

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: Peptidase C30

Chain A: 



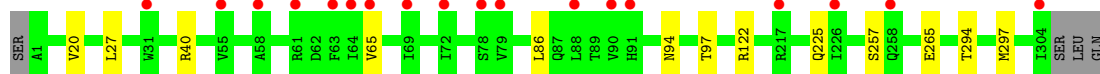
- Molecule 1: Peptidase C30

Chain B: 



- Molecule 1: Peptidase C30

Chain C: 




- Molecule 1: Peptidase C30

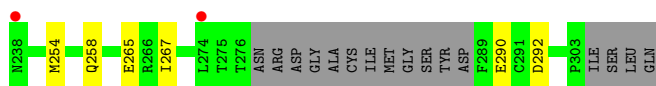
Chain D: 



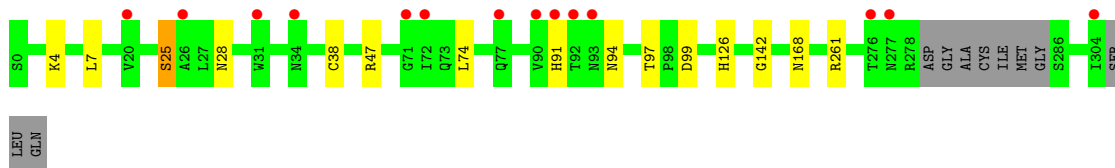
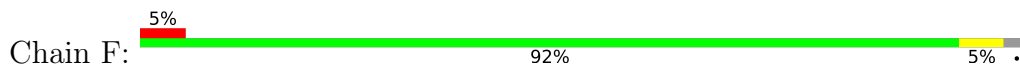
- Molecule 1: Peptidase C30

Chain E: 

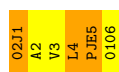




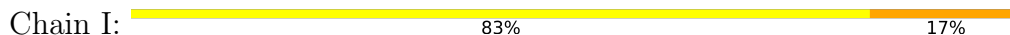
- Molecule 1: Peptidase C30



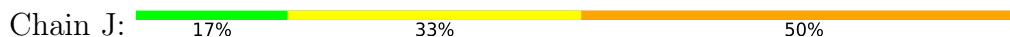
- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE



- 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



- 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



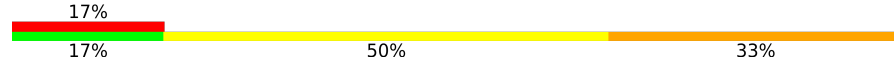
- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE

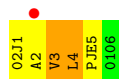
EUCINAMIDE

Chain L:  17% 67% 17%



• 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 M:  17% 50% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	122.29Å 122.29Å 289.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 2.60 49.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.74-2.60) 99.5 (49.74-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.191 , 0.241 0.192 , 0.239	Depositor DCC
R_{free} test set	3733 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14877	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% 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	0.32	0/2477	0.48	0/3375
1	B	0.33	0/2443	0.51	1/3328 (0.0%)
1	C	0.32	0/2429	0.48	0/3313
1	D	0.35	0/2416	0.51	0/3291
1	E	0.33	0/2331	0.51	2/3178 (0.1%)
1	F	0.33	0/2383	0.49	0/3253
2	H	2.54	2/19 (10.5%)	1.16	0/25
2	I	2.62	2/19 (10.5%)	1.07	0/25
2	J	2.57	2/19 (10.5%)	0.97	0/25
2	K	2.56	2/19 (10.5%)	1.21	0/25
2	L	2.58	2/19 (10.5%)	0.93	0/25
2	M	2.58	2/19 (10.5%)	0.88	0/25
All	All	0.40	12/14593 (0.1%)	0.50	3/19888 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	VAL	C-N	8.39	1.53	1.34
2	M	3	VAL	C-N	8.33	1.53	1.34
2	J	3	VAL	C-N	8.31	1.53	1.34
2	K	3	VAL	C-N	8.26	1.53	1.34
2	L	3	VAL	C-N	8.24	1.53	1.34
2	H	3	VAL	C-N	8.14	1.52	1.34
2	I	2	ALA	C-N	5.82	1.47	1.34
2	J	2	ALA	C-N	5.74	1.47	1.34
2	L	2	ALA	C-N	5.73	1.47	1.34
2	K	2	ALA	C-N	5.71	1.47	1.34
2	M	2	ALA	C-N	5.71	1.47	1.34
2	H	2	ALA	C-N	5.64	1.47	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	218	PRO	N-CA-C	5.48	126.34	112.10
1	E	27	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	27	LEU	CA-CB-CG	5.02	126.85	115.30

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	2412	0	2350	10	0
1	B	2382	0	2323	12	0
1	C	2371	0	2279	5	0
1	D	2359	0	2270	8	0
1	E	2276	0	2202	17	0
1	F	2322	0	2198	6	0
2	H	49	0	45	6	0
2	I	49	0	45	1	0
2	J	49	0	45	2	0
2	K	49	0	45	1	0
2	L	49	0	45	0	0
2	M	49	0	45	2	0
3	A	149	0	0	0	0
3	B	152	0	0	0	0
3	C	35	0	0	0	0
3	D	31	0	0	0	0
3	E	44	0	0	0	0
3	F	47	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
All	All	14877	0	13892	57	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 2.

All (57) 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:225:GLN:HG2	1:B:266:ARG:HG3	1.70	0.72
1:B:15:ARG:HA	1:B:69:ILE:HG21	1.75	0.69
1:D:285:GLY:HA2	1:E:290:GLU:HG3	1.85	0.58
1:C:225:GLN:HB3	1:C:265:GLU:HB3	1.83	0.58
1:D:91:HIS:CD2	1:D:91:HIS:H	2.22	0.56
2:H:5:PJE:H4	2:H:6:010:H5	1.88	0.54
1:B:225:GLN:HB3	1:B:265:GLU:HB3	1.89	0.54
1:D:15:ARG:HA	1:D:69:ILE:HG21	1.88	0.54
1:F:28[A]:ASN:ND2	1:F:142:GLY:O	2.43	0.51
1:E:167:ASN:HD21	2:H:1:02J:H4	1.75	0.51
1:D:225:GLN:HG2	1:D:266:ARG:HG3	1.92	0.50
1:A:165:GLU:HB2	2:J:5:PJE:O8	2.12	0.49
1:A:40:ARG:HA	1:A:86:LEU:HG	1.95	0.49
1:A:188:GLU:HG3	2:J:4:LEU:HD22	1.95	0.47
1:A:47:ARG:O	1:A:50:GLN:HG2	2.13	0.47
1:B:110:SER:HB2	1:B:126:HIS:CE1	2.49	0.47
1:E:226:ILE:O	1:E:265:GLU:HG3	2.15	0.47
1:A:46:PHE:HB3	1:A:50:GLN:HG3	1.96	0.47
1:A:274:LEU:HA	1:A:277[B]:ASN:HD22	1.79	0.47
1:B:287:TYR:CZ	1:B:289:PHE:HA	2.50	0.47
1:E:188:GLU:HG3	2:H:4:LEU:HD22	1.97	0.46
1:F:25:SER:HB2	2:I:6:010:H1	1.97	0.46
1:F:94:ASN:HB3	1:F:97:THR:OG1	2.16	0.46
1:E:165:GLU:HB2	2:H:5:PJE:O8	2.15	0.46
1:E:150:THR:OG1	1:E:159:HIS:HE1	2.00	0.45
1:C:20:VAL:HG22	1:C:65:VAL:HG12	1.98	0.45
1:B:110:SER:HB2	1:B:126:HIS:HE1	1.81	0.45
1:E:225:GLN:HB2	1:E:265:GLU:HB3	1.99	0.45
1:E:218:PRO:HB3	1:E:221:LEU:HD23	1.99	0.44
1:D:7:LEU:HD22	1:E:7:LEU:HD22	1.99	0.44
2:M:4:LEU:HD13	2:M:4:LEU:HA	1.75	0.44
1:B:40:ARG:HA	1:B:86:LEU:HG	2.00	0.44
1:A:94:ASN:HB3	1:A:97:THR:OG1	2.18	0.44
1:A:256:LEU:HD21	1:A:299:TYR:HA	2.00	0.44
1:B:166:PHE:HB2	1:B:170:THR:OG1	2.18	0.44
1:E:31:TRP:CE2	1:E:94:ASN:HB2	2.52	0.44
1:B:94:ASN:HB3	1:B:97:THR:OG1	2.18	0.43
1:E:25:SER:HA	2:H:6:010:H1	1.99	0.43
1:A:186:ASP:OD1	1:A:186:ASP:N	2.49	0.43
1:A:49:ASP:HB2	1:B:254:MET:CE	2.48	0.43
1:E:45:LYS:HG2	2:H:4:LEU:HD23	2.01	0.43
1:D:168:ASN:OD1	1:D:168:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HG	1:B:178:GLY:HA2	2.00	0.43
1:E:254:MET:O	1:E:258:GLN:HG2	2.18	0.43
1:B:162:HIS:NE2	2:K:5:PJE:O8	2.48	0.42
1:E:40:ARG:HA	1:E:86:LEU:HG	2.01	0.42
1:E:208:TYR:CZ	1:E:267:ILE:HG13	2.55	0.42
1:C:40:ARG:HA	1:C:86:LEU:HG	2.01	0.41
1:D:10:SER:O	1:D:14:GLU:HG3	2.19	0.41
1:C:294:THR:OG1	1:C:297:MET:HG3	2.20	0.41
1:D:165:GLU:O	2:M:3:VAL:N	2.48	0.41
1:F:7:LEU:HG	1:F:126:HIS:HB2	2.02	0.41
1:E:218:PRO:HB3	1:E:221:LEU:CD2	2.51	0.41
1:F:74:LEU:HA	1:F:91:HIS:HE1	1.86	0.41
1:E:151:LEU:HD23	1:E:156:LEU:HA	2.03	0.41
1:C:94:ASN:HB3	1:C:97:THR:OG1	2.21	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	304/308 (99%)	291 (96%)	13 (4%)	0	100	100
1	B	296/308 (96%)	282 (95%)	14 (5%)	0	100	100
1	C	302/308 (98%)	286 (95%)	16 (5%)	0	100	100
1	D	296/308 (96%)	287 (97%)	9 (3%)	0	100	100
1	E	285/308 (92%)	275 (96%)	10 (4%)	0	100	100
1	F	295/308 (96%)	287 (97%)	8 (3%)	0	100	100
2	H	1/6 (17%)	1 (100%)	0	0	100	100
2	I	1/6 (17%)	1 (100%)	0	0	100	100
2	J	1/6 (17%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	1/6 (17%)	1 (100%)	0	0	100	100
2	L	1/6 (17%)	1 (100%)	0	0	100	100
2	M	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1784/1884 (95%)	1714 (96%)	70 (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	265/268 (99%)	261 (98%)	4 (2%)	65	83
1	B	263/268 (98%)	259 (98%)	4 (2%)	65	83
1	C	255/268 (95%)	252 (99%)	3 (1%)	71	87
1	D	254/268 (95%)	246 (97%)	8 (3%)	40	66
1	E	247/268 (92%)	239 (97%)	8 (3%)	39	65
1	F	248/268 (92%)	242 (98%)	6 (2%)	49	74
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	I	2/2 (100%)	0	2 (100%)	0	0
2	J	2/2 (100%)	0	2 (100%)	0	0
2	K	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	L	2/2 (100%)	0	2 (100%)	0	0
2	M	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1544/1620 (95%)	1502 (97%)	42 (3%)	44	71

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	111	MET

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	266	ARG
1	B	27	LEU
1	B	141	ASN
1	B	152	LYS
1	B	194	THR
1	C	27	LEU
1	C	122	ARG
1	C	257	SER
1	D	12	VAL
1	D	17	MET
1	D	54	MET
1	D	79	VAL
1	D	101	LYS
1	D	218	PRO
1	D	237	ASN
1	D	284	MET
1	E	4	LYS
1	E	27	LEU
1	E	110	SER
1	E	111	MET
1	E	154	LYS
1	E	169	LYS
1	E	194	THR
1	E	292	ASP
1	F	4	LYS
1	F	25	SER
1	F	38	CYS
1	F	47	ARG
1	F	99	ASP
1	F	168	ASN
2	H	4	LEU
2	I	3	VAL
2	I	4	LEU
2	J	3	VAL
2	J	4	LEU
2	K	4	LEU
2	L	3	VAL
2	L	4	LEU
2	M	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	70	GLN
1	D	94	ASN
1	E	159	HIS
1	F	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	02J	K	1	2	6,8,9	5.01	4 (66%)	4,10,12	2.14	1 (25%)
2	PJE	M	5	1,2	12,13,14	5.57	7 (58%)	12,16,18	5.43	5 (41%)
2	02J	H	1	2	6,8,9	4.98	4 (66%)	4,10,12	1.96	1 (25%)
2	02J	I	1	2	6,8,9	5.14	4 (66%)	4,10,12	3.73	2 (50%)
2	PJE	I	5	1,2	12,13,14	5.60	7 (58%)	12,16,18	5.38	5 (41%)
2	02J	L	1	2	6,8,9	4.76	4 (66%)	4,10,12	2.36	1 (25%)
2	02J	J	1	2	6,8,9	4.97	4 (66%)	4,10,12	2.07	1 (25%)
2	PJE	K	5	1,2	12,13,14	5.49	7 (58%)	12,16,18	5.63	5 (41%)
2	PJE	J	5	1,2	12,13,14	5.50	7 (58%)	12,16,18	5.54	5 (41%)
2	02J	M	1	2	6,8,9	4.89	4 (66%)	4,10,12	2.40	1 (25%)
2	PJE	H	5	1,2	12,13,14	5.54	7 (58%)	12,16,18	5.53	5 (41%)
2	PJE	L	5	1,2	12,13,14	5.55	7 (58%)	12,16,18	5.54	5 (41%)

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	02J	K	1	2	-	0/0/2/4	0/1/1/1
2	PJE	M	5	1,2	-	1/7/18/19	0/1/1/1
2	02J	H	1	2	-	0/0/2/4	0/1/1/1
2	02J	I	1	2	-	0/0/2/4	0/1/1/1
2	PJE	I	5	1,2	-	1/7/18/19	0/1/1/1
2	02J	L	1	2	-	0/0/2/4	0/1/1/1
2	02J	J	1	2	-	0/0/2/4	0/1/1/1
2	PJE	K	5	1,2	-	1/7/18/19	0/1/1/1
2	PJE	J	5	1,2	-	2/7/18/19	0/1/1/1
2	02J	M	1	2	-	0/0/2/4	0/1/1/1
2	PJE	H	5	1,2	-	1/7/18/19	0/1/1/1
2	PJE	L	5	1,2	-	1/7/18/19	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	5	PJE	C27-C28	-11.25	1.35	1.53
2	H	5	PJE	C27-C28	-11.20	1.35	1.53
2	L	5	PJE	C27-C28	-11.19	1.35	1.53
2	M	5	PJE	C27-C28	-11.15	1.35	1.53
2	J	5	PJE	C27-C28	-11.11	1.35	1.53
2	K	5	PJE	C27-C28	-11.01	1.36	1.53
2	M	5	PJE	O8-C29	10.49	1.44	1.23
2	I	5	PJE	O8-C29	10.48	1.44	1.23
2	H	5	PJE	O8-C29	10.41	1.44	1.23
2	L	5	PJE	O8-C29	10.40	1.44	1.23
2	J	5	PJE	O8-C29	10.38	1.44	1.23
2	K	5	PJE	O8-C29	10.38	1.44	1.23
2	I	1	02J	C3-C41	9.18	1.58	1.48
2	K	1	02J	C3-C41	8.63	1.57	1.48
2	H	1	02J	C3-C41	8.58	1.57	1.48
2	J	1	02J	C3-C41	8.54	1.57	1.48
2	M	1	02J	C3-C41	8.39	1.57	1.48
2	L	1	02J	C3-C41	8.23	1.57	1.48
2	L	5	PJE	C28-N6	7.71	1.62	1.46
2	K	5	PJE	C28-N6	7.70	1.62	1.46
2	M	5	PJE	C28-N6	7.69	1.62	1.46
2	J	5	PJE	C28-N6	7.64	1.62	1.46
2	I	5	PJE	C28-N6	7.64	1.62	1.46
2	H	5	PJE	C28-N6	7.62	1.62	1.46
2	K	1	02J	C6-C5	6.75	1.56	1.48
2	I	1	02J	C6-C5	6.74	1.56	1.48
2	J	1	02J	C6-C5	6.74	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	02J	C6-C5	6.73	1.56	1.48
2	M	1	02J	C6-C5	6.72	1.56	1.48
2	L	1	02J	C6-C5	6.49	1.56	1.48
2	I	5	PJE	C26-C29	5.10	1.58	1.52
2	M	5	PJE	C26-C29	5.02	1.58	1.52
2	L	5	PJE	C26-C29	4.95	1.58	1.52
2	I	5	PJE	C19-C20	4.87	1.56	1.50
2	M	5	PJE	C19-C20	4.83	1.56	1.50
2	H	5	PJE	C26-C29	4.78	1.58	1.52
2	H	5	PJE	C19-C20	4.73	1.56	1.50
2	L	5	PJE	C19-C20	4.71	1.56	1.50
2	J	5	PJE	C26-C29	4.69	1.57	1.52
2	K	5	PJE	C26-C29	4.69	1.57	1.52
2	K	5	PJE	C19-C20	4.60	1.56	1.50
2	J	5	PJE	C19-C20	4.55	1.56	1.50
2	I	5	PJE	C21-C22	4.38	1.57	1.44
2	M	5	PJE	C21-C22	4.30	1.57	1.44
2	H	5	PJE	C21-C22	4.29	1.57	1.44
2	L	5	PJE	C21-C22	4.24	1.57	1.44
2	J	5	PJE	C21-C22	4.24	1.57	1.44
2	K	5	PJE	C21-C22	4.20	1.57	1.44
2	I	1	02J	C4-C3	4.11	1.47	1.39
2	K	1	02J	C4-C3	4.07	1.47	1.39
2	H	1	02J	C4-C3	4.06	1.47	1.39
2	J	1	02J	C4-C3	4.05	1.47	1.39
2	M	1	02J	C4-C3	4.03	1.47	1.39
2	L	1	02J	C4-C3	3.88	1.46	1.39
2	K	1	02J	C4-C5	3.52	1.44	1.39
2	J	1	02J	C4-C5	3.46	1.44	1.39
2	H	1	02J	C4-C5	3.45	1.44	1.39
2	M	1	02J	C4-C5	3.24	1.44	1.39
2	I	1	02J	C4-C5	3.19	1.44	1.39
2	L	1	02J	C4-C5	3.14	1.43	1.39
2	K	5	PJE	C25-C26	-2.71	1.47	1.53
2	L	5	PJE	C25-C26	-2.71	1.47	1.53
2	H	5	PJE	C25-C26	-2.68	1.47	1.53
2	M	5	PJE	C25-C26	-2.67	1.47	1.53
2	I	5	PJE	C25-C26	-2.67	1.47	1.53
2	J	5	PJE	C25-C26	-2.65	1.47	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	5	PJE	O8-C29-C26	-14.04	109.72	126.23
2	H	5	PJE	O8-C29-C26	-13.97	109.80	126.23
2	L	5	PJE	O8-C29-C26	-13.82	109.98	126.23
2	J	5	PJE	O8-C29-C26	-13.73	110.09	126.23
2	I	5	PJE	O8-C29-C26	-13.68	110.15	126.23
2	M	5	PJE	O8-C29-C26	-13.45	110.41	126.23
2	L	5	PJE	O8-C29-N6	-11.07	110.18	125.54
2	I	5	PJE	O8-C29-N6	-10.95	110.35	125.54
2	M	5	PJE	O8-C29-N6	-10.82	110.52	125.54
2	J	5	PJE	O8-C29-N6	-10.77	110.60	125.54
2	H	5	PJE	O8-C29-N6	-10.73	110.65	125.54
2	K	5	PJE	O8-C29-N6	-10.48	110.99	125.54
2	I	1	02J	O42-C41-C3	-6.99	117.60	124.22
2	K	5	PJE	C19-C20-C21	-6.89	114.56	124.41
2	J	5	PJE	C19-C20-C21	-6.02	115.81	124.41
2	M	5	PJE	C19-C20-C21	-5.75	116.20	124.41
2	H	5	PJE	C19-C20-C21	-5.72	116.24	124.41
2	L	5	PJE	C19-C20-C21	-5.65	116.34	124.41
2	I	5	PJE	C19-C20-C21	-4.38	118.15	124.41
2	M	1	02J	O42-C41-C3	-4.11	120.33	124.22
2	L	1	02J	O42-C41-C3	-4.02	120.42	124.22
2	K	1	02J	O42-C41-C3	-3.47	120.93	124.22
2	J	5	PJE	C28-N6-C29	-3.37	107.22	113.84
2	K	5	PJE	C28-N6-C29	-3.32	107.32	113.84
2	J	1	02J	O42-C41-C3	-3.30	121.09	124.22
2	M	5	PJE	C28-N6-C29	-3.14	107.67	113.84
2	L	5	PJE	C28-N6-C29	-3.08	107.79	113.84
2	H	1	02J	O42-C41-C3	-3.01	121.37	124.22
2	H	5	PJE	C28-N6-C29	-2.99	107.96	113.84
2	I	5	PJE	C28-N6-C29	-2.95	108.04	113.84
2	K	5	PJE	C27-C28-N6	2.63	107.28	103.43
2	J	5	PJE	C27-C28-N6	2.50	107.09	103.43
2	M	5	PJE	C27-C28-N6	2.49	107.08	103.43
2	H	5	PJE	C27-C28-N6	2.44	107.00	103.43
2	L	5	PJE	C27-C28-N6	2.35	106.87	103.43
2	I	5	PJE	C27-C28-N6	2.25	106.72	103.43
2	I	1	02J	C4-C3-N2	-2.17	106.01	109.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	5	PJE	C20-C21-C22-O7

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Mol	Chain	Res	Type	Atoms
2	I	5	PJE	C20-C21-C22-O7
2	J	5	PJE	C20-C21-C22-O7
2	K	5	PJE	C20-C21-C22-O7
2	L	5	PJE	C20-C21-C22-O7
2	M	5	PJE	C20-C21-C22-O7
2	J	5	PJE	C25-C19-C20-C21

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	02J	1	0
2	K	5	PJE	1	0
2	J	5	PJE	1	0
2	H	5	PJE	2	0

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

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	304/308 (98%)	-0.31	0 100 100	24, 40, 66, 85	0
1	B	299/308 (97%)	-0.39	2 (0%) 87 86	24, 39, 69, 100	0
1	C	304/308 (98%)	0.24	18 (5%) 22 17	40, 64, 94, 108	0
1	D	302/308 (98%)	-0.03	7 (2%) 60 54	44, 63, 89, 106	0
1	E	291/308 (94%)	0.04	9 (3%) 49 42	38, 58, 93, 116	0
1	F	298/308 (96%)	0.13	14 (4%) 31 25	37, 65, 102, 112	0
2	H	3/6 (50%)	-0.05	0 100 100	48, 48, 49, 55	0
2	I	3/6 (50%)	0.12	0 100 100	72, 72, 77, 92	0
2	J	3/6 (50%)	-0.41	0 100 100	37, 37, 40, 52	0
2	K	3/6 (50%)	-0.00	0 100 100	32, 32, 33, 42	0
2	L	3/6 (50%)	-0.10	0 100 100	55, 55, 56, 61	0
2	M	3/6 (50%)	1.30	1 (33%) 0 0	61, 61, 69, 79	0
All	All	1816/1884 (96%)	-0.05	51 (2%) 53 46	24, 55, 92, 116	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	71	GLY	4.1
1	F	92	THR	4.0
1	E	218	PRO	3.9
1	E	220	TRP	3.9
1	C	58	ALA	3.8
1	F	91	HIS	3.8
1	F	90	VAL	3.7
1	F	72	ILE	3.7
1	C	65	VAL	3.5
1	C	79	VAL	3.5
1	F	77	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	207	LEU	3.4
1	E	0	SER	3.4
1	C	88	LEU	3.4
1	C	304	ILE	3.4
1	F	26	ALA	3.3
1	D	278	ARG	3.3
1	C	226	ILE	3.2
1	C	217	ARG	3.2
1	E	72	ILE	3.0
1	D	91	HIS	3.0
1	F	31	TRP	2.8
1	E	222	ALA	2.8
1	F	20	VAL	2.8
1	D	77	GLN	2.7
2	M	2	ALA	2.7
1	C	55	VAL	2.7
1	D	90	VAL	2.7
1	F	34	ASN	2.6
1	E	208	TYR	2.5
1	C	258	GLN	2.4
1	C	91	HIS	2.4
1	C	63	PHE	2.4
1	D	190	ILE	2.4
1	F	276	THR	2.4
1	C	90	VAL	2.3
1	D	74	LEU	2.3
1	C	61	ARG	2.3
1	F	277	ASN	2.2
1	C	64	ILE	2.2
1	C	72	ILE	2.2
1	D	72	ILE	2.2
1	E	238	ASN	2.2
1	B	215	ASP	2.2
1	F	93	ASN	2.1
1	E	274	LEU	2.1
1	C	69	ILE	2.1
1	F	304	ILE	2.1
1	C	31	TRP	2.1
1	C	78	SER	2.1
1	B	304	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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(\AA^2)	Q<0.9
2	02J	I	1	8/9	0.44	0.63	92,109,116,120	0
2	02J	J	1	8/9	0.63	0.40	68,90,106,109	0
2	02J	H	1	8/9	0.73	0.47	84,92,111,115	0
2	02J	M	1	8/9	0.78	0.61	90,98,116,119	0
2	02J	K	1	8/9	0.83	0.33	72,82,92,99	0
2	PJE	M	5	13/14	0.92	0.17	44,59,81,84	0
2	PJE	I	5	13/14	0.94	0.13	66,78,99,103	0
2	PJE	L	5	13/14	0.95	0.18	45,53,74,82	0
2	PJE	J	5	13/14	0.95	0.15	35,39,59,65	0
2	PJE	K	5	13/14	0.96	0.15	23,36,48,49	0
2	02J	L	1	8/9	0.96	0.23	55,65,83,86	0
2	PJE	H	5	13/14	0.96	0.20	41,49,60,65	0

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.