wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 05:43 PM JST

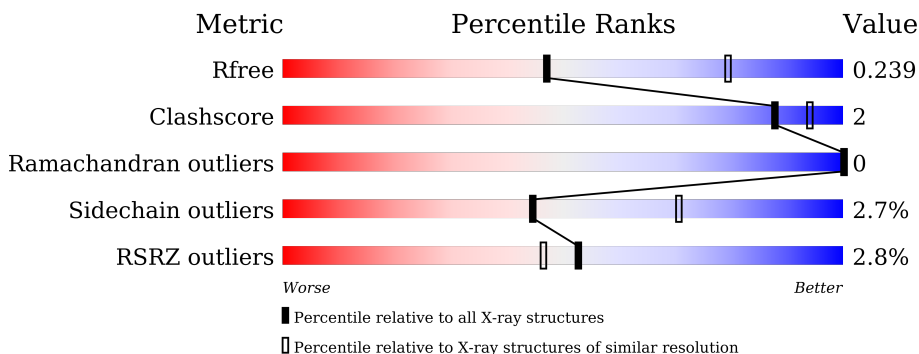|		
PDB ID	:	7WKU
Title	:	Structure of PDCoV Mpro in complex with an inhibitor
Authors	:	Wang, F.H.; Yang, H.T.
Deposited on	:	2022-01-11
Resolution	:	2.60 Å(reported)

---

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.
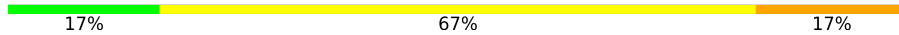
Metric	Percentile Ranks	Value
Rfree		0.239
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		2.7%
RSRZ outliers		2.8%

Worse ———————————— Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
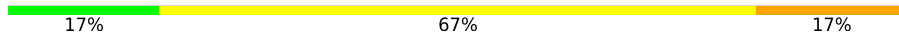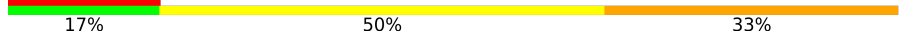
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	6% 94% · ·
1	D	308	2% 92% 6% ·
1	E	308	3% 84% 9% · 6%
1	F	308	5% 92% 5% ·

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	6	67% 33%
2	I	6	83% 17%
2	J	6	17% 33% 50%
2	K	6	17% 67% 17%
2	L	6	17% 67% 17%
2	M	6	17% 17% 50% 33%

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

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

Continued on next page...

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Peptidase C30
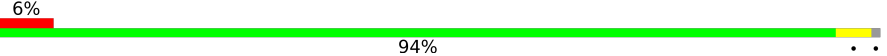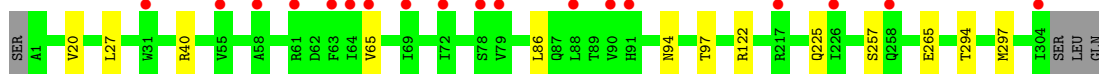
Chain A:

- Molecule 1: Peptidase C30

Chain B:
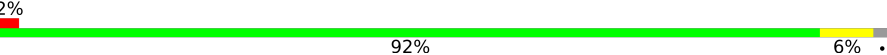
- Molecule 1: Peptidase C30

Chain C:

- Molecule 1: Peptidase C30

Chain D:

- Molecule 1: Peptidase C30

Chain E:

M254 Q258 E265 R266 I267 L274 T275 T276 ASN ARG ASP GLY ALA CYS ILE MET GLY SER TYR ASP F289 E290 C291 D292 P303 ILE SER LEU GLN

• Molecule 1: Peptidase C30

Chain F:

5%

92%   5%

S0 K4 L7 V20 S25 A26 L27 N28 W31 N34 C38 R47 G71 I72 Q73 L74 Q77 V90 H91 T92 N93 N94 T97 P98 D99 H126 G142 N168 R261 T276 N277 R278 ASP GLY ALA CYS ILE MET GLY S286 I304 SER
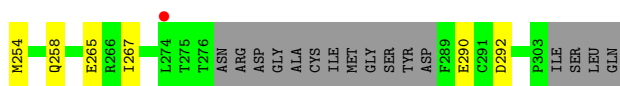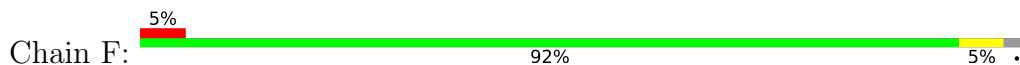
LEU GLN

• 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 H:

67%   33%

O2J1 A2 V3 L4 PJE5 0106

• 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 I:

83%   17%

O2J1 A2 V3 L4 PJE5 0106

• 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 J:

17%   33%   50%

O2J1 A2 V3 L4 PJE5 0106

• 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 K:

17%   67%   17%

O2J1 A2 V3 L4 PJE5 0106

• 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 L:

17%   67%   17%

O2J1 A2 V3 L4 PJE5 O106

• 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%

17%   50%   33%

O2J1 A2 V3 L4 PJE5 O106
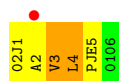
4   Data and refinement statistics   ⓘ

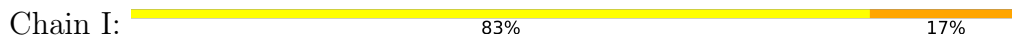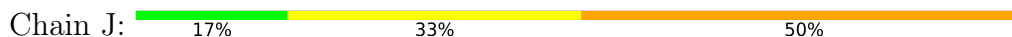| Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	122.29Å 122.29Å 289.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 2.60 49.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.74-2.60) 99.5 (49.74-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

---

[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 02J, 010, PJE

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%)

The worst 5 of 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

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	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	16	0
1	F	2322	0	2198	6	0
2	H	49	0	41	4	0
2	I	49	0	41	1	0
2	J	49	0	41	2	0
2	K	49	0	41	1	0
2	L	49	0	41	0	0
2	M	49	0	41	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	13868	55	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.

The worst 5 of 55 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	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	3/6 (50%)	3 (100%)	0	0	100	100
2	I	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	J	3/6 (50%)	3 (100%)	0	0	100	100
2	K	3/6 (50%)	3 (100%)	0	0	100	100
2	L	3/6 (50%)	3 (100%)	0	0	100	100
2	M	3/6 (50%)	3 (100%)	0	0	100	100
All	All	1796/1884 (95%)	1725 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	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

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	25	SER
2	I	4	LEU
1	F	38	CYS
1	F	168	ASN
2	J	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 (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PJE	I	5	2,1	-	1/7/18/19	0/1/1/1
2	PJE	J	5	2,1	-	2/7/18/19	0/1/1/1
2	02J	I	1	2	-	0/0/2/4	0/1/1/1
2	PJE	L	5	2,1	-	1/7/18/19	0/1/1/1
2	PJE	M	5	2,1	-	1/7/18/19	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PJE	K	5	2,1	-	1/7/18/19	0/1/1/1
2	PJE	H	5	2,1	-	1/7/18/19	0/1/1/1
2	02J	K	1	2	-	0/0/2/4	0/1/1/1
2	02J	L	1	2	-	0/0/2/4	0/1/1/1
2	02J	M	1	2	-	0/0/2/4	0/1/1/1
2	02J	J	1	2	-	0/0/2/4	0/1/1/1
2	02J	H	1	2	-	0/0/2/4	0/1/1/1

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	5	PJE	O-C-C21-C20
2	I	5	PJE	O-C-C21-C20
2	J	5	PJE	O-C-C21-C20
2	K	5	PJE	O-C-C21-C20
2	L	5	PJE	O-C-C21-C20

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

Continued on next page...

Continued from previous page...

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

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, 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

The worst 5 of 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

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	02J	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 ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.