



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 08:50 am GMT

PDB ID : 3D23  
Title : Main protease of HCoV-HKU1  
Authors : Zhao, Q.; Chen, C.; Li, S.; Zou, Y.  
Deposited on : 2008-05-07  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

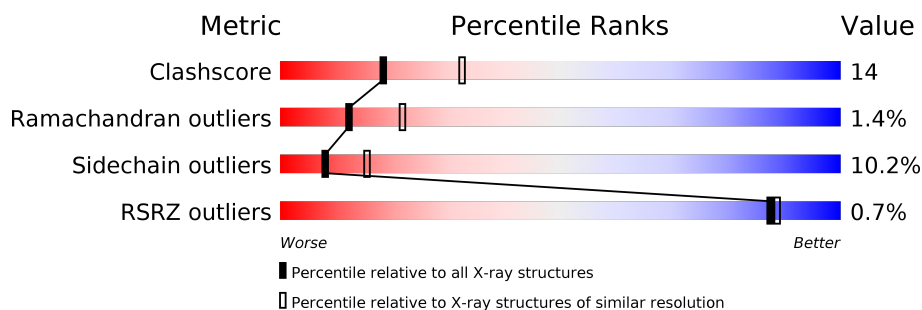
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	302	<div> <div>73% 21% 5% .</div> </div>
1	B	302	<div> <div>2% 71% 23% 6%</div> </div>
1	C	302	<div> <div>72% 23% . .</div> </div>
1	D	302	<div> <div>75% 20% . .</div> </div>
2	E	6	<div> <div>50% 33% 17%</div> </div>
2	F	6	<div> <div>67% 17% 17%</div> </div>
2	G	6	<div> <div>50% 33% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	6	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (67%), yellow (17%), and orange (17%). The percentages are labeled below the segments.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9579 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	301	Total	C	N	O	S	0	1	0
			2312	1472	377	441	22			
1	A	299	Total	C	N	O	S	0	0	0
			2288	1461	372	433	22			
1	C	298	Total	C	N	O	S	0	0	0
			2285	1457	372	434	22			
1	D	299	Total	C	N	O	S	0	0	0
			2290	1460	372	436	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ALA	-	EXPRESSION TAG	UNP Q5MQD2
B	0	SER	-	EXPRESSION TAG	UNP Q5MQD2
A	-1	ALA	-	EXPRESSION TAG	UNP Q5MQD2
A	0	SER	-	EXPRESSION TAG	UNP Q5MQD2
C	-1	ALA	-	EXPRESSION TAG	UNP Q5MQD2
C	0	SER	-	EXPRESSION TAG	UNP Q5MQD2
D	-1	ALA	-	EXPRESSION TAG	UNP Q5MQD2
D	0	SER	-	EXPRESSION TAG	UNP Q5MQD2

- 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	F	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	E	6	Total	C	N	O	0	0	0
			49	35	6	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	0
			49	35	6	8			

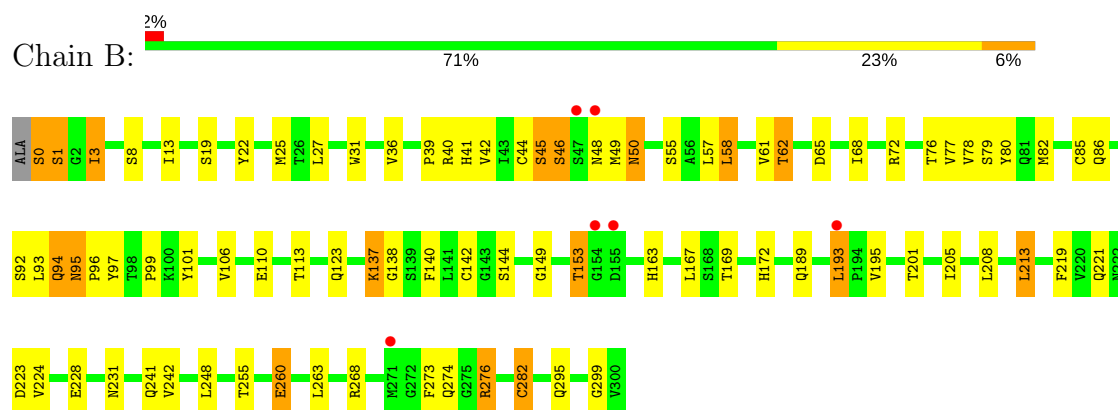
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	56	Total	O	0	0
			56	56		
3	A	56	Total	O	0	0
			56	56		
3	C	41	Total	O	0	0
			41	41		
3	D	55	Total	O	0	0
			55	55		

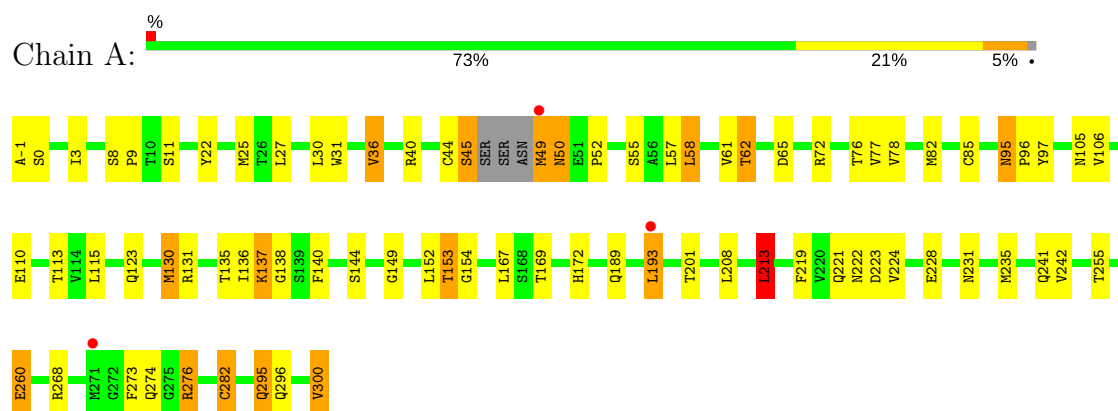
### 3 Residue-property plots [i](#)

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

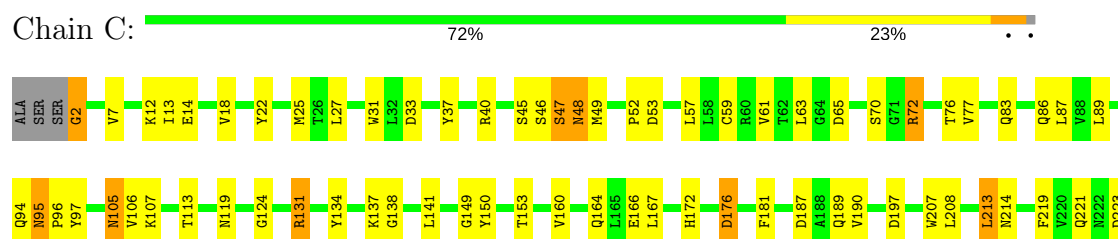
#### • Molecule 1: 3C-like proteinase



#### • Molecule 1: 3C-like proteinase



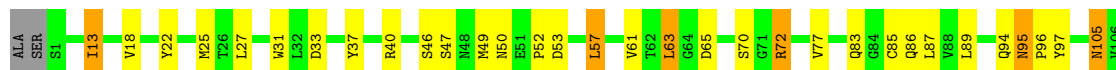
#### • Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase

Chain D: 75% 20%



- 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% 17% 17%



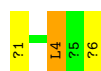
- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE

Chain F: 67% 17% 17%



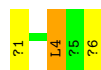
- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE

Chain E: 50% 33% 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 G: 50% 33% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.77Å 91.77Å 187.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 41.04 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.50) 63.2 (41.04-1.97)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.77 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.229 , 0.285 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0991e-14. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.99	2/2338 (0.1%)	0.99	4/3181 (0.1%)
1	B	1.02	3/2363 (0.1%)	0.94	0/3216
1	C	1.07	6/2336 (0.3%)	1.01	7/3179 (0.2%)
1	D	1.03	0/2341	0.99	5/3185 (0.2%)
2	E	0.65	0/19	1.99	0/25
2	F	0.59	0/19	1.38	0/25
2	G	0.70	0/19	1.82	0/25
2	H	0.65	0/19	1.50	0/25
All	All	1.03	11/9454 (0.1%)	0.99	16/12861 (0.1%)

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	1	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	TYR	CD1-CE1	7.23	1.50	1.39
1	A	44	CYS	CB-SG	-6.63	1.71	1.82
1	C	166	GLU	CB-CG	6.38	1.64	1.52
1	B	44	CYS	CB-SG	-5.58	1.72	1.81
1	B	137	LYS	CE-NZ	5.56	1.62	1.49

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLN	CB-CA-C	18.50	147.41	110.40
1	A	50	ASN	N-CA-C	6.52	128.60	111.00
1	D	268	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	164	GLN	N-CA-C	6.09	127.44	111.00
1	D	268	ARG	NE-CZ-NH2	-5.81	117.39	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	274	GLN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	MET	Peptide

## 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	2288	0	2249	68	0
1	B	2312	0	2269	76	0
1	C	2285	0	2242	71	0
1	D	2290	0	2246	58	0
2	E	49	0	45	11	0
2	F	49	0	45	6	0
2	G	49	0	45	9	0
2	H	49	0	45	6	0
3	A	56	0	0	3	0
3	B	56	0	0	2	0
3	C	41	0	0	5	0
3	D	55	0	0	5	0
All	All	9579	0	9186	265	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 14.

The worst 5 of 265 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.06	1.15
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.13	1.07
1:B:189:GLN:HE21	2:H:4:LEU:H	1.08	0.99
1:B:0:SER:O	1:B:1:SER:HB3	1.64	0.97
1:A:130:MET:HA	1:A:130:MET:HE3	1.46	0.97

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	295/302 (98%)	280 (95%)	12 (4%)	3 (1%)	17	31
1	B	300/302 (99%)	276 (92%)	15 (5%)	9 (3%)	5	7
1	C	296/302 (98%)	272 (92%)	22 (7%)	2 (1%)	24	42
1	D	297/302 (98%)	272 (92%)	21 (7%)	4 (1%)	13	23
2	E	1/6 (17%)	1 (100%)	0	0	100	100
2	F	1/6 (17%)	1 (100%)	0	0	100	100
2	G	1/6 (17%)	1 (100%)	0	0	100	100
2	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1192/1232 (97%)	1104 (93%)	70 (6%)	18 (2%)	12	20

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	SER
1	B	50[A]	ASN
1	B	50[B]	ASN
1	B	299	GLY
1	C	47	SER

### 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	254/258 (98%)	226 (89%)	28 (11%)	7	13
1	B	259/258 (100%)	232 (90%)	27 (10%)	8	15
1	C	255/258 (99%)	232 (91%)	23 (9%)	10	20
1	D	255/258 (99%)	232 (91%)	23 (9%)	10	20
2	E	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	F	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	G	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1031/1040 (99%)	926 (90%)	105 (10%)	8	15

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
1	C	72	ARG
1	D	235	MET
1	A	208	LEU
1	A	295	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	C	86	GLN
1	D	221	GLN
1	A	241	GLN
1	A	295	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	E	1	2	6,8,9	2.76	3 (50%)	4,10,12	2.79	3 (75%)
2	PJE	E	5	2	12,13,14	4.30	6 (50%)	10,16,18	3.33	4 (40%)
2	02J	F	1	2	6,8,9	1.52	2 (33%)	4,10,12	2.78	1 (25%)
2	PJE	F	5	2	12,13,14	2.62	4 (33%)	10,16,18	1.48	1 (10%)
2	02J	G	1	2	6,8,9	1.83	3 (50%)	4,10,12	0.99	0
2	PJE	G	5	2	12,13,14	2.30	3 (25%)	10,16,18	2.49	4 (40%)
2	02J	H	1	2	6,8,9	1.49	2 (33%)	4,10,12	3.20	1 (25%)
2	PJE	H	5	2	12,13,14	3.01	4 (33%)	10,16,18	2.54	4 (40%)

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	E	1	2	-	0/0/2/4	0/1/1/1
2	PJE	E	5	2	-	1/7/18/19	0/1/1/1
2	02J	F	1	2	-	0/0/2/4	0/1/1/1
2	PJE	F	5	2	-	1/7/18/19	0/1/1/1
2	02J	G	1	2	-	0/0/2/4	0/1/1/1
2	PJE	G	5	2	-	1/7/18/19	0/1/1/1
2	02J	H	1	2	-	0/0/2/4	0/1/1/1
2	PJE	H	5	2	-	1/7/18/19	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	PJE	C19-C20	2.08	1.52	1.50
2	G	5	PJE	O8-C29	2.20	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	PJE	C25-C26	2.25	1.59	1.53
2	G	1	02J	C6-C5	2.29	1.51	1.48
2	H	1	02J	C6-C5	2.31	1.51	1.48

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	PJE	C27-C28-N6	-8.93	89.40	103.48
2	H	5	PJE	C27-C28-N6	-6.04	93.96	103.48
2	H	1	02J	O42-C41-C3	-5.92	119.50	124.30
2	G	5	PJE	O8-C29-C26	-5.35	119.96	126.26
2	F	1	02J	O42-C41-C3	-4.81	120.40	124.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	02J	3	0
2	G	1	02J	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/302 (99%)	-0.40	3 (1%) 82 84	22, 36, 60, 82	0
1	B	301/302 (99%)	-0.37	6 (1%) 65 67	21, 36, 61, 84	0
1	C	298/302 (98%)	-0.56	0 100 100	19, 36, 61, 72	0
1	D	299/302 (99%)	-0.56	0 100 100	21, 36, 62, 72	0
2	E	3/6 (50%)	-0.37	0 100 100	27, 27, 28, 35	0
2	F	3/6 (50%)	-0.98	0 100 100	36, 36, 37, 42	0
2	G	3/6 (50%)	-0.61	0 100 100	26, 26, 27, 31	0
2	H	3/6 (50%)	-0.79	0 100 100	38, 38, 39, 42	0
All	All	1209/1232 (98%)	-0.47	9 (0%) 87 88	19, 36, 61, 84	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	3.8
1	A	271	MET	3.6
1	B	48	ASN	3.2
1	B	155	ASP	2.7
1	B	271	MET	2.6

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	02J	G	1	8/9	0.89	0.16	49,53,56,57	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	02J	E	1	8/9	0.89	0.18	51,55,58,59	0
2	02J	F	1	8/9	0.89	0.23	47,57,60,62	0
2	02J	H	1	8/9	0.90	0.22	46,57,60,61	0
2	PJE	E	5	13/14	0.91	0.24	30,37,50,52	0
2	PJE	G	5	13/14	0.91	0.19	19,25,50,50	0
2	PJE	F	5	13/14	0.92	0.12	30,36,62,65	0
2	PJE	H	5	13/14	0.92	0.14	30,38,64,66	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.