



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID : 4J04  
Title : Crystal structure of hcv ns5b polymerase in complex with 4-CHLORO-2-[(2,4,5-TRICHLOROPHENYL)SULFONYL]AMINO}BENZOIC ACID  
Authors : Coulombe, R.  
Deposited on : 2013-01-30  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

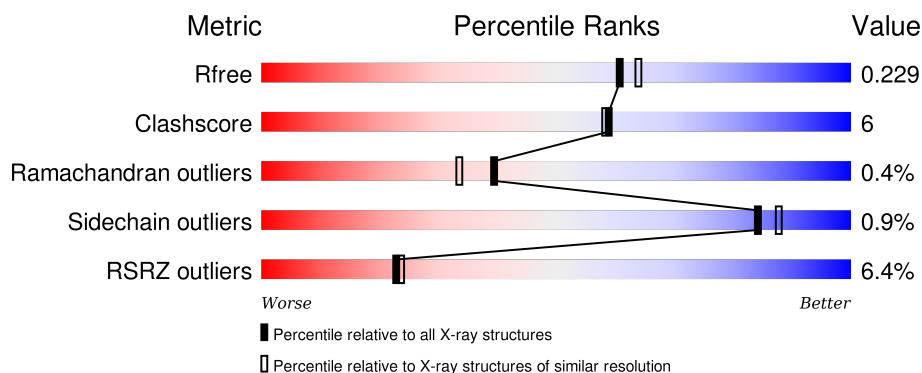
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

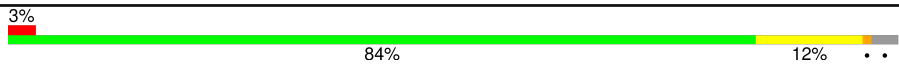
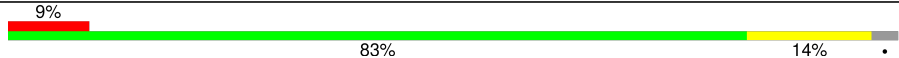
The reported resolution of this entry is 2.00 Å.

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	576	
1	B	576	

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	1JF	A	601	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9434 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.

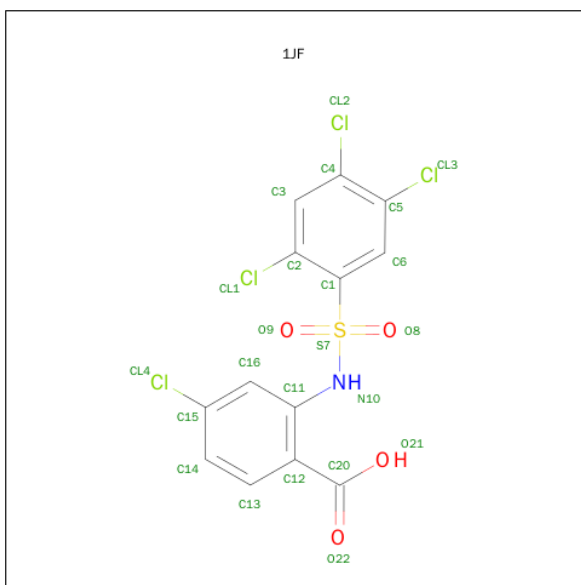
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	558	Total	C	N	O	S	0	0	0
			4346	2737	768	809	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is 4-CHLORO-2-([(2,4,5-TRICHLOROPHENYL)SULFONYL]AMINO)BENZOIC ACID (three-letter code: 1JF) (formula: C<sub>13</sub>H<sub>7</sub>Cl<sub>4</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	C 13	Cl 4	N 1	O 4	S 1	0	0
2	A	1	Total 23	C 13	Cl 4	N 1	O 4	S 1	0	0
2	B	1	Total 23	C 13	Cl 4	N 1	O 4	S 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

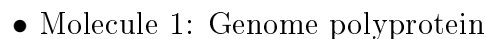
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	364	Total	O	0	0
			364	364		
4	B	293	Total	O	0	0
			293	293		



- Molecule 1: Genome polyprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.97Å 107.97Å 133.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 38.35 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.00) 98.3 (38.35-1.99)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.00Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.206 , 0.232 0.203 , 0.229	Depositor DCC
$R_{free}$ test set	10325 reflections (11.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.1	EDS
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 103030 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN, 1JF

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	0.28	0/4453	0.58	0/6044
1	B	0.26	0/4440	0.55	0/6025
All	All	0.27	0/8893	0.57	0/12069

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

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	4358	0	4369	52	0
1	B	4346	0	4357	52	0
2	A	46	0	11	0	0
2	B	23	0	5	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	364	0	0	7	0
4	B	293	0	0	3	0
All	All	9434	0	8742	101	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 6.



All (101) 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:106:LYS:HE3	1:A:106:LYS:HA	1.46	0.94
1:A:505:ARG:HB3	1:A:505:ARG:HH11	1.47	0.79
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.22	0.70
1:B:106:LYS:NZ	1:B:110:ASN:HD21	1.93	0.67
1:A:230:GLU:HG2	4:A:914:HOH:O	1.95	0.66
1:A:309:GLN:O	1:A:324:CYS:HB2	1.95	0.66
1:B:85:ILE:HD13	1:B:116:VAL:HG13	1.82	0.62
1:B:309:GLN:O	1:B:324:CYS:HB2	2.01	0.61
1:B:394:ARG:O	1:B:398:GLU:HG3	1.99	0.61
1:B:337:ARG:O	1:B:341:GLU:HG3	2.02	0.60
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.84	0.59
1:A:106:LYS:HA	1:A:106:LYS:CE	2.29	0.59
1:B:470:SER:O	1:B:474:LEU:HG	2.02	0.59
1:B:27:SER:HB2	1:B:400:ALA:HB2	1.86	0.58
1:A:143:GLU:OE1	1:A:158:ARG:HD3	2.04	0.58
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.85	0.58
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.86	0.57
1:A:85:ILE:HG12	1:A:173:MET:SD	2.46	0.56
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.87	0.56
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.88	0.56
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.87	0.56
1:B:40:THR:HB	1:B:157:ALA:HB2	1.88	0.55
1:A:440:GLU:HG2	1:A:457:LEU:CD1	2.38	0.54
1:A:40:THR:HB	1:A:157:ALA:HB2	1.90	0.53
1:A:100:LYS:HE3	4:A:998:HOH:O	2.07	0.53
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.89	0.53
1:B:346:TYR:O	1:B:347:SER:HB3	2.08	0.53
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.49	0.53
1:B:439:LEU:HB3	1:B:457:LEU:HD21	1.91	0.53
1:B:465:ARG:NH1	1:B:545:LEU:HB3	2.25	0.51
1:A:234:ARG:HD3	1:B:247:PRO:HG3	1.93	0.51
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.93	0.51
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.91	0.51
1:B:459:LEU:O	1:B:463:ILE:HG13	2.11	0.51
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.93	0.50
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.93	0.50
1:A:361:GLU:HG3	1:A:370:VAL:O	2.12	0.50
1:A:57:LEU:HD23	1:A:57:LEU:C	2.32	0.50
1:A:247:PRO:HG3	1:B:234:ARG:HD3	1.94	0.49
1:B:178:VAL:HG23	4:B:916:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:HIS:NE2	4:A:702:HOH:O	2.35	0.49
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.94	0.49
1:B:434:LEU:HD21	1:B:511:LEU:HD23	1.94	0.49
1:B:22:PRO:HB2	1:B:25:PRO:CD	2.42	0.49
1:A:394:ARG:O	1:A:398:GLU:HG3	2.13	0.49
1:B:191:TYR:O	1:B:194:GLN:HG2	2.13	0.47
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.95	0.47
1:A:248:GLU:HG3	4:A:704:HOH:O	2.15	0.47
1:A:461:GLN:HB2	1:A:545:LEU:HD11	1.95	0.47
1:B:83:LEU:HB2	1:B:173:MET:HA	1.97	0.47
1:B:508:ARG:HD2	1:B:526:PHE:O	2.15	0.47
1:B:31:LEU:O	1:B:31:LEU:HD12	2.15	0.46
1:B:534:LEU:HD12	1:B:534:LEU:N	2.31	0.46
1:A:306:ALA:O	1:A:307:LYS:HB2	2.15	0.46
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.55	0.46
1:A:251:GLN:NE2	1:B:254:ARG:HG2	2.31	0.46
1:A:184:GLN:HB2	4:A:763:HOH:O	2.15	0.46
1:A:485:VAL:O	1:A:489:LEU:HG	2.16	0.46
1:A:440:GLU:HG2	1:A:457:LEU:HD11	1.99	0.45
1:A:52:VAL:HB	1:A:226:SER:OG	2.17	0.45
1:B:106:LYS:HZ3	1:B:110:ASN:HD21	1.64	0.45
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.99	0.45
1:A:505:ARG:NH1	1:A:505:ARG:HB3	2.25	0.45
1:B:131:GLU:HG3	4:B:939:HOH:O	2.16	0.45
1:B:496:PRO:HG2	1:B:499:THR:HG23	1.98	0.45
1:B:84:SER:OG	1:B:87:GLU:HG3	2.17	0.45
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.99	0.45
1:B:22:PRO:HB2	1:B:25:PRO:HG3	1.98	0.44
1:A:233:ILE:HD13	1:A:262:ILE:HA	1.99	0.44
1:A:24:ASN:HB3	1:A:27:SER:OG	2.17	0.44
1:B:501:ARG:HE	1:B:505:ARG:NH2	2.14	0.44
1:B:501:ARG:HE	1:B:505:ARG:HH21	1.63	0.44
1:B:466:LEU:HD21	1:B:547:LEU:HD13	2.00	0.44
1:A:455:GLU:HB3	4:A:838:HOH:O	2.18	0.43
1:A:176:TYR:OH	1:A:562:HIS:HE1	2.01	0.43
1:A:313:MET:SD	1:A:322:VAL:HG22	2.58	0.43
1:A:184:GLN:HG3	4:A:876:HOH:O	2.19	0.43
1:B:233:ILE:HD13	1:B:261:TYR:O	2.19	0.43
1:B:80:ALA:HB3	1:B:245:LEU:HD23	2.01	0.42
1:B:485:VAL:O	1:B:489:LEU:HG	2.18	0.42
1:A:172:LYS:HE3	1:A:560:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TRP:CE2	1:A:401:ARG:HD2	2.54	0.42
1:B:527:ASN:OD1	1:B:534:LEU:HD13	2.19	0.42
1:A:545:LEU:HB3	1:A:547:LEU:HD13	2.02	0.42
1:A:470:SER:O	1:A:474:LEU:HG	2.19	0.42
1:B:501:ARG:NE	1:B:505:ARG:HH21	2.17	0.42
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.42
1:B:527:ASN:HD21	1:B:534:LEU:H	1.67	0.41
1:A:148:GLN:HA	1:A:149:PRO:HD3	1.91	0.41
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.60	0.41
1:B:82:LEU:HD13	1:B:249:ALA:HB2	2.02	0.41
1:B:501:ARG:O	1:B:505:ARG:HG3	2.21	0.41
1:B:390:THR:HB	1:B:391:PRO:HD3	2.02	0.41
1:B:31:LEU:HB3	1:B:494:VAL:HG22	2.03	0.41
1:B:20:LYS:HB2	4:B:800:HOH:O	2.20	0.41
1:B:106:LYS:HZ2	1:B:110:ASN:HD21	1.66	0.41
1:A:388:PRO:C	1:A:391:PRO:HD2	2.41	0.41
1:A:544:GLN:HG2	1:A:544:GLN:O	2.22	0.40
1:B:116:VAL:HG12	1:B:120:ARG:NH1	2.36	0.40
1:B:465:ARG:HG3	1:B:465:ARG:HH11	1.85	0.40
1:B:433:LEU:HB3	1:B:439:LEU:HD23	2.03	0.40

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	555/576 (96%)	545 (98%)	10 (2%)	0	100	100
1	B	554/576 (96%)	537 (97%)	13 (2%)	4 (1%)	26	19
All	All	1109/1152 (96%)	1082 (98%)	23 (2%)	4 (0%)	39	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	PRO
1	B	27	SER
1	B	154	ARG
1	B	23	ILE

### 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	477/491 (97%)	471 (99%)	6 (1%)	76	79
1	B	475/491 (97%)	472 (99%)	3 (1%)	90	93
All	All	952/982 (97%)	943 (99%)	9 (1%)	84	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LYS
1	A	184	GLN
1	A	336	LEU
1	A	402	HIS
1	A	505	ARG
1	A	531	ARG
1	B	273	ASN
1	B	303	CYS
1	B	310	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	273	ASN
1	A	438	GLN
1	A	514	GLN
1	A	544	GLN
1	A	562	HIS

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Mol	Chain	Res	Type
1	B	110	ASN
1	B	251	GLN
1	B	273	ASN
1	B	309	GLN
1	B	406	ASN
1	B	436	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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	1JF	A	601	-	21,24,24	2.28	10 (47%)	31,36,36	1.67	6 (19%)
2	1JF	A	602	3	21,24,24	2.16	11 (52%)	31,36,36	1.41	2 (6%)
2	1JF	B	601	3	21,24,24	2.17	14 (66%)	31,36,36	1.55	5 (16%)

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	1JF	A	601	-	-	1/11/15/15	0/2/2/2
2	1JF	A	602	3	-	0/11/15/15	0/2/2/2
2	1JF	B	601	3	-	0/11/15/15	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	1JF	C4-C5	2.02	1.44	1.39
2	B	601	1JF	C2-C1	2.05	1.43	1.40
2	A	602	1JF	C13-C14	2.08	1.42	1.38
2	A	601	1JF	C6-C5	2.09	1.42	1.38
2	B	601	1JF	C13-C14	2.15	1.42	1.38
2	B	601	1JF	O8-S7	2.15	1.45	1.43
2	A	602	1JF	O8-S7	2.15	1.45	1.43
2	A	602	1JF	C16-C11	2.17	1.42	1.39
2	B	601	1JF	C14-C15	2.18	1.42	1.38
2	B	601	1JF	O9-S7	2.22	1.45	1.43
2	A	602	1JF	C6-C5	2.23	1.42	1.38
2	B	601	1JF	C13-C12	2.35	1.43	1.39
2	A	602	1JF	C13-C12	2.36	1.43	1.39
2	B	601	1JF	C6-C5	2.43	1.42	1.38
2	A	601	1JF	C2-C1	2.49	1.43	1.40
2	B	601	1JF	C16-C11	2.52	1.43	1.39
2	A	602	1JF	C3-C4	2.57	1.42	1.38
2	A	601	1JF	C12-C11	2.61	1.44	1.40
2	B	601	1JF	C3-C4	2.67	1.43	1.38
2	A	601	1JF	O9-S7	2.74	1.46	1.43
2	A	601	1JF	C16-C15	2.75	1.43	1.38
2	A	601	1JF	C3-C4	2.76	1.43	1.38
2	A	602	1JF	C6-C1	2.76	1.43	1.39
2	B	601	1JF	C12-C11	2.88	1.44	1.40
2	B	601	1JF	C6-C1	2.98	1.43	1.39
2	A	602	1JF	C3-C2	2.99	1.43	1.38
2	B	601	1JF	C3-C2	3.05	1.43	1.38
2	A	601	1JF	C3-C2	3.06	1.43	1.38
2	A	602	1JF	O9-S7	3.06	1.46	1.43
2	A	601	1JF	C6-C1	3.09	1.44	1.39
2	A	601	1JF	C16-C11	3.22	1.44	1.39
2	A	602	1JF	C12-C11	3.42	1.45	1.40
2	B	601	1JF	S7-N10	3.57	1.69	1.63
2	A	602	1JF	S7-N10	3.87	1.70	1.63
2	A	601	1JF	S7-N10	4.16	1.70	1.63

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	1JF	O9-S7-O8	-3.10	115.43	119.54
2	B	601	1JF	O9-S7-O8	-3.09	115.44	119.54
2	A	601	1JF	O9-S7-O8	-3.02	115.53	119.54
2	A	601	1JF	C3-C2-CL1	-2.45	114.73	118.50
2	B	601	1JF	C3-C2-CL1	-2.35	114.87	118.50
2	B	601	1JF	O8-S7-C1	2.02	110.97	107.63
2	A	601	1JF	O8-S7-C1	2.11	111.10	107.63
2	B	601	1JF	C2-C1-S7	2.19	124.64	123.30
2	A	601	1JF	C2-C1-S7	2.22	124.66	123.30
2	A	601	1JF	O8-S7-N10	2.23	112.36	106.69
2	A	602	1JF	C1-C2-CL1	4.22	124.61	121.54
2	B	601	1JF	C1-C2-CL1	5.19	125.31	121.54
2	A	601	1JF	C1-C2-CL1	5.76	125.73	121.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	1JF	C2-C1-S7-N10

There are no ring outliers.

No monomer is involved in short contacts.

## 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	559/576 (97%)	0.20	19 (3%)	49 50	20, 31, 52, 76	0
1	B	558/576 (96%)	0.58	52 (9%)	11 11	21, 37, 70, 87	0
All	All	1117/1152 (96%)	0.39	71 (6%)	23 24	20, 33, 63, 87	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	LEU	11.0
1	B	548	SER	8.4
1	B	25	PRO	8.4
1	B	23	ILE	7.3
1	B	153	GLY	7.2
1	B	29	SER	6.5
1	B	546	ASP	6.4
1	B	511	LEU	5.6
1	A	548	SER	4.9
1	A	544	GLN	4.8
1	B	24	ASN	4.3
1	B	545	LEU	4.1
1	B	14	CYS	4.1
1	B	534	LEU	4.0
1	B	535	LYS	4.0
1	A	16	ALA	3.8
1	B	531	ARG	3.8
1	A	541	ALA	3.5
1	B	563	SER	3.5
1	B	544	GLN	3.5
1	B	513	SER	3.4
1	A	15	ALA	3.4
1	A	95	HIS	3.4
1	A	546	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	515	GLY	3.3
1	B	523	ARG	3.3
1	B	514	GLN	3.2
1	B	95	HIS	3.2
1	B	57	LEU	3.2
1	A	543	SER	3.2
1	B	22	PRO	3.1
1	A	148	GLN	3.0
1	A	14	CYS	2.9
1	B	85	ILE	2.9
1	B	547	LEU	2.8
1	B	530	VAL	2.8
1	A	438	GLN	2.8
1	B	512	LEU	2.8
1	A	563	SER	2.7
1	A	402	HIS	2.7
1	A	540	PRO	2.7
1	B	16	ALA	2.7
1	B	330	GLN	2.7
1	B	402	HIS	2.7
1	A	149	PRO	2.7
1	B	435	ALA	2.7
1	A	545	LEU	2.6
1	B	437	GLU	2.6
1	B	15	ALA	2.6
1	B	377	SER	2.4
1	A	535	LYS	2.4
1	B	20	LYS	2.4
1	B	289	CYS	2.3
1	B	436	GLN	2.3
1	B	469	LEU	2.3
1	B	290	GLY	2.3
1	B	287	THR	2.2
1	A	286	THR	2.2
1	B	540	PRO	2.2
1	B	440	GLU	2.2
1	B	443	LEU	2.1
1	B	293	LEU	2.1
1	B	110	ASN	2.1
1	B	516	GLY	2.1
1	B	543	SER	2.1
1	A	320	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	309	GLN	2.1
1	B	502	HIS	2.1
1	B	212	LYS	2.0
1	B	127	LEU	2.0
1	B	465	ARG	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 carbohydrates in this entry.

## 6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	1JF	A	601	23/23	0.88	0.20	3.70	43,55,66,72	0
2	1JF	B	601	23/23	0.91	0.16	0.79	41,48,58,63	0
2	1JF	A	602	23/23	0.95	0.11	-0.68	30,33,38,47	0
3	MN	A	604	1/1	0.91	0.11	-	51,51,51,51	0
3	MN	B	603	1/1	0.93	0.13	-	54,54,54,54	0
3	MN	B	602	1/1	0.96	0.08	-	55,55,55,55	0
3	MN	A	603	1/1	0.99	0.05	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.