



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:27 am GMT

PDB ID : 3I5K  
Title : Crystal structure of the NS5B polymerase from Hepatitis C Virus (HCV) strain JFH1  
Authors : Simister, P.C.; Schmitt, M.; Lohmann, V.; Bressanelli, S.  
Deposited on : 2009-07-05  
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

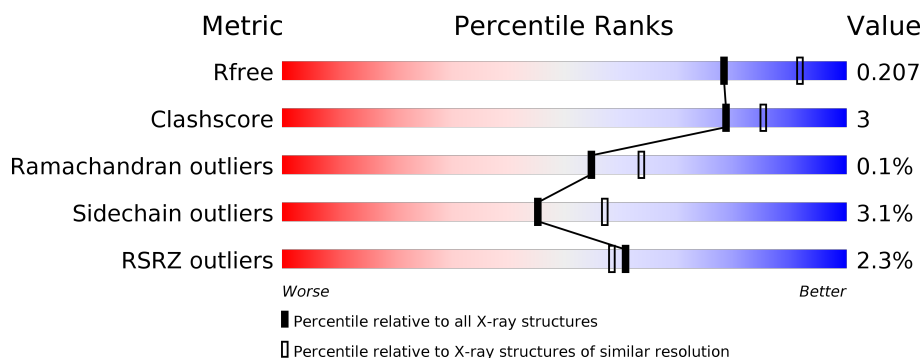
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	566	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	B	566	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	C	566	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	D	566	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	567	-	-	-	X
2	PO4	A	570	-	-	-	X
2	PO4	B	567	-	-	-	X
2	PO4	C	567	-	-	-	X
2	PO4	C	570	-	-	-	X
2	PO4	D	568	-	-	-	X
2	PO4	D	570	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19549 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4416	2794	778	816	28			
1	B	566	Total	C	N	O	S	0	0	0
			4416	2794	778	816	28			
1	C	566	Total	C	N	O	S	0	0	0
			4416	2794	778	816	28			
1	D	566	Total	C	N	O	S	0	0	0
			4416	2794	778	816	28			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	VAL	-	EXPRESSION TAG	UNP Q99IB8
B	566	VAL	-	EXPRESSION TAG	UNP Q99IB8
C	566	VAL	-	EXPRESSION TAG	UNP Q99IB8
D	566	VAL	-	EXPRESSION TAG	UNP Q99IB8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

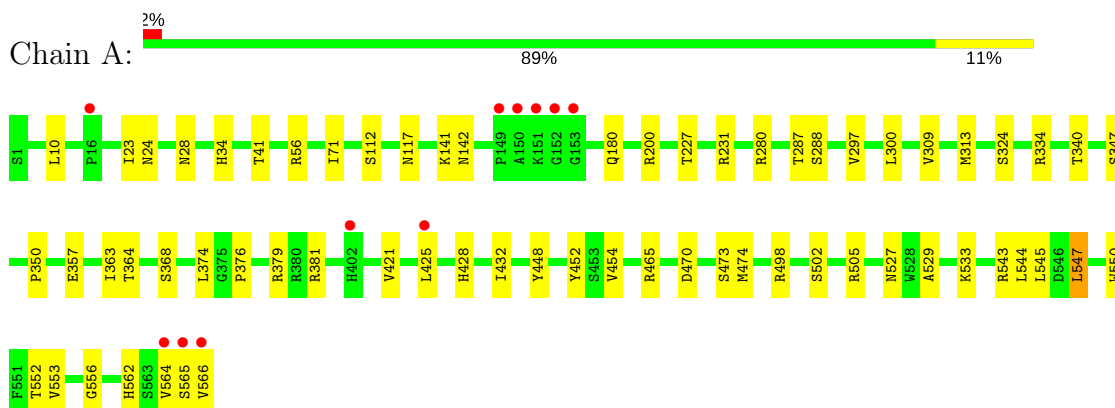
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	467	Total	O	0	0
			467	467		
3	B	505	Total	O	0	0
			505	505		
3	C	405	Total	O	0	0
			405	405		
3	D	423	Total	O	0	0
			423	423		

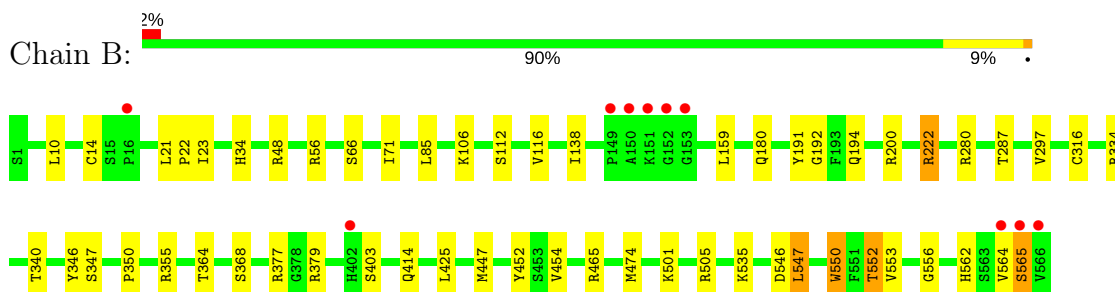
### 3 Residue-property plots [i](#)

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.

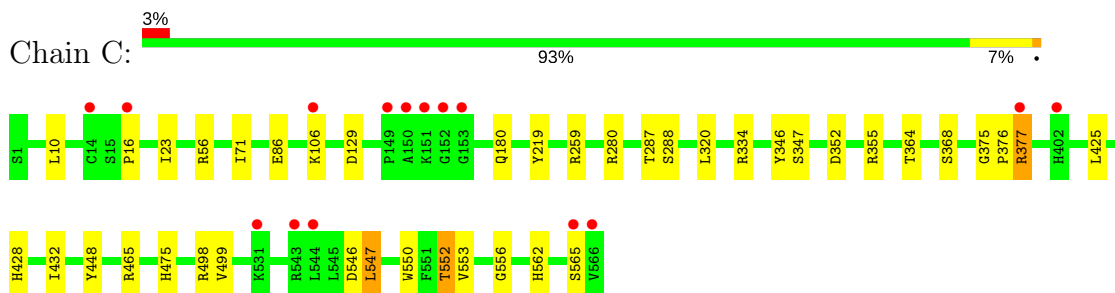
#### • Molecule 1: RNA-directed RNA polymerase



#### • Molecule 1: RNA-directed RNA polymerase

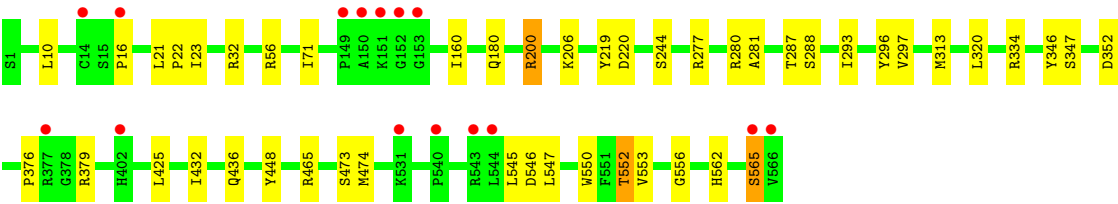


#### • Molecule 1: RNA-directed RNA polymerase



#### • Molecule 1: RNA-directed RNA polymerase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.56Å 115.73Å 133.16Å 90.00° 107.18° 90.00°	Depositor
Resolution (Å)	29.65 – 2.20 28.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.65-2.20) 99.8 (28.93-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.228 0.197 , 0.207	Depositor DCC
$R_{free}$ test set	4017 reflections (2.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 46.13 % 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 1.1965e-04. 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: PO4

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	0.56	0/4518	0.63	0/6135
1	B	0.58	0/4518	0.64	0/6135
1	C	0.51	0/4518	0.60	0/6135
1	D	0.53	0/4518	0.61	0/6135
All	All	0.54	0/18072	0.62	0/24540

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	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	556	GLY	Peptide
1	B	556	GLY	Peptide
1	C	556	GLY	Peptide
1	D	556	GLY	Peptide

## 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	4416	0	4446	38	0
1	B	4416	0	4446	35	0
1	C	4416	0	4446	22	0
1	D	4416	0	4446	25	0
2	A	25	0	0	1	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	467	0	0	6	0
3	B	505	0	0	8	0
3	C	405	0	0	7	0
3	D	423	0	0	6	0
All	All	19549	0	17784	117	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 3.

All (117) 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:71:ILE:CD1	1:A:297:VAL:HG22	1.88	1.03
1:B:71:ILE:CD1	1:B:297:VAL:HG22	2.03	0.88
1:A:71:ILE:HD13	1:A:297:VAL:HG22	1.52	0.88
1:D:220:ASP:HB2	3:D:717:HOH:O	1.75	0.87
1:D:552:THR:HG21	3:D:666:HOH:O	1.79	0.83
1:A:465:ARG:NH1	1:A:547:LEU:H	1.75	0.83
1:C:465:ARG:NH1	1:C:547:LEU:H	1.80	0.79
1:A:465:ARG:HH12	1:A:547:LEU:H	1.27	0.79
1:A:543:ARG:HA	1:D:379:ARG:HH22	1.51	0.74
1:C:465:ARG:HH12	1:C:547:LEU:H	1.34	0.74
1:B:71:ILE:HD12	1:B:297:VAL:HG22	1.69	0.74
1:B:552:THR:HG21	3:B:785:HOH:O	1.88	0.73
1:C:552:THR:HG21	3:C:698:HOH:O	1.90	0.71
1:C:448:TYR:OH	3:C:1400:HOH:O	2.08	0.70
1:A:448:TYR:OH	3:A:1479:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:PRO:HG3	1:A:473:SER:HB3	1.76	0.68
1:A:71:ILE:HD13	1:A:297:VAL:CG2	2.26	0.66
1:A:543:ARG:HA	1:D:379:ARG:NH2	2.11	0.65
1:A:376:PRO:HG3	1:A:473:SER:CB	2.27	0.65
1:D:71:ILE:CD1	1:D:297:VAL:HG22	2.28	0.64
1:A:562:HIS:HD2	3:A:603:HOH:O	1.81	0.64
1:C:562:HIS:HE1	3:C:928:HOH:O	1.81	0.63
1:A:180:GLN:HE22	1:A:553:VAL:HA	1.63	0.63
1:B:71:ILE:HD13	1:B:297:VAL:HG22	1.81	0.63
1:A:379:ARG:HD3	1:A:381:ARG:NH2	2.14	0.62
1:D:71:ILE:HD13	1:D:297:VAL:HG22	1.83	0.61
1:D:465:ARG:NH1	1:D:545:LEU:O	2.34	0.61
1:D:180:GLN:HE22	1:D:553:VAL:HA	1.65	0.60
1:A:470:ASP:O	1:A:474:MET:HG2	2.03	0.58
1:A:231:ARG:NH2	2:A:571:PO4:O1	2.36	0.58
1:B:562:HIS:HE1	3:B:873:HOH:O	1.87	0.58
1:B:562:HIS:HD2	3:B:672:HOH:O	1.87	0.57
1:A:300:LEU:HD13	1:A:313:MET:HE2	1.88	0.56
1:A:545:LEU:HD23	1:A:566:VAL:HG22	1.89	0.54
1:B:106:LYS:HD2	3:B:1482:HOH:O	2.08	0.54
1:B:501:LYS:HE3	1:B:505:ARG:NH1	2.23	0.54
1:C:219:TYR:HB3	1:C:320:LEU:HD23	1.89	0.53
1:B:546:ASP:O	1:B:565:SER:HB2	2.08	0.53
1:C:180:GLN:HE22	1:C:553:VAL:HA	1.74	0.53
1:A:71:ILE:HD12	1:A:297:VAL:HG22	1.81	0.53
1:D:280:ARG:HD2	1:D:287:THR:HA	1.92	0.52
1:C:498:ARG:NH1	3:C:1352:HOH:O	2.43	0.52
1:C:376:PRO:O	1:C:377:ARG:HB2	2.11	0.51
1:B:403:SER:OG	3:B:1485:HOH:O	2.20	0.50
1:A:180:GLN:NE2	1:A:553:VAL:HA	2.27	0.49
1:A:280:ARG:HD2	1:A:287:THR:HA	1.95	0.48
1:B:535:LYS:HE3	3:C:965:HOH:O	2.13	0.48
1:A:527:ASN:O	1:A:533:LYS:HD3	2.13	0.48
1:B:364:THR:HA	1:B:368:SER:O	2.14	0.48
1:B:552:THR:HG22	3:B:760:HOH:O	2.13	0.48
1:A:200:ARG:NE	3:A:1479:HOH:O	2.46	0.47
1:C:280:ARG:HD2	1:C:287:THR:HA	1.97	0.47
1:C:355:ARG:HG2	3:C:1534:HOH:O	2.15	0.47
1:A:357:GLU:OE1	1:A:363:ILE:HD13	2.15	0.47
1:A:428:HIS:O	1:A:432:ILE:HG12	2.15	0.47
1:A:364:THR:HA	1:A:368:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:TYR:HA	1:B:562:HIS:O	2.15	0.47
1:B:85:LEU:HD21	1:B:116:VAL:HG22	1.97	0.46
1:D:32:ARG:HD2	3:D:641:HOH:O	2.14	0.46
1:A:421:VAL:HA	1:A:425:LEU:HB2	1.98	0.46
1:B:340:THR:CG2	1:B:350:PRO:HG3	2.46	0.46
1:B:222:ARG:HE	1:B:222:ARG:HB3	1.47	0.46
1:A:502:SER:HB2	3:A:1610:HOH:O	2.16	0.45
1:A:374:LEU:HD21	1:B:379:ARG:HD2	1.98	0.45
1:A:452:TYR:HA	1:A:562:HIS:O	2.16	0.45
1:B:180:GLN:HE22	1:B:553:VAL:HA	1.82	0.45
1:B:454:VAL:HG22	1:B:564:VAL:CG2	2.47	0.45
1:D:180:GLN:NE2	1:D:553:VAL:HA	2.29	0.45
1:B:138:ILE:HD11	1:B:159:LEU:HD13	1.99	0.45
1:C:129:ASP:O	1:C:259:ARG:HD2	2.18	0.44
1:B:180:GLN:NE2	1:B:553:VAL:HA	2.32	0.44
1:B:346:TYR:O	1:B:347:SER:HB3	2.18	0.44
1:A:227:THR:HB	1:A:347:SER:O	2.17	0.44
1:A:309:VAL:O	1:A:324:SER:HB2	2.18	0.44
1:C:498:ARG:HG3	1:C:499:VAL:N	2.32	0.44
1:D:346:TYR:O	1:D:347:SER:HB3	2.17	0.44
1:A:41:THR:HA	1:A:142:ASN:ND2	2.33	0.43
1:B:501:LYS:HE3	1:B:505:ARG:HH12	1.83	0.43
1:C:498:ARG:HH11	1:C:498:ARG:HG2	1.83	0.43
1:D:562:HIS:HD2	3:D:624:HOH:O	2.00	0.43
1:C:180:GLN:NE2	1:C:553:VAL:HA	2.34	0.43
1:D:296:TYR:CD1	1:D:313:MET:CE	3.00	0.43
1:D:465:ARG:HH12	1:D:546:ASP:HA	1.84	0.43
1:C:375:GLY:O	1:C:475:HIS:HE1	2.01	0.43
1:D:200:ARG:NH2	1:D:448:TYR:CE2	2.87	0.43
1:B:192:GLY:HA3	1:B:316:CYS:SG	2.59	0.43
1:D:432:ILE:O	1:D:436:GLN:HG3	2.19	0.42
1:A:505:ARG:HD2	1:A:529:ALA:O	2.18	0.42
1:D:219:TYR:HB3	1:D:320:LEU:HD23	2.01	0.42
1:D:552:THR:HG22	3:D:591:HOH:O	2.20	0.42
1:D:376:PRO:HD3	1:D:473:SER:OG	2.19	0.42
1:D:546:ASP:O	1:D:565:SER:HB2	2.19	0.42
1:C:346:TYR:O	1:C:347:SER:HB3	2.18	0.42
1:A:340:THR:CG2	1:A:350:PRO:HG3	2.50	0.42
1:B:454:VAL:HG22	1:B:564:VAL:HG23	2.02	0.42
1:C:364:THR:HA	1:C:368:SER:O	2.20	0.41
1:D:293:ILE:O	1:D:297:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:HG2	1:B:159:LEU:HG	2.02	0.41
1:D:206:LYS:HE3	3:D:1586:HOH:O	2.19	0.41
1:D:277:ARG:CZ	1:D:281:ALA:HB2	2.51	0.41
1:B:280:ARG:HD2	1:B:287:THR:HA	2.02	0.41
1:B:355:ARG:HG2	3:B:1317:HOH:O	2.19	0.41
1:B:21:LEU:HA	1:B:22:PRO:HD3	1.95	0.41
1:D:21:LEU:HA	1:D:22:PRO:HD3	1.89	0.41
1:B:414:GLN:HE21	1:B:447:MET:HG3	1.86	0.41
1:B:191:TYR:O	1:B:194:GLN:HG2	2.21	0.41
1:B:34:HIS:HD2	3:B:1443:HOH:O	2.04	0.41
1:B:547:LEU:O	1:B:550:TRP:HB2	2.21	0.41
1:A:454:VAL:HG22	1:A:564:VAL:CG2	2.51	0.41
1:C:428:HIS:O	1:C:432:ILE:HG12	2.21	0.41
1:C:562:HIS:HD2	3:C:668:HOH:O	2.04	0.41
1:A:24:ASN:O	1:A:28:ASN:HB2	2.20	0.40
1:A:34:HIS:HD2	3:A:1269:HOH:O	2.04	0.40
1:A:117:ASN:ND2	3:A:1616:HOH:O	2.54	0.40
1:B:465:ARG:HG2	1:B:547:LEU:HD22	2.03	0.40
1:C:465:ARG:HH12	1:C:547:LEU:N	2.11	0.40
1:C:465:ARG:HH12	1:C:546:ASP:HA	1.87	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	564/566 (100%)	554 (98%)	10 (2%)	0	100	100
1	B	564/566 (100%)	555 (98%)	9 (2%)	0	100	100
1	C	564/566 (100%)	552 (98%)	11 (2%)	1 (0%)	51	58
1	D	564/566 (100%)	552 (98%)	11 (2%)	1 (0%)	51	58
All	All	2256/2264 (100%)	2213 (98%)	41 (2%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	16	PRO
1	C	16	PRO

### 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	482/482 (100%)	469 (97%)	13 (3%)	50	62
1	B	482/482 (100%)	466 (97%)	16 (3%)	43	54
1	C	482/482 (100%)	467 (97%)	15 (3%)	45	57
1	D	482/482 (100%)	467 (97%)	15 (3%)	45	57
All	All	1928/1928 (100%)	1869 (97%)	59 (3%)	45	57

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	23	ILE
1	A	56	ARG
1	A	112	SER
1	A	141	LYS
1	A	288	SER
1	A	334	ARG
1	A	498	ARG
1	A	544	LEU
1	A	547	LEU
1	A	550	TRP
1	A	552	THR
1	A	565	SER
1	B	10	LEU
1	B	14	CYS
1	B	23	ILE
1	B	56	ARG
1	B	66	SER

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Mol	Chain	Res	Type
1	B	112	SER
1	B	200	ARG
1	B	222	ARG
1	B	334	ARG
1	B	377	ARG
1	B	425	LEU
1	B	474	MET
1	B	547	LEU
1	B	550	TRP
1	B	552	THR
1	B	565	SER
1	C	10	LEU
1	C	23	ILE
1	C	56	ARG
1	C	71	ILE
1	C	86	GLU
1	C	106	LYS
1	C	288	SER
1	C	334	ARG
1	C	352	ASP
1	C	377	ARG
1	C	425	LEU
1	C	547	LEU
1	C	550	TRP
1	C	552	THR
1	C	565	SER
1	D	10	LEU
1	D	23	ILE
1	D	56	ARG
1	D	160	ILE
1	D	200	ARG
1	D	244	SER
1	D	288	SER
1	D	334	ARG
1	D	352	ASP
1	D	425	LEU
1	D	474	MET
1	D	547	LEU
1	D	550	TRP
1	D	552	THR
1	D	565	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	90	GLN
1	A	180	GLN
1	A	475	HIS
1	A	562	HIS
1	B	34	HIS
1	B	180	GLN
1	B	414	GLN
1	B	444	ASN
1	B	475	HIS
1	B	562	HIS
1	C	28	ASN
1	C	180	GLN
1	C	414	GLN
1	C	444	ASN
1	C	475	HIS
1	C	562	HIS
1	D	180	GLN
1	D	414	GLN
1	D	444	ASN
1	D	475	HIS
1	D	562	HIS

### 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 ⓘ

17 ligands 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	PO4	A	567	-	4,4,4	0.70	0	6,6,6	0.48	0
2	PO4	A	568	-	4,4,4	0.59	0	6,6,6	0.63	0
2	PO4	A	569	-	4,4,4	0.76	0	6,6,6	0.46	0
2	PO4	A	570	-	4,4,4	0.73	0	6,6,6	0.59	0
2	PO4	A	571	-	4,4,4	0.65	0	6,6,6	0.51	0
2	PO4	B	567	-	4,4,4	0.67	0	6,6,6	0.54	0
2	PO4	B	568	-	4,4,4	0.63	0	6,6,6	0.53	0
2	PO4	B	569	-	4,4,4	0.77	0	6,6,6	0.40	0
2	PO4	B	570	-	4,4,4	0.70	0	6,6,6	0.54	0
2	PO4	C	567	-	4,4,4	0.71	0	6,6,6	0.43	0
2	PO4	C	568	-	4,4,4	0.73	0	6,6,6	0.44	0
2	PO4	C	569	-	4,4,4	0.75	0	6,6,6	0.43	0
2	PO4	C	570	-	4,4,4	0.69	0	6,6,6	0.51	0
2	PO4	D	567	-	4,4,4	0.70	0	6,6,6	0.44	0
2	PO4	D	568	-	4,4,4	0.62	0	6,6,6	0.57	0
2	PO4	D	569	-	4,4,4	0.70	0	6,6,6	0.39	0
2	PO4	D	570	-	4,4,4	0.78	0	6,6,6	0.37	0

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	PO4	A	567	-	-	0/0/0/0	0/0/0/0
2	PO4	A	568	-	-	0/0/0/0	0/0/0/0
2	PO4	A	569	-	-	0/0/0/0	0/0/0/0
2	PO4	A	570	-	-	0/0/0/0	0/0/0/0
2	PO4	A	571	-	-	0/0/0/0	0/0/0/0
2	PO4	B	567	-	-	0/0/0/0	0/0/0/0
2	PO4	B	568	-	-	0/0/0/0	0/0/0/0
2	PO4	B	569	-	-	0/0/0/0	0/0/0/0
2	PO4	B	570	-	-	0/0/0/0	0/0/0/0
2	PO4	C	567	-	-	0/0/0/0	0/0/0/0
2	PO4	C	568	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	C	569	-	-	0/0/0/0	0/0/0/0
2	PO4	C	570	-	-	0/0/0/0	0/0/0/0
2	PO4	D	567	-	-	0/0/0/0	0/0/0/0
2	PO4	D	568	-	-	0/0/0/0	0/0/0/0
2	PO4	D	569	-	-	0/0/0/0	0/0/0/0
2	PO4	D	570	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	571	PO4	1	0

## 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	566/566 (100%)	-0.38	11 (1%) 67 65	12, 20, 31, 49	0
1	B	566/566 (100%)	-0.37	10 (1%) 69 66	12, 20, 32, 49	0
1	C	566/566 (100%)	-0.36	15 (2%) 55 52	12, 20, 31, 48	0
1	D	566/566 (100%)	-0.36	15 (2%) 55 52	12, 20, 31, 48	0
All	All	2264/2264 (100%)	-0.37	51 (2%) 61 58	12, 20, 31, 49	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	VAL	7.7
1	B	566	VAL	7.2
1	B	150	ALA	5.2
1	A	150	ALA	5.1
1	B	565	SER	5.1
1	C	150	ALA	5.1
1	A	565	SER	4.8
1	C	566	VAL	4.3
1	D	543	ARG	3.9
1	C	149	PRO	3.8
1	A	153	GLY	3.8
1	D	150	ALA	3.8
1	C	16	PRO	3.7
1	B	564	VAL	3.6
1	B	153	GLY	3.6
1	D	149	PRO	3.5
1	D	566	VAL	3.5
1	A	149	PRO	3.4
1	A	564	VAL	3.4
1	C	544	LEU	3.4
1	D	402	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	149	PRO	3.3
1	D	377	ARG	3.1
1	B	16	PRO	3.1
1	D	152	GLY	3.0
1	B	151	LYS	3.0
1	C	543	ARG	3.0
1	C	151	LYS	2.9
1	A	151	LYS	2.9
1	A	152	GLY	2.9
1	D	544	LEU	2.9
1	C	377	ARG	2.6
1	D	151	LYS	2.6
1	D	16	PRO	2.6
1	C	531	LYS	2.6
1	D	565	SER	2.5
1	A	16	PRO	2.4
1	C	565	SER	2.4
1	C	14	CYS	2.4
1	C	152	GLY	2.3
1	D	531	LYS	2.3
1	C	402	HIS	2.3
1	A	425	LEU	2.2
1	D	153	GLY	2.2
1	C	153	GLY	2.2
1	B	152	GLY	2.2
1	B	402	HIS	2.1
1	A	402	HIS	2.1
1	D	14	CYS	2.1
1	D	540	PRO	2.1
1	C	106	LYS	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	PO4	D	570	5/5	0.84	0.28	3.88	81,81,82,83	0
2	PO4	C	570	5/5	0.89	0.31	3.85	77,77,78,78	0
2	PO4	A	567	5/5	0.93	0.16	3.23	58,61,61,61	0
2	PO4	C	567	5/5	0.93	0.16	3.05	71,73,73,73	0
2	PO4	B	567	5/5	0.95	0.15	2.88	61,63,63,63	0
2	PO4	D	568	5/5	0.95	0.14	2.04	62,63,64,64	0
2	PO4	A	570	5/5	0.97	0.19	2.04	52,53,54,55	0
2	PO4	A	568	5/5	0.93	0.18	1.87	83,83,83,84	0
2	PO4	D	567	5/5	0.99	0.20	1.70	45,45,46,46	0
2	PO4	B	569	5/5	0.88	0.17	1.23	77,77,79,79	0
2	PO4	A	569	5/5	0.98	0.17	0.75	48,48,48,49	0
2	PO4	B	568	5/5	0.96	0.17	0.38	47,47,48,48	0
2	PO4	C	568	5/5	0.97	0.12	-0.23	53,53,54,55	0
2	PO4	C	569	5/5	0.92	0.24	-	102,102,102,103	0
2	PO4	A	571	5/5	0.87	0.26	-	92,92,92,92	0
2	PO4	B	570	5/5	0.91	0.24	-	78,78,79,80	0
2	PO4	D	569	5/5	0.93	0.20	-	80,80,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.