



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:29 am BST

PDB ID : 3MHZ  
Title : 1.7A structure of 2-fluorohistidine labeled Protective Antigen  
Authors : Lovell, S.; Battaille, K.P.; Wimalasena, D.S.; Janowiak, B.E.; Miyagi, M.; Sun, J.; Hajduch, J.; Pooput, C.; Kirk, K.L.; Bann, J.G.  
Deposited on : 2010-04-09  
Resolution : 1.70 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

<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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

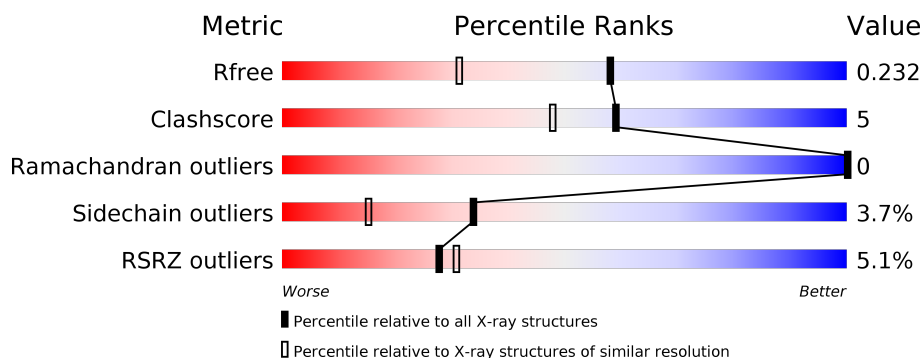
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	735	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5722 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.

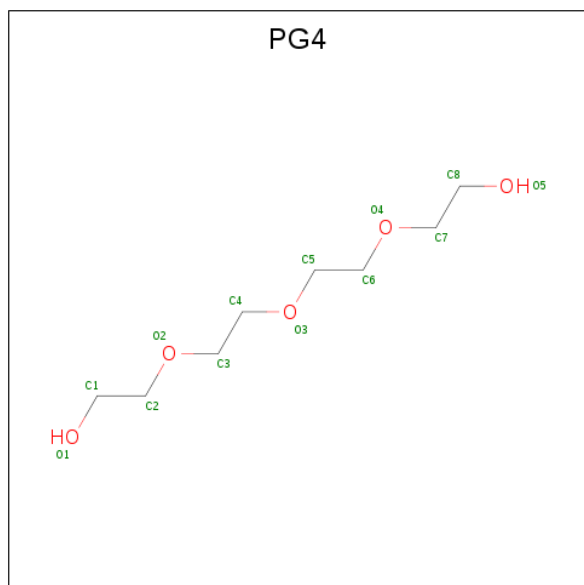
- Molecule 1 is a protein called Protective antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	S			
1	A	673	5307	3335	7	882	1074	9	0	7	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

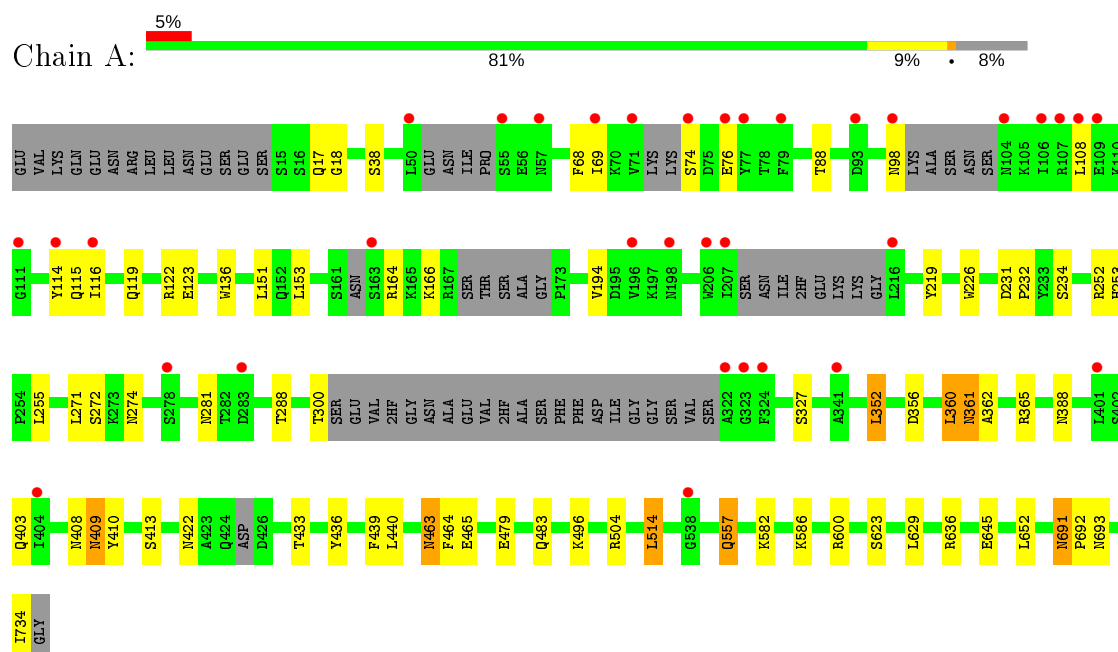
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	400	Total 400	O 400	0	0

### 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 ( $\text{RSRZ} > 2$ ). 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: Protective antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.37Å 93.97Å 119.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 46.99 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.70) 98.7 (46.99-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.70Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0109	Depositor
R, $R_{free}$	0.192 , 0.222 0.202 , 0.232	Depositor DCC
$R_{free}$ test set	4400 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, 0.333 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: CA, PG4, 2HF

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	0.75	1/5325 (0.0%)	0.82	9/7213 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	645	GLU	CB-CG	-5.73	1.41	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	LEU	CA-CB-CG	8.09	133.91	115.30
1	A	252	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	164	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	514	LEU	CB-CG-CD2	6.49	122.03	111.00
1	A	360	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	A	365	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	504	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	164	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	636	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5307	0	5132	49	0
2	A	2	0	0	0	0
3	A	13	0	18	0	0
4	A	400	0	0	4	0
All	All	5722	0	5150	49	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 5.

All (49) 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:409:ASN:HD22	1:A:410:TYR:H	1.15	0.89
1:A:272:SER:HB3	1:A:288:THR:HG22	1.61	0.83
1:A:433[B]:THR:HG21	4:A:1058:HOH:O	1.79	0.82
1:A:17:GLN:OE1	1:A:153:LEU:HD23	1.88	0.73
1:A:691:ASN:HD22	1:A:693:ASN:H	1.39	0.68
1:A:69:ILE:HD11	1:A:114:TYR:HB2	1.76	0.67
1:A:691:ASN:ND2	1:A:693:ASN:H	1.92	0.67
1:A:408:ASN:HD21	1:A:496:LYS:NZ	1.94	0.65
1:A:69:ILE:CD1	1:A:114:TYR:HB2	2.28	0.64
1:A:403:GLN:HE22	1:A:413[A]:SER:H	1.45	0.64
1:A:327:SER:O	4:A:984:HOH:O	2.14	0.64
1:A:361:ASN:HD21	1:A:422:ASN:H	1.47	0.63
1:A:403:GLN:HE22	1:A:413[B]:SER:H	1.46	0.63
1:A:352:LEU:HD22	1:A:356:ASP:CB	2.30	0.61
1:A:557:GLN:H	1:A:557:GLN:CD	2.04	0.60
1:A:17:GLN:HA	1:A:153:LEU:CD2	2.31	0.60
1:A:352:LEU:HD22	1:A:356:ASP:HB2	1.84	0.60
1:A:691:ASN:HD22	1:A:691:ASN:C	2.07	0.56
1:A:253:2HF:HND1	1:A:255:LEU:H	1.55	0.54
1:A:17:GLN:HA	1:A:153:LEU:HD23	1.88	0.54
1:A:18:GLY:H	1:A:153:LEU:HD22	1.72	0.54
1:A:69:ILE:HG22	1:A:151:LEU:HD23	1.90	0.53
1:A:361:ASN:HD22	1:A:362:ALA:H	1.58	0.52
1:A:409:ASN:ND2	1:A:410:TYR:H	1.96	0.52
1:A:623:SER:HA	1:A:734:ILE:HG22	1.91	0.51
1:A:586:LYS:NZ	4:A:1102:HOH:O	2.42	0.51
1:A:18:GLY:N	1:A:153:LEU:HD22	2.26	0.51
1:A:436:TYR:CE2	1:A:440:LEU:HD11	2.46	0.50
1:A:17:GLN:OE1	1:A:153:LEU:CD2	2.57	0.50
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD22	1:A:356:ASP:HB3	1.95	0.47
1:A:18:GLY:O	1:A:153:LEU:HD22	2.15	0.47
1:A:194:VAL:HG22	1:A:219:TYR:HE2	1.79	0.47
1:A:122:ARG:NH2	4:A:881:HOH:O	2.48	0.47
1:A:88:THR:HB	1:A:119:GLN:HG2	1.97	0.46
1:A:226:TRP:CZ2	1:A:234:SER:HB3	2.51	0.46
1:A:463:ASN:ND2	1:A:465:GLU:H	2.14	0.46
1:A:463:ASN:HD22	1:A:463:ASN:C	2.20	0.45
1:A:274:ASN:HD21	1:A:433[B]:THR:HG22	1.80	0.45
1:A:623:SER:HA	1:A:734:ILE:CG2	2.47	0.45
1:A:463:ASN:HD22	1:A:464:PHE:N	2.15	0.44
1:A:18:GLY:HA3	1:A:38:SER:O	2.17	0.43
1:A:300:THR:HG23	1:A:600:ARG:O	2.18	0.43
1:A:68:PHE:CE1	1:A:115:GLN:HG2	2.55	0.42
1:A:479:GLU:O	1:A:483:GLN:NE2	2.39	0.42
1:A:69:ILE:HG12	1:A:116:ILE:HD11	2.02	0.42
1:A:691:ASN:HD22	1:A:692:PRO:N	2.18	0.42
1:A:409:ASN:HD22	1:A:410:TYR:N	1.98	0.41
1:A:352:LEU:HD12	1:A:439:PHE:CD2	2.56	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	655/735 (89%)	642 (98%)	13 (2%)	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	581/651 (89%)	560 (96%)	21 (4%)	35	16

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	76	GLU
1	A	98	ASN
1	A	108	LEU
1	A	123	GLU
1	A	136	TRP
1	A	166	LYS
1	A	271	LEU
1	A	281	ASN
1	A	352	LEU
1	A	360	LEU
1	A	361	ASN
1	A	388	ASN
1	A	409	ASN
1	A	463	ASN
1	A	514	LEU
1	A	557	GLN
1	A	582	LYS
1	A	629	LEU
1	A	652	LEU
1	A	691	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	58	GLN
1	A	85	ASN
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	98	ASN
1	A	115	GLN
1	A	124	ASN
1	A	150	ASN
1	A	180	ASN
1	A	361	ASN
1	A	388	ASN
1	A	400	GLN
1	A	403	GLN
1	A	408	ASN
1	A	409	ASN
1	A	437	ASN
1	A	463	ASN
1	A	539	ASN
1	A	541	GLN
1	A	630	ASN
1	A	691	ASN
1	A	697	ASN
1	A	709	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	$\# Z  > 2$
1	2HF	A	263	1	8,11,12	0.81	0	2,14,16	0.53	0
1	2HF	A	616	1	8,11,12	0.90	0	2,14,16	1.06	0
1	2HF	A	299	1	8,11,12	1.21	1 (12%)	2,14,16	0.62	0
1	2HF	A	253	1	8,11,12	1.34	3 (37%)	2,14,16	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2HF	A	336	1	8,11,12	1.46	1 (12%)	2,14,16	1.23	0
1	2HF	A	86	1	8,11,12	1.12	1 (12%)	2,14,16	1.52	1 (50%)
1	2HF	A	597	1	8,11,12	1.03	0	2,14,16	1.18	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
1	2HF	A	263	1	-	0/5/6/8	0/1/1/1
1	2HF	A	616	1	-	1/5/6/8	0/1/1/1
1	2HF	A	299	1	-	0/5/6/8	0/1/1/1
1	2HF	A	253	1	-	1/5/6/8	0/1/1/1
1	2HF	A	336	1	-	0/5/6/8	0/1/1/1
1	2HF	A	86	1	-	2/5/6/8	0/1/1/1
1	2HF	A	597	1	-	1/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	2HF	CE1-NE2	-3.38	1.29	1.34
1	A	86	2HF	F1-CE1	2.65	1.40	1.33
1	A	299	2HF	F1-CE1	2.50	1.39	1.33
1	A	253	2HF	CE1-NE2	-2.10	1.31	1.34
1	A	253	2HF	F1-CE1	2.09	1.38	1.33
1	A	253	2HF	CE1-ND1	-2.06	1.31	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	2HF	CB-CA-C	-2.05	107.63	111.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	616	2HF	O-C-CA-CB
1	A	86	2HF	O-C-CA-CB
1	A	86	2HF	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
1	A	597	2HF	CA-CB-CG-CD2
1	A	253	2HF	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	253	2HF	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
3	PG4	A	738	-	12,12,12	0.52	0	11,11,11	0.46	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
3	PG4	A	738	-	-	7/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	738	PG4	O3-C5-C6-O4
3	A	738	PG4	O1-C1-C2-O2
3	A	738	PG4	O4-C7-C8-O5
3	A	738	PG4	O2-C3-C4-O3
3	A	738	PG4	C1-C2-O2-C3
3	A	738	PG4	C6-C5-O3-C4
3	A	738	PG4	C5-C6-O4-C7

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	666/735 (90%)	0.16	34 (5%)	28 31	19, 32, 61, 87	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	PHE	8.3
1	A	322	ALA	7.4
1	A	207	ILE	4.6
1	A	106	ILE	4.3
1	A	198	ASN	4.2
1	A	111	GLY	3.7
1	A	77	TYR	3.4
1	A	71	VAL	3.3
1	A	74	SER	3.2
1	A	206	TRP	3.1
1	A	55	SER	3.1
1	A	538	GLY	3.1
1	A	57	ASN	3.1
1	A	196	VAL	2.9
1	A	404	ILE	2.9
1	A	323	GLY	2.7
1	A	76	GLU	2.6
1	A	278	SER	2.6
1	A	69	ILE	2.5
1	A	108	LEU	2.5
1	A	114	TYR	2.5
1	A	104	ASN	2.4
1	A	216	LEU	2.4
1	A	163	SER	2.4
1	A	401	LEU	2.4
1	A	341	ALA	2.3
1	A	93	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	116	ILE	2.2
1	A	283	ASP	2.2
1	A	79	PHE	2.2
1	A	98	ASN	2.2
1	A	50	LEU	2.0
1	A	107	ARG	2.0
1	A	109	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	2HF	A	299	11/12	0.92	0.10	25,30,38,44	0
1	2HF	A	86	11/12	0.93	0.11	41,46,56,62	0
1	2HF	A	336	11/12	0.94	0.08	24,26,30,33	0
1	2HF	A	597	11/12	0.96	0.08	24,25,30,32	0
1	2HF	A	263	11/12	0.97	0.08	20,21,23,23	0
1	2HF	A	616	11/12	0.97	0.06	24,26,30,30	0
1	2HF	A	253	11/12	0.99	0.07	20,22,24,26	0

## 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. 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
3	PG4	A	738	13/13	0.70	0.21	50,56,60,60	0
2	CA	A	737	1/1	0.98	0.09	24,24,24,24	0
2	CA	A	736	1/1	1.00	0.07	22,22,22,22	0



## 6.5 Other polymers

There are no such residues in this entry.