



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:49 AM GMT

PDB ID : 4KPQ  
Title : Structure and receptor binding specificity of the hemagglutinin H13 from avian influenza A virus H13N6  
Authors : Lu, X.; Qi, J.; Shi, Y.; Gao, G.  
Deposited on : 2013-05-14  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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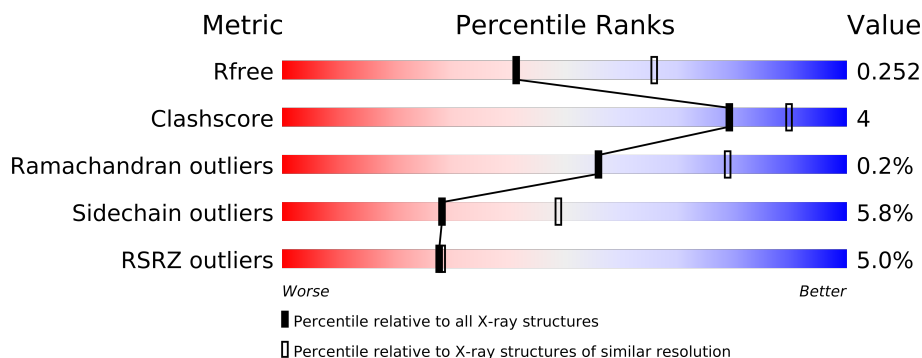
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	C	327	
1	E	327	
2	B	175	
2	D	175	
2	F	175	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11841 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2555	1610	448	485	12			
1	C	324	Total	C	N	O	S	0	0	0
			2555	1610	448	485	12			
1	E	324	Total	C	N	O	S	0	0	0
			2555	1610	448	485	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ILE	-	EXPRESSION TAG	UNP P13103
A	5	GLN	-	EXPRESSION TAG	UNP P13103
C	4	ILE	-	EXPRESSION TAG	UNP P13103
C	5	GLN	-	EXPRESSION TAG	UNP P13103
E	4	ILE	-	EXPRESSION TAG	UNP P13103
E	5	GLN	-	EXPRESSION TAG	UNP P13103

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1312	811	229	265	7			
2	D	165	Total	C	N	O	S	0	0	0
			1312	811	229	265	7			
2	F	165	Total	C	N	O	S	0	0	0
			1312	811	229	265	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

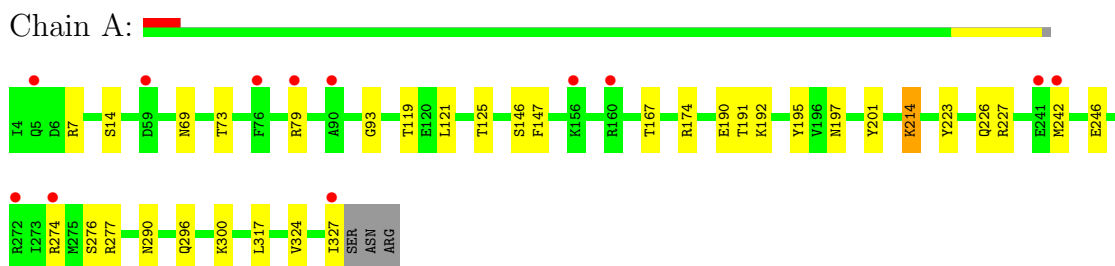
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	31	Total	O	0	0
			31	31		
4	C	58	Total	O	0	0
			58	58		
4	D	33	Total	O	0	0
			33	33		
4	E	43	Total	O	0	0
			43	43		
4	F	19	Total	O	0	0
			19	19		

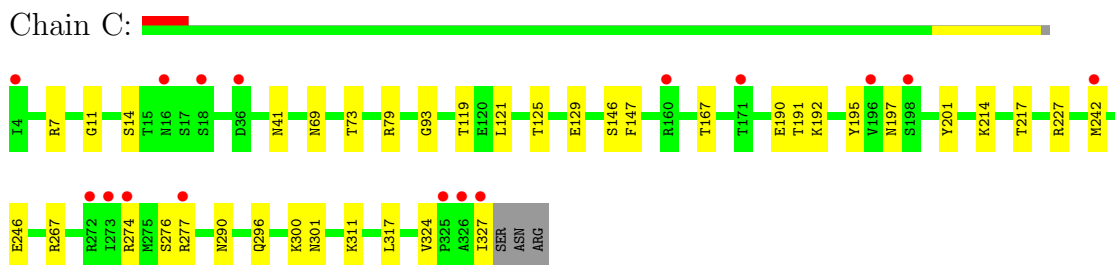
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

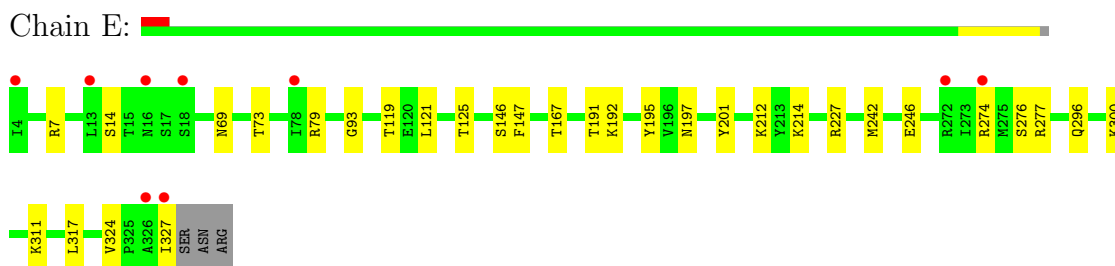
#### • Molecule 1: Hemagglutinin



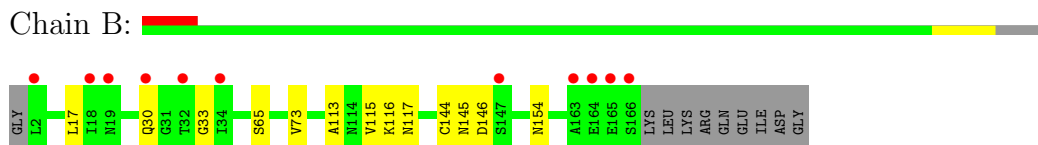
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin

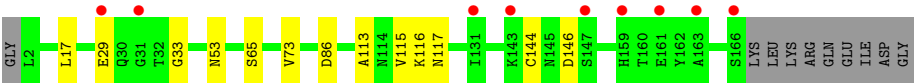


#### • Molecule 2: Hemagglutinin



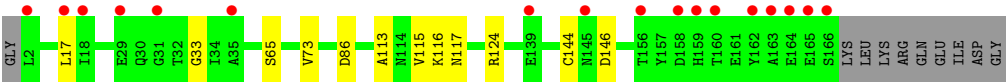
#### • Molecule 2: Hemagglutinin





● Molecule 2: Hemagglutinin

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.11Å 77.06Å 76.47Å 85.50° 82.55° 87.37°	Depositor
Resolution (Å)	42.35 – 2.50 42.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.35-2.50) 97.6 (42.35-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.224 , 0.257 0.220 , 0.252	Depositor DCC
$R_{free}$ test set	2880 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.2	EDS
Estimated twinning fraction	0.003 for -l,-k,-h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57001 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.24	0/2619	0.43	0/3560
1	C	0.24	0/2619	0.43	0/3560
1	E	0.24	0/2619	0.43	0/3560
2	B	0.25	0/1333	0.42	0/1798
2	D	0.24	0/1333	0.42	0/1798
2	F	0.24	0/1333	0.41	0/1798
All	All	0.24	0/11856	0.43	0/16074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2555	0	0	11	1
1	C	2555	0	0	14	0
1	E	2555	0	0	8	0
2	B	1312	0	0	5	0
2	D	1312	0	0	4	1
2	F	1312	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	14	0	0	1	0
4	A	42	0	0	5	0
4	B	31	0	0	3	0
4	C	58	0	0	6	0
4	D	33	0	0	1	0
4	E	43	0	0	0	0
4	F	19	0	0	1	0
All	All	11841	0	0	41	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:267:ARG:NH1	4:C:441:HOH:O	2.10	0.85
1:A:226:GLN:O	4:A:419:HOH:O	1.93	0.84
1:A:214:LYS:NZ	4:A:405:HOH:O	2.22	0.72
2:B:30:GLN:NE2	4:B:207:HOH:O	2.25	0.70
1:A:223:TYR:O	4:A:419:HOH:O	2.10	0.69
2:B:154:ASN:ND2	4:B:213:HOH:O	2.31	0.64
1:C:11:GLY:O	4:C:450:HOH:O	2.15	0.63
1:C:300:LYS:O	2:D:65:SER:OG	2.18	0.61
1:E:300:LYS:O	2:F:65:SER:OG	2.19	0.59
1:C:301:ASN:OD1	4:C:441:HOH:O	2.15	0.59
1:E:201:TYR:OH	1:E:246:GLU:OE2	2.24	0.56
1:C:41:ASN:ND2	4:C:405:HOH:O	2.39	0.55
2:D:113:ALA:O	2:D:117:ASN:ND2	2.39	0.55
1:A:201:TYR:OH	1:A:246:GLU:OE2	2.24	0.55
1:C:201:TYR:OH	1:C:246:GLU:OE2	2.24	0.55
1:A:223:TYR:N	4:A:419:HOH:O	2.42	0.53
2:B:113:ALA:O	2:B:117:ASN:ND2	2.41	0.53
1:A:195:TYR:O	1:A:197:ASN:N	2.43	0.52
1:E:195:TYR:O	1:E:197:ASN:N	2.43	0.51
2:B:145:ASN:ND2	4:B:223:HOH:O	2.43	0.51
1:C:129:GLU:N	4:C:433:HOH:O	2.44	0.51
1:A:300:LYS:O	2:B:65:SER:OG	2.28	0.50
2:D:53:ASN:ND2	4:D:208:HOH:O	2.44	0.50
2:F:113:ALA:O	2:F:117:ASN:ND2	2.44	0.50
1:C:195:TYR:O	1:C:197:ASN:N	2.44	0.50
1:C:276:SER:OG	1:C:277:ARG:N	2.44	0.50
3:E:601:NAG:O3	3:E:601:NAG:O7	2.30	0.50
2:F:124:ARG:NE	4:F:207:HOH:O	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:276:SER:OG	1:E:277:ARG:N	2.46	0.49
1:A:276:SER:OG	1:A:277:ARG:N	2.45	0.49
1:C:290:ASN:ND2	4:C:424:HOH:O	2.47	0.46
1:C:311:LYS:NZ	2:D:86:ASP:OD2	2.50	0.45
1:C:146:SER:OG	1:C:147:PHE:N	2.51	0.43
1:E:69:ASN:ND2	1:E:93:GLY:O	2.52	0.42
1:E:146:SER:OG	1:E:147:PHE:N	2.53	0.42
1:A:146:SER:OG	1:A:147:PHE:N	2.53	0.41
1:A:69:ASN:ND2	1:A:93:GLY:O	2.53	0.41
1:E:311:LYS:NZ	2:F:86:ASP:OD2	2.53	0.41
1:A:290:ASN:N	4:A:406:HOH:O	2.53	0.41
1:C:217:THR:O	1:E:212:LYS:NZ	2.54	0.41
1:C:69:ASN:ND2	1:C:93:GLY:O	2.54	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:ARG:NH2	2:D:29:GLU:O[1_564]	2.11	0.09

## 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	322/327 (98%)	305 (95%)	17 (5%)	0	100	100
1	C	322/327 (98%)	306 (95%)	16 (5%)	0	100	100
1	E	322/327 (98%)	305 (95%)	17 (5%)	0	100	100
2	B	163/175 (93%)	156 (96%)	6 (4%)	1 (1%)	33	55
2	D	163/175 (93%)	155 (95%)	7 (4%)	1 (1%)	33	55
2	F	163/175 (93%)	155 (95%)	7 (4%)	1 (1%)	33	55
All	All	1455/1506 (97%)	1382 (95%)	70 (5%)	3 (0%)	56	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	33	GLY
2	F	33	GLY
2	B	33	GLY

### 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	285/288 (99%)	266 (93%)	19 (7%)	23	40
1	C	285/288 (99%)	266 (93%)	19 (7%)	23	40
1	E	285/288 (99%)	267 (94%)	18 (6%)	25	44
2	B	140/148 (95%)	134 (96%)	6 (4%)	40	65
2	D	140/148 (95%)	134 (96%)	6 (4%)	40	65
2	F	140/148 (95%)	134 (96%)	6 (4%)	40	65
All	All	1275/1308 (98%)	1201 (94%)	74 (6%)	28	49

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	14	SER
1	A	73	THR
1	A	79	ARG
1	A	119	THR
1	A	121	LEU
1	A	125	THR
1	A	167	THR
1	A	190	GLU
1	A	191	THR
1	A	192	LYS
1	A	214	LYS
1	A	227	ARG
1	A	242	MET
1	A	274	ARG
1	A	296	GLN
1	A	317	LEU

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Mol	Chain	Res	Type
1	A	324	VAL
1	A	327	ILE
2	B	17	LEU
2	B	73	VAL
2	B	115	VAL
2	B	116	LYS
2	B	144	CYS
2	B	146	ASP
1	C	7	ARG
1	C	14	SER
1	C	73	THR
1	C	79	ARG
1	C	119	THR
1	C	121	LEU
1	C	125	THR
1	C	167	THR
1	C	190	GLU
1	C	191	THR
1	C	192	LYS
1	C	214	LYS
1	C	227	ARG
1	C	242	MET
1	C	274	ARG
1	C	296	GLN
1	C	317	LEU
1	C	324	VAL
1	C	327	ILE
2	D	17	LEU
2	D	73	VAL
2	D	115	VAL
2	D	116	LYS
2	D	144	CYS
2	D	146	ASP
1	E	7	ARG
1	E	14	SER
1	E	73	THR
1	E	79	ARG
1	E	119	THR
1	E	121	LEU
1	E	125	THR
1	E	167	THR
1	E	191	THR

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Mol	Chain	Res	Type
1	E	192	LYS
1	E	214	LYS
1	E	227	ARG
1	E	242	MET
1	E	274	ARG
1	E	296	GLN
1	E	317	LEU
1	E	324	VAL
1	E	327	ILE
2	F	17	LEU
2	F	73	VAL
2	F	115	VAL
2	F	116	LYS
2	F	144	CYS
2	F	146	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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	$\# Z  > 2$
3	NAG	E	601	1	12,14,15	0.47	0	15,19,21	0.83	1 (6%)

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	NAG	E	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAG	O5-C5-C6	2.35	109.45	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	324/327 (99%)	0.21	12 (3%)	39 41	39, 72, 115, 145	0
1	C	324/327 (99%)	0.38	16 (4%)	28 29	42, 78, 113, 162	0
1	E	324/327 (99%)	0.23	9 (2%)	50 53	39, 73, 114, 160	0
2	B	165/175 (94%)	0.48	11 (6%)	17 17	35, 61, 109, 207	0
2	D	165/175 (94%)	0.42	9 (5%)	24 24	35, 70, 129, 159	0
2	F	165/175 (94%)	0.67	17 (10%)	7 6	35, 77, 158, 196	0
All	All	1467/1506 (97%)	0.36	74 (5%)	28 28	35, 73, 127, 207	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	ILE	20.5
1	C	326	ALA	8.7
1	E	327	ILE	7.3
2	B	164	GLU	7.0
1	E	4	ILE	6.7
2	D	29	GLU	6.5
2	F	166	SER	5.3
2	F	162	TYR	4.6
1	E	16	ASN	4.6
2	B	163	ALA	4.5
2	F	18	ILE	4.4
2	F	17	LEU	4.3
1	C	272	ARG	4.2
1	E	274	ARG	4.1
2	F	160	THR	4.1
2	F	29	GLU	4.0
1	C	277	ARG	3.9
2	F	163	ALA	3.9
1	C	18	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	160	ARG	3.7
2	B	34	ILE	3.7
2	F	164	GLU	3.5
1	A	242	MET	3.4
2	D	147	SER	3.4
1	A	76	PHE	3.3
1	A	160	ARG	3.3
2	F	31	GLY	3.3
2	F	158	ASP	3.3
1	E	326	ALA	3.2
2	B	19	ASN	3.2
1	C	274	ARG	3.1
1	A	272	ARG	3.1
2	B	147	SER	3.0
2	D	166	SER	3.0
2	F	156	THR	3.0
1	E	78	ILE	3.0
2	F	159	HIS	2.9
1	C	325	PRO	2.9
2	B	166	SER	2.9
1	E	272	ARG	2.9
1	C	4	ILE	2.9
1	C	16	ASN	2.8
1	A	274	ARG	2.7
1	A	90	ALA	2.7
1	A	327	ILE	2.6
2	B	2	LEU	2.5
2	D	31	GLY	2.5
1	C	242	MET	2.5
1	A	79	ARG	2.5
1	A	241	GLU	2.5
1	E	18	SER	2.5
2	D	161	GLU	2.5
2	D	163	ALA	2.4
2	D	131	ILE	2.4
2	B	165	GLU	2.4
2	F	145	ASN	2.3
2	F	2	LEU	2.3
2	B	18	ILE	2.3
2	F	165	GLU	2.3
1	C	171	THR	2.2
1	C	198	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	13	LEU	2.2
2	B	32	THR	2.2
2	D	143	LYS	2.1
2	D	159	HIS	2.1
1	A	59	ASP	2.1
1	A	5	GLN	2.1
2	F	139	GLU	2.1
2	F	35	ALA	2.1
2	B	30	GLN	2.0
1	A	156	LYS	2.0
1	C	196	VAL	2.0
1	C	273	ILE	2.0
1	C	36	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	E	601	14/15	0.27	0.74	87,94,99,102	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.