



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:09 PM 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 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

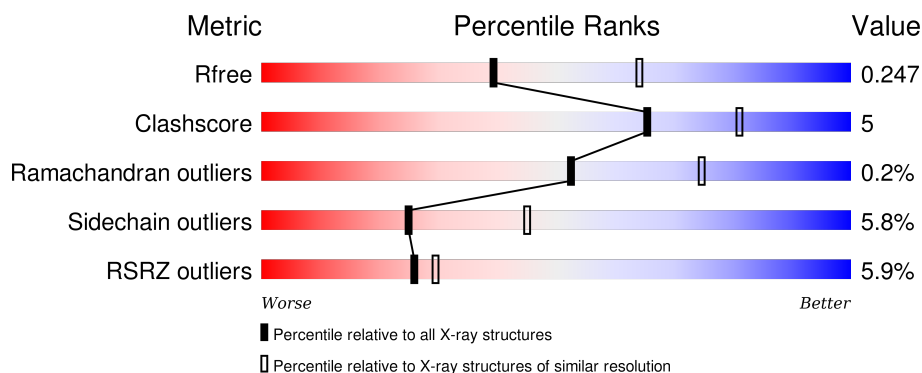
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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	327	<div> <div>5%</div> <div>82% 15% ..</div> </div>
1	C	327	<div> <div>5%</div> <div>81% 15% ..</div> </div>
1	E	327	<div> <div>3%</div> <div>83% 13% ..</div> </div>
2	B	175	<div> <div>7%</div> <div>79% 14% • 6%</div> </div>
2	D	175	<div> <div>6%</div> <div>82% 11% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	175	<div><div></div><div>11%</div><div>82%</div><div>12%</div><div>• 6%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11841 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 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<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

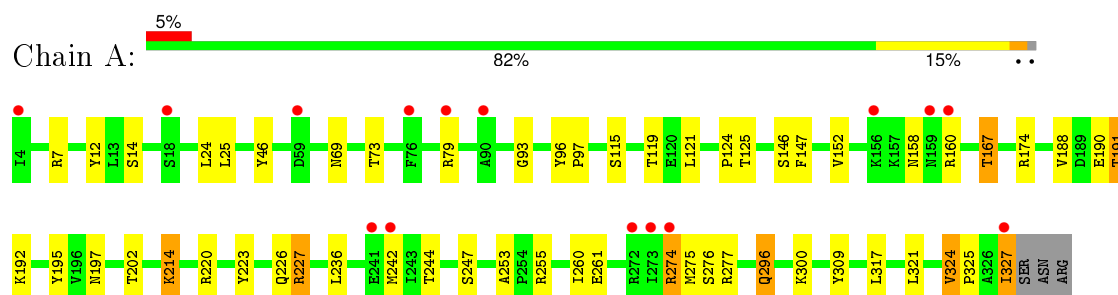
- Molecule 4 is water.

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		

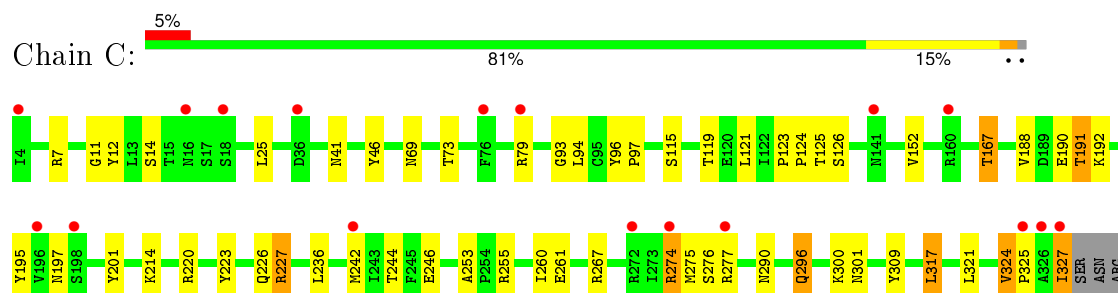
### 3 Residue-property plots [i](#)

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

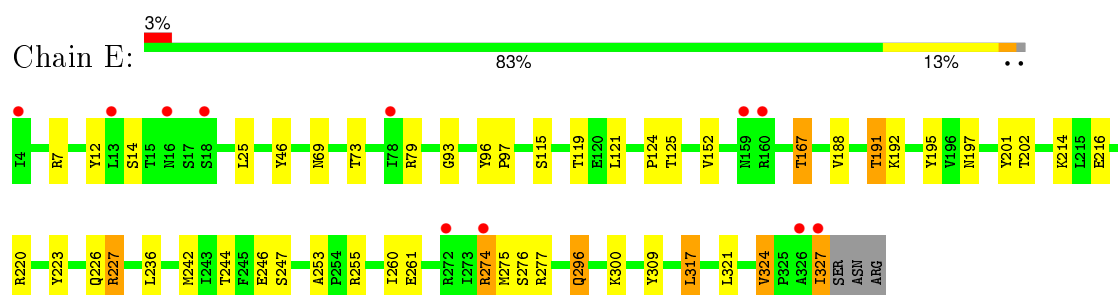
#### • Molecule 1: Hemagglutinin



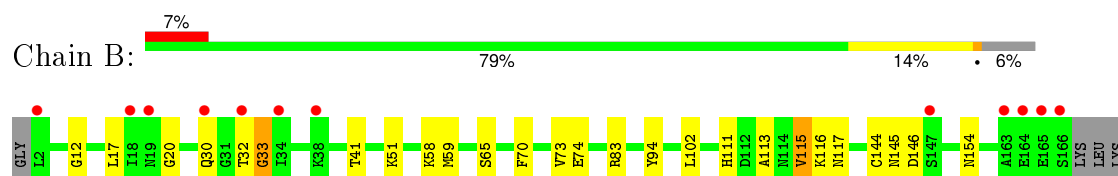
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin

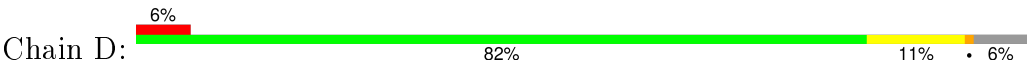


#### • Molecule 2: Hemagglutinin



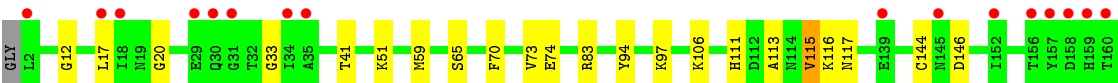
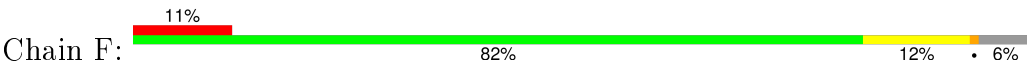
ARG  
GLN  
GLU  
ILE  
ASP  
GLY

● Molecule 2: Hemagglutinin



ILE  
ASP  
GLY

● Molecule 2: Hemagglutinin



## 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) 95.5 (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 0.210 , 0.247	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> )	0.29 , 36.4	EDS
Estimated twinning fraction	0.003 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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.

<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 [i](#)

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

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 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	2555	0	2476	31	1
1	C	2555	0	2476	32	0
1	E	2555	0	2474	25	0
2	B	1312	0	1240	17	0
2	D	1312	0	1240	12	1
2	F	1312	0	1240	12	0
3	E	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	42	0	0	6	0
4	B	31	0	0	3	0
4	C	58	0	0	7	0
4	D	33	0	0	0	0
4	E	43	0	0	0	0
4	F	19	0	0	0	0
All	All	11841	0	11159	114	1

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 (114) 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: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
1:E:167:THR:HB	1:E:244:THR:HG22	1.79	0.65
1:A:167:THR:HB	1:A:244:THR:HG22	1.79	0.65
4:C:450:HOH:O	2:D:115:VAL:HB	1.97	0.64
1:C:11:GLY:O	4:C:450:HOH:O	2.15	0.63
1:C:167:THR:HB	1:C:244:THR:HG22	1.81	0.63
1:C:300:LYS:O	2:D:65:SER:OG	2.18	0.61
1:C:236:LEU:HD21	1:C:260:ILE:HD11	1.84	0.60
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
2:F:70:PHE:HB3	2:F:74:GLU:HG3	1.85	0.58
1:E:236:LEU:HD21	1:E:260:ILE:HD11	1.86	0.58
1:A:236:LEU:HD21	1:A:260:ILE:HD11	1.85	0.58
2:D:70:PHE:HB3	2:D:74:GLU:HG3	1.85	0.57
2:B:70:PHE:HB3	2:B:74:GLU:HG3	1.86	0.57
2:B:154:ASN:ND2	4:B:213:HOH:O	2.31	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: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:160:ARG:HA	4:A:413:HOH:O	2.09	0.52
1:C:327:ILE:HG13	2:D:12:GLY:HA3	1.92	0.51
2:D:20:GLY:HA2	2:D:41:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ARG:HG3	1:E:275:MET:N	2.25	0.51
1:E:195:TYR:O	1:E:197:ASN:N	2.43	0.51
2:F:113:ALA:O	2:F:117:ASN:ND2	2.44	0.50
1:C:274:ARG:HG3	1:C:275:MET:N	2.27	0.50
1:C:276:SER:OG	1:C:277:ARG:N	2.44	0.50
1:A:300:LYS:O	2:B:65:SER:OG	2.28	0.49
2:F:20:GLY:HA2	2:F:41:THR:HG21	1.94	0.49
1:A:274:ARG:HG3	1:A:275:MET:N	2.26	0.49
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:25:LEU:HD21	2:F:51:LYS:HE3	1.93	0.49
1:A:195:TYR:O	1:A:197:ASN:N	2.43	0.49
1:C:96:TYR:CE1	1:C:226:GLN:HG3	2.48	0.49
2:B:20:GLY:HA2	2:B:41:THR:HG21	1.94	0.48
1:A:96:TYR:CE1	1:A:226:GLN:HG3	2.48	0.48
2:B:59:MET:HG3	2:F:94:TYR:CE1	2.48	0.48
1:E:152:VAL:HG23	1:E:253:ALA:HB3	1.96	0.48
1:A:152:VAL:HG23	1:A:253:ALA:HB3	1.96	0.48
1:C:115:SER:HB2	1:C:261:GLU:HB3	1.97	0.47
1:E:96:TYR:CE1	1:E:226:GLN:HG3	2.50	0.47
1:E:327:ILE:HG13	2:F:12:GLY:HA3	1.96	0.47
1:C:290:ASN:ND2	4:C:424:HOH:O	2.47	0.46
2:B:145:ASN:ND2	4:B:223:HOH:O	2.43	0.46
1:C:152:VAL:HG23	1:C:253:ALA:HB3	1.96	0.46
3:E:601:NAG:O7	3:E:601:NAG:O3	2.30	0.46
1:C:97:PRO:HA	1:C:223:TYR:CZ	2.50	0.46
2:B:51:LYS:HE3	1:E:25:LEU:HD21	1.98	0.46
1:A:115:SER:HB2	1:A:261:GLU:HB3	1.98	0.46
1:E:220:ARG:O	1:E:227:ARG:HG3	2.16	0.45
2:D:111:HIS:O	2:D:115:VAL:HG13	2.15	0.45
1:E:97:PRO:HA	1:E:223:TYR:CZ	2.52	0.45
1:A:12:TYR:HE2	1:A:324:VAL:HG13	1.82	0.45
1:E:188:VAL:HA	1:E:191:THR:HG23	1.98	0.45
1:C:94:LEU:HG	4:C:455:HOH:O	2.15	0.45
1:A:188:VAL:HA	1:A:191:THR:HG23	1.99	0.45
2:B:32:THR:HA	2:B:33:GLY:HA3	1.75	0.45
1:C:46:TYR:HB2	1:C:275:MET:HA	1.99	0.45
1:E:115:SER:HB2	1:E:261:GLU:HB3	1.98	0.45
2:B:94:TYR:CE1	2:D:59:MET:HG3	2.51	0.45
1:A:46:TYR:HB2	1:A:275:MET:HA	1.99	0.45
1:C:220:ARG:O	1:C:227:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HA	1:A:223:TYR:CZ	2.52	0.44
1:C:123:PRO:HA	1:C:124:PRO:HD3	1.81	0.44
2:D:94:TYR:CE1	2:F:59:MET:HG3	2.51	0.44
1:E:12:TYR:HE2	1:E:324:VAL:HG13	1.82	0.44
1:E:201:TYR:OH	1:E:246:GLU:OE2	2.24	0.44
1:C:124:PRO:HG3	1:C:255:ARG:HG3	2.00	0.44
1:C:188:VAL:HA	1:C:191:THR:HG23	1.98	0.44
1:C:12:TYR:HE2	1:C:324:VAL:HG13	1.82	0.44
1:E:317:LEU:HA	1:E:317:LEU:HD23	1.89	0.44
1:A:220:ARG:O	1:A:227:ARG:HG3	2.18	0.44
1:E:124:PRO:HG3	1:E:255:ARG:HG3	1.99	0.43
1:E:46:TYR:HB2	1:E:275:MET:HA	2.00	0.43
1:A:321:LEU:H	1:A:321:LEU:HD23	1.82	0.43
1:C:296:GLN:HB3	1:C:296:GLN:HE21	1.70	0.43
1:A:124:PRO:HG3	1:A:255:ARG:HG3	2.01	0.43
2:F:111:HIS:O	2:F:115:VAL:HG13	2.19	0.43
1:C:324:VAL:HA	1:C:325:PRO:HD3	1.77	0.43
1:C:296:GLN:O	1:C:309:TYR:HA	2.18	0.43
1:A:25:LEU:HD21	2:D:51:LYS:HE3	1.99	0.43
1:C:195:TYR:O	1:C:197:ASN:N	2.44	0.43
2:B:51:LYS:HB2	1:E:25:LEU:HD23	2.00	0.42
4:A:405:HOH:O	1:E:216:GLU:HA	2.19	0.42
1:E:69:ASN:ND2	1:E:93:GLY:O	2.52	0.42
1:A:296:GLN:HE21	1:A:296:GLN:HB3	1.71	0.42
1:C:201:TYR:OH	1:C:246:GLU:OE2	2.24	0.42
2:B:58:LYS:HD2	2:F:97:LYS:HD3	2.02	0.41
1:E:202:THR:HG23	1:E:247:SER:HB2	2.02	0.41
1:A:327:ILE:HG13	2:B:12:GLY:HA3	2.01	0.41
1:C:321:LEU:H	1:C:321:LEU:HD23	1.84	0.41
1:A:158:ASN:O	1:A:160:ARG:HG3	2.20	0.41
2:D:32:THR:HA	2:D:33:GLY:HA3	1.75	0.41
1:A:24:LEU:HD22	2:B:102:LEU:HD23	2.02	0.41
2:B:111:HIS:O	2:B:115:VAL:HG13	2.20	0.41
1:A:146:SER:OG	1:A:147:PHE:N	2.53	0.41
1:E:321:LEU:HD23	1:E:321:LEU:H	1.85	0.41
1:E:296:GLN:O	1:E:309:TYR:HA	2.20	0.41
1:C:69:ASN:ND2	1:C:93:GLY:O	2.54	0.41
2:B:83:ARG:HA	2:B:83:ARG:HD2	1.92	0.41
2:F:83:ARG:HD2	2:F:83:ARG:HA	1.91	0.41
1:A:324:VAL:HA	1:A:325:PRO:HD3	1.76	0.40
1:C:123:PRO:HB2	1:C:126:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLN:O	1:A:309:TYR:HA	2.20	0.40
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.90	0.40
1:A:69:ASN:ND2	1:A:93:GLY:O	2.53	0.40
1:A:202:THR:HG23	1:A:247:SER:HB2	2.03	0.40
2:D:102:LEU:HD22	2:F:106:LYS:NZ	2.37	0.40

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	Interatomic distance (Å)	Clash overlap (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%)	30	50
2	D	163/175 (93%)	155 (95%)	7 (4%)	1 (1%)	30	50
2	F	163/175 (93%)	155 (95%)	7 (4%)	1 (1%)	30	50
All	All	1455/1506 (97%)	1382 (95%)	70 (5%)	3 (0%)	52	75

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%)	20	37
1	C	285/288 (99%)	266 (93%)	19 (7%)	20	37
1	E	285/288 (99%)	267 (94%)	18 (6%)	22	40
2	B	140/148 (95%)	134 (96%)	6 (4%)	35	61
2	D	140/148 (95%)	134 (96%)	6 (4%)	35	61
2	F	140/148 (95%)	134 (96%)	6 (4%)	35	61
All	All	1275/1308 (98%)	1201 (94%)	74 (6%)	25	45

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
1	A	324	VAL
1	A	327	ILE
2	B	17	LEU
2	B	73	VAL
2	B	115	VAL

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Mol	Chain	Res	Type
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
1	E	192	LYS
1	E	214	LYS
1	E	227	ARG
1	E	242	MET
1	E	274	ARG

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Mol	Chain	Res	Type
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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	121	GLN
2	D	121	GLN
2	F	121	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	14,14,15	0.27	0	15,19,21	0.53	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	NAG	E	601	1	-	0/6/23/26	0/1/1/1

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
3	E	601	NAG	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	324/327 (99%)	0.27	15 (4%)	36 41	39, 72, 115, 145	0
1	C	324/327 (99%)	0.41	17 (5%)	31 35	42, 78, 113, 162	0
1	E	324/327 (99%)	0.29	11 (3%)	49 54	39, 73, 114, 160	0
2	B	165/175 (94%)	0.55	12 (7%)	18 20	35, 61, 109, 207	0
2	D	165/175 (94%)	0.50	11 (6%)	21 23	35, 70, 129, 159	0
2	F	165/175 (94%)	0.77	20 (12%)	6 5	35, 77, 158, 196	0
All	All	1467/1506 (97%)	0.42	86 (5%)	26 29	35, 73, 127, 207	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	ILE	17.1
1	C	326	ALA	8.0
1	E	4	ILE	7.9
1	E	327	ILE	6.8
2	D	29	GLU	6.7
2	B	164	GLU	6.7
2	F	162	TYR	5.1
1	C	18	SER	5.0
2	F	166	SER	4.9
1	E	274	ARG	4.8
1	E	16	ASN	4.7
2	F	29	GLU	4.6
1	C	277	ARG	4.5
2	B	163	ALA	4.5
2	F	18	ILE	4.4
2	F	17	LEU	4.2
2	F	31	GLY	4.1
2	F	163	ALA	4.1
2	F	160	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	158	ASP	4.0
1	A	242	MET	4.0
1	C	160	ARG	3.9
1	E	326	ALA	3.9
1	A	272	ARG	3.8
1	C	272	ARG	3.8
2	D	163	ALA	3.7
2	B	34	ILE	3.7
1	E	18	SER	3.6
1	C	274	ARG	3.5
1	A	76	PHE	3.4
2	D	166	SER	3.3
2	F	156	THR	3.3
2	D	161	GLU	3.2
1	C	4	ILE	3.2
2	B	147	SER	3.2
2	B	2	LEU	3.2
2	B	19	ASN	3.1
1	A	274	ARG	3.1
1	A	79	ARG	3.1
2	F	164	GLU	3.1
2	B	165	GLU	3.0
1	A	241	GLU	3.0
2	F	2	LEU	3.0
2	F	159	HIS	2.9
1	C	325	PRO	2.9
2	D	159	HIS	2.9
2	D	147	SER	2.8
2	B	166	SER	2.8
1	A	273	ILE	2.8
2	F	145	ASN	2.7
2	D	31	GLY	2.7
2	D	164	GLU	2.7
1	C	16	ASN	2.7
1	A	160	ARG	2.7
1	A	159	ASN	2.7
1	E	272	ARG	2.5
1	C	196	VAL	2.5
2	D	143	LYS	2.5
1	C	242	MET	2.5
2	B	18	ILE	2.4
1	A	4	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	30	GLN	2.4
2	F	30	GLN	2.4
1	E	78	ILE	2.4
1	C	198	SER	2.4
1	A	59	ASP	2.4
1	A	327	ILE	2.4
1	A	18	SER	2.3
2	F	35	ALA	2.3
1	C	141	ASN	2.3
2	D	2	LEU	2.3
1	E	160	ARG	2.2
2	B	32	THR	2.2
2	D	160	THR	2.2
2	F	157	TYR	2.2
1	C	76	PHE	2.2
1	A	90	ALA	2.1
2	B	38	LYS	2.1
1	E	13	LEU	2.1
1	C	36	ASP	2.1
2	F	152	ILE	2.1
1	C	79	ARG	2.1
2	F	34	ILE	2.1
1	A	156	LYS	2.1
1	E	159	ASN	2.0
2	F	139	GLU	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	601	14/15	0.70	0.26	-	87,94,99,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.