



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:49 PM GMT

PDB ID : 4K62
Title : Structure of an avian influenza H5 hemagglutinin from the influenza virus A/Indonesia/5/2005
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-15
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

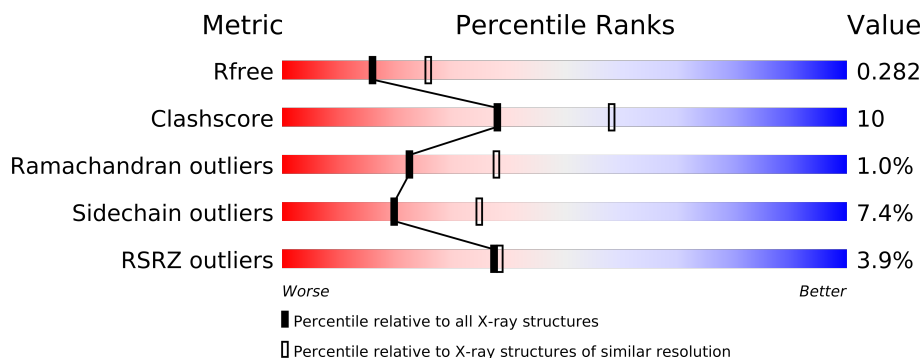
The following versions of software and data (see [references](#)) were used in the production of this report:

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 ≥ 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	321	
1	C	321	
1	E	321	
1	G	321	
2	B	164	
2	D	164	
2	F	164	
2	H	164	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15877 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	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	C	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	E	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	G	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	EXPRESSION TAG	UNP A8HWY8
C	4	GLN	-	EXPRESSION TAG	UNP A8HWY8
E	4	GLN	-	EXPRESSION TAG	UNP A8HWY8
G	4	GLN	-	EXPRESSION TAG	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	D	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	F	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	H	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	23	Total	O	0	0
			23	23		
4	C	120	Total	O	0	0
			120	120		
4	D	19	Total	O	0	0
			19	19		
4	E	36	Total	O	0	0
			36	36		
4	F	24	Total	O	0	0
			24	24		
4	G	23	Total	O	0	0
			23	23		
4	H	23	Total	O	0	0
			23	23		

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.

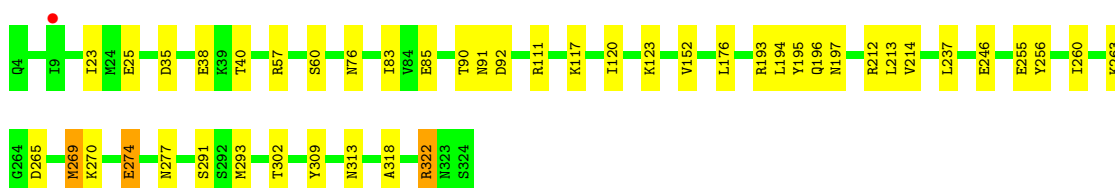
• Molecule 1: Hemagglutinin

Chain A:



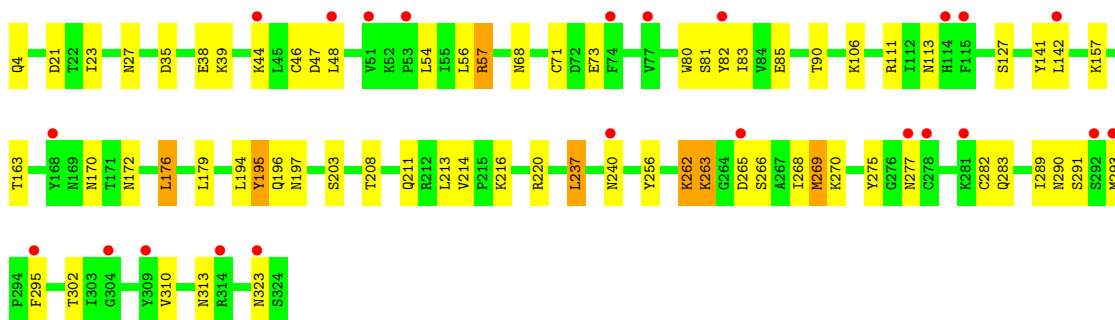
• Molecule 1: Hemagglutinin

Chain C:



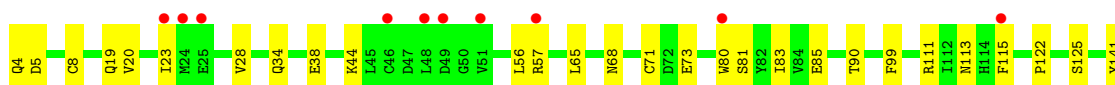
• Molecule 1: Hemagglutinin

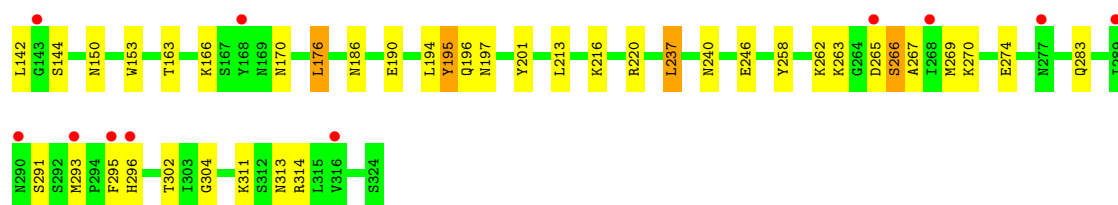
Chain E:



• Molecule 1: Hemagglutinin

Chain G:





• Molecule 2: Hemagglutinin

Chain B:



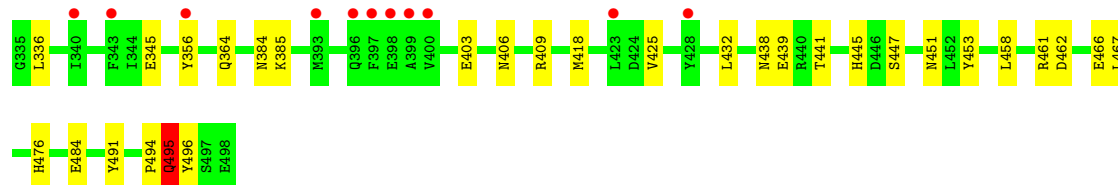
• Molecule 2: Hemagglutinin

Chain D:



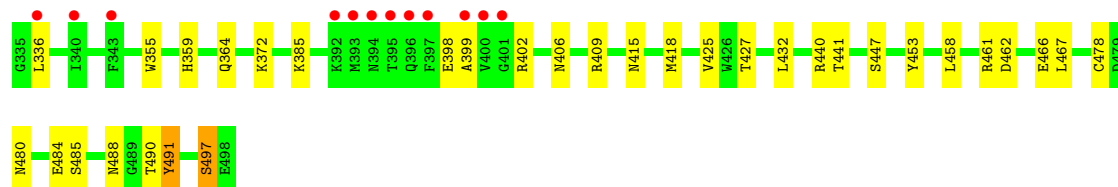
• Molecule 2: Hemagglutinin

Chain F:



• Molecule 2: Hemagglutinin

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.51Å 70.51Å 489.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 2.50 48.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (48.89-2.50) 91.2 (48.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.235 , 0.279 0.238 , 0.282	Depositor DCC
R_{free} test set	4281 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 5.8	EDS
Estimated twinning fraction	0.410 for -h,-k,l 0.428 for -h,-k,l 0.095 for h,-h-k,-l 0.095 for -k,-h,-l	Xtriage
Reported twinning fraction	0.410 for -h,-k,l	Depositor
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 85815 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15877	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.37	0/2603	0.57	0/3537
1	C	0.37	0/2603	0.58	0/3537
1	E	0.31	0/2603	0.55	0/3537
1	G	0.32	0/2603	0.56	0/3537
2	B	0.37	0/1355	0.54	0/1823
2	D	0.46	1/1355 (0.1%)	0.60	1/1823 (0.1%)
2	F	0.53	2/1355 (0.1%)	0.56	0/1823
2	H	0.35	0/1355	0.54	0/1823
All	All	0.38	3/15832 (0.0%)	0.56	1/21440 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	496	TYR	CE1-CZ	-6.71	1.29	1.38
2	F	496	TYR	CE1-CZ	-5.81	1.30	1.38
2	F	496	TYR	CG-CD2	-5.05	1.32	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	496	TYR	N-CA-C	-5.01	97.46	111.00

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	2541	0	18	25	0
1	C	2541	0	34	22	0
1	E	2541	0	42	35	0
1	G	2541	0	23	31	0
2	B	1328	0	23	16	2
2	D	1328	0	26	10	1
2	F	1328	0	26	13	1
2	H	1328	0	37	13	1
3	A	14	0	13	0	0
3	C	14	0	13	0	0
4	A	105	0	0	16	0
4	B	23	0	0	8	0
4	C	120	0	0	13	1
4	D	19	0	0	4	1
4	E	36	0	0	8	0
4	F	24	0	0	4	0
4	G	23	0	0	5	0
4	H	23	0	0	4	0
All	All	15877	0	255	156	6

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 10.

All (156) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:TYR:OH	4:C:750:HOH:O	1.84	0.94
1:C:212:ARG:NH2	4:C:808:HOH:O	2.02	0.93
2:H:372:LYS:NZ	4:H:514:HOH:O	2.06	0.88
1:A:308:LYS:NZ	2:B:398:GLU:OE2	2.08	0.87
2:D:440:ARG:NH1	4:D:515:HOH:O	2.09	0.84
1:G:166:LYS:NZ	4:G:407:HOH:O	2.10	0.84
2:F:384:ASN:ND2	4:F:517:HOH:O	2.13	0.81
1:G:4:GLN:NE2	4:G:410:HOH:O	2.14	0.81
1:C:120:ILE:O	4:C:762:HOH:O	1.99	0.80
2:D:493:TYR:O	2:D:495:GLN:N	2.15	0.80
1:E:4:GLN:NE2	4:E:433:HOH:O	2.15	0.78
1:A:212:ARG:NH2	4:A:754:HOH:O	2.15	0.78
1:A:58:ASP:OD2	4:A:791:HOH:O	2.01	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:141:TYR:O	4:E:419:HOH:O	2.03	0.77
2:B:400:VAL:O	4:B:511:HOH:O	2.02	0.77
2:B:454:ASP:OD2	4:B:521:HOH:O	2.03	0.76
1:A:91:ASN:ND2	4:A:705:HOH:O	2.20	0.74
1:E:203:SER:OG	4:E:432:HOH:O	2.05	0.74
1:A:120:ILE:O	4:A:751:HOH:O	2.06	0.73
1:A:76:ASN:OD1	4:A:779:HOH:O	2.07	0.73
2:B:409:ARG:O	4:B:510:HOH:O	2.05	0.73
1:A:110:SER:OG	4:A:800:HOH:O	2.06	0.73
1:A:244:ASN:ND2	4:A:745:HOH:O	2.23	0.72
1:E:113:ASN:N	1:E:262:LYS:O	2.22	0.72
1:C:40:THR:O	4:C:812:HOH:O	2.07	0.71
2:F:439:GLU:O	4:F:516:HOH:O	2.07	0.71
1:A:173:GLN:NE2	4:A:778:HOH:O	2.22	0.71
2:D:495:GLN:NE2	4:D:503:HOH:O	2.23	0.71
1:C:76:ASN:OD1	4:C:765:HOH:O	2.08	0.70
1:G:81:SER:O	1:G:266:SER:OG	2.09	0.70
2:F:451:ASN:OD1	4:F:505:HOH:O	2.10	0.69
1:C:246:GLU:OE1	4:C:780:HOH:O	2.11	0.68
1:G:216:LYS:O	1:G:220:ARG:NH2	2.27	0.67
1:G:85:GLU:OE2	1:G:270:LYS:NZ	2.27	0.67
1:C:255:GLU:OE2	4:C:742:HOH:O	2.13	0.66
2:B:493:TYR:O	2:B:495:GLN:N	2.28	0.66
1:C:260:ILE:O	4:C:809:HOH:O	2.15	0.65
2:B:407:LEU:O	4:B:501:HOH:O	2.15	0.65
1:C:83:ILE:O	1:C:269:MET:N	2.29	0.65
2:D:400:VAL:O	4:D:512:HOH:O	2.15	0.65
1:A:72:ASP:OD1	1:A:149:ARG:NH1	2.30	0.64
1:G:57:ARG:NE	1:G:73:GLU:OE2	2.30	0.64
2:F:356:TYR:OH	2:F:445:HIS:ND1	2.31	0.64
1:C:91:ASN:ND2	4:C:810:HOH:O	2.30	0.63
1:E:80:TRP:N	1:E:113:ASN:O	2.32	0.63
1:E:47:ASP:OD1	1:E:275:TYR:OH	2.15	0.63
1:E:216:LYS:O	1:E:220:ARG:NH2	2.32	0.63
2:B:488:ASN:ND2	4:B:523:HOH:O	2.32	0.63
1:A:238:LYS:N	4:A:718:HOH:O	2.32	0.62
1:E:85:GLU:OE2	1:E:270:LYS:NZ	2.32	0.62
1:C:193:ARG:NH2	4:C:754:HOH:O	2.33	0.61
2:F:364:GLN:NE2	4:F:519:HOH:O	2.34	0.61
1:E:54:LEU:N	1:E:82:TYR:O	2.34	0.61
1:E:179:LEU:N	4:E:421:HOH:O	2.32	0.60
2:D:408:GLU:OE2	4:D:513:HOH:O	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:315:LEU:N	4:A:728:HOH:O	2.35	0.58
1:G:186:ASN:N	1:G:190:GLU:OE1	2.36	0.58
1:C:35:ASP:OD1	4:C:728:HOH:O	2.17	0.58
1:E:111:ARG:HB2	4:E:402:HOH:O	2.03	0.58
2:B:356:TYR:OH	2:B:445:HIS:ND1	2.37	0.58
1:C:195:TYR:O	1:C:197:ASN:N	2.36	0.58
2:H:402:ARG:NH1	2:H:415:ASN:OD1	2.37	0.57
1:A:79:GLU:OE2	1:A:262:LYS:NZ	2.37	0.57
1:A:106:LYS:NZ	2:B:403:GLU:OE2	2.38	0.57
1:G:170:ASN:O	1:G:240:ASN:N	2.38	0.57
2:D:356:TYR:OH	2:D:445:HIS:ND1	2.38	0.57
1:C:318:ALA:O	4:C:730:HOH:O	2.17	0.56
1:E:211:GLN:OE1	4:E:410:HOH:O	2.18	0.56
1:G:34:GLN:N	4:G:423:HOH:O	2.38	0.55
1:E:127:SER:O	1:E:157:LYS:NZ	2.39	0.55
2:F:453:TYR:OH	2:F:466:GLU:OE2	2.23	0.55
1:C:60:SER:OG	1:C:92:ASP:OD2	2.24	0.55
1:G:65:LEU:O	1:G:150:ASN:ND2	2.40	0.55
1:A:156:LYS:NZ	4:A:772:HOH:O	2.40	0.55
1:A:149:ARG:NH2	4:A:719:HOH:O	2.40	0.54
1:E:256:TYR:O	4:E:424:HOH:O	2.19	0.54
1:G:80:TRP:N	1:G:113:ASN:O	2.41	0.54
2:F:385:LYS:NZ	2:F:441:THR:OG1	2.41	0.54
1:E:57:ARG:NE	1:E:73:GLU:OE2	2.41	0.53
1:G:83:ILE:N	1:G:267:ALA:O	2.41	0.53
1:G:304:GLY:N	4:G:420:HOH:O	2.41	0.53
2:B:450:LYS:NZ	4:B:522:HOH:O	2.42	0.53
1:G:122:PRO:O	1:G:125:SER:OG	2.27	0.53
1:E:21:ASP:O	2:F:438:ASN:ND2	2.42	0.53
1:C:38:GLU:OE1	1:C:291:SER:OG	2.27	0.52
1:E:46:CYS:N	1:E:283:GLN:OE1	2.42	0.52
1:E:38:GLU:N	1:E:295:PHE:O	2.43	0.51
1:E:106:LYS:NZ	2:F:403:GLU:OE2	2.44	0.51
2:D:450:LYS:NZ	2:D:454:ASP:OD2	2.44	0.51
2:H:497:SER:O	4:H:508:HOH:O	2.19	0.51
1:G:311:LYS:N	2:H:427:THR:OG1	2.44	0.51
1:G:141:TYR:N	1:G:144:SER:O	2.44	0.50
1:E:38:GLU:OE1	1:E:291:SER:OG	2.29	0.50
1:A:263:LYS:NZ	4:A:739:HOH:O	2.44	0.50
1:A:83:ILE:O	1:A:269:MET:N	2.44	0.50
1:G:5:ASP:OD1	2:H:478:CYS:N	2.44	0.50
2:F:494:PRO:O	2:F:494:PRO:CG	2.60	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:38:GLU:N	1:G:295:PHE:O	2.45	0.49
1:E:111:ARG:O	1:E:263:LYS:NZ	2.45	0.49
1:G:240:ASN:ND2	4:G:417:HOH:O	2.46	0.49
1:E:21:ASP:OD1	1:E:27:ASN:N	2.45	0.49
2:B:453:TYR:OH	2:B:466:GLU:OE2	2.30	0.49
2:H:490:THR:OG1	2:H:491:TYR:N	2.44	0.49
1:G:19:GLN:O	1:G:314:ARG:NH2	2.46	0.49
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.45	0.49
2:D:496:TYR:C	2:D:496:TYR:CD1	2.78	0.49
1:C:85:GLU:N	1:C:269:MET:O	2.46	0.49
1:G:44:LYS:O	1:G:283:GLN:NE2	2.46	0.48
2:H:406:ASN:OD1	2:H:409:ARG:NH2	2.47	0.48
1:E:263:LYS:NZ	4:E:402:HOH:O	2.47	0.47
1:A:195:TYR:O	1:A:197:ASN:N	2.48	0.47
1:E:35:ASP:OD2	1:E:39:LYS:NZ	2.47	0.47
1:E:81:SER:O	1:E:266:SER:OG	2.32	0.47
1:G:38:GLU:OE1	1:G:291:SER:OG	2.32	0.47
2:H:385:LYS:NZ	2:H:441:THR:OG1	2.47	0.47
1:A:38:GLU:OE1	1:A:291:SER:OG	2.32	0.47
1:A:41:HIS:N	4:A:768:HOH:O	2.48	0.46
1:E:111:ARG:NH1	1:E:265:ASP:OD1	2.47	0.46
1:G:8:CYS:N	2:H:359:HIS:O	2.48	0.46
2:D:496:TYR:O	2:D:496:TYR:CD1	2.69	0.46
2:F:406:ASN:OD1	2:F:409:ARG:NH2	2.50	0.45
1:E:282:CYS:O	1:E:289:ILE:N	2.50	0.45
1:E:170:ASN:O	1:E:240:ASN:N	2.50	0.45
1:G:68:ASN:O	1:G:71:CYS:N	2.50	0.45
1:E:83:ILE:O	1:E:269:MET:N	2.50	0.45
1:E:44:LYS:O	1:E:283:GLN:NE2	2.50	0.45
2:F:495:GLN:O	2:F:495:GLN:CG	2.61	0.45
1:G:176:LEU:O	1:G:237:LEU:N	2.49	0.45
1:E:68:ASN:O	1:E:71:CYS:N	2.51	0.44
2:H:453:TYR:OH	2:H:466:GLU:OE2	2.35	0.44
1:E:195:TYR:O	1:E:197:ASN:N	2.51	0.44
1:A:34:GLN:NE2	4:A:773:HOH:O	2.51	0.44
1:E:265:ASP:O	1:E:266:SER:OG	2.35	0.44
1:C:85:GLU:OE2	1:C:270:LYS:NZ	2.28	0.44
2:B:440:ARG:NH1	4:B:503:HOH:O	2.50	0.44
1:G:150:ASN:ND2	1:G:258:TYR:OH	2.51	0.44
1:G:20:VAL:O	1:G:28:VAL:N	2.50	0.44
1:G:195:TYR:O	1:G:197:ASN:N	2.52	0.43
1:C:309:TYR:O	2:D:396:GLN:NE2	2.50	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:440:ARG:NH1	4:H:504:HOH:O	2.52	0.42
2:B:482:CYS:O	2:B:485:SER:OG	2.37	0.42
1:G:113:ASN:N	1:G:262:LYS:O	2.53	0.41
1:C:57:ARG:NH1	1:C:274:GLU:OE2	2.53	0.41
1:A:60:SER:OG	1:A:92:ASP:OD2	2.38	0.41
2:B:426:TRP:NE1	4:B:513:HOH:O	2.36	0.41
1:G:201:TYR:OH	1:G:246:GLU:OE1	2.37	0.41
1:A:309:TYR:O	2:B:396:GLN:NE2	2.53	0.41
1:E:170:ASN:OD1	1:E:172:ASN:ND2	2.54	0.41
1:E:176:LEU:O	1:E:237:LEU:N	2.54	0.41
2:H:488:ASN:ND2	4:H:505:HOH:O	2.54	0.41
2:F:476:HIS:NE2	2:F:491:TYR:OH	2.54	0.41
1:G:153:TRP:NE1	1:G:195:TYR:OH	2.53	0.40
2:H:364:GLN:OE1	2:H:480:ASN:N	2.55	0.40
1:C:123:LYS:NZ	4:C:740:HOH:O	2.54	0.40
1:A:52:LYS:N	4:A:729:HOH:O	2.54	0.40
2:B:463:ASN:ND2	2:B:491:TYR:OH	2.55	0.40

All (6) 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)
2:B:398:GLU:O	2:B:417:LYS:NZ[3.675]	1.79	0.41
2:B:398:GLU:O	2:B:417:LYS:CE[3.675]	1.89	0.31
4:C:761:HOH:O	4:C:764:HOH:O[3.685]	2.00	0.20
2:F:336:LEU:O	2:F:447:SER:OG[2.865]	2.12	0.08
2:D:439:GLU:OE2	4:D:515:HOH:O[2.875]	2.13	0.07
2:H:336:LEU:O	2:H:447:SER:OG[2.865]	2.13	0.07

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	319/321 (99%)	306 (96%)	12 (4%)	1 (0%)	50 73
1	C	319/321 (99%)	305 (96%)	13 (4%)	1 (0%)	50 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	319/321 (99%)	300 (94%)	17 (5%)	2 (1%)	33	55
1	G	319/321 (99%)	301 (94%)	17 (5%)	1 (0%)	50	73
2	B	162/164 (99%)	149 (92%)	10 (6%)	3 (2%)	12	19
2	D	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	9	12
2	F	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	19	32
2	H	162/164 (99%)	149 (92%)	8 (5%)	5 (3%)	7	8
All	All	1924/1940 (99%)	1814 (94%)	91 (5%)	19 (1%)	22	38

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
2	B	461	ARG
2	B	496	TYR
1	C	196	GLN
2	D	461	ARG
1	E	196	GLN
2	F	461	ARG
2	F	495	GLN
1	G	196	GLN
2	H	398	GLU
2	H	461	ARG
2	H	491	TYR
2	B	494	PRO
2	D	398	GLU
2	D	494	PRO
2	H	497	SER
2	D	399	ALA
2	H	399	ALA
1	E	268	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	288/288 (100%)	260 (90%)	28 (10%)	12	21
1	C	288/288 (100%)	269 (93%)	19 (7%)	24	41
1	E	288/288 (100%)	264 (92%)	24 (8%)	16	29
1	G	288/288 (100%)	266 (92%)	22 (8%)	19	33
2	B	140/140 (100%)	129 (92%)	11 (8%)	18	31
2	D	140/140 (100%)	135 (96%)	5 (4%)	47	73
2	F	140/140 (100%)	131 (94%)	9 (6%)	25	43
2	H	140/140 (100%)	131 (94%)	9 (6%)	25	43
All	All	1712/1712 (100%)	1585 (93%)	127 (7%)	20	35

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	16	SER
1	A	23	ILE
1	A	56	LEU
1	A	57	ARG
1	A	90	THR
1	A	149	ARG
1	A	152	VAL
1	A	158	ASN
1	A	163	THR
1	A	167	SER
1	A	173	GLN
1	A	176	LEU
1	A	194	LEU
1	A	195	TYR
1	A	208	THR
1	A	213	LEU
1	A	214	VAL
1	A	237	LEU
1	A	263	LYS
1	A	274	GLU
1	A	277	ASN
1	A	284	THR
1	A	293	MET
1	A	302	THR
1	A	313	ASN
1	A	322	ARG

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Mol	Chain	Res	Type
1	A	323	ASN
2	B	355	TRP
2	B	356	TYR
2	B	398	GLU
2	B	418	MET
2	B	425	VAL
2	B	432	LEU
2	B	458	LEU
2	B	467	LEU
2	B	481	GLU
2	B	496	TYR
2	B	497	SER
1	C	23	ILE
1	C	90	THR
1	C	111	ARG
1	C	117	LYS
1	C	152	VAL
1	C	176	LEU
1	C	194	LEU
1	C	213	LEU
1	C	214	VAL
1	C	237	LEU
1	C	263	LYS
1	C	265	ASP
1	C	269	MET
1	C	274	GLU
1	C	277	ASN
1	C	293	MET
1	C	302	THR
1	C	313	ASN
1	C	322	ARG
2	D	418	MET
2	D	425	VAL
2	D	432	LEU
2	D	458	LEU
2	D	467	LEU
1	E	23	ILE
1	E	48	LEU
1	E	56	LEU
1	E	57	ARG
1	E	90	THR
1	E	142	LEU

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Mol	Chain	Res	Type
1	E	163	THR
1	E	176	LEU
1	E	194	LEU
1	E	195	TYR
1	E	208	THR
1	E	213	LEU
1	E	214	VAL
1	E	237	LEU
1	E	262	LYS
1	E	263	LYS
1	E	269	MET
1	E	277	ASN
1	E	290	ASN
1	E	293	MET
1	E	302	THR
1	E	310	VAL
1	E	313	ASN
1	E	323	ASN
2	F	345	GLU
2	F	418	MET
2	F	425	VAL
2	F	432	LEU
2	F	458	LEU
2	F	462	ASP
2	F	467	LEU
2	F	484	GLU
2	F	495	GLN
1	G	23	ILE
1	G	56	LEU
1	G	90	THR
1	G	99	PHE
1	G	111	ARG
1	G	115	PHE
1	G	142	LEU
1	G	163	THR
1	G	176	LEU
1	G	194	LEU
1	G	195	TYR
1	G	213	LEU
1	G	237	LEU
1	G	263	LYS
1	G	265	ASP

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Mol	Chain	Res	Type
1	G	266	SER
1	G	269	MET
1	G	274	GLU
1	G	293	MET
1	G	296	HIS
1	G	302	THR
1	G	313	ASN
2	H	355	TRP
2	H	418	MET
2	H	425	VAL
2	H	432	LEU
2	H	458	LEU
2	H	462	ASP
2	H	467	LEU
2	H	484	GLU
2	H	485	SER

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 ⓘ

2 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	$\# Z > 2$
3	NAG	A	601	1	12,14,15	0.71	0	15,19,21	0.99	0
3	NAG	C	601	1	12,14,15	0.65	0	15,19,21	1.03	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	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	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	C	601	NAG	O5-C5-C6	3.07	110.20	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, 95th 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 ²)	Q<0.9
1	A	321/321 (100%)	0.02	0 100 100	2, 15, 41, 64	0
1	C	321/321 (100%)	-0.04	1 (0%) 91 93	4, 16, 39, 57	0
1	E	321/321 (100%)	0.54	23 (7%) 15 15	15, 43, 84, 103	0
1	G	321/321 (100%)	0.47	21 (6%) 18 18	17, 44, 83, 100	0
2	B	164/164 (100%)	0.25	5 (3%) 48 50	8, 35, 57, 67	0
2	D	164/164 (100%)	0.22	2 (1%) 75 77	6, 36, 55, 72	0
2	F	164/164 (100%)	0.48	11 (6%) 17 17	19, 39, 71, 96	0
2	H	164/164 (100%)	0.54	12 (7%) 15 14	20, 39, 71, 98	0
All	All	1940/1940 (100%)	0.29	75 (3%) 37 38	2, 32, 73, 103	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	397	PHE	8.7
2	H	397	PHE	6.6
2	F	399	ALA	6.0
2	H	401	GLY	5.5
1	E	82	TYR	4.7
1	E	74	PHE	4.6
1	G	143	GLY	4.3
1	G	48	LEU	4.0
1	E	304	GLY	3.9
1	G	277	ASN	3.8
2	H	340	ILE	3.7
2	H	400	VAL	3.6
1	E	277	ASN	3.5
1	G	293	MET	3.5
1	E	115	PHE	3.5
1	E	314	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	168	TYR	3.5
2	F	343	PHE	3.4
2	H	399	ALA	3.3
2	H	336	LEU	3.3
1	E	114	HIS	3.2
1	E	51	VAL	3.2
1	E	77	VAL	3.2
2	H	393	MET	3.1
1	G	168	TYR	3.1
1	G	25	GLU	3.0
1	G	115	PHE	3.0
2	H	395	THR	3.0
1	G	290	ASN	2.9
1	E	278	CYS	2.9
2	D	335	GLY	2.8
2	B	497	SER	2.8
1	E	295	PHE	2.8
2	B	496	TYR	2.8
2	F	423	LEU	2.7
2	F	393	MET	2.7
1	G	295	PHE	2.7
1	E	323	ASN	2.7
1	E	142	LEU	2.6
2	H	396	GLN	2.6
1	E	309	TYR	2.6
1	G	51	VAL	2.6
1	E	265	ASP	2.6
1	E	240	ASN	2.5
2	D	496	TYR	2.5
1	G	316	VAL	2.5
1	E	48	LEU	2.5
2	F	396	GLN	2.5
1	E	293	MET	2.5
1	G	49	ASP	2.4
2	F	340	ILE	2.4
1	G	289	ILE	2.4
2	F	428	TYR	2.4
2	F	400	VAL	2.4
1	G	265	ASP	2.4
1	E	53	PRO	2.3
1	E	281	LYS	2.3
2	H	394	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	24	MET	2.3
1	C	9	ILE	2.3
1	G	80	TRP	2.3
1	G	46	CYS	2.2
1	G	57	ARG	2.2
1	G	23	ILE	2.2
2	B	396	GLN	2.2
1	E	44	LYS	2.2
2	B	367	GLY	2.2
1	G	296	HIS	2.2
1	E	292	SER	2.1
2	B	366	SER	2.1
1	G	268	ILE	2.1
2	F	356	TYR	2.0
2	F	398	GLU	2.0
2	H	392	LYS	2.0
2	H	343	PHE	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, 95th 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 ²)	Q<0.9
3	NAG	A	601	14/15	0.14	0.28	11,19,28,35	0
3	NAG	C	601	14/15	0.14	-0.97	15,20,25,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.