



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:00 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 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

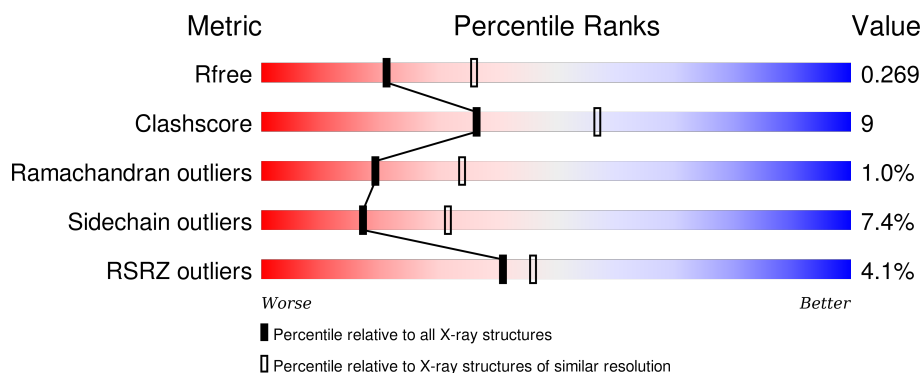
# 1 Overall quality at a glance

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	321	<div> <div></div> <div>75% 23% .</div> </div>
1	C	321	<div> <div></div> <div>76% 23% .</div> </div>
1	E	321	<div> <div>8%</div> <div>70% 27% .</div> </div>
1	G	321	<div> <div>7%</div> <div>70% 27% .</div> </div>
2	B	164	<div> <div>3%</div> <div>73% 24% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	164	<div><div>%</div><div><div></div><div>74%</div><div>24%</div><div></div></div><div></div></div>
2	F	164	<div><div>7%</div><div><div></div><div>75%</div><div>22%</div><div></div></div><div></div></div>
2	H	164	<div><div>8%</div><div><div></div><div>81%</div><div>15%</div><div></div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15877 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	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:  $C_8H_{15}NO_6$ ).



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		

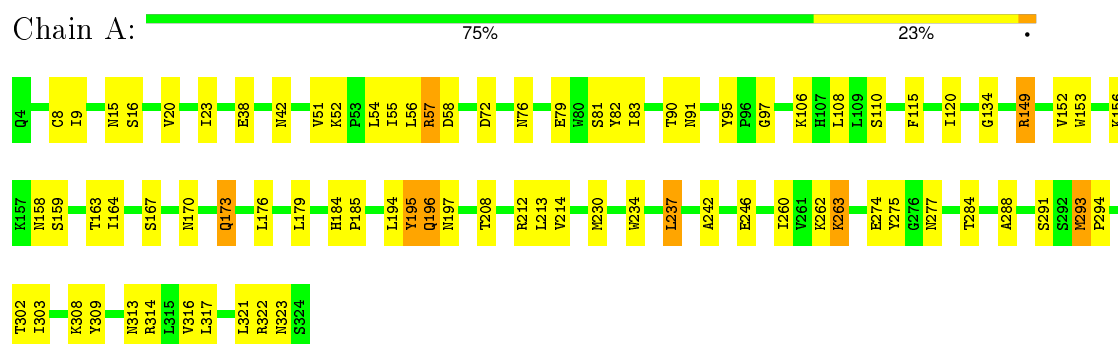
- Molecule 4 is water.

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		

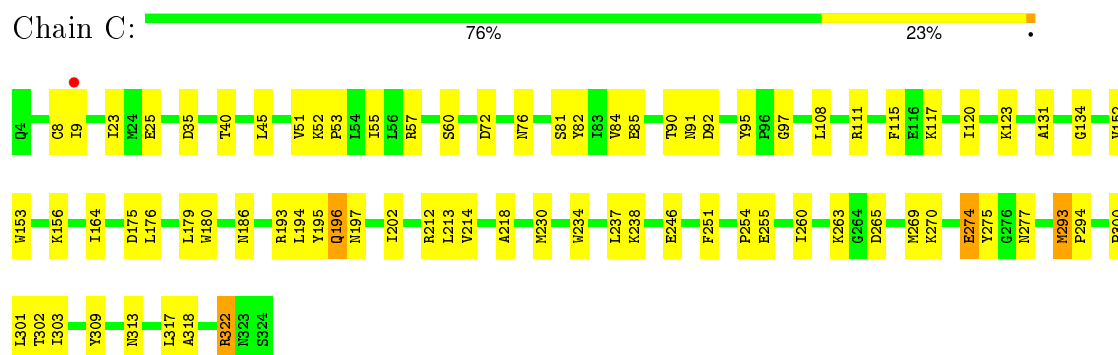
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

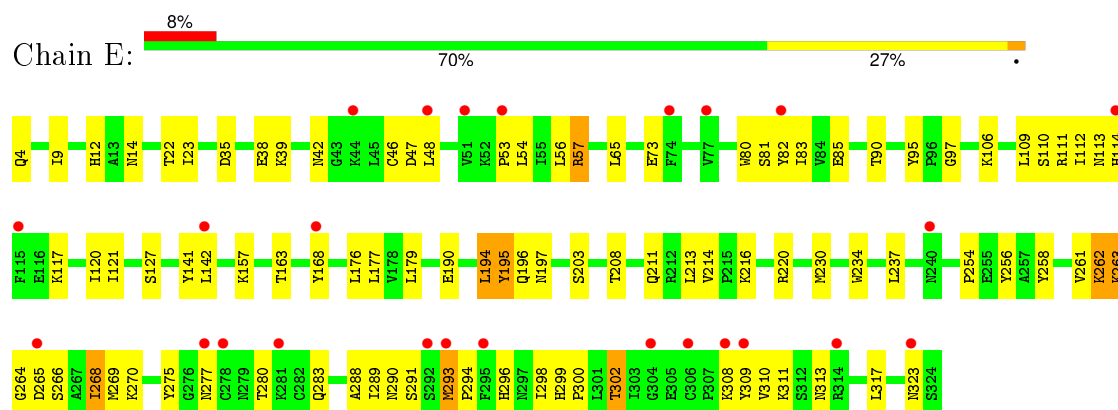
#### • Molecule 1: Hemagglutinin



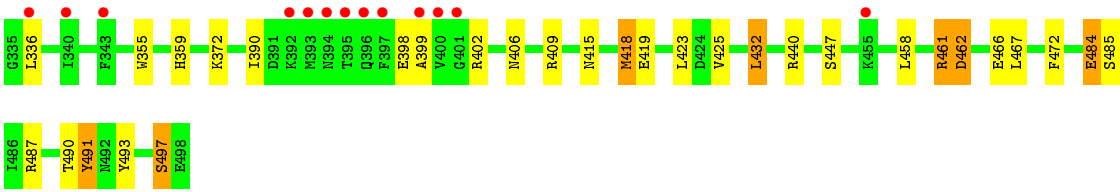
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.235 , 0.279 0.238 , 0.269	Depositor DCC
$R_{free}$ test set	4284 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 6.4	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 <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<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	0.37	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 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	2541	0	2478	44	0
1	C	2541	0	2478	45	0
1	E	2541	0	2479	67	0
1	G	2541	0	2479	60	0
2	B	1328	0	1231	25	2
2	D	1328	0	1231	25	1
2	F	1328	0	1231	35	1
2	H	1328	0	1231	19	1
3	A	14	0	13	1	0
3	C	14	0	13	0	0
4	A	105	0	0	12	0
4	B	23	0	0	5	0
4	C	120	0	0	12	1
4	D	19	0	0	4	1
4	E	36	0	0	6	0
4	F	24	0	0	4	0
4	G	23	0	0	4	0
4	H	23	0	0	3	0
All	All	15877	0	14864	288	6

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 9.

All (288) 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: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: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
1:E:4:GLN:NE2	4:E:433:HOH:O	2.15	0.78
2:D:493:TYR:O	2:D:495:GLN:N	2.15	0.78
2:F:384:ASN:ND2	4:F:517:HOH:O	2.13	0.77
1:G:309:TYR:HE2	2:H:423:LEU:HD21	1.48	0.77
1:A:58:ASP:OD2	4:A:791:HOH:O	2.01	0.77
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:G:51:VAL:HG13	1:G:81:SER:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:203:SER:OG	4:E:432:HOH:O	2.05	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
2:F:451:ASN:OD1	4:F:505:HOH:O	2.10	0.69
1:A:110:SER:OG	4:A:800:HOH:O	2.06	0.69
1:E:308:LYS:HD3	2:F:396:GLN:HB3	1.75	0.69
1:C:246:GLU:OE1	4:C:780:HOH:O	2.11	0.68
1:E:54:LEU:HD23	1:E:83:ILE:HG12	1.75	0.68
1:G:81:SER:O	1:G:266:SER:OG	2.09	0.68
2:F:495:GLN:O	2:F:495:GLN:HG3	1.92	0.68
2:H:372:LYS:NZ	4:H:514:HOH:O	2.06	0.68
1:G:54:LEU:HD23	1:G:83:ILE:HG12	1.75	0.68
1:G:309:TYR:CE2	2:H:423:LEU:HD21	2.29	0.68
1:G:216:LYS:O	1:G:220:ARG:NH2	2.27	0.67
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.76	0.67
1:G:85:GLU:OE2	1:G:270:LYS:NZ	2.27	0.67
1:G:120:ILE:HD11	1:G:254:PRO:HB2	1.77	0.67
2:F:462:ASP:HB2	2:F:493:TYR:OH	1.95	0.67
1:E:65:LEU:HD11	1:E:109:LEU:HD11	1.75	0.66
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:51:VAL:HG13	1:C:81:SER:HB3	1.78	0.65
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
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:C:212:ARG:NH2	4:C:808:HOH:O	2.02	0.64
1:E:309:TYR:CE2	2:F:423:LEU:HD21	2.32	0.64
1:G:166:LYS:NZ	4:G:407:HOH:O	2.10	0.64
1:G:57:ARG:NE	1:G:73:GLU:OE2	2.30	0.64
1:C:91:ASN:ND2	4:C:810:HOH:O	2.30	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:E:85:GLU:OE2	1:E:270:LYS:NZ	2.32	0.62
1:E:114:HIS:HB3	1:E:262:LYS:HB2	1.81	0.61
1:G:42:ASN:HD21	1:G:288:ALA:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:494:PRO:O	2:F:494:PRO:HG2	2.01	0.61
1:G:82:TYR:OH	1:G:283:GLN:HG2	2.01	0.61
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.81	0.60
1:A:51:VAL:HG13	1:A:81:SER:HB3	1.84	0.59
2:D:408:GLU:OE2	4:D:513:HOH:O	2.17	0.59
1:A:55:ILE:HD12	1:A:275:TYR:HB2	1.85	0.59
1:C:35:ASP:OD1	4:C:728:HOH:O	2.17	0.58
2:B:418:MET:HG3	2:B:419:GLU:N	2.17	0.58
1:E:111:ARG:HB2	4:E:402:HOH:O	2.03	0.58
1:A:212:ARG:NH2	4:A:754:HOH:O	2.15	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
2:D:418:MET:HG3	2:D:419:GLU:N	2.18	0.57
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.85	0.57
1:A:164:ILE:O	1:A:246:GLU:HA	2.05	0.57
1:E:113:ASN:N	1:E:262:LYS:O	2.22	0.57
2:D:385:LYS:HD3	2:D:437:GLU:HB3	1.87	0.57
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.86	0.57
1:C:318:ALA:O	4:C:730:HOH:O	2.17	0.56
1:E:309:TYR:HE2	2:F:423:LEU:HD21	1.70	0.56
1:A:321:LEU:HD13	2:B:340:ILE:HD13	1.88	0.56
1:E:211:GLN:OE1	4:E:410:HOH:O	2.18	0.56
1:E:9:ILE:HD11	2:F:456:VAL:HG21	1.87	0.56
1:E:110:SER:O	1:E:266:SER:HB2	2.06	0.55
1:E:302:THR:HG22	2:F:399:ALA:HB3	1.88	0.55
1:E:293:MET:HG3	1:E:294:PRO:HD2	1.89	0.55
1:E:38:GLU:HB2	1:E:293:MET:HB3	1.88	0.55
1:G:311:LYS:HG3	2:H:423:LEU:HG	1.88	0.54
2:F:418:MET:HG3	2:F:419:GLU:N	2.21	0.54
1:E:256:TYR:O	4:E:424:HOH:O	2.19	0.54
1:C:60:SER:OG	1:C:92:ASP:OD2	2.24	0.54
1:A:97:GLY:HA3	1:A:230:MET:O	2.08	0.54
1:E:82:TYR:OH	1:E:283:GLN:HG2	2.08	0.54
1:A:317:LEU:HD13	2:B:434:VAL:HG22	1.90	0.54
2:B:356:TYR:OH	2:B:445:HIS:ND1	2.37	0.54
1:G:34:GLN:HB3	4:G:423:HOH:O	2.08	0.54
1:G:79:GLU:HG3	1:G:114:HIS:HB2	1.90	0.53
1:G:113:ASN:HB2	1:G:262:LYS:HG2	1.91	0.53
1:G:306:CYS:O	1:G:308:LYS:HE3	2.08	0.53
1:E:80:TRP:N	1:E:113:ASN:O	2.32	0.53
2:H:484:GLU:HG2	2:H:487:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.91	0.52
1:G:296:HIS:HE1	1:G:309:TYR:HB2	1.74	0.52
1:E:22:THR:HG22	2:F:438:ASN:HB3	1.92	0.52
1:A:91:ASN:ND2	4:A:705:HOH:O	2.20	0.52
1:A:106:LYS:NZ	2:B:403:GLU:OE2	2.38	0.52
1:A:149:ARG:NH2	4:A:719:HOH:O	2.40	0.52
1:G:186:ASN:N	1:G:190:GLU:OE1	2.36	0.52
1:E:114:HIS:CB	1:E:262:LYS:HB2	2.40	0.52
1:E:120:ILE:HG13	1:E:121:ILE:HG13	1.91	0.52
1:A:309:TYR:HE2	2:B:423:LEU:HD21	1.75	0.52
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.91	0.52
2:F:396:GLN:HG3	2:F:426:TRP:CE2	2.46	0.51
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.90	0.51
2:H:497:SER:O	4:H:508:HOH:O	2.19	0.51
1:E:42:ASN:HD21	1:E:288:ALA:HB3	1.75	0.51
1:E:47:ASP:OD1	1:E:275:TYR:OH	2.15	0.51
1:C:164:ILE:O	1:C:246:GLU:HA	2.10	0.51
1:A:9:ILE:HG23	2:B:452:LEU:HD23	1.92	0.51
1:C:193:ARG:NH2	4:C:754:HOH:O	2.33	0.51
1:E:106:LYS:NZ	2:F:403:GLU:OE2	2.44	0.51
1:G:120:ILE:HG13	1:G:121:ILE:HG13	1.92	0.50
1:G:289:ILE:HD11	1:G:298:ILE:HD12	1.92	0.50
1:E:296:HIS:HB2	1:E:298:ILE:HD13	1.93	0.50
1:E:22:THR:HB	2:F:439:GLU:HB2	1.94	0.50
2:H:418:MET:HG3	2:H:419:GLU:N	2.25	0.50
1:G:38:GLU:HB2	1:G:293:MET:HB3	1.93	0.50
1:G:55:ILE:HG12	1:G:84:VAL:HB	1.92	0.50
2:F:466:GLU:HG2	2:F:472:PHE:CE2	2.46	0.50
2:F:492:ASN:ND2	2:F:495:GLN:HE21	2.10	0.50
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.94	0.49
2:B:338:GLY:O	2:B:342:GLY:HA3	2.12	0.49
1:G:82:TYR:HA	1:G:266:SER:OG	2.13	0.49
2:F:494:PRO:O	2:F:494:PRO:CG	2.60	0.49
1:C:9:ILE:HG23	2:D:452:LEU:HD23	1.94	0.49
1:E:38:GLU:OE1	1:E:291:SER:OG	2.29	0.49
1:E:120:ILE:HD11	1:E:254:PRO:HB2	1.93	0.49
2:H:466:GLU:HG2	2:H:472:PHE:CE2	2.48	0.49
1:G:65:LEU:HD11	1:G:109:LEU:HD11	1.95	0.49
2:D:496:TYR:C	2:D:496:TYR:CD1	2.78	0.49
1:C:309:TYR:HE2	2:D:423:LEU:HD21	1.78	0.49
2:D:356:TYR:OH	2:D:445:HIS:ND1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:HG3	1:A:294:PRO:HD2	1.95	0.49
2:H:490:THR:OG1	2:H:491:TYR:N	2.44	0.49
2:B:385:LYS:HD3	2:B:437:GLU:HB3	1.93	0.48
2:B:396:GLN:HG3	2:B:426:TRP:CD2	2.48	0.48
1:G:38:GLU:HB3	1:G:296:HIS:HB3	1.96	0.48
1:E:308:LYS:HD3	2:F:396:GLN:CB	2.41	0.48
1:E:83:ILE:HB	1:E:268:ILE:HG12	1.96	0.48
1:A:8:CYS:O	2:B:358:TYR:HA	2.13	0.48
1:E:53:PRO:HB3	1:E:82:TYR:CD2	2.48	0.48
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.45	0.48
1:A:79:GLU:OE2	1:A:262:LYS:NZ	2.37	0.48
2:H:406:ASN:OD1	2:H:409:ARG:NH2	2.47	0.48
2:F:493:TYR:HB3	2:F:494:PRO:HD3	1.96	0.48
1:G:114:HIS:HB3	1:G:262:LYS:HB3	1.96	0.48
1:A:173:GLN:NE2	4:A:778:HOH:O	2.22	0.47
2:D:466:GLU:HG2	2:D:472:PHE:CE2	2.49	0.47
1:A:195:TYR:O	1:A:197:ASN:N	2.48	0.47
1:G:296:HIS:CE1	1:G:309:TYR:HB2	2.49	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:A:42:ASN:HD21	1:A:288:ALA:HB3	1.80	0.47
2:D:396:GLN:HG3	2:D:426:TRP:CD2	2.50	0.47
1:G:45:LEU:HA	1:G:283:GLN:NE2	2.30	0.47
1:E:97:GLY:HA3	1:E:230:MET:O	2.15	0.47
1:A:82:TYR:HB3	1:A:303:ILE:HD13	1.96	0.47
2:F:463:ASN:HB3	2:F:476:HIS:HD2	1.80	0.47
2:F:463:ASN:HB3	2:F:476:HIS:CD2	2.50	0.46
1:C:317:LEU:HD11	2:D:389:ILE:HD13	1.97	0.46
1:E:57:ARG:NE	1:E:73:GLU:OE2	2.41	0.46
1:A:263:LYS:NZ	4:A:739:HOH:O	2.44	0.46
1:E:111:ARG:NH1	1:E:265:ASP:OD1	2.47	0.46
1:E:46:CYS:HB2	1:E:280:THR:HG22	1.97	0.46
1:C:97:GLY:HA3	1:C:230:MET:O	2.15	0.46
1:A:115:PHE:HE2	1:A:260:ILE:HG12	1.81	0.46
2:D:450:LYS:NZ	2:D:454:ASP:OD2	2.44	0.46
1:A:170:ASN:HB2	1:A:237:LEU:HD13	1.97	0.46
1:C:82:TYR:HB3	1:C:303:ILE:HD13	1.97	0.46
1:G:293:MET:HG3	1:G:294:PRO:HD2	1.97	0.46
1:C:300:PRO:HB2	1:C:301:LEU:HD12	1.96	0.46
1:A:159:SER:O	1:A:196:GLN:HG3	2.16	0.46
2:D:463:ASN:HA	2:D:497:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:HB2	1:E:80:TRP:CG	2.51	0.46
2:D:496:TYR:CD1	2:D:496:TYR:O	2.69	0.46
1:C:123:LYS:HE2	1:C:131:ALA:O	2.16	0.46
2:B:398:GLU:HG2	2:B:398:GLU:H	1.48	0.45
2:F:406:ASN:OD1	2:F:409:ARG:NH2	2.50	0.45
2:D:389:ILE:HG23	2:D:433:LEU:HD23	1.98	0.45
1:G:317:LEU:HB3	4:G:423:HOH:O	2.16	0.45
1:E:54:LEU:N	1:E:82:TYR:O	2.34	0.45
1:E:109:LEU:HD23	1:E:112:ILE:HD12	1.98	0.45
1:A:52:LYS:HE3	1:A:275:TYR:CE2	2.52	0.45
1:E:120:ILE:HB	1:E:168:TYR:CZ	2.51	0.45
1:E:127:SER:O	1:E:157:LYS:NZ	2.39	0.45
1:E:261:VAL:HG23	1:E:262:LYS:HD2	1.98	0.45
2:D:338:GLY:O	2:D:342:GLY:HA3	2.17	0.45
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.98	0.45
2:B:427:THR:O	2:B:431:GLU:HG3	2.17	0.45
1:E:296:HIS:CE1	1:E:309:TYR:HB2	2.52	0.45
1:G:317:LEU:HD12	1:G:317:LEU:HA	1.84	0.45
2:H:466:GLU:HG2	2:H:472:PHE:HE2	1.81	0.45
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.80	0.45
1:C:317:LEU:HD13	2:D:434:VAL:HG22	1.98	0.45
1:G:237:LEU:HA	1:G:237:LEU:HD23	1.79	0.44
1:C:8:CYS:O	2:D:358:TYR:HA	2.17	0.44
1:A:57:ARG:HB3	1:A:58:ASP:H	1.64	0.44
1:E:12:HIS:NE2	1:E:14:ASN:HB3	2.32	0.44
1:E:309:TYR:CD2	2:F:423:LEU:HD21	2.52	0.44
1:A:54:LEU:HD23	1:A:83:ILE:HG12	2.00	0.44
1:E:113:ASN:ND2	1:E:264:GLY:HA3	2.32	0.44
2:B:436:MET:O	2:B:440:ARG:HG2	2.17	0.44
1:E:195:TYR:O	1:E:197:ASN:N	2.51	0.44
1:G:44:LYS:O	1:G:283:GLN:NE2	2.46	0.44
1:C:85:GLU:OE2	1:C:270:LYS:NZ	2.28	0.44
1:G:150:ASN:ND2	1:G:258:TYR:OH	2.51	0.44
1:G:95:TYR:CD2	1:G:230:MET:HG2	2.53	0.43
1:E:95:TYR:CD2	1:E:230:MET:HG2	2.53	0.43
1:A:314:ARG:HA	4:A:728:HOH:O	2.17	0.43
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.99	0.43
1:G:120:ILE:HB	1:G:168:TYR:CZ	2.52	0.43
2:F:453:TYR:OH	2:F:466:GLU:OE2	2.23	0.43
2:F:458:LEU:HD13	2:F:458:LEU:HA	1.89	0.43
1:G:195:TYR:O	1:G:197:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:461:ARG:HB2	2:H:462:ASP:H	1.70	0.43
2:F:477:LYS:HD3	2:F:477:LYS:HA	1.73	0.43
1:C:55:ILE:HD12	1:C:275:TYR:HB2	1.99	0.43
1:G:105:LEU:O	1:G:109:LEU:HG	2.19	0.43
1:C:45:LEU:HD13	1:C:84:VAL:HG21	2.01	0.43
1:G:294:PRO:HB3	2:H:390:ILE:HG23	2.01	0.43
1:A:38:GLU:OE1	1:A:291:SER:OG	2.32	0.43
1:G:300:PRO:HB2	1:G:301:LEU:HD12	1.99	0.43
1:G:176:LEU:HA	1:G:176:LEU:HD23	1.88	0.43
1:G:169:ASN:HA	1:G:242:ALA:HA	2.01	0.43
1:G:47:ASP:HB2	1:G:279:ASN:HA	2.00	0.43
1:G:112:ILE:HG12	1:G:263:LYS:HD2	2.01	0.43
2:H:440:ARG:NH1	4:H:504:HOH:O	2.52	0.42
1:C:175:ASP:OD1	1:C:238:LYS:HD3	2.19	0.42
2:D:477:LYS:HA	2:D:477:LYS:HD3	1.73	0.42
1:A:184:HIS:HA	1:A:185:PRO:HD3	1.84	0.42
1:C:186:ASN:HA	1:C:218:ALA:O	2.18	0.42
1:E:299:HIS:HA	1:E:300:PRO:HD3	1.93	0.42
1:E:317:LEU:HD13	2:F:434:VAL:HG22	2.01	0.42
2:H:432:LEU:HD22	2:H:432:LEU:HA	1.68	0.42
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.70	0.42
1:A:156:LYS:NZ	4:A:772:HOH:O	2.40	0.42
1:E:289:ILE:HG23	1:E:291:SER:HB2	2.01	0.42
1:A:95:TYR:CD2	1:A:230:MET:HG2	2.55	0.42
1:E:177:LEU:HB3	1:E:258:TYR:HB2	2.02	0.42
1:C:95:TYR:CD2	1:C:230:MET:HG2	2.55	0.42
1:C:72:ASP:HB2	4:C:769:HOH:O	2.19	0.42
1:G:311:LYS:HE3	2:H:423:LEU:HD23	2.02	0.41
1:G:97:GLY:HA3	1:G:230:MET:O	2.20	0.41
1:E:117:LYS:HG3	1:E:258:TYR:CE1	2.55	0.41
1:C:57:ARG:NH1	1:C:274:GLU:OE2	2.53	0.41
1:A:242:ALA:H	3:A:601:NAG:H82	1.85	0.41
1:A:58:ASP:HA	4:A:791:HOH:O	2.20	0.41
1:A:42:ASN:ND2	1:A:288:ALA:HB3	2.35	0.41
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.55	0.41
1:A:20:VAL:HG12	1:A:316:VAL:HG12	2.03	0.41
1:G:182:ILE:HD12	1:G:213:LEU:HB3	2.02	0.41
2:H:462:ASP:HB2	2:H:493:TYR:OH	2.21	0.41
1:C:180:TRP:HB3	1:C:254:PRO:HD3	2.02	0.41
1:C:293:MET:HG3	1:C:294:PRO:HD2	2.02	0.41
1:G:110:SER:O	1:G:266:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:LEU:HA	1:E:317:LEU:HD12	1.86	0.41
1:E:311:LYS:HG3	2:F:423:LEU:HG	2.03	0.41
1:G:275:TYR:CE2	1:G:277:ASN:HA	2.55	0.41
1:C:202:ILE:HD11	1:C:251:PHE:HA	2.02	0.41
1:G:296:HIS:O	1:G:309:TYR:HA	2.20	0.41
1:C:115:PHE:HE2	1:C:260:ILE:HG12	1.85	0.41
1:E:112:ILE:HA	1:E:263:LYS:HA	2.03	0.41
2:F:466:GLU:HG2	2:F:472:PHE:HE2	1.84	0.41
2:B:396:GLN:HG3	2:B:426:TRP:CG	2.55	0.41
1:C:85:GLU:O	1:C:270:LYS:HA	2.21	0.41
1:C:52:LYS:HE3	1:C:275:TYR:CE2	2.55	0.41
2:F:389:ILE:HG12	2:F:433:LEU:HD21	2.03	0.41
2:D:421:GLY:O	2:D:425:VAL:HG12	2.20	0.41
2:B:461:ARG:HB2	2:B:462:ASP:H	1.77	0.41
2:D:364:GLN:OE1	2:D:479:ASP:HB2	2.21	0.41
1:G:164:ILE:O	1:G:246:GLU:HA	2.21	0.41
1:E:111:ARG:HA	1:E:264:GLY:O	2.21	0.41
1:G:8:CYS:N	2:H:359:HIS:O	2.48	0.41
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.56	0.40
2:F:481:GLU:HB2	4:F:515:HOH:O	2.21	0.40
1:G:113:ASN:HB2	1:G:262:LYS:CG	2.51	0.40
2:F:484:GLU:HG2	2:F:487:ARG:HH21	1.86	0.40
2:B:453:TYR:OH	2:B:466:GLU:OE2	2.30	0.40
2:B:389:ILE:HG23	2:B:433:LEU:HD23	2.03	0.40
1:E:294:PRO:HB3	2:F:390:ILE:HG23	2.03	0.40
1:C:9:ILE:HD13	2:D:453:TYR:CD1	2.57	0.40
1:G:39:LYS:HG2	1:G:297:ASN:OD1	2.22	0.40
1:E:190:GLU:HG2	1:E:194:LEU:HD22	2.02	0.40
1:G:267:ALA:HB3	1:G:303:ILE:HD12	2.03	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	Interatomic distance (Å)	Clash overlap (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%)	46	68
1	C	319/321 (99%)	305 (96%)	13 (4%)	1 (0%)	46	68
1	E	319/321 (99%)	300 (94%)	17 (5%)	2 (1%)	30	50
1	G	319/321 (99%)	301 (94%)	17 (5%)	1 (0%)	46	68
2	B	162/164 (99%)	149 (92%)	10 (6%)	3 (2%)	10	16
2	D	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	7	10
2	F	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	16	29
2	H	162/164 (99%)	149 (92%)	8 (5%)	5 (3%)	5	7
All	All	1924/1940 (99%)	1814 (94%)	91 (5%)	19 (1%)	19	34

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

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Mol	Chain	Res	Type
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%)	10	19
1	C	288/288 (100%)	269 (93%)	19 (7%)	21	38
1	E	288/288 (100%)	264 (92%)	24 (8%)	14	26
1	G	288/288 (100%)	266 (92%)	22 (8%)	16	30
2	B	140/140 (100%)	129 (92%)	11 (8%)	15	28
2	D	140/140 (100%)	135 (96%)	5 (4%)	42	69
2	F	140/140 (100%)	131 (94%)	9 (6%)	22	39
2	H	140/140 (100%)	131 (94%)	9 (6%)	22	39
All	All	1712/1712 (100%)	1585 (93%)	127 (7%)	17	31

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	113	ASN
1	C	76	ASN
1	C	186	ASN
1	E	4	GLN
1	E	114	HIS
2	F	495	GLN
1	G	4	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	14,14,15	0.58	0	15,19,21	1.29	2 (13%)
3	NAG	C	601	1	14,14,15	0.52	0	15,19,21	0.95	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 (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	C2-N2-C7	-2.32	120.06	123.04
3	C	601	NAG	C1-O5-C5	2.06	114.86	112.25
3	A	601	NAG	C1-O5-C5	3.48	116.67	112.25

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	A	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	321/321 (100%)	-0.01	0 100 100	2, 15, 41, 64	0
1	C	321/321 (100%)	-0.06	1 (0%) 94 95	4, 16, 39, 57	0
1	E	321/321 (100%)	0.53	25 (7%) 16 17	15, 43, 84, 103	0
1	G	321/321 (100%)	0.46	22 (6%) 20 22	17, 44, 83, 100	0
2	B	164/164 (100%)	0.24	5 (3%) 54 59	8, 35, 57, 67	0
2	D	164/164 (100%)	0.20	2 (1%) 81 83	6, 36, 55, 72	0
2	F	164/164 (100%)	0.47	11 (6%) 21 23	19, 39, 71, 96	0
2	H	164/164 (100%)	0.55	13 (7%) 15 17	20, 39, 71, 98	0
All	All	1940/1940 (100%)	0.28	79 (4%) 41 46	2, 32, 73, 103	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	397	PHE	9.3
2	H	397	PHE	6.7
2	F	399	ALA	6.4
2	H	401	GLY	6.1
1	E	82	TYR	4.9
1	E	74	PHE	4.8
1	G	143	GLY	4.5
1	G	48	LEU	4.2
1	E	304	GLY	4.1
2	H	400	VAL	4.0
2	H	340	ILE	4.0
1	G	293	MET	3.9
1	G	277	ASN	3.9
1	E	314	ARG	3.7
2	H	399	ALA	3.6
1	E	115	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	51	VAL	3.5
1	E	277	ASN	3.5
1	E	168	TYR	3.5
2	H	336	LEU	3.5
1	E	114	HIS	3.5
2	F	343	PHE	3.5
1	E	77	VAL	3.5
2	H	393	MET	3.4
1	G	25	GLU	3.3
1	G	290	ASN	3.1
2	B	497	SER	3.1
1	G	168	TYR	3.0
1	E	278	CYS	3.0
1	G	115	PHE	3.0
2	F	393	MET	3.0
2	H	395	THR	3.0
2	D	335	GLY	3.0
1	E	295	PHE	2.8
2	F	423	LEU	2.8
1	G	295	PHE	2.8
2	B	496	TYR	2.8
1	G	51	VAL	2.8
1	G	265	ASP	2.7
1	G	316	VAL	2.7
1	E	142	LEU	2.7
1	E	309	TYR	2.7
2	H	396	GLN	2.7
1	E	265	ASP	2.6
1	G	289	ILE	2.6
2	F	400	VAL	2.6
2	F	396	GLN	2.6
1	E	293	MET	2.6
1	E	323	ASN	2.6
1	G	24	MET	2.6
1	E	240	ASN	2.6
1	E	44	LYS	2.5
1	E	48	LEU	2.5
2	F	428	TYR	2.5
1	G	49	ASP	2.5
2	D	496	TYR	2.5
1	E	53	PRO	2.5
2	F	340	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	394	ASN	2.5
2	B	367	GLY	2.4
1	G	80	TRP	2.4
2	B	396	GLN	2.4
1	E	281	LYS	2.4
1	G	296	HIS	2.4
1	G	57	ARG	2.4
1	G	23	ILE	2.3
2	B	366	SER	2.3
1	C	9	ILE	2.2
1	G	46	CYS	2.2
1	E	292	SER	2.1
2	H	392	LYS	2.1
1	G	268	ILE	2.1
2	H	343	PHE	2.1
2	F	356	TYR	2.1
1	G	301	LEU	2.1
1	E	306	CYS	2.0
2	F	435	LEU	2.0
1	E	308	LYS	2.0
2	H	455	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	601	14/15	0.92	0.14	-0.52	15,20,25,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	601	14/15	0.90	0.14	-	11,19,28,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.