



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:25 PM GMT

PDB ID : 4XQU  
Title : Crystal structure of hemagglutinin from Jiangxi-Donghu (2013) H10N8 influenza virus in complex with 3'-SLN  
Authors : Tzarum, N.; Zhang, H.; Zhu, X.; Wilson, I.A.  
Deposited on : 2015-01-20  
Resolution : 3.25 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

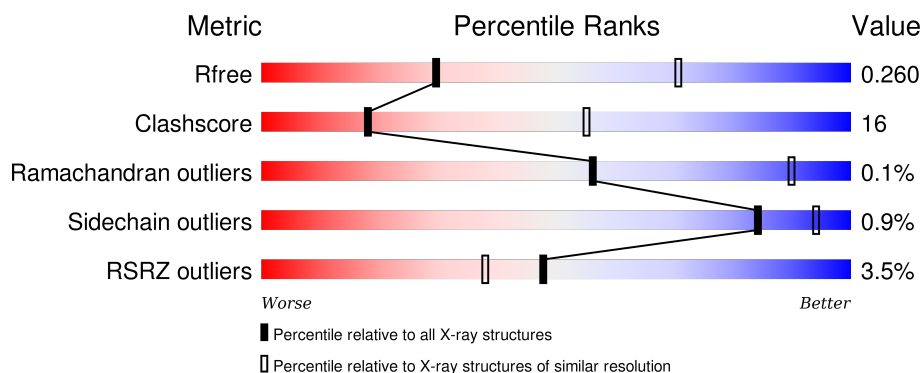
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	326	<div> <div>0%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>..</div> </div> </div>
1	C	326	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	E	326	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>..</div> </div> </div>
2	B	181	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>7%</div> </div> </div>
2	D	181	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	181	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SIA	C	401	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11593 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	C	318	Total	C	N	O	S	0	0	0
			2441	1510	449	465	17			
1	E	317	Total	C	N	O	S	0	0	0
			2433	1504	448	464	17			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	-	expression tag	UNP A0A059T4A1
A	9	ASP	-	expression tag	UNP A0A059T4A1
A	10	PRO	-	expression tag	UNP A0A059T4A1
C	8	ALA	-	expression tag	UNP A0A059T4A1
C	9	ASP	-	expression tag	UNP A0A059T4A1
C	10	PRO	-	expression tag	UNP A0A059T4A1
E	8	ALA	-	expression tag	UNP A0A059T4A1
E	9	ASP	-	expression tag	UNP A0A059T4A1
E	10	PRO	-	expression tag	UNP A0A059T4A1

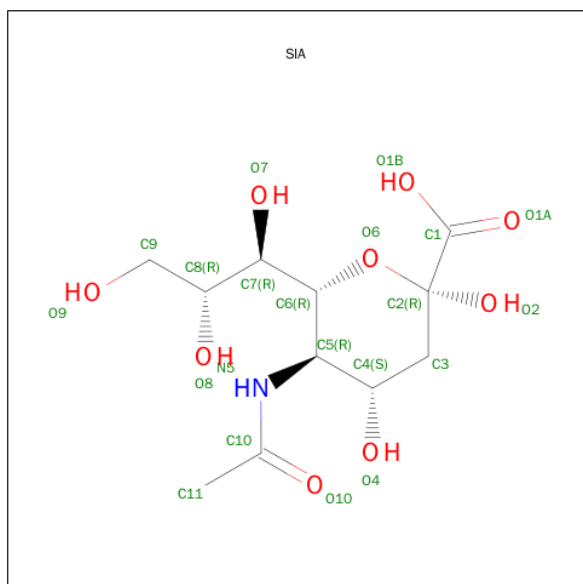
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1363	839	237	279	8			
2	D	165	Total	C	N	O	S	0	0	0
			1347	836	232	271	8			
2	F	166	Total	C	N	O	S	0	0	0
			1350	838	234	271	7			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A059T4A1
B	176	GLY	-	expression tag	UNP A0A059T4A1
B	177	ARG	-	expression tag	UNP A0A059T4A1
B	178	LEU	-	expression tag	UNP A0A059T4A1
B	179	VAL	-	expression tag	UNP A0A059T4A1
B	180	PRO	-	expression tag	UNP A0A059T4A1
B	181	ARG	-	expression tag	UNP A0A059T4A1
D	175	SER	-	expression tag	UNP A0A059T4A1
D	176	GLY	-	expression tag	UNP A0A059T4A1
D	177	ARG	-	expression tag	UNP A0A059T4A1
D	178	LEU	-	expression tag	UNP A0A059T4A1
D	179	VAL	-	expression tag	UNP A0A059T4A1
D	180	PRO	-	expression tag	UNP A0A059T4A1
D	181	ARG	-	expression tag	UNP A0A059T4A1
F	175	SER	-	expression tag	UNP A0A059T4A1
F	176	GLY	-	expression tag	UNP A0A059T4A1
F	177	ARG	-	expression tag	UNP A0A059T4A1
F	178	LEU	-	expression tag	UNP A0A059T4A1
F	179	VAL	-	expression tag	UNP A0A059T4A1
F	180	PRO	-	expression tag	UNP A0A059T4A1
F	181	ARG	-	expression tag	UNP A0A059T4A1

- Molecule 3 is O-SIALIC ACID (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



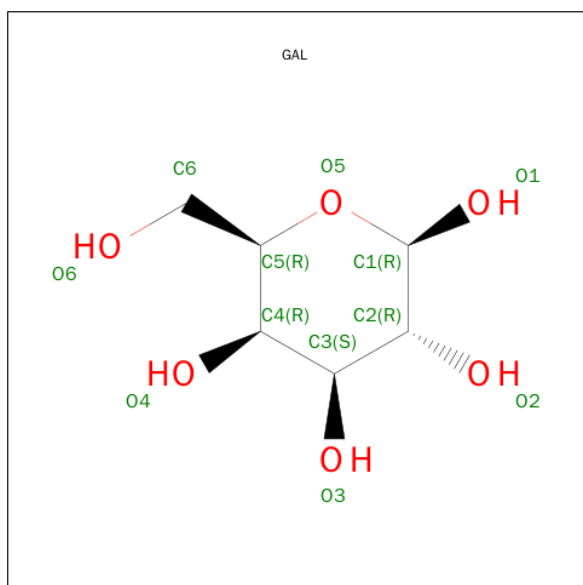
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	O	
			20	11	1	8	

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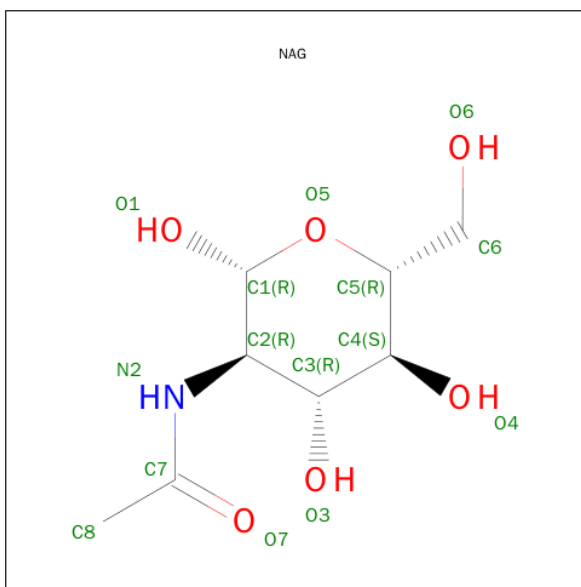
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			20	11	1	8		
3	E	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			12	6	6		

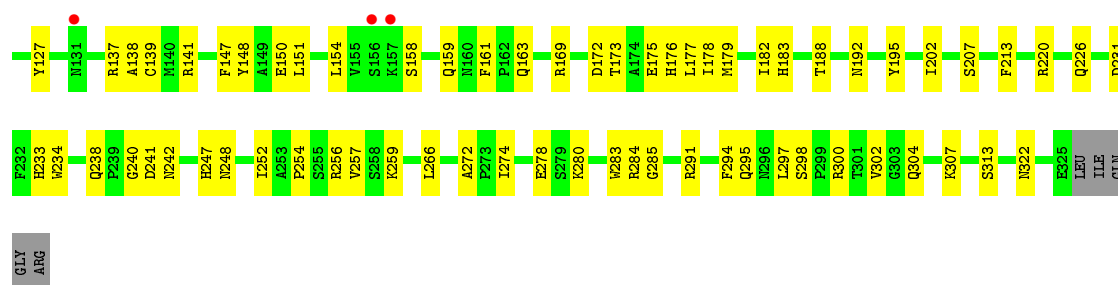
- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



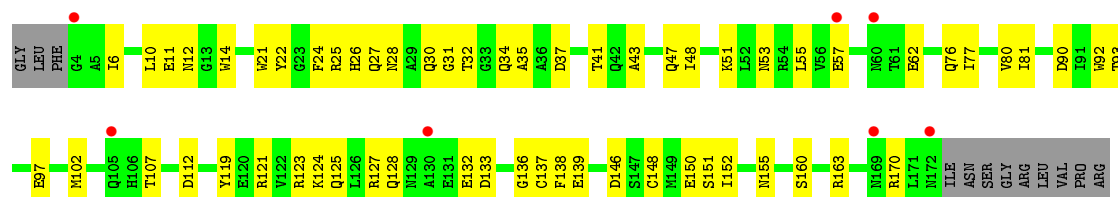
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			15	8	1	6		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		



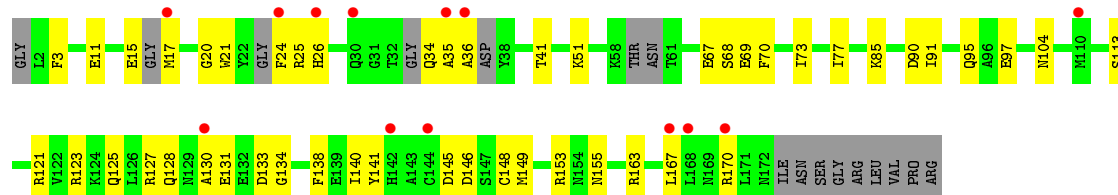




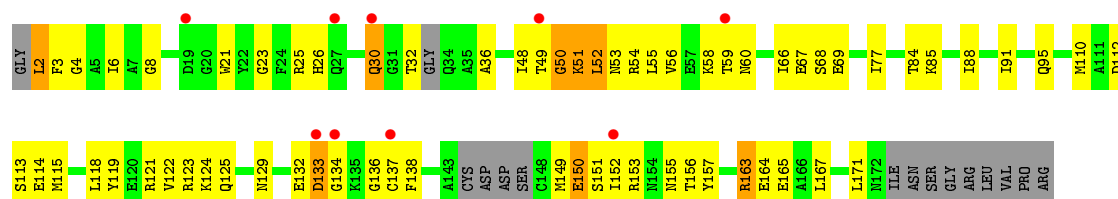
- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.87Å 245.85Å 71.00Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	48.39 – 3.25 48.39 – 3.21	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.39-3.25) 86.5 (48.39-3.21)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.217 , 0.261 0.217 , 0.260	Depositor DCC
$R_{free}$ test set	1450 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 17.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 31183 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	0.33	0/2486	0.61	1/3368 (0.0%)
1	C	0.29	0/2489	0.59	1/3371 (0.0%)
1	E	0.31	0/2481	0.58	1/3360 (0.0%)
2	B	0.28	0/1387	0.58	1/1872 (0.1%)
2	D	0.29	0/1367	0.59	0/1837
2	F	0.30	0/1373	0.76	4/1850 (0.2%)
All	All	0.30	0/11583	0.61	8/15658 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	B	0	1
2	F	0	3
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASN	N-CA-C	-12.10	78.33	111.00
2	F	149	MET	CB-CA-C	-10.49	89.42	110.40
2	F	150	GLU	N-CA-CB	-7.11	97.79	110.60
1	E	51	LEU	CA-CB-CG	6.02	129.14	115.30
2	F	52	LEU	N-CA-C	-5.35	96.56	111.00
2	F	2	LEU	CA-CB-CG	5.34	127.59	115.30
1	C	285	GLY	N-CA-C	-5.25	99.97	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	GLU	CB-CA-C	-5.13	100.13	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	150	GLU	Peptide
1	E	31	ASN	Peptide
2	F	163	ARG	Peptide
2	F	50	GLY	Peptide
2	F	51	LYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2385	101	0
1	C	2441	0	2392	72	0
1	E	2433	0	2382	75	0
2	B	1363	0	1259	47	0
2	D	1347	0	1248	40	0
2	F	1350	0	1258	69	0
3	A	20	0	17	1	0
3	C	20	0	17	1	0
3	E	20	0	17	1	0
4	A	11	0	9	1	0
4	C	11	0	9	1	0
4	E	12	0	11	0	0
5	A	57	0	52	1	0
5	C	57	0	52	1	0
5	E	14	0	13	2	0
All	All	11593	0	11121	357	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (357) 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:48:ILE:HD11	1:C:50:ARG:NH1	1.19	1.41
1:C:48:ILE:CD1	1:C:50:ARG:NH1	2.05	1.19
1:E:284:ARG:HD2	2:F:69:GLU:OE1	1.46	1.16
1:A:137:ARG:HA	1:A:145:ASN:ND2	1.62	1.15
1:A:137:ARG:CA	1:A:145:ASN:HD21	1.63	1.12
1:A:137:ARG:CA	1:A:145:ASN:ND2	2.16	1.09
1:C:48:ILE:HD11	1:C:50:ARG:CZ	1.88	1.02
1:C:48:ILE:HD11	1:C:50:ARG:HH12	1.25	1.00
1:A:136:THR:C	1:A:145:ASN:HD22	1.64	0.99
1:A:137:ARG:N	1:A:145:ASN:ND2	2.14	0.95
2:F:132:GLU:O	2:F:137:CYS:O	1.83	0.94
1:A:141:ARG:HH21	1:A:149:ALA:HB2	1.28	0.93
1:C:48:ILE:CD1	1:C:50:ARG:HH12	1.74	0.93
1:A:141:ARG:NH2	1:A:149:ALA:HB2	1.82	0.93
1:C:226:GLN:NE2	3:C:401:SIA:O1B	2.05	0.89
1:A:141:ARG:C	1:A:142:ASN:O	1.98	0.86
1:E:226:GLN:NE2	3:E:401:SIA:O1A	2.13	0.81
1:C:25:ILE:HD11	1:C:33:GLN:HB2	1.62	0.81
1:A:136:THR:C	1:A:145:ASN:ND2	2.34	0.81
2:F:51:LYS:CG	2:F:52:LEU:H	1.89	0.79
1:A:144:GLY:O	1:A:145:ASN:O	2.00	0.78
2:F:51:LYS:HG3	2:F:52:LEU:H	1.47	0.78
2:D:134:GLY:HA2	2:F:124:LYS:HB3	1.64	0.78
1:C:283:TRP:O	1:C:285:GLY:O	2.02	0.78
1:A:44:GLU:OE2	1:A:46:THR:OG1	2.05	0.74
2:D:125:GLN:NE2	2:D:155:ASN:OD1	2.21	0.74
1:E:176:HIS:HD2	1:E:259:LYS:HB2	1.53	0.74
2:D:95:GLN:NE2	2:F:95:GLN:OE1	2.21	0.74
2:B:25:ARG:NH2	2:B:34:GLN:OE1	2.21	0.73
1:E:188:THR:O	1:E:192:ASN:ND2	2.22	0.73
1:C:187:SER:HB2	1:C:190:GLU:H	1.53	0.73
1:C:50:ARG:O	1:C:286:GLY:HA3	1.89	0.72
2:F:30:GLN:HE21	2:F:30:GLN:C	1.93	0.72
1:A:18:HIS:CD2	2:B:21:TRP:HA	2.24	0.72
1:A:74:PRO:HG3	1:A:141:ARG:NH1	2.05	0.71
1:E:163:GLN:NE2	1:E:248:ASN:OD1	2.24	0.70
1:A:123:THR:HG22	1:A:257:VAL:HG13	1.74	0.70
2:F:123:ARG:HD3	2:F:132:GLU:OE2	1.91	0.69
1:C:51:LEU:HD12	1:C:286:GLY:HA2	1.73	0.69
1:E:291:ARG:HG2	2:F:58:LYS:HE3	1.75	0.69
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.56	0.69
2:B:125:GLN:NE2	2:B:155:ASN:OD1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:N	1:A:145:ASN:HD21	1.83	0.67
1:A:296:ASN:HD22	1:A:312:ARG:HA	1.59	0.67
2:F:21:TRP:HH2	2:F:48:ILE:HG13	1.61	0.66
2:D:25:ARG:HB3	2:D:34:GLN:HE21	1.60	0.66
2:B:6:ILE:HD13	2:B:112:ASP:HA	1.77	0.65
1:C:172:ASP:OD1	1:C:173:THR:N	2.30	0.65
1:A:50:ARG:O	1:A:287:SER:OG	2.13	0.65
2:F:49:THR:HA	2:F:51:LYS:HB3	1.77	0.65
2:F:6:ILE:HG13	2:F:112:ASP:HB3	1.78	0.65
2:B:128:GLN:O	2:B:170:ARG:NH1	2.29	0.65
1:A:220:ARG:NH1	1:A:227:SER:O	2.30	0.65
1:C:317:ALA:N	2:D:104:ASN:OD1	2.28	0.64
1:A:97:CYS:O	1:A:224:ASN:ND2	2.29	0.64
1:C:120:LYS:HD2	1:C:150:GLU:OE2	1.97	0.64
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.62	0.64
2:B:30:GLN:OE1	2:B:30:GLN:N	2.30	0.64
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.28	0.64
1:E:108:LEU:HD11	1:E:177:LEU:HD11	1.78	0.64
1:A:65:HIS:HB3	1:A:95:ALA:HB2	1.80	0.64
2:D:90:ASP:OD2	1:E:307:LYS:NZ	2.32	0.63
1:E:300:ARG:NH1	2:F:67:GLU:OE2	2.24	0.63
1:E:20:VAL:H	1:E:322:ASN:ND2	1.96	0.63
1:E:175:GLU:OE1	1:E:238:GLN:NE2	2.27	0.63
1:A:137:ARG:CB	1:A:145:ASN:HD21	2.09	0.63
1:A:30:THR:HG22	2:D:51:LYS:HE2	1.79	0.63
2:F:110:MET:O	2:F:113:SER:OG	2.16	0.63
2:D:91:ILE:HD13	2:F:91:ILE:HG21	1.81	0.63
1:A:295:GLN:NE2	1:A:298:SER:H	1.97	0.63
1:A:241:ASP:OD1	1:A:242:ASN:N	2.31	0.62
1:A:303:GLY:HA2	2:B:62:GLU:HG3	1.81	0.62
1:E:60:ASP:HB2	1:E:274:ILE:HD11	1.81	0.62
1:E:172:ASP:OD1	1:E:173:THR:N	2.31	0.62
1:A:172:ASP:OD1	1:A:173:THR:N	2.33	0.61
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.83	0.61
1:E:280:LYS:HE2	1:E:304:GLN:HE21	1.65	0.61
1:E:51:LEU:HD12	1:E:272:ALA:HB3	1.83	0.61
2:F:151:SER:HA	2:F:156:THR:HB	1.82	0.60
1:E:178:ILE:HG13	1:E:257:VAL:HG22	1.82	0.60
1:E:41:GLU:OE1	1:E:313:SER:OG	2.18	0.60
2:D:24:PHE:N	2:D:35:ALA:O	2.35	0.60
2:B:125:GLN:HE22	2:B:155:ASN:HA	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:HA	1:A:256:ARG:HG2	1.82	0.60
1:A:144:GLY:C	1:A:145:ASN:O	2.40	0.59
1:A:172:ASP:OD2	1:A:259:LYS:NZ	2.35	0.59
1:A:63:ASN:O	1:A:93:ALA:HA	2.03	0.59
1:E:102:THR:HB	1:E:105:VAL:HB	1.84	0.59
1:E:14:CYS:HB2	2:F:25:ARG:HB3	1.83	0.59
1:C:295:GLN:HG2	1:C:306:PRO:HG2	1.85	0.59
1:A:271:ASP:OD2	1:A:284:ARG:CG	2.51	0.58
1:E:176:HIS:CD2	1:E:259:LYS:HB2	2.36	0.58
1:C:281:CYS:SG	1:C:288:ILE:HD12	2.42	0.58
1:A:144:GLY:O	1:A:145:ASN:C	2.37	0.58
1:A:48:ILE:HG22	1:A:49:ASN:N	2.19	0.58
2:B:127:ARG:HG2	2:B:128:GLN:HG2	1.86	0.57
1:A:15:LEU:HD13	2:B:119:TYR:HA	1.85	0.57
1:A:311:ARG:NE	2:B:97:GLU:OE1	2.31	0.57
1:E:109:ARG:NH2	2:F:68:SER:HB2	2.19	0.57
1:A:58:HIS:HE1	1:A:276:ASN:HD22	1.53	0.56
1:E:123:THR:HG22	1:E:257:VAL:HG23	1.86	0.56
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.87	0.56
1:E:48:ILE:HG22	1:E:50:ARG:HG2	1.86	0.56
1:A:74:PRO:HG3	1:A:141:ARG:HH12	1.70	0.56
2:F:150:GLU:HG3	2:F:153:ARG:HD2	1.88	0.56
2:D:20:GLY:HA2	2:D:41:THR:HG21	1.88	0.56
1:C:187:SER:HB2	1:C:190:GLU:HB2	1.88	0.56
2:F:23:GLY:HA2	2:F:36:ALA:HA	1.88	0.56
2:D:134:GLY:CA	2:F:124:LYS:HB3	2.34	0.56
1:A:141:ARG:N	1:A:142:ASN:O	2.39	0.55
1:C:107:ALA:O	1:C:111:LYS:HG3	2.06	0.55
2:F:129:ASN:ND2	2:F:157:TYR:OH	2.39	0.55
1:A:60:ASP:HB2	1:A:274:ILE:HD11	1.89	0.55
1:A:160:ASN:HA	1:A:196:GLY:HA3	1.89	0.55
1:E:179:MET:O	1:E:254:PRO:HB3	2.07	0.55
1:A:141:ARG:CG	1:A:141:ARG:HH11	2.20	0.55
2:B:11:GLU:O	2:B:12:ASN:ND2	2.40	0.55
1:E:127:TYR:CD1	1:E:154:LEU:HD21	2.41	0.55
2:B:22:TYR:H	2:B:41:THR:HG22	1.73	0.54
1:C:269:GLN:NE2	2:D:69:GLU:H	2.05	0.54
1:E:141:ARG:NH2	1:E:147:PHE:O	2.41	0.54
2:F:48:ILE:O	2:F:51:LYS:HB3	2.08	0.54
1:E:179:MET:HG2	1:E:234:TRP:HB3	1.88	0.54
2:B:37:ASP:OD2	2:B:121:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:GLN:NE2	1:E:298:SER:H	2.06	0.54
2:F:4:GLY:O	2:F:8:GLY:HA3	2.08	0.53
1:C:25:ILE:HD11	1:C:33:GLN:CB	2.36	0.53
1:A:106:GLU:O	1:A:110:GLN:HG3	2.08	0.53
1:E:213:PHE:HE2	1:E:233:HIS:CD2	2.26	0.53
1:A:84:TRP:CE2	1:A:87:LEU:HD13	2.43	0.53
1:A:202:ILE:HG21	1:A:251:LEU:HD13	1.91	0.53
1:C:20:VAL:H	1:C:322:ASN:ND2	2.06	0.53
1:A:42:THR:HA	1:A:292:LEU:HD22	1.90	0.53
1:C:18:HIS:CD2	2:D:21:TRP:HA	2.44	0.53
2:D:3:PHE:HE2	2:D:113:SER:HB2	1.73	0.53
1:C:57:LYS:O	1:C:85:ASP:N	2.29	0.53
1:A:108:LEU:O	1:A:112:ILE:HD12	2.10	0.52
1:C:41:GLU:OE1	1:C:313:SER:OG	2.27	0.52
1:C:48:ILE:CG2	1:C:287:SER:O	2.58	0.52
1:C:44:GLU:HG2	1:C:292:LEU:HD12	1.92	0.52
2:F:123:ARG:CD	2:F:132:GLU:OE2	2.57	0.52
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.25	0.51
1:C:266:LEU:HD11	1:C:302:VAL:HG13	1.92	0.51
1:A:48:ILE:CG2	1:A:49:ASN:N	2.73	0.51
1:E:283:TRP:CH2	1:E:285:GLY:HA3	2.46	0.51
4:C:402:GAL:C1	5:C:403:NAG:O6	2.59	0.51
1:C:150:GLU:CD	1:C:256:ARG:HE	2.12	0.51
2:F:122:VAL:HG22	2:F:152:ILE:HG22	1.91	0.51
1:E:154:LEU:HD22	1:E:247:HIS:HE1	1.76	0.51
1:A:220:ARG:HD3	1:C:210:ARG:HG3	1.92	0.51
2:F:119:TYR:HE2	2:F:136:GLY:HA2	1.75	0.51
1:E:150:GLU:HG3	1:E:256:ARG:HE	1.75	0.51
4:A:402:GAL:C1	5:A:403:NAG:O6	2.59	0.51
1:E:182:ILE:HD12	1:E:202:ILE:HD13	1.93	0.51
1:E:43:VAL:HG22	1:E:294:PHE:HB2	1.92	0.51
2:B:28:ASN:HB3	2:B:31:GLY:O	2.10	0.51
2:F:2:LEU:HD12	2:F:3:PHE:N	2.25	0.51
1:A:271:ASP:OD2	1:A:284:ARG:HG3	2.12	0.50
1:E:48:ILE:CG2	1:E:50:ARG:NH2	2.74	0.50
1:E:97:CYS:O	1:E:138:ALA:HB1	2.11	0.50
1:C:38:ASN:OD1	1:C:39:ALA:N	2.43	0.50
1:A:41:GLU:OE2	1:A:42:THR:N	2.44	0.50
2:B:123:ARG:HB2	2:B:138:PHE:CZ	2.46	0.50
2:B:160:SER:O	2:B:163:ARG:HB2	2.10	0.50
1:C:98:TYR:CE1	1:C:230:ILE:HG13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:HG22	1:A:270:SER:HB2	1.92	0.50
2:F:125:GLN:HE22	2:F:155:ASN:HA	1.76	0.50
1:C:18:HIS:CE1	1:C:37:THR:HG21	2.47	0.50
1:A:210:ARG:HG3	1:E:220:ARG:HE	1.76	0.50
2:F:51:LYS:HB2	2:F:52:LEU:HG	1.92	0.50
2:D:15:GLU:O	2:D:17:MET:N	2.43	0.50
2:B:148:CYS:O	2:B:151:SER:HB3	2.12	0.50
1:A:104:ASN:HB2	1:A:234:TRP:HE1	1.76	0.49
1:C:28:THR:O	2:F:54:ARG:NH2	2.42	0.49
1:C:48:ILE:HD12	1:C:50:ARG:HH12	1.69	0.49
1:A:179:MET:HG2	1:A:234:TRP:HB3	1.94	0.49
2:B:27:GLN:HA	2:B:32:THR:HG22	1.94	0.49
2:F:110:MET:HE1	2:F:114:GLU:HG2	1.93	0.49
1:A:58:HIS:CE1	1:A:276:ASN:HD22	2.28	0.49
1:A:82:GLY:HA3	1:A:84:TRP:HZ3	1.77	0.49
1:E:68:GLY:HA2	1:E:71:ILE:HG22	1.94	0.49
1:E:77:ASP:OD2	1:E:141:ARG:NH1	2.42	0.49
1:C:59:LYS:HE3	1:C:79:HIS:CD2	2.47	0.49
1:A:48:ILE:HG22	1:A:50:ARG:H	1.76	0.49
2:F:119:TYR:CE2	2:F:136:GLY:HA2	2.48	0.49
1:A:36:VAL:HG11	1:A:317:ALA:HB1	1.95	0.48
2:B:43:ALA:O	2:B:47:GLN:HG3	2.12	0.48
2:D:141:TYR:CD2	2:D:170:ARG:HG3	2.48	0.48
1:A:141:ARG:NH1	1:A:141:ARG:CG	2.73	0.48
2:B:21:TRP:N	2:B:21:TRP:CD1	2.81	0.48
1:C:102:THR:HB	1:C:105:VAL:HB	1.95	0.48
2:F:51:LYS:HG3	2:F:52:LEU:N	2.23	0.48
2:B:148:CYS:O	2:B:152:ILE:HG13	2.14	0.48
1:E:137:ARG:HG3	1:E:137:ARG:O	2.13	0.48
1:E:54:LYS:HB2	1:E:278:GLU:HA	1.95	0.48
2:D:3:PHE:HE1	2:F:3:PHE:CZ	2.31	0.48
1:C:30:THR:O	2:F:50:GLY:HA3	2.14	0.48
1:C:132:SER:HA	1:C:154:LEU:HD23	1.96	0.48
1:E:151:LEU:HD23	1:E:254:PRO:HA	1.96	0.48
1:E:295:GLN:HE21	1:E:297:LEU:N	2.12	0.48
1:E:13:ILE:CG2	2:F:138:PHE:HB2	2.44	0.48
2:F:21:TRP:CH2	2:F:48:ILE:HG13	2.46	0.47
1:E:283:TRP:CZ2	1:E:285:GLY:HA3	2.48	0.47
2:F:84:THR:O	2:F:88:ILE:HG12	2.13	0.47
1:E:280:LYS:HE3	1:E:304:GLN:HG3	1.95	0.47
1:A:31:ASN:HB3	1:A:34:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:164:GLU:CD	2:F:165:GLU:HG2	2.34	0.47
1:A:141:ARG:NH1	1:A:141:ARG:HG2	2.27	0.47
1:C:13:ILE:HG13	2:D:26:HIS:HB3	1.96	0.47
1:C:110:GLN:O	1:C:114:GLU:HG3	2.15	0.47
1:C:48:ILE:HG22	1:C:287:SER:O	2.13	0.47
2:F:133:ASP:OD2	2:F:137:CYS:HB2	2.15	0.47
2:B:14:TRP:CH2	2:B:25:ARG:HG2	2.49	0.47
2:D:97:GLU:HG2	2:F:54:ARG:NH1	2.29	0.47
1:C:241:ASP:OD1	1:C:242:ASN:N	2.48	0.47
2:D:131:GLU:CD	2:F:163:ARG:HH22	2.17	0.47
1:A:74:PRO:HD2	1:A:97:CYS:SG	2.55	0.47
1:A:48:ILE:HB	1:A:287:SER:O	2.15	0.47
1:E:70:LEU:HD11	1:E:112:ILE:HD11	1.97	0.47
1:E:158:SER:HB2	1:E:159:GLN:HG3	1.97	0.47
1:E:266:LEU:HD11	1:E:302:VAL:HG12	1.96	0.47
1:E:20:VAL:H	1:E:322:ASN:HD22	1.63	0.46
2:B:28:ASN:ND2	2:B:146:ASP:OD1	2.48	0.46
2:F:51:LYS:HG3	2:F:53:ASN:H	1.81	0.46
2:D:127:ARG:HG2	2:D:128:GLN:HG2	1.97	0.46
2:B:124:LYS:HD2	2:F:134:GLY:HA2	1.97	0.46
1:C:36:VAL:HG11	1:C:317:ALA:HB1	1.97	0.46
1:E:291:ARG:HB3	2:F:56:VAL:HB	1.97	0.46
1:A:295:GLN:HE21	1:A:298:SER:H	1.62	0.46
1:C:18:HIS:HE1	1:C:37:THR:HG21	1.80	0.46
1:C:169:ARG:HG2	1:C:242:ASN:CG	2.35	0.46
2:F:112:ASP:O	2:F:115:MET:N	2.49	0.46
1:A:65:HIS:CE1	1:A:67:ILE:HG12	2.51	0.46
1:A:161:PHE:O	1:A:198:GLN:NE2	2.45	0.46
1:A:29:LEU:HD11	2:B:102:MET:HG3	1.97	0.46
1:C:65:HIS:ND1	1:C:66:PRO:HD2	2.29	0.46
1:E:207:SER:HB2	1:E:241:ASP:OD2	2.16	0.46
1:A:184:HIS:HB3	1:A:216:VAL:O	2.16	0.46
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.51	0.46
2:B:76:GLN:O	2:B:80:VAL:HG23	2.16	0.45
2:F:49:THR:C	2:F:51:LYS:HG2	2.37	0.45
2:F:164:GLU:CD	2:F:165:GLU:H	2.19	0.45
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.51	0.45
1:A:200:LEU:O	1:A:214:VAL:HG13	2.16	0.45
1:A:18:HIS:HD2	2:B:21:TRP:HA	1.76	0.45
2:B:77:ILE:O	2:B:81:ILE:HG13	2.16	0.45
1:E:172:ASP:HB3	1:E:176:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD21	2:B:24:PHE:CE1	2.51	0.45
1:E:240:GLY:O	5:E:403:NAG:H82	2.17	0.45
1:C:46:THR:O	1:C:46:THR:OG1	2.30	0.45
2:F:77:ILE:HA	2:F:77:ILE:HD12	1.79	0.45
1:A:48:ILE:CG2	1:A:49:ASN:H	2.29	0.45
2:D:123:ARG:HB2	2:D:138:PHE:CZ	2.51	0.45
2:F:52:LEU:HA	2:F:55:LEU:HB3	1.99	0.45
2:D:3:PHE:HE1	2:F:3:PHE:HZ	1.65	0.45
2:B:53:ASN:O	2:B:57:GLU:HG3	2.16	0.45
1:A:178:ILE:HD11	1:A:254:PRO:HG3	1.98	0.45
1:E:151:LEU:HB3	1:E:252:ILE:HG22	1.98	0.45
1:C:38:ASN:HB3	1:C:318:THR:HG23	1.98	0.44
2:F:125:GLN:NE2	2:F:155:ASN:HA	2.32	0.44
2:F:51:LYS:HD2	2:F:52:LEU:HB2	1.99	0.44
1:C:311:ARG:NH2	2:F:59:THR:HG22	2.33	0.44
2:F:112:ASP:N	2:F:112:ASP:OD1	2.50	0.44
1:A:283:TRP:CZ2	1:A:285:GLY:HA3	2.52	0.44
2:F:85:LYS:HE3	2:F:85:LYS:HB2	1.69	0.44
1:A:112:ILE:O	1:A:115:SER:OG	2.21	0.44
2:D:163:ARG:O	2:D:167:LEU:HD13	2.18	0.44
1:C:62:GLY:O	1:C:90:ARG:HB2	2.17	0.44
2:D:11:GLU:N	2:D:11:GLU:OE1	2.51	0.44
2:B:10:LEU:HD21	2:B:136:GLY:HA3	1.99	0.44
2:D:141:TYR:HD2	2:D:170:ARG:HG3	1.82	0.44
1:C:118:ILE:HG12	1:C:260:LEU:HD23	1.99	0.44
1:E:56:ARG:HH22	1:E:280:LYS:HZ2	1.66	0.44
1:A:130:ILE:HG12	1:A:161:PHE:CZ	2.52	0.44
2:F:164:GLU:CG	2:F:165:GLU:H	2.31	0.44
2:B:51:LYS:NZ	2:B:107:THR:OG1	2.41	0.44
1:C:60:ASP:HA	1:C:88:ILE:HB	2.00	0.44
2:B:24:PHE:HB2	2:B:35:ALA:HB3	1.99	0.44
2:B:77:ILE:HD12	2:B:77:ILE:HA	1.83	0.44
1:A:84:TRP:CZ2	1:A:87:LEU:HD13	2.53	0.43
1:C:161:PHE:HB3	1:C:248:ASN:O	2.17	0.43
1:C:121:ILE:N	1:C:121:ILE:HD12	2.32	0.43
2:B:125:GLN:HE22	2:B:155:ASN:CA	2.29	0.43
1:A:226:GLN:NE2	3:A:401:SIA:O1A	2.52	0.43
1:C:266:LEU:HD12	1:C:267:GLY:H	1.84	0.43
1:E:241:ASP:HA	5:E:403:NAG:H82	1.99	0.43
2:D:121:ARG:HD3	2:D:121:ARG:O	2.18	0.43
1:C:42:THR:OG1	1:C:314:LEU:O	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:MET:O	2:D:153:ARG:HG3	2.19	0.43
1:A:13:ILE:HG13	2:B:26:HIS:HB3	1.99	0.43
1:C:315:MET:O	2:D:104:ASN:ND2	2.49	0.43
1:C:61:LEU:HD21	1:C:87:LEU:HD11	2.00	0.43
1:C:61:LEU:HD23	1:C:79:HIS:CD2	2.53	0.43
1:C:278:GLU:HG3	1:C:278:GLU:O	2.19	0.43
1:E:161:PHE:HB3	1:E:248:ASN:O	2.18	0.42
1:C:325:GLU:OE1	1:C:325:GLU:N	2.36	0.42
1:E:53:MET:HG3	1:E:274:ILE:HG23	2.01	0.42
2:D:20:GLY:HA3	2:D:36:ALA:HB1	2.00	0.42
1:C:314:LEU:HA	1:C:314:LEU:HD23	1.85	0.42
1:E:44:GLU:HG2	1:E:46:THR:O	2.19	0.42
1:E:304:GLN:HB3	2:F:60:ASN:HB3	1.99	0.42
2:D:130:ALA:HB2	2:D:140:ILE:HG22	2.00	0.42
1:C:200:LEU:HD13	1:C:249:GLY:O	2.19	0.42
1:E:57:LYS:O	1:E:85:ASP:N	2.46	0.42
1:A:17:HIS:HB2	1:A:320:MET:SD	2.59	0.42
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.68	0.42
1:A:152:LYS:HG3	1:A:255:SER:HB3	2.02	0.42
1:E:73:THR:HG23	1:E:74:PRO:HD2	2.01	0.42
1:C:18:HIS:HD2	2:D:21:TRP:HA	1.83	0.42
1:A:104:ASN:HB3	1:A:107:ALA:HB3	2.02	0.42
1:A:125:PHE:CD2	1:A:166:ASN:HB3	2.55	0.42
1:E:154:LEU:HD23	1:E:161:PHE:HZ	1.83	0.42
1:E:13:ILE:HG23	2:F:138:PHE:HB2	2.01	0.42
1:A:137:ARG:HB2	1:A:145:ASN:HD21	1.80	0.42
2:D:73:ILE:HD11	2:D:77:ILE:HG23	2.00	0.42
1:A:15:LEU:CD1	2:B:119:TYR:HA	2.48	0.42
1:A:42:THR:HG22	2:B:55:LEU:HD21	2.02	0.42
1:A:203:SER:OG	1:A:246:SER:HB2	2.19	0.42
2:F:26:HIS:O	2:F:32:THR:HA	2.20	0.41
1:E:18:HIS:CD2	2:F:21:TRP:HA	2.55	0.41
1:E:48:ILE:HG21	1:E:50:ARG:CZ	2.50	0.41
1:A:14:CYS:HB2	2:B:25:ARG:O	2.20	0.41
1:C:269:GLN:NE2	2:D:68:SER:OG	2.54	0.41
1:C:60:ASP:CG	1:C:90:ARG:HH21	2.24	0.41
1:A:29:LEU:HG	2:B:102:MET:HA	2.03	0.41
1:C:184:HIS:HA	1:C:185:PRO:HD3	1.88	0.41
2:F:66:ILE:HG12	2:F:66:ILE:H	1.70	0.41
2:B:133:ASP:HB3	2:B:137:CYS:O	2.20	0.41
2:B:127:ARG:HG2	2:B:128:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:HB3	1:A:198:GLN:NE2	2.35	0.41
2:F:167:LEU:O	2:F:171:LEU:HG	2.21	0.41
2:D:146:ASP:OD1	2:D:146:ASP:N	2.54	0.41
1:A:185:PRO:C	1:A:220:ARG:HH22	2.24	0.41
1:E:148:TYR:HB2	1:E:151:LEU:HB2	2.02	0.41
2:F:114:GLU:HA	2:F:114:GLU:OE1	2.20	0.41
2:F:151:SER:HB2	2:F:157:TYR:HB2	2.02	0.41
2:F:163:ARG:HG2	2:F:167:LEU:HD11	2.02	0.41
2:F:133:ASP:CG	2:F:137:CYS:HB2	2.41	0.41
1:A:210:ARG:NH1	1:E:231:ASP:OD2	2.52	0.41
2:B:133:ASP:HB2	2:B:139:GLU:OE2	2.21	0.41
2:F:118:LEU:CD1	2:F:121:ARG:HH21	2.34	0.41
1:A:120:LYS:HA	1:A:257:VAL:O	2.21	0.41
2:D:67:GLU:OE2	2:D:85:LYS:NZ	2.42	0.41
1:C:91:GLU:HA	2:D:70:PHE:CD2	2.55	0.41
1:E:74:PRO:HA	1:E:141:ARG:NH1	2.36	0.40
1:E:266:LEU:HD11	1:E:302:VAL:CG1	2.50	0.40
2:B:90:ASP:O	2:B:93:THR:HG22	2.21	0.40
1:C:50:ARG:O	1:C:286:GLY:CA	2.64	0.40
1:A:63:ASN:O	1:A:94:ILE:N	2.45	0.40
1:C:109:ARG:NH2	2:D:68:SER:HB2	2.36	0.40
2:D:145:ASP:O	2:D:148:CYS:HB3	2.22	0.40
1:E:169:ARG:HG2	1:E:242:ASN:CG	2.41	0.40
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.02	0.40
1:A:65:HIS:HB2	1:A:93:ALA:HB1	2.03	0.40
1:E:56:ARG:HH21	1:E:280:LYS:HD2	1.86	0.40
1:C:48:ILE:HG23	1:C:287:SER:O	2.21	0.40
1:E:97:CYS:SG	1:E:139:CYS:N	2.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/326 (97%)	305 (96%)	10 (3%)	1 (0%)	46	83
1	C	314/326 (96%)	306 (98%)	7 (2%)	1 (0%)	46	83
1	E	313/326 (96%)	294 (94%)	19 (6%)	0	100	100
2	B	167/181 (92%)	159 (95%)	8 (5%)	0	100	100
2	D	153/181 (84%)	148 (97%)	5 (3%)	0	100	100
2	F	160/181 (88%)	142 (89%)	18 (11%)	0	100	100
All	All	1423/1521 (94%)	1354 (95%)	67 (5%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	C	286	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	269/275 (98%)	266 (99%)	3 (1%)	80	92
1	C	270/275 (98%)	266 (98%)	4 (2%)	72	90
1	E	269/275 (98%)	268 (100%)	1 (0%)	93	97
2	B	144/154 (94%)	144 (100%)	0	100	100
2	D	143/154 (93%)	142 (99%)	1 (1%)	88	96
2	F	142/154 (92%)	140 (99%)	2 (1%)	74	90
All	All	1237/1287 (96%)	1226 (99%)	11 (1%)	84	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	MET
1	A	141	ARG
1	A	287	SER

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Mol	Chain	Res	Type
1	C	48	ILE
1	C	85	ASP
1	C	210	ARG
1	C	287	SER
2	D	133	ASP
1	E	46	THR
2	F	30	GLN
2	F	133	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	145	ASN
1	A	222	GLN
1	A	226	GLN
1	A	276	ASN
1	A	295	GLN
2	B	53	ASN
2	B	95	GLN
2	B	125	GLN
2	B	155	ASN
1	C	79	HIS
1	C	159	GLN
1	C	226	GLN
1	C	269	GLN
1	C	322	ASN
2	D	34	GLN
2	D	95	GLN
2	D	125	GLN
1	E	176	HIS
1	E	247	HIS
1	E	269	GLN
1	E	276	ASN
1	E	295	GLN
1	E	304	GLN
1	E	322	ASN
2	F	12	ASN
2	F	30	GLN
2	F	95	GLN
2	F	105	GLN
2	F	117	ASN

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Mol	Chain	Res	Type
2	F	129	ASN
2	F	155	ASN
2	F	172	ASN

### 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 ⓘ

15 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	SIA	A	401	4	16,20,21	0.33	0	18,28,31	0.82	1 (5%)
4	GAL	A	402	3,5	11,11,12	0.50	0	14,15,17	1.41	3 (21%)
5	NAG	A	403	4	15,15,15	0.77	0	17,21,21	1.50	2 (11%)
5	NAG	A	404	1	14,14,15	0.62	1 (7%)	15,19,21	0.51	0
5	NAG	A	405	1,5	14,14,15	0.73	1 (7%)	15,19,21	0.78	0
5	NAG	A	406	5	14,14,15	0.43	0	15,19,21	0.95	1 (6%)
3	SIA	C	401	4	16,20,21	0.33	0	18,28,31	0.82	1 (5%)
4	GAL	C	402	3,5	11,11,12	0.50	0	14,15,17	1.40	3 (21%)
5	NAG	C	403	4	15,15,15	0.78	0	17,21,21	1.51	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	404	1	14,14,15	0.67	1 (7%)	15,19,21	1.02	1 (6%)
5	NAG	C	405	1,5	14,14,15	0.74	1 (7%)	15,19,21	0.76	0
5	NAG	C	406	5	14,14,15	0.22	0	15,19,21	0.45	0
3	SIA	E	401	4	16,20,21	0.34	0	18,28,31	0.82	1 (5%)
4	GAL	E	402	3	12,12,12	0.44	0	17,17,17	2.91	2 (11%)
5	NAG	E	403	1	14,14,15	0.71	1 (7%)	15,19,21	0.77	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	SIA	A	401	4	-	0/14/34/38	0/1/1/1
4	GAL	A	402	3,5	-	0/2/19/22	0/1/1/1
5	NAG	A	403	4	-	0/6/26/26	0/1/1/1
5	NAG	A	404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	406	5	-	0/6/23/26	0/1/1/1
3	SIA	C	401	4	-	0/14/34/38	0/1/1/1
4	GAL	C	402	3,5	-	0/2/19/22	0/1/1/1
5	NAG	C	403	4	-	0/6/26/26	0/1/1/1
5	NAG	C	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	406	5	-	0/6/23/26	0/1/1/1
3	SIA	E	401	4	-	0/14/34/38	0/1/1/1
4	GAL	E	402	3	-	0/2/22/22	0/1/1/1
5	NAG	E	403	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	403	NAG	O5-C1	-2.34	1.39	1.43
5	A	405	NAG	O5-C1	-2.32	1.39	1.43
5	C	405	NAG	O5-C1	-2.29	1.39	1.43
5	C	404	NAG	O5-C1	-2.25	1.40	1.43
5	A	404	NAG	O5-C1	-2.23	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	NAG	O4-C4-C3	-4.97	99.14	110.34
5	A	403	NAG	O4-C4-C3	-4.96	99.16	110.34
5	A	406	NAG	C2-N2-C7	-2.81	119.43	123.04
5	C	404	NAG	O5-C5-C6	-2.35	102.27	107.35
5	A	403	NAG	C2-N2-C7	-2.29	117.22	123.10
5	C	403	NAG	C2-N2-C7	-2.28	117.24	123.10
4	E	402	GAL	O1-C1-C2	-2.22	103.25	109.21
4	A	402	GAL	O3-C3-C2	-2.11	106.18	110.00
4	C	402	GAL	O3-C3-C2	-2.11	106.18	110.00
3	C	401	SIA	O6-C6-C5	2.43	112.46	108.48
3	A	401	SIA	O6-C6-C5	2.46	112.50	108.48
3	E	401	SIA	O6-C6-C5	2.46	112.52	108.48
4	C	402	GAL	C1-O5-C5	2.68	115.65	112.25
4	A	402	GAL	C1-O5-C5	2.71	115.69	112.25
4	C	402	GAL	C1-C2-C3	3.17	113.29	109.54
4	A	402	GAL	C1-C2-C3	3.17	113.29	109.54
4	E	402	GAL	O1-C1-O5	11.18	140.81	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SIA	1	0
4	A	402	GAL	1	0
5	A	403	NAG	1	0
3	C	401	SIA	1	0
4	C	402	GAL	1	0
5	C	403	NAG	1	0
3	E	401	SIA	1	0
5	E	403	NAG	2	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	318/326 (97%)	-0.13	4 (1%) 79 71	51, 69, 104, 125	0
1	C	318/326 (97%)	-0.00	11 (3%) 48 38	53, 76, 120, 140	0
1	E	317/326 (97%)	-0.11	7 (2%) 65 55	46, 73, 108, 132	0
2	B	169/181 (93%)	0.28	7 (4%) 41 31	54, 101, 132, 141	0
2	D	165/181 (91%)	0.44	13 (7%) 15 11	58, 110, 145, 154	0
2	F	166/181 (91%)	0.41	9 (5%) 29 22	53, 107, 130, 139	0
All	All	1453/1521 (95%)	0.08	51 (3%) 48 38	46, 81, 128, 154	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	24	PHE	5.5
1	E	11	ASP	4.5
2	F	27	GLN	4.3
2	D	170	ARG	4.3
1	C	47	GLY	4.2
1	A	24	THR	4.1
2	B	4	GLY	3.9
1	A	21	ALA	3.8
1	E	12	LYS	3.7
2	D	36	ALA	3.3
1	E	13	ILE	3.3
2	F	49	THR	3.1
2	D	35	ALA	3.1
2	F	137	CYS	3.0
1	E	131	ASN	3.0
1	A	23	GLY	3.0
1	A	22	ASN	3.0
1	C	326	LEU	3.0
1	E	14	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	20	VAL	2.9
1	C	16	GLY	2.8
1	C	42	THR	2.7
2	B	57	GLU	2.7
2	D	167	LEU	2.7
2	B	172	ASN	2.6
1	C	136	THR	2.6
2	D	17	MET	2.6
2	F	30	GLN	2.6
2	D	144	CYS	2.5
1	E	157	LYS	2.5
2	B	130	ALA	2.5
2	F	59	THR	2.4
2	F	152	ILE	2.4
2	D	110	MET	2.3
2	D	168	LEU	2.3
2	B	60	ASN	2.3
2	D	130	ALA	2.2
1	C	253	ALA	2.2
2	D	30	GLN	2.2
2	D	26	HIS	2.2
1	E	156	SER	2.2
2	F	134	GLY	2.2
2	B	169	ASN	2.1
1	C	21	ALA	2.1
2	F	19	ASP	2.1
2	D	142	HIS	2.1
2	B	105	GLN	2.1
1	C	129	SER	2.0
2	F	133	ASP	2.0
1	C	43	VAL	2.0
1	C	310	ASN	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	SIA	C	401	20/21	0.85	0.43	2.67	74,97,111,117	0
5	NAG	C	405	14/15	0.85	0.29	1.86	89,101,121,137	0
5	NAG	E	403	14/15	0.85	0.22	0.83	74,93,108,114	0
5	NAG	A	405	14/15	0.87	0.19	0.76	89,101,119,119	0
3	SIA	E	401	20/21	0.83	0.27	0.74	76,91,106,107	0
3	SIA	A	401	20/21	0.87	0.17	-0.28	67,77,97,97	0
5	NAG	A	406	14/15	0.74	0.37	-	112,126,141,143	0
5	NAG	C	404	14/15	0.82	0.24	-	125,138,145,156	0
5	NAG	C	406	14/15	0.85	0.24	-	100,123,132,138	0
4	GAL	E	402	12/12	0.89	0.20	-	98,114,122,128	0
4	GAL	C	402	11/12	0.81	0.24	-	115,129,142,151	0
5	NAG	A	403	15/15	0.81	0.43	-	116,134,154,155	0
5	NAG	A	404	14/15	0.82	0.18	-	101,116,126,129	0
5	NAG	C	403	15/15	0.72	0.37	-	152,172,181,196	0
4	GAL	A	402	11/12	0.92	0.12	-	87,98,111,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.