



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DJ8  
Title : Structure of the hemagglutinin complexed with 6SLN from a highly pathogenic H7N7 influenza virus  
Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.  
Deposited on : 2012-02-01  
Resolution : 2.80 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

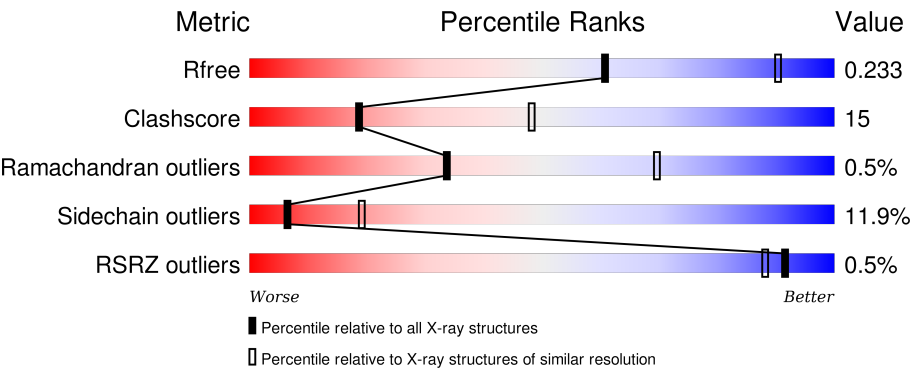
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 <sub>free</sub>	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	
1	C	327	
1	E	327	
2	B	177	
2	D	177	

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Mol	Chain	Length	Quality of chain
2	F	177	

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
4	SIA	A	404	-	-	-	X
4	SIA	C	404	-	-	-	X
4	SIA	E	404	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11749 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	316	Total	C	N	O	S	4	0	0
			2422	1502	435	471	14			
1	C	316	Total	C	N	O	S	4	0	0
			2422	1502	435	471	14			
1	E	317	Total	C	N	O	S	3	1	0
			2437	1510	440	473	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	EXPRESSION TAG	UNP Q6VMK1
A	-2	ASP	-	EXPRESSION TAG	UNP Q6VMK1
A	-1	PRO	-	EXPRESSION TAG	UNP Q6VMK1
A	0	GLY	-	EXPRESSION TAG	UNP Q6VMK1
C	-3	ALA	-	EXPRESSION TAG	UNP Q6VMK1
C	-2	ASP	-	EXPRESSION TAG	UNP Q6VMK1
C	-1	PRO	-	EXPRESSION TAG	UNP Q6VMK1
C	0	GLY	-	EXPRESSION TAG	UNP Q6VMK1
E	-3	ALA	-	EXPRESSION TAG	UNP Q6VMK1
E	-2	ASP	-	EXPRESSION TAG	UNP Q6VMK1
E	-1	PRO	-	EXPRESSION TAG	UNP Q6VMK1
E	0	GLY	-	EXPRESSION TAG	UNP Q6VMK1

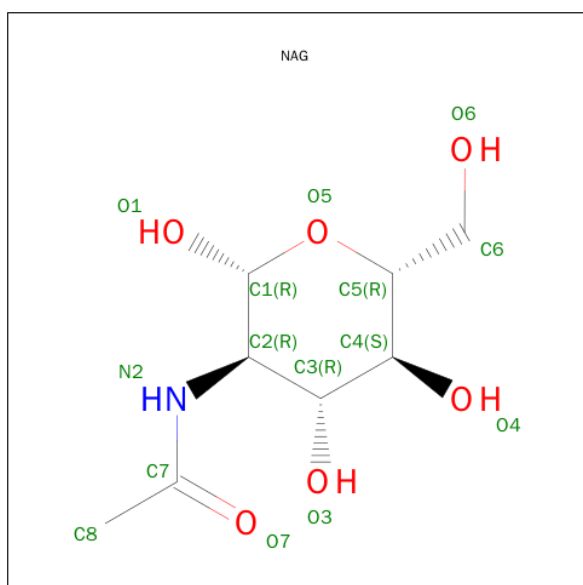
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	4	0	0
			1380	851	243	279	7			
2	D	171	Total	C	N	O	S	0	0	0
			1388	857	244	280	7			
2	F	169	Total	C	N	O	S	0	0	0
			1369	845	239	278	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP Q6VMK1
B	176	GLY	-	EXPRESSION TAG	UNP Q6VMK1
B	177	ARG	-	EXPRESSION TAG	UNP Q6VMK1
D	175	SER	-	EXPRESSION TAG	UNP Q6VMK1
D	176	GLY	-	EXPRESSION TAG	UNP Q6VMK1
D	177	ARG	-	EXPRESSION TAG	UNP Q6VMK1
F	175	SER	-	EXPRESSION TAG	UNP Q6VMK1
F	176	GLY	-	EXPRESSION TAG	UNP Q6VMK1
F	177	ARG	-	EXPRESSION TAG	UNP Q6VMK1

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



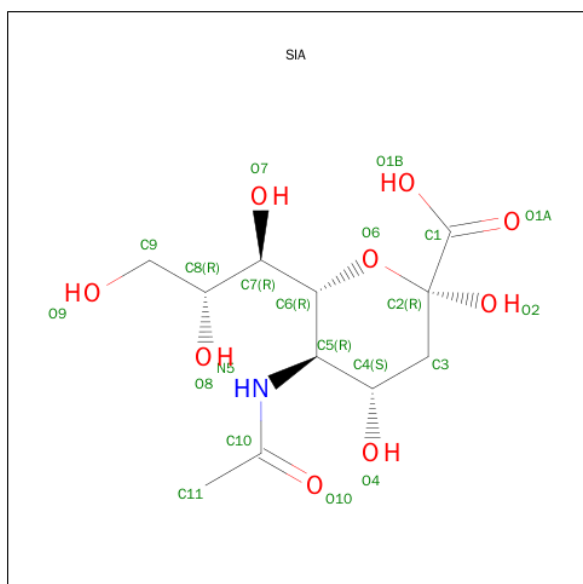
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



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

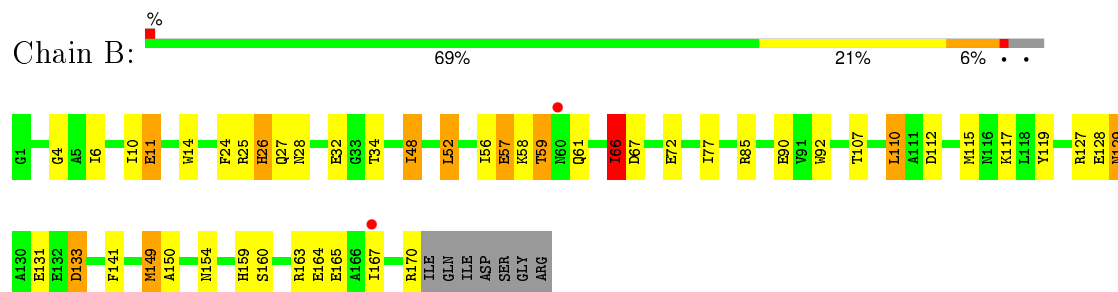
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	14	Total 14	O 14	0	0
5	C	25	Total 25	O 25	0	0
5	D	11	Total 11	O 11	0	0
5	E	18	Total 18	O 18	0	0
5	F	13	Total 13	O 13	0	0





## • Molecule 2: Hemagglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.77Å 117.60Å 120.46Å 90.00° 124.15° 90.00°	Depositor
Resolution (Å)	48.23 – 2.80 48.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.23-2.80) 99.2 (48.23-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, $R_{free}$	0.190 , 0.235 0.189 , 0.233	Depositor DCC
$R_{free}$ test set	2938 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.1	EDS
Estimated twinning fraction	0.001 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2 *h+1/2*k 0.000 for 1/2*h+1/2*k+2*1,1/2*h+1/2*k,-1 /2*h+1/2*k-l 0.010 for 1/2*h-1/2*k+2*1,-1/2*h+1/2*k,-1 /2*h-1/2*k-l 0.003 for -1/2*h+3/2*k-l,1/2*h+1/2*k+1,1 /2*h-1/2*k 0.000 for -h-k-l,1,k 0.013 for -h+k-l,-l,-k 0.000 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-l,1/2 *h-1/2*k 0.012 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1 /2*h+1/2*k 0.438 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.448 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l 0.010 for -h-2*1,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 57923 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11749	wwPDB-VP

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<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.

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Property	Value	Source
Average B, all atoms ( $\text{\AA}^2$ )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, 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	0.91	4/2468 (0.2%)	0.93	2/3337 (0.1%)
1	C	0.99	8/2468 (0.3%)	1.04	8/3337 (0.2%)
1	E	0.96	4/2483 (0.2%)	0.93	3/3356 (0.1%)
2	B	0.87	1/1404 (0.1%)	0.85	1/1892 (0.1%)
2	D	0.87	1/1412 (0.1%)	0.86	1/1903 (0.1%)
2	F	0.90	1/1393 (0.1%)	0.84	1/1878 (0.1%)
All	All	0.93	19/11628 (0.2%)	0.93	16/15703 (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
2	B	0	1
2	F	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	164	LYS	CG-CD	-11.97	1.11	1.52
1	C	148	ASP	CA-CB	-10.29	1.31	1.53
1	C	225	TRP	CD2-CE2	10.07	1.53	1.41
1	C	148	ASP	CB-CG	7.50	1.67	1.51
1	E	171	TRP	CD2-CE2	7.07	1.49	1.41
1	C	171	TRP	CD2-CE2	6.97	1.49	1.41
1	E	225	TRP	NE1-CE2	-6.52	1.29	1.37
1	A	225	TRP	NE1-CE2	-6.39	1.29	1.37
1	C	2	LYS	CG-CD	-6.20	1.31	1.52
2	B	14	TRP	CD2-CE2	6.00	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	TRP	CD2-CE3	-5.69	1.31	1.40
1	A	171	TRP	CD2-CE2	5.66	1.48	1.41
2	F	14	TRP	CD2-CE2	5.59	1.48	1.41
1	C	225	TRP	CD1-NE1	-5.58	1.28	1.38
1	A	142	TRP	CD2-CE2	5.45	1.47	1.41
2	D	14	TRP	CD2-CE2	5.42	1.47	1.41
1	E	142	TRP	CD2-CE2	5.32	1.47	1.41
1	A	129	CYS	CB-SG	-5.23	1.73	1.81
1	C	142	TRP	CD2-CE2	5.09	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	ASP	CB-CG-OD2	-15.69	104.18	118.30
1	C	225	TRP	CE2-CD2-CG	-12.13	97.60	107.30
1	C	148	ASP	CB-CG-OD1	12.03	129.13	118.30
1	C	225	TRP	CG-CD2-CE3	8.81	141.83	133.90
1	E	148	ASP	C-N-CA	7.57	140.62	121.70
1	C	225	TRP	CA-CB-CG	-6.59	101.18	113.70
1	C	225	TRP	CB-CG-CD1	-6.09	119.08	127.00
1	E	164	LYS	CB-CG-CD	6.00	127.19	111.60
2	B	110	LEU	CA-CB-CG	5.94	128.96	115.30
2	D	110	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	40	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	F	110	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	256	MET	CA-CB-CG	5.07	121.92	113.30
1	E	256	MET	CA-CB-CG	5.04	121.87	113.30
1	C	148	ASP	CB-CA-C	-5.03	100.35	110.40
1	C	121	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	66	ILE	Peptide
2	F	66	ILE	Peptide

## 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	2422	0	2369	80	0
1	C	2422	0	2369	81	0
1	E	2437	0	2384	72	0
2	B	1380	0	1283	54	0
2	D	1388	0	1294	51	0
2	F	1369	0	1270	52	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
3	C	42	0	39	0	0
3	D	14	0	13	2	0
3	E	42	0	39	0	0
3	F	14	0	13	2	0
4	A	20	0	17	0	0
4	C	20	0	17	0	0
4	E	20	0	17	0	0
5	A	22	0	0	3	0
5	B	14	0	0	1	0
5	C	25	0	0	4	0
5	D	11	0	0	1	0
5	E	18	0	0	0	0
5	F	13	0	0	3	0
All	All	11749	0	11176	351	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 15.

All (351) 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:98:LEU:HD13	1:C:225:TRP:CE3	1.79	1.17
1:C:98:LEU:HD13	1:C:225:TRP:HE3	1.13	1.07
2:B:165:GLU:HG2	5:B:313:HOH:O	1.59	1.02
2:B:59:THR:HG23	2:B:61:GLN:H	1.21	1.02
1:C:225:TRP:O	1:C:225:TRP:CD1	2.12	1.01
2:D:59:THR:HG23	2:D:61:GLN:H	1.23	1.00
2:F:59:THR:HG23	2:F:61:GLN:H	1.24	0.99
1:E:120:ILE:HG22	1:E:121:ARG:N	1.83	0.92
2:F:165:GLU:HG2	5:F:310:HOH:O	1.68	0.92
1:A:5:LEU:H	1:A:5:LEU:HD22	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:HD22	1:E:5:LEU:H	1.34	0.92
2:B:25:ARG:HE	2:B:34:THR:CG2	1.82	0.92
1:C:5:LEU:HD22	1:C:5:LEU:H	1.32	0.91
1:E:120:ILE:HG22	1:E:121:ARG:H	1.36	0.91
1:C:225:TRP:C	1:C:225:TRP:CD1	2.39	0.91
1:C:120:ILE:HG22	1:C:121:ARG:N	1.86	0.91
1:A:120:ILE:HG22	1:A:121:ARG:N	1.85	0.89
2:D:25:ARG:HE	2:D:34:THR:CG2	1.86	0.87
2:B:57:GLU:HG2	2:B:58:LYS:H	1.40	0.86
2:F:25:ARG:HE	2:F:34:THR:CG2	1.88	0.86
2:B:66:ILE:HD12	2:B:66:ILE:H	1.40	0.86
2:B:25:ARG:HE	2:B:34:THR:HG22	1.38	0.85
2:D:57:GLU:HG2	2:D:58:LYS:H	1.41	0.85
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.41	0.85
2:F:25:ARG:HE	2:F:34:THR:HG22	1.40	0.84
2:D:25:ARG:HE	2:D:34:THR:HG22	1.40	0.84
2:F:66:ILE:HD12	2:F:66:ILE:H	1.42	0.84
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.44	0.83
2:F:57:GLU:HG2	2:F:58:LYS:H	1.44	0.82
2:D:66:ILE:H	2:D:66:ILE:HD12	1.43	0.82
1:A:120:ILE:HG22	1:A:121:ARG:H	1.40	0.81
1:A:183:THR:HA	1:A:187:GLY:O	1.81	0.80
1:C:120:ILE:HG22	1:C:121:ARG:H	1.42	0.80
1:C:183:THR:HA	1:C:187:GLY:O	1.81	0.80
1:A:120:ILE:CG2	1:A:144:LEU:O	2.31	0.79
1:E:183:THR:HA	1:E:187:GLY:O	1.82	0.79
1:E:120:ILE:CG2	1:E:144:LEU:O	2.31	0.78
1:C:120:ILE:CG2	1:C:144:LEU:O	2.33	0.77
2:D:59:THR:CG2	2:D:61:GLN:H	1.98	0.77
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.49	0.75
1:C:92:PHE:HE2	1:C:170:ILE:HD11	1.50	0.75
1:A:82:GLU:OE2	5:A:507:HOH:O	2.03	0.75
1:C:98:LEU:CD1	1:C:225:TRP:HE3	1.97	0.75
3:F:201:NAG:H83	5:F:305:HOH:O	1.85	0.75
1:E:120:ILE:HG21	1:E:144:LEU:O	1.86	0.74
1:A:120:ILE:HG21	1:A:144:LEU:O	1.88	0.74
2:D:163:ARG:O	2:D:167:ILE:HG13	1.88	0.74
3:D:201:NAG:H83	5:D:305:HOH:O	1.87	0.73
1:C:178:SER:HB2	1:C:181:GLU:H	1.53	0.72
2:B:59:THR:CG2	2:B:61:GLN:H	1.99	0.72
1:C:120:ILE:HG21	1:C:144:LEU:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ARG:HH11	1:E:121:ARG:CG	2.04	0.71
1:E:92:PHE:HE2	1:E:170:ILE:HD11	1.55	0.70
2:B:128:GLU:OE2	2:B:170:ARG:NH1	2.23	0.70
2:B:163:ARG:O	2:B:167:ILE:HG13	1.90	0.70
1:C:38:VAL:HG21	1:C:280:ILE:HD12	1.71	0.70
1:A:92:PHE:HE2	1:A:170:ILE:HD11	1.54	0.70
1:C:98:LEU:HD13	1:C:225:TRP:CZ3	2.27	0.70
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.73	0.70
2:F:59:THR:CG2	2:F:61:GLN:H	2.02	0.69
2:F:59:THR:HG23	2:F:61:GLN:N	2.05	0.69
2:D:59:THR:HG23	2:D:61:GLN:N	2.05	0.68
1:A:38:VAL:HG21	1:A:280:ILE:HD12	1.76	0.68
1:E:178:SER:HB2	1:E:181:GLU:H	1.58	0.68
2:B:59:THR:HG23	2:B:61:GLN:N	2.04	0.68
2:F:25:ARG:HH21	2:F:34:THR:HG21	1.59	0.67
2:D:25:ARG:HH21	2:D:34:THR:HG21	1.58	0.67
1:C:1:ASP:OD2	5:C:514:HOH:O	2.11	0.67
1:C:225:TRP:H	1:C:225:TRP:HD1	1.41	0.67
2:D:57:GLU:HG2	2:D:58:LYS:N	2.10	0.67
2:F:66:ILE:N	2:F:66:ILE:HD12	2.07	0.67
1:C:82:GLU:OE2	5:C:522:HOH:O	2.12	0.67
2:B:57:GLU:HG2	2:B:58:LYS:N	2.10	0.67
1:A:178:SER:HB2	1:A:181:GLU:H	1.59	0.67
2:B:25:ARG:HE	2:B:34:THR:HG21	1.59	0.67
2:F:163:ARG:O	2:F:167:ILE:HG13	1.94	0.67
1:C:201:GLN:NE2	1:E:222:ASP:OD1	2.23	0.66
1:A:201:GLN:NE2	1:C:222:ASP:OD1	2.24	0.66
1:A:121:ARG:NH1	1:A:145:SER:O	2.26	0.65
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.08	0.65
1:E:120:ILE:CG2	1:E:121:ARG:N	2.57	0.65
2:F:164:GLU:HG3	2:F:165:GLU:N	2.12	0.65
2:F:164:GLU:HG3	2:F:165:GLU:H	1.62	0.65
2:B:25:ARG:HH21	2:B:34:THR:HG21	1.60	0.65
1:A:120:ILE:CG2	1:A:121:ARG:N	2.60	0.64
1:A:140:MET:HE2	1:A:245:PRO:HA	1.78	0.64
1:E:140:MET:HE2	1:E:245:PRO:HA	1.79	0.64
1:C:140:MET:HE2	1:C:245:PRO:HA	1.79	0.64
1:C:98:LEU:CD1	1:C:225:TRP:CE3	2.70	0.64
1:C:154:GLN:OE1	1:C:239:ASN:HB3	1.97	0.63
1:E:38:VAL:HG21	1:E:280:ILE:HD12	1.79	0.63
1:A:282:ASN:HB3	2:B:56:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:OE2	2:D:170:ARG:NH1	2.29	0.63
1:E:154:GLN:OE1	1:E:239:ASN:HB3	1.99	0.63
1:C:298:ARG:HG2	2:D:92:TRP:CD2	2.34	0.63
2:D:117:LYS:HE3	2:F:4:GLY:HA2	1.80	0.63
2:D:164:GLU:HG3	2:D:165:GLU:N	2.14	0.63
1:A:88:TYR:CE1	1:A:217:GLN:HG2	2.33	0.63
2:F:57:GLU:HG2	2:F:58:LYS:N	2.12	0.63
1:C:121:ARG:HH11	1:C:121:ARG:CG	2.11	0.63
1:C:121:ARG:NH1	1:C:145:SER:O	2.31	0.62
1:C:88:TYR:CE1	1:C:217:GLN:HG2	2.35	0.62
2:B:4:GLY:HA2	2:F:117:LYS:HE3	1.82	0.62
1:C:291:ARG:NH1	2:D:67:ASP:HB3	2.13	0.62
2:D:66:ILE:N	2:D:66:ILE:HD12	2.10	0.62
2:B:117:LYS:HE3	2:D:4:GLY:HA2	1.80	0.62
1:A:154:GLN:OE1	1:A:239:ASN:HB3	2.00	0.62
2:D:25:ARG:HE	2:D:34:THR:HG21	1.65	0.62
2:B:141:PHE:CD1	2:B:170:ARG:HG2	2.35	0.62
2:B:164:GLU:HG3	2:B:165:GLU:N	2.14	0.62
1:C:291:ARG:HD2	2:D:67:ASP:OD2	2.00	0.62
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.14	0.61
1:E:88:TYR:CE1	1:E:217:GLN:HG2	2.35	0.61
1:C:225:TRP:O	1:C:225:TRP:HD1	1.76	0.60
2:B:160:SER:HA	2:B:163:ARG:HB2	1.81	0.60
1:A:298:ARG:HG2	2:B:92:TRP:CD2	2.35	0.60
1:C:225:TRP:N	1:C:225:TRP:HD1	1.97	0.60
2:D:164:GLU:HG3	2:D:165:GLU:H	1.67	0.60
1:C:225:TRP:N	1:C:225:TRP:CD1	2.65	0.59
2:F:160:SER:HA	2:F:163:ARG:HB2	1.82	0.59
1:E:282:ASN:HB3	2:F:56:ILE:HG23	1.84	0.59
1:A:119:GLY:C	1:A:120:ILE:HG13	2.22	0.59
1:E:121:ARG:HG3	1:E:121:ARG:NH1	2.11	0.59
1:A:291:ARG:NH1	2:B:67:ASP:HB3	2.17	0.59
1:A:170:ILE:HD12	1:A:225:TRP:HB3	1.83	0.59
1:E:120:ILE:CG2	1:E:121:ARG:H	2.13	0.59
2:B:66:ILE:HD12	2:B:66:ILE:N	2.05	0.59
1:C:119:GLY:C	1:C:120:ILE:HG13	2.23	0.58
1:A:158:SER:OG	1:A:235:THR:HB	2.03	0.58
2:D:160:SER:HA	2:D:163:ARG:HB2	1.84	0.58
1:A:140:MET:CE	1:A:245:PRO:HA	2.33	0.58
1:C:147:THR:CG2	1:C:148:ASP:N	2.67	0.58
1:E:298:ARG:HG2	2:F:92:TRP:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.86	0.57
1:E:119:GLY:C	1:E:120:ILE:HG13	2.24	0.57
2:F:25:ARG:HE	2:F:34:THR:HG21	1.67	0.57
1:A:99:ARG:O	1:A:103:ARG:HG3	2.04	0.57
1:C:282:ASN:HB3	2:D:56:ILE:HG23	1.86	0.57
1:C:147:THR:CG2	1:C:148:ASP:H	2.17	0.57
1:A:298:ARG:NE	5:A:521:HOH:O	2.37	0.57
1:A:32:THR:HG22	1:A:33:VAL:HG23	1.86	0.57
1:C:98:LEU:HA	1:C:225:TRP:HZ3	1.70	0.57
1:E:291:ARG:HD2	2:F:67:ASP:OD2	2.05	0.56
2:D:141:PHE:CD1	2:D:170:ARG:HG2	2.40	0.56
1:E:291:ARG:NH1	2:F:67:ASP:HB3	2.20	0.56
2:F:67:ASP:OD2	2:F:85:ARG:NH2	2.38	0.56
2:D:6:ILE:HD12	2:D:112:ASP:HA	1.88	0.56
1:E:121:ARG:NH1	1:E:145:SER:O	2.35	0.56
1:E:1:ASP:HB2	2:F:28:ASN:HA	1.87	0.56
1:A:147:THR:CG2	1:A:148:ASP:N	2.69	0.56
2:B:164:GLU:HG3	2:B:165:GLU:H	1.69	0.56
1:E:170:ILE:HD12	1:E:225:TRP:HB3	1.87	0.56
1:E:41:ILE:HD11	1:E:260:SER:OG	2.06	0.56
1:C:147:THR:HG22	1:C:148:ASP:N	2.21	0.55
1:E:32:THR:HG22	1:E:33:VAL:HG23	1.88	0.55
1:C:120:ILE:CG2	1:C:121:ARG:H	2.17	0.55
1:C:203:SER:OG	1:E:207:SER:HB3	2.07	0.55
1:C:120:ILE:CG2	1:C:121:ARG:N	2.60	0.55
2:F:75:ARG:HD3	3:F:201:NAG:H81	1.89	0.55
1:C:191:LYS:HA	1:C:239:ASN:HD21	1.72	0.55
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.19	0.54
2:D:163:ARG:NH2	2:F:131:GLU:OE1	2.37	0.54
1:A:120:ILE:CG2	1:A:121:ARG:H	2.17	0.54
1:C:298:ARG:NE	5:C:519:HOH:O	2.39	0.54
1:E:140:MET:CE	1:E:245:PRO:HA	2.37	0.54
1:C:140:MET:CE	1:C:245:PRO:HA	2.37	0.54
1:A:191:LYS:O	1:A:205:VAL:HG13	2.08	0.54
1:A:291:ARG:HD2	2:B:67:ASP:OD2	2.08	0.54
1:C:158:SER:OG	1:C:235:THR:HB	2.08	0.54
1:A:147:THR:HG22	1:A:148:ASP:N	2.23	0.54
2:B:26:HIS:HB2	2:B:149:MET:CE	2.38	0.54
1:E:120:ILE:HG23	1:E:144:LEU:O	2.07	0.53
1:E:191:LYS:HA	1:E:239:ASN:HD21	1.72	0.53
1:C:41:ILE:HD11	1:C:260:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:OE1	2:F:163:ARG:NH2	2.41	0.53
1:C:32:THR:HG22	1:C:33:VAL:HG23	1.91	0.53
1:A:147:THR:CG2	1:A:148:ASP:H	2.22	0.53
1:A:120:ILE:HG23	1:A:144:LEU:O	2.06	0.52
1:C:191:LYS:O	1:C:205:VAL:HG13	2.09	0.52
1:A:191:LYS:HA	1:A:239:ASN:HD21	1.74	0.52
1:C:92:PHE:CE2	1:C:170:ILE:HD11	2.40	0.52
1:A:1:ASP:HB2	2:B:28:ASN:HA	1.92	0.52
1:A:203:SER:OG	1:C:207:SER:HB3	2.09	0.52
2:D:26:HIS:HB2	2:D:149:MET:CE	2.39	0.52
2:F:26:HIS:HB2	2:F:149:MET:CE	2.40	0.52
1:E:158:SER:OG	1:E:235:THR:HB	2.09	0.52
1:E:191:LYS:O	1:E:205:VAL:HG13	2.10	0.52
1:C:120:ILE:HG23	1:C:144:LEU:O	2.06	0.51
1:C:59:THR:HG22	1:C:60:ILE:HG12	1.91	0.51
2:D:75:ARG:HD3	3:D:201:NAG:H81	1.91	0.51
1:A:222:ASP:OD1	1:E:201:GLN:NE2	2.32	0.51
1:E:56:LEU:O	1:E:59:THR:HB	2.11	0.51
1:C:213:GLN:HA	1:C:217:GLN:O	2.10	0.51
2:B:133:ASP:C	2:B:133:ASP:OD2	2.49	0.51
1:A:41:ILE:HD11	1:A:260:SER:OG	2.11	0.51
2:F:24:PHE:O	2:F:34:THR:HA	2.11	0.51
1:A:12:ASN:HB3	5:A:522:HOH:O	2.11	0.51
2:D:61:GLN:OE1	2:F:90:GLU:OE2	2.29	0.51
5:C:514:HOH:O	2:D:144:CYS:N	2.20	0.51
1:E:86:VAL:HG22	1:E:137:TYR:OH	2.11	0.51
2:D:133:ASP:OD2	2:D:133:ASP:C	2.49	0.51
1:E:5:LEU:H	1:E:5:LEU:CD2	2.17	0.50
1:C:1:ASP:HB2	2:D:28:ASN:HA	1.94	0.50
1:C:56:LEU:O	1:C:59:THR:HB	2.11	0.50
2:B:25:ARG:NH2	2:B:34:THR:HG21	2.26	0.50
1:E:225:TRP:N	1:E:225:TRP:CD1	2.79	0.50
2:B:24:PHE:O	2:B:34:THR:HA	2.13	0.49
1:E:123:ASN:O	1:E:125:THR:HG23	2.12	0.49
1:E:171:TRP:CH2	1:E:195:VAL:HG11	2.47	0.49
1:A:5:LEU:H	1:A:5:LEU:CD2	2.18	0.49
1:C:86:VAL:HG22	1:C:137:TYR:OH	2.13	0.49
2:B:56:ILE:HG22	2:B:56:ILE:O	2.13	0.49
1:C:123:ASN:O	1:C:125:THR:HG23	2.13	0.49
2:B:67:ASP:OD2	2:B:85:ARG:NH2	2.44	0.48
2:F:133:ASP:C	2:F:133:ASP:OD2	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:ILE:HG22	2:F:56:ILE:O	2.13	0.48
2:D:56:ILE:O	2:D:56:ILE:HG22	2.13	0.48
2:D:24:PHE:O	2:D:34:THR:HA	2.14	0.48
1:C:163:ARG:HD3	1:C:250:PHE:CZ	2.49	0.48
1:A:59:THR:HG22	1:A:60:ILE:HG12	1.96	0.48
1:A:119:GLY:O	1:A:120:ILE:HG13	2.14	0.48
1:A:152:PHE:CD2	1:A:239:ASN:C	2.88	0.48
1:A:207:SER:HB3	1:E:203:SER:OG	2.13	0.48
2:B:61:GLN:OE1	2:D:90:GLU:OE2	2.31	0.47
1:A:213:GLN:HA	1:A:217:GLN:O	2.15	0.47
1:A:86:VAL:HG22	1:A:137:TYR:OH	2.14	0.47
2:B:163:ARG:NH2	2:D:131:GLU:OE1	2.45	0.47
1:A:225:TRP:CD1	1:A:225:TRP:N	2.82	0.47
1:E:152:PHE:CD2	1:E:239:ASN:C	2.87	0.47
2:B:11:GLU:H	2:B:11:GLU:HG2	1.49	0.47
1:E:106:GLY:HA2	1:E:255:SER:HB3	1.96	0.47
1:C:103:ARG:HB3	1:C:257:GLY:HA3	1.96	0.47
2:B:61:GLN:OE1	2:D:90:GLU:HG2	2.15	0.47
2:F:25:ARG:NH2	2:F:34:THR:HG21	2.28	0.47
2:D:25:ARG:NH2	2:D:34:THR:HG21	2.26	0.47
2:D:57:GLU:CG	2:D:58:LYS:N	2.75	0.47
1:C:119:GLY:O	1:C:120:ILE:HG13	2.14	0.47
1:C:152:PHE:CD2	1:C:239:ASN:C	2.88	0.47
1:C:99:ARG:O	1:C:103:ARG:HG3	2.15	0.47
2:B:57:GLU:CG	2:B:58:LYS:N	2.74	0.46
1:E:119:GLY:O	1:E:120:ILE:HG13	2.14	0.46
1:C:171:TRP:CH2	1:C:195:VAL:HG11	2.50	0.46
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.50	0.46
2:B:90:GLU:OE2	2:F:61:GLN:OE1	2.34	0.46
2:B:150:ALA:O	2:B:154:ASN:ND2	2.49	0.46
2:B:25:ARG:NE	2:B:34:THR:HG21	2.28	0.46
1:A:171:TRP:CH2	1:A:195:VAL:HG11	2.51	0.46
1:E:149:ASN:OD1	1:E:183:THR:HG22	2.16	0.46
2:F:165:GLU:CG	5:F:310:HOH:O	2.44	0.46
1:A:42:CYS:HB2	1:A:278:THR:HG21	1.98	0.46
1:A:92:PHE:CE2	1:A:170:ILE:HD11	2.42	0.45
1:E:103:ARG:HB3	1:E:257:GLY:HA3	1.97	0.45
1:C:186:TYR:CZ	1:C:241:ALA:HA	2.51	0.45
1:A:200:TYR:CD2	1:A:200:TYR:C	2.89	0.45
1:C:98:LEU:HA	1:C:225:TRP:CZ3	2.49	0.45
1:E:192:LEU:N	1:E:239:ASN:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:CYS:HB2	1:C:278:THR:HG21	1.98	0.45
1:E:186:TYR:CZ	1:E:241:ALA:HA	2.52	0.45
2:F:77:ILE:HA	2:F:77:ILE:HD12	1.78	0.45
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.51	0.45
1:E:213:GLN:HA	1:E:217:GLN:O	2.15	0.45
2:B:52:LEU:HA	2:B:52:LEU:HD12	1.84	0.45
1:A:192:LEU:HD22	1:A:193:ILE:H	1.81	0.45
2:B:26:HIS:HB2	2:B:149:MET:HE2	1.99	0.45
1:C:5:LEU:HD22	1:C:5:LEU:N	2.12	0.44
1:A:5:LEU:HD21	2:B:119:TYR:HD1	1.82	0.44
1:E:99:ARG:O	1:E:103:ARG:HG3	2.17	0.44
1:C:165:ASP:HB3	1:C:166:PRO:CD	2.48	0.44
2:F:150:ALA:O	2:F:154:ASN:ND2	2.50	0.44
1:A:57:LEU:HD21	1:A:99:ARG:HG2	2.00	0.44
1:E:230:PRO:O	1:E:231:ASN:HB2	2.17	0.44
1:E:165:ASP:HB3	1:E:166:PRO:CD	2.48	0.44
1:A:165:ASP:HB3	1:A:166:PRO:CD	2.48	0.44
1:A:291:ARG:HH12	2:B:67:ASP:HB3	1.82	0.44
2:F:26:HIS:ND1	2:F:26:HIS:C	2.71	0.44
1:A:230:PRO:O	1:A:231:ASN:HB2	2.18	0.44
1:E:152:PHE:HA	1:E:153:PRO:HD3	1.87	0.43
1:A:103:ARG:HB3	1:A:257:GLY:HA3	1.99	0.43
2:D:26:HIS:HB2	2:D:149:MET:HE2	2.00	0.43
1:C:200:TYR:C	1:C:200:TYR:CD2	2.91	0.43
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.99	0.43
1:E:200:TYR:CD2	1:E:200:TYR:C	2.90	0.43
1:A:120:ILE:HG23	1:A:145:SER:HA	2.01	0.43
1:E:88:TYR:CD2	1:E:221:ILE:HD12	2.53	0.43
1:E:1:ASP:HB2	2:F:27:GLN:O	2.19	0.43
1:A:207:SER:O	1:A:211:ARG:NH2	2.46	0.43
1:A:226:LEU:C	1:A:226:LEU:HD12	2.39	0.43
1:E:226:LEU:C	1:E:226:LEU:HD12	2.38	0.43
1:E:92:PHE:CE2	1:E:170:ILE:HD11	2.44	0.43
1:E:41:ILE:HD11	1:E:260:SER:CB	2.49	0.43
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.99	0.43
1:A:232:ASP:OD2	1:A:233:THR:N	2.49	0.43
2:B:25:ARG:NE	2:B:34:THR:CG2	2.66	0.43
1:A:213:GLN:OE1	1:A:216:GLY:HA2	2.19	0.43
1:A:191:LYS:HE3	1:A:191:LYS:HB3	1.88	0.43
2:D:88:MET:HB3	2:D:88:MET:HE2	1.88	0.43
2:D:25:ARG:NE	2:D:34:THR:HG21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:GLN:OE1	2:F:90:GLU:HG2	2.19	0.42
2:D:67:ASP:OD2	2:D:85:ARG:NH2	2.50	0.42
2:F:107:THR:HA	2:F:110:LEU:HD13	2.01	0.42
1:C:5:LEU:HD21	2:D:119:TYR:HD1	1.83	0.42
2:B:26:HIS:C	2:B:26:HIS:ND1	2.73	0.42
1:E:232:ASP:OD2	1:E:233:THR:N	2.49	0.42
2:D:52:LEU:HD12	2:D:52:LEU:HA	1.84	0.42
1:E:90:GLY:HA3	1:E:221:ILE:O	2.19	0.42
1:A:32:THR:HB	1:A:305:LEU:O	2.20	0.42
2:D:57:GLU:OE1	2:D:57:GLU:N	2.53	0.42
1:E:163:ARG:HD3	1:E:250:PHE:CZ	2.54	0.42
1:E:265:ASP:OD2	1:E:268:CYS:SG	2.78	0.42
1:C:230:PRO:O	1:C:231:ASN:HB2	2.20	0.42
2:F:26:HIS:HB2	2:F:149:MET:HE2	2.01	0.42
1:A:56:LEU:O	1:A:59:THR:HB	2.19	0.42
2:F:57:GLU:CG	2:F:58:LYS:N	2.77	0.42
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.02	0.42
2:D:107:THR:HA	2:D:110:LEU:HD13	2.02	0.42
1:E:120:ILE:HG23	1:E:145:SER:HA	2.01	0.41
2:D:26:HIS:C	2:D:26:HIS:ND1	2.74	0.41
1:E:147:THR:CG2	1:E:148:ASP:N	2.83	0.41
1:C:192:LEU:N	1:C:239:ASN:OD1	2.50	0.41
2:D:150:ALA:O	2:D:154:ASN:ND2	2.54	0.41
2:F:122:VAL:O	2:F:123:LYS:C	2.59	0.41
1:A:164:LYS:HB2	1:A:164:LYS:HE3	1.75	0.41
1:A:181:GLU:OE1	1:A:181:GLU:HA	2.21	0.41
1:A:235:THR:HG22	1:C:212:PRO:HG3	2.02	0.41
2:B:129:ASN:OD1	2:B:129:ASN:N	2.53	0.41
2:F:25:ARG:NE	2:F:34:THR:HG21	2.35	0.41
1:A:192:LEU:N	1:A:239:ASN:OD1	2.53	0.41
1:E:314:VAL:HA	1:E:315:PRO:HD3	1.84	0.41
2:F:158:ASP:OD2	2:F:161:LYS:HB2	2.20	0.41
2:B:57:GLU:OE1	2:B:57:GLU:N	2.53	0.41
1:E:31:GLU:HG3	1:E:32:THR:N	2.35	0.41
2:B:77:ILE:HD12	2:B:77:ILE:HA	1.80	0.41
2:F:57:GLU:N	2:F:57:GLU:OE1	2.54	0.41
1:E:181:GLU:OE1	1:E:181:GLU:HA	2.20	0.41
2:F:88:MET:HE2	2:F:88:MET:HB3	1.85	0.41
1:C:291:ARG:HH12	2:D:67:ASP:HB3	1.83	0.41
1:A:1:ASP:HB2	2:B:27:GLN:O	2.21	0.41
1:E:5:LEU:HD22	1:E:5:LEU:N	2.13	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:HD21	2:F:119:TYR:HD1	1.86	0.40
2:F:159:HIS:CG	2:F:160:SER:N	2.89	0.40
1:A:32:THR:HG23	1:A:285:PHE:HD1	1.86	0.40
2:B:10:ILE:N	2:B:10:ILE:HD12	2.36	0.40
1:C:41:ILE:HD11	1:C:260:SER:CB	2.51	0.40
1:A:123:ASN:O	1:A:125:THR:HG23	2.21	0.40
2:D:77:ILE:HD12	2:D:77:ILE:HA	1.75	0.40
2:B:159:HIS:CG	2:B:160:SER:N	2.89	0.40
1:A:212:PRO:HG3	1:E:235:THR:HG22	2.03	0.40
2:F:126:LEU:O	2:F:127:ARG:C	2.60	0.40
1:C:152:PHE:HA	1:C:153:PRO:HD3	1.86	0.40
1:C:81:ARG:NH1	1:C:261:GLU:OE2	2.53	0.40
1:C:314:VAL:HA	1:C:315:PRO:HD3	1.83	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	314/327 (96%)	287 (91%)	26 (8%)	1 (0%)	46	79
1	C	314/327 (96%)	285 (91%)	28 (9%)	1 (0%)	46	79
1	E	316/327 (97%)	288 (91%)	26 (8%)	2 (1%)	30	65
2	B	168/177 (95%)	158 (94%)	9 (5%)	1 (1%)	30	65
2	D	169/177 (96%)	157 (93%)	11 (6%)	1 (1%)	30	65
2	F	167/177 (94%)	155 (93%)	11 (7%)	1 (1%)	30	65
All	All	1448/1512 (96%)	1330 (92%)	111 (8%)	7 (0%)	34	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	127	ARG
1	C	148	ASP
1	A	148	ASP
2	B	127	ARG
1	E	150	ALA
2	F	127	ARG
1	E	52	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	268/277 (97%)	236 (88%)	32 (12%)	6	19
1	C	268/277 (97%)	234 (87%)	34 (13%)	5	16
1	E	269/277 (97%)	235 (87%)	34 (13%)	5	17
2	B	145/151 (96%)	131 (90%)	14 (10%)	10	29
2	D	146/151 (97%)	129 (88%)	17 (12%)	7	20
2	F	144/151 (95%)	128 (89%)	16 (11%)	8	23
All	All	1240/1284 (97%)	1093 (88%)	147 (12%)	6	19

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	HIS
1	A	14	THR
1	A	20	THR
1	A	24	VAL
1	A	32	THR
1	A	59	THR
1	A	65	GLN
1	A	73	SER
1	A	82	GLU
1	A	86	VAL
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	122	THR
1	A	126	THR
1	A	143	LEU
1	A	162	THR
1	A	165	ASP
1	A	170	ILE
1	A	176	SER
1	A	178	SER
1	A	180	THR
1	A	182	GLN
1	A	192	LEU
1	A	194	THR
1	A	200	TYR
1	A	203	SER
1	A	207	SER
1	A	217	GLN
1	A	235	THR
1	A	261	GLU
1	A	263	GLN
1	A	298	ARG
2	B	11	GLU
2	B	26	HIS
2	B	32	GLU
2	B	48	ILE
2	B	52	LEU
2	B	57	GLU
2	B	59	THR
2	B	66	ILE
2	B	72	GLU
2	B	110	LEU
2	B	115	MET
2	B	129	ASN
2	B	133	ASP
2	B	149	MET
1	C	5	LEU
1	C	8	HIS
1	C	14	THR
1	C	20	THR
1	C	24	VAL
1	C	32	THR
1	C	59	THR
1	C	65	GLN

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Mol	Chain	Res	Type
1	C	73	SER
1	C	82	GLU
1	C	86	VAL
1	C	121	ARG
1	C	122	THR
1	C	126	THR
1	C	129	CYS
1	C	143	LEU
1	C	165	ASP
1	C	170	ILE
1	C	176	SER
1	C	178	SER
1	C	182	GLN
1	C	194	THR
1	C	200	TYR
1	C	203	SER
1	C	205	VAL
1	C	217	GLN
1	C	225	TRP
1	C	235	THR
1	C	251	LEU
1	C	261	GLU
1	C	263	GLN
1	C	291	ARG
1	C	298	ARG
1	C	312	LYS
2	D	11	GLU
2	D	26	HIS
2	D	32	GLU
2	D	39	LYS
2	D	48	ILE
2	D	52	LEU
2	D	57	GLU
2	D	59	THR
2	D	66	ILE
2	D	72	GLU
2	D	110	LEU
2	D	115	MET
2	D	121	ARG
2	D	129	ASN
2	D	133	ASP
2	D	149	MET

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Mol	Chain	Res	Type
2	D	171	ILE
1	E	5	LEU
1	E	8	HIS
1	E	14	THR
1	E	20	THR
1	E	24	VAL
1	E	32	THR
1	E	59	THR
1	E	65	GLN
1	E	73	SER
1	E	82	GLU
1	E	86	VAL
1	E	121	ARG
1	E	122	THR
1	E	126	THR
1	E	129	CYS
1	E	143	LEU
1	E	148	ASP
1	E	164	LYS
1	E	165	ASP
1	E	170	ILE
1	E	176	SER
1	E	178	SER
1	E	180	THR
1	E	182	GLN
1	E	192	LEU
1	E	194	THR
1	E	200	TYR
1	E	203	SER
1	E	207	SER
1	E	217	GLN
1	E	263	GLN
1	E	291	ARG
1	E	298	ARG
1	E	312	LYS
2	F	11	GLU
2	F	26	HIS
2	F	32	GLU
2	F	39	LYS
2	F	48	ILE
2	F	52	LEU
2	F	57	GLU

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Mol	Chain	Res	Type
2	F	59	THR
2	F	66	ILE
2	F	72	GLU
2	F	110	LEU
2	F	115	MET
2	F	129	ASN
2	F	133	ASP
2	F	149	MET
2	F	169	ASN

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	NAG	A	401	1	14,14,15	0.45	0	15,19,21	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	402	1	14,14,15	0.50	0	15,19,21	2.60	4 (26%)
3	NAG	A	403	1	14,14,15	0.64	0	15,19,21	1.63	1 (6%)
4	SIA	A	404	-	16,20,21	1.09	1 (6%)	18,28,31	1.63	3 (16%)
3	NAG	B	201	2	14,14,15	0.57	0	15,19,21	2.37	4 (26%)
3	NAG	C	401	1	14,14,15	0.47	0	15,19,21	1.66	2 (13%)
3	NAG	C	402	1	14,14,15	0.52	0	15,19,21	2.35	3 (20%)
3	NAG	C	403	1	14,14,15	0.53	0	15,19,21	1.48	3 (20%)
4	SIA	C	404	-	16,20,21	1.08	1 (6%)	18,28,31	1.90	5 (27%)
3	NAG	D	201	2	14,14,15	0.55	0	15,19,21	2.16	6 (40%)
3	NAG	E	401	1	14,14,15	0.61	0	15,19,21	1.32	1 (6%)
3	NAG	E	402	1	14,14,15	0.51	0	15,19,21	2.33	3 (20%)
3	NAG	E	403	1	14,14,15	0.48	0	15,19,21	1.18	1 (6%)
4	SIA	E	404	-	16,20,21	1.13	1 (6%)	18,28,31	1.60	5 (27%)
3	NAG	F	201	2	14,14,15	0.70	0	15,19,21	1.96	6 (40%)

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	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	SIA	A	404	-	-	0/14/34/38	0/1/1/1
3	NAG	B	201	2	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	403	1	-	0/6/23/26	0/1/1/1
4	SIA	C	404	-	-	0/14/34/38	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	E	403	1	-	0/6/23/26	0/1/1/1
4	SIA	E	404	-	-	0/14/34/38	0/1/1/1
3	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	404	SIA	C7-C6	2.85	1.56	1.52
4	A	404	SIA	C7-C6	3.17	1.57	1.52
4	E	404	SIA	C7-C6	3.26	1.57	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	SIA	C3-C4-C5	-4.04	106.97	111.47
3	A	402	NAG	O3-C3-C2	-3.81	101.57	109.11
4	A	404	SIA	C3-C4-C5	-3.53	107.54	111.47
3	C	402	NAG	O3-C3-C2	-3.08	103.02	109.11
3	A	402	NAG	C2-N2-C7	-3.06	119.11	123.04
4	E	404	SIA	C3-C4-C5	-2.73	108.43	111.47
3	E	402	NAG	C2-N2-C7	-2.70	119.57	123.04
3	E	402	NAG	O3-C3-C2	-2.60	103.96	109.11
3	C	402	NAG	C6-C5-C4	-2.47	106.93	113.02
3	A	402	NAG	C6-C5-C4	-2.19	107.62	113.02
3	A	401	NAG	C3-C2-N2	-2.16	105.40	110.56
3	B	201	NAG	C8-C7-N2	-2.15	112.00	116.11
3	C	403	NAG	O7-C7-C8	-2.14	118.14	122.06
3	D	201	NAG	C4-C3-C2	-2.10	107.97	111.23
3	F	201	NAG	O6-C6-C5	-2.00	104.71	111.33
4	A	404	SIA	C11-C10-N5	2.00	119.94	116.11
3	F	201	NAG	O3-C3-C4	2.03	114.91	110.34
3	C	403	NAG	C3-C2-N2	2.08	115.55	110.56
3	D	201	NAG	O4-C4-C3	2.10	115.07	110.34
3	D	201	NAG	O7-C7-N2	2.12	126.18	121.86
4	E	404	SIA	C11-C10-N5	2.17	120.26	116.11
3	C	401	NAG	O5-C5-C6	2.18	112.06	107.35
4	E	404	SIA	O9-C9-C8	2.37	116.24	111.10
3	F	201	NAG	O7-C7-N2	2.38	126.72	121.86
4	C	404	SIA	C11-C10-N5	2.42	120.74	116.11
3	F	201	NAG	O4-C4-C3	2.56	116.10	110.34
3	D	201	NAG	O3-C3-C4	2.57	116.12	110.34
4	E	404	SIA	O6-C2-C3	2.58	114.82	109.86
3	B	201	NAG	O3-C3-C4	2.60	116.19	110.34
3	B	201	NAG	O4-C4-C3	2.66	116.31	110.34
4	C	404	SIA	O9-C9-C8	2.81	117.21	111.10
4	C	404	SIA	O6-C2-C3	2.95	115.52	109.86
3	D	201	NAG	C2-N2-C7	3.11	127.03	123.04
3	C	403	NAG	C1-O5-C5	3.23	116.34	112.25
3	E	403	NAG	C1-O5-C5	3.25	116.38	112.25
3	A	401	NAG	C1-O5-C5	3.57	116.78	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404	SIA	C8-C7-C6	3.70	120.44	113.01
3	F	201	NAG	C2-N2-C7	3.77	127.89	123.04
3	F	201	NAG	C1-O5-C5	3.80	117.07	112.25
4	C	404	SIA	C8-C7-C6	3.86	120.77	113.01
4	A	404	SIA	C8-C7-C6	3.91	120.87	113.01
3	E	401	NAG	C1-O5-C5	3.96	117.27	112.25
3	C	401	NAG	C1-O5-C5	4.78	118.32	112.25
3	A	403	NAG	C1-O5-C5	5.51	119.24	112.25
3	D	201	NAG	C1-O5-C5	5.52	119.26	112.25
3	B	201	NAG	C1-O5-C5	6.92	121.03	112.25
3	C	402	NAG	C1-O5-C5	7.43	121.68	112.25
3	E	402	NAG	C1-O5-C5	7.63	121.94	112.25
3	A	402	NAG	C1-O5-C5	7.96	122.35	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	NAG	2	0
3	F	201	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	316/327 (96%)	-0.36	0 <span>100</span> <span>100</span>	19, 46, 88, 114	1 (0%)
1	C	316/327 (96%)	-0.33	1 (0%) <span>94</span> <span>92</span>	19, 47, 89, 112	3 (0%)
1	E	317/327 (96%)	-0.35	0 <span>100</span> <span>100</span>	20, 45, 86, 115	2 (0%)
2	B	170/177 (96%)	-0.28	2 (1%) <span>81</span> <span>73</span>	17, 64, 107, 118	1 (0%)
2	D	171/177 (96%)	-0.27	3 (1%) <span>71</span> <span>61</span>	17, 64, 106, 118	0
2	F	169/177 (95%)	-0.29	1 (0%) <span>90</span> <span>86</span>	18, 62, 108, 113	0
All	All	1459/1512 (96%)	-0.32	7 (0%) <span>91</span> <span>88</span>	17, 52, 98, 118	7 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	SER	3.3
2	D	60	ASN	2.4
2	D	168	GLN	2.4
2	B	167	ILE	2.3
2	F	60	ASN	2.3
2	D	3	PHE	2.2
2	B	60	ASN	2.1

### 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 ⓘ

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
4	SIA	E	404	20/21	0.84	0.43	6.90	99,130,177,200	0
4	SIA	A	404	20/21	0.82	0.41	6.70	119,147,190,237	0
4	SIA	C	404	20/21	0.80	0.38	6.57	111,138,176,195	0
3	NAG	B	201	14/15	0.91	0.14	-1.00	57,74,98,107	0
3	NAG	F	201	14/15	0.92	0.14	-1.25	58,80,95,101	0
3	NAG	D	201	14/15	0.90	0.14	-1.47	61,83,94,97	0
3	NAG	A	401	14/15	0.89	0.16	-	103,123,143,145	0
3	NAG	A	403	14/15	0.77	0.22	-	92,129,157,166	0
3	NAG	C	403	14/15	0.81	0.18	-	103,126,148,157	0
3	NAG	E	401	14/15	0.88	0.16	-	94,114,131,138	0
3	NAG	C	402	14/15	0.87	0.16	-	83,114,141,143	0
3	NAG	A	402	14/15	0.82	0.17	-	76,118,143,150	0
3	NAG	C	401	14/15	0.84	0.21	-	98,123,145,154	0
3	NAG	E	402	14/15	0.90	0.16	-	84,121,148,151	0
3	NAG	E	403	14/15	0.82	0.18	-	96,128,156,157	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.