



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:41 PM UTC

PDB ID : 6D8B / pdb_00006d8b
Title : The crystal structure of hemagglutinin from A/Hong Kong/125/2017 H7N9 influenza virus
Authors : Yang, H.; Stevens, J.
Deposited on : 2018-04-26
Resolution : 2.95 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

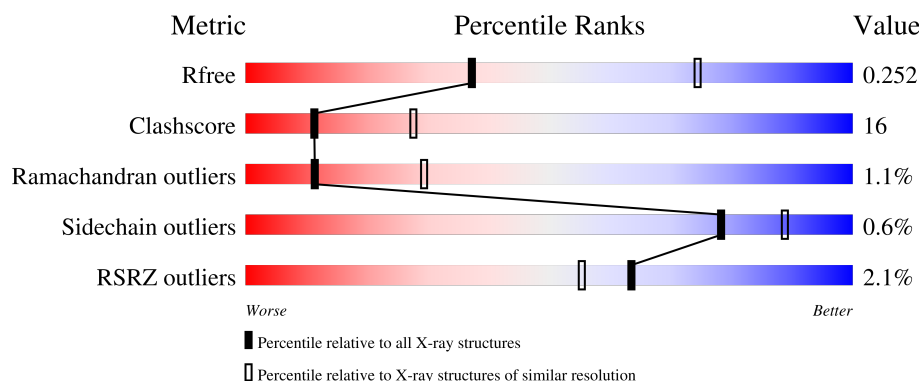
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	3% 70% 27% ...
1	C	321	2% 70% 27% ..
1	E	321	% 70% 27% ..
2	B	221	3% 52% 24% • 23%
2	D	221	56% 21% • 23%

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Mol	Chain	Length	Quality of chain
2	F	221	% 50% 27% 23%

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	NAG	E	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11499 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.

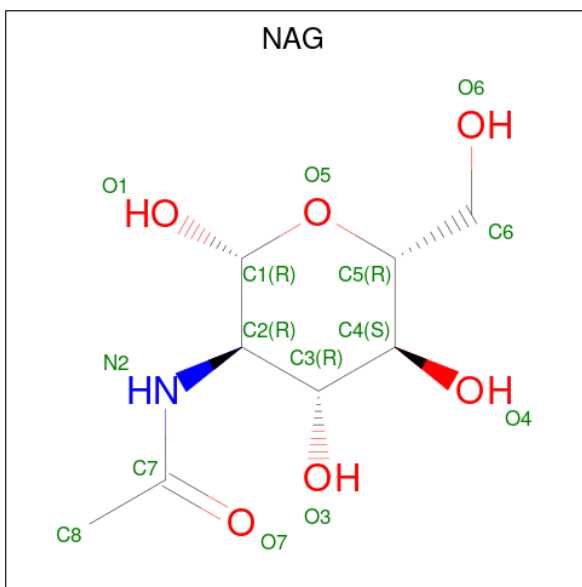
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			
1	C	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			
1	E	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			
2	D	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			
2	F	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

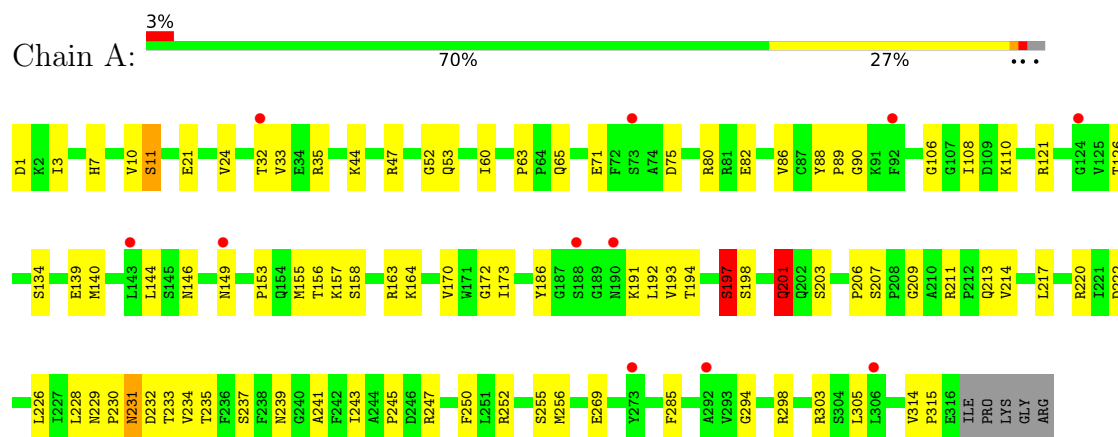


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

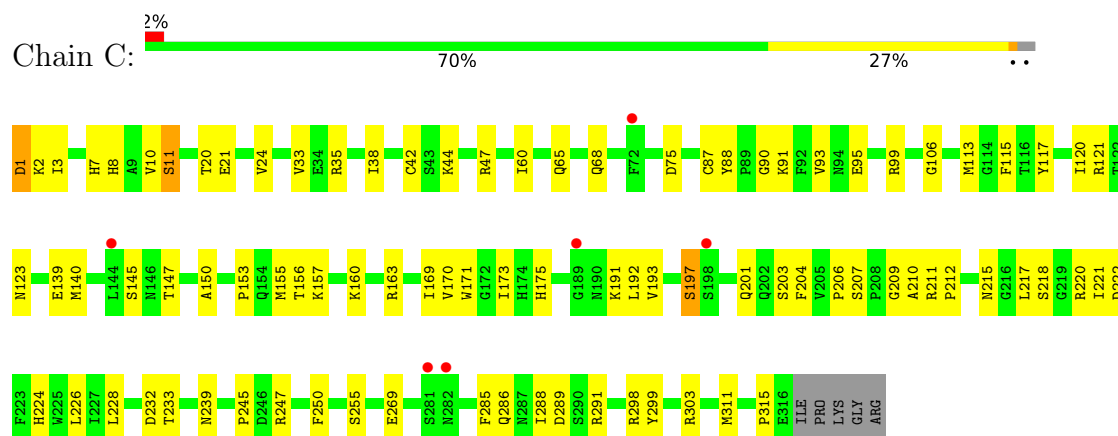
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

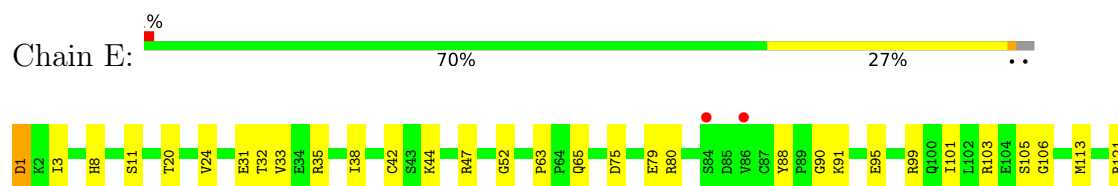
- Molecule 1: Hemagglutinin HA1 chain

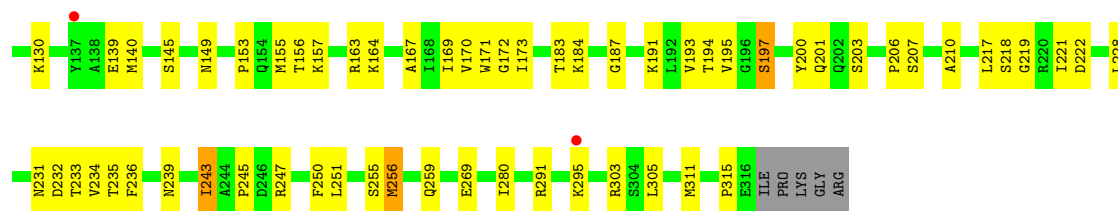


- Molecule 1: Hemagglutinin HA1 chain

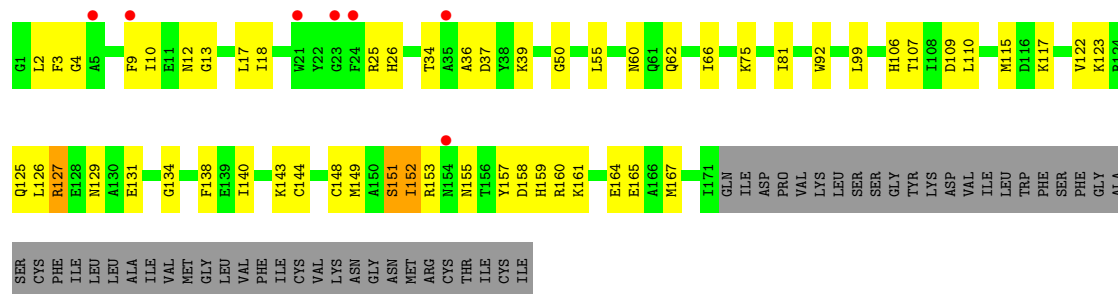


- Molecule 1: Hemagglutinin HA1 chain

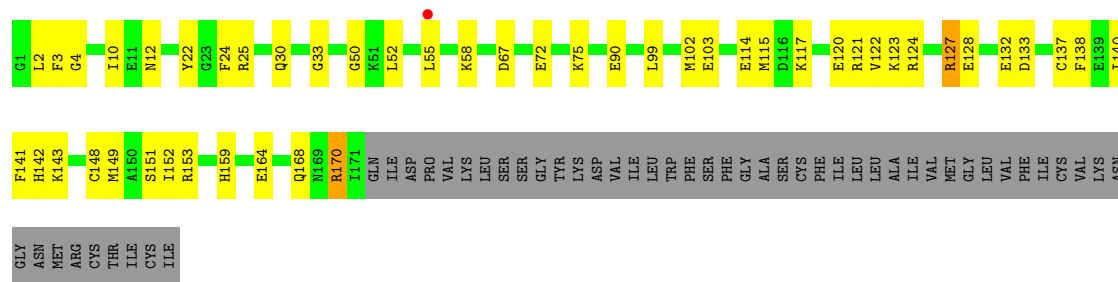




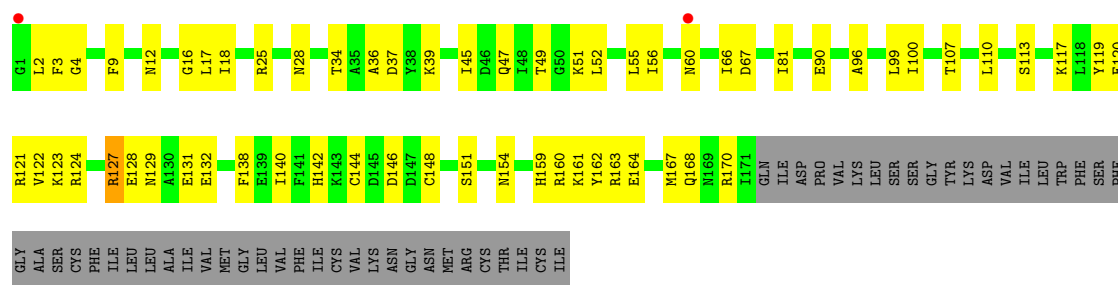
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.64Å 116.89Å 119.63Å 90.00° 124.16° 90.00°	Depositor
Resolution (Å)	39.15 – 2.95 39.15 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.15-2.95) 98.6 (39.15-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.96Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.234 , 0.279 (Not available) , 0.252	Depositor DCC
R_{free} test set	2675 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 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*l,1/2*h+1/2*k,-1 /2*h+1/2*k-l 0.000 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1 /2*h-1/2*k-l 0.000 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1 /2*h-1/2*k 0.000 for -h-k-l,l,k 0.003 for -h+k-l,-l,-k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2* *h-1/2*k 0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1 /2*h+1/2*k 0.427 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.409 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l 0.000 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11499	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: 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	0/2462	0.70	5/3329 (0.2%)
1	C	0.30	0/2462	0.68	1/3329 (0.0%)
1	E	0.33	0/2462	0.73	6/3329 (0.2%)
2	B	0.34	0/1413	0.79	4/1903 (0.2%)
2	D	0.36	0/1413	0.80	4/1903 (0.2%)
2	F	0.37	0/1413	0.91	2/1903 (0.1%)
All	All	0.34	0/11625	0.75	22/15696 (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	A	0	2
1	C	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	ASP	N-CA-C	-9.62	84.06	111.00
1	C	1	ASP	N-CA-C	-8.93	85.99	111.00
1	E	130	LYS	CA-CB-CG	8.79	131.68	114.10
2	F	164	GLU	CA-CB-CG	7.36	128.83	114.10
1	A	164	LYS	CD-CE-NZ	-7.24	88.73	111.90
2	F	164	GLU	CB-CA-C	-6.88	99.80	110.81
1	E	130	LYS	N-CA-CB	6.47	120.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	ILE	CG1-CB-CG2	-6.26	91.91	110.70
2	B	149	MET	CA-CB-CG	-6.13	101.83	114.10
1	A	164	LYS	CG-CD-CE	6.08	125.29	111.30
2	D	30	GLN	CA-CB-CG	5.97	126.03	114.10
1	A	201	GLN	N-CA-C	-5.90	100.17	109.50
1	E	130	LYS	CB-CA-C	-5.54	100.39	109.53
2	B	152	ILE	CB-CA-C	-5.46	104.89	112.04
2	D	143	LYS	CA-C-N	5.44	131.60	123.23
2	D	143	LYS	C-N-CA	5.44	131.60	123.23
2	D	170	ARG	CB-CG-CD	5.40	123.72	111.30
1	E	243	ILE	CB-CA-C	5.35	118.77	110.96
2	B	152	ILE	CB-CG1-CD1	-5.28	102.70	113.80
1	A	231	ASN	N-CA-CB	-5.16	101.78	110.49
1	A	243	ILE	CA-CB-CG1	5.15	119.16	110.40
1	E	24	VAL	CG1-CB-CG2	5.01	121.82	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	SER	Peptide
1	A	201	GLN	Sidechain
1	C	197	SER	Peptide
1	E	197	SER	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	2416	0	2382	76	0
1	C	2416	0	2382	90	0
1	E	2416	0	2382	77	0
2	B	1389	0	1300	65	0
2	D	1389	0	1300	38	0
2	F	1389	0	1300	70	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	8	0
3	F	14	0	13	0	0
All	All	11499	0	11124	366	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 (366) 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:256:MET:HE1	1:A:294:GLY:HA2	1.27	1.15
1:C:191:LYS:HA	1:C:239:ASN:HD21	1.15	1.01
2:B:9:PHE:HB2	2:F:121:ARG:CZ	1.90	1.01
2:F:121:ARG:HH11	2:F:124:ARG:HD2	1.24	1.00
1:A:191:LYS:HA	1:A:239:ASN:HD21	1.22	1.00
1:E:191:LYS:HA	1:E:239:ASN:HD21	1.24	1.00
2:B:164:GLU:HG2	2:B:165:GLU:N	1.81	0.94
1:A:256:MET:HE1	1:A:294:GLY:CA	1.98	0.93
2:B:107:THR:HA	2:B:110:LEU:HD22	1.51	0.92
2:F:121:ARG:NH1	2:F:124:ARG:HD2	1.84	0.90
1:E:31:GLU:OE1	1:E:32:THR:N	2.05	0.90
1:A:201:GLN:HE21	1:C:91:LYS:HB2	1.36	0.90
1:E:194:THR:HG23	1:E:203:SER:HB2	1.55	0.89
1:E:31:GLU:OE1	1:E:33:VAL:N	2.06	0.88
1:A:32:THR:HG22	1:A:305:LEU:O	1.74	0.88
2:B:164:GLU:HG2	2:B:165:GLU:H	1.38	0.88
2:F:37:ASP:OD1	2:F:39:LYS:HD2	1.72	0.88
1:C:191:LYS:HA	1:C:239:ASN:ND2	1.89	0.88
1:A:201:GLN:NE2	1:C:91:LYS:HB2	1.88	0.87
2:F:120:GLU:O	2:F:124:ARG:NH1	2.11	0.84
2:B:107:THR:HA	2:B:110:LEU:CD2	2.09	0.82
2:F:131:GLU:OE2	2:F:170:ARG:NH1	2.11	0.82
1:A:211:ARG:HD2	1:A:220:ARG:HG2	1.60	0.81
2:F:66:ILE:HD12	2:F:67:ASP:HB2	1.62	0.80
1:A:194:THR:HG23	1:A:237:SER:HB3	1.63	0.79
1:C:38:ILE:HD11	1:C:42:CYS:SG	2.24	0.78
2:F:127:ARG:HB2	2:F:159:HIS:ND1	1.99	0.77
2:B:26:HIS:HD2	2:B:153:ARG:HH12	1.34	0.75
2:B:134:GLY:O	2:F:121:ARG:NH2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LYS:CA	1:C:239:ASN:HD21	1.98	0.74
1:E:164:LYS:CD	3:E:401:NAG:H81	2.18	0.74
1:A:3:ILE:CD1	2:B:152:ILE:HD11	2.17	0.74
2:B:9:PHE:HB2	2:F:121:ARG:NH2	2.03	0.73
1:E:38:ILE:HD11	1:E:42:CYS:SG	2.28	0.73
2:F:60:ASN:ND2	2:F:60:ASN:O	2.21	0.73
1:E:195:VAL:HG12	1:E:200:TYR:HE2	1.55	0.72
2:F:127:ARG:HB2	2:F:159:HIS:CE1	2.25	0.72
2:D:127:ARG:NH2	2:F:131:GLU:OE1	2.22	0.72
1:A:256:MET:CE	1:A:294:GLY:HA2	2.15	0.71
1:A:149:ASN:O	1:A:149:ASN:ND2	2.24	0.71
2:B:107:THR:O	2:B:110:LEU:HD23	1.90	0.71
2:D:168:GLN:O	2:D:168:GLN:HG2	1.90	0.71
1:A:173:ILE:HD11	1:A:193:VAL:HG21	1.73	0.70
1:A:201:GLN:OE1	1:C:222:ASP:HB3	1.93	0.69
1:A:35:ARG:HD3	1:A:303:ARG:HG3	1.73	0.68
2:F:129:ASN:OD1	2:F:159:HIS:NE2	2.27	0.68
1:E:95:GLU:OE1	1:E:99:ARG:NH2	2.27	0.68
1:E:172:GLY:HA3	1:E:243:ILE:HD11	1.75	0.67
2:D:120:GLU:O	2:D:124:ARG:NH1	2.28	0.67
2:B:37:ASP:OD1	2:B:39:LYS:NZ	2.22	0.66
2:D:149:MET:O	2:D:153:ARG:HG3	1.96	0.66
1:E:3:ILE:HG22	2:F:138:PHE:HB2	1.78	0.66
1:A:191:LYS:HA	1:A:239:ASN:ND2	2.04	0.65
1:C:121:ARG:NH1	1:C:145:SER:O	2.30	0.65
2:B:164:GLU:O	2:B:167:MET:HG2	1.97	0.64
2:B:152:ILE:HG13	2:B:153:ARG:H	1.61	0.64
2:B:122:VAL:HA	2:B:125:GLN:HG3	1.79	0.64
1:A:194:THR:HG21	1:C:209:GLY:HA3	1.80	0.64
2:B:50:GLY:HA3	1:C:20:THR:O	1.97	0.64
1:C:191:LYS:HD3	1:C:239:ASN:ND2	2.13	0.64
2:D:10:ILE:HD12	2:D:115:MET:SD	2.37	0.64
2:F:128:GLU:H	2:F:159:HIS:CE1	2.15	0.64
1:E:164:LYS:NZ	3:E:401:NAG:C8	2.61	0.63
2:D:152:ILE:HD12	2:D:153:ARG:N	2.13	0.63
1:C:140:MET:HE1	1:C:170:VAL:O	1.97	0.63
2:F:160:ARG:HA	2:F:163:ARG:HB2	1.80	0.63
1:E:217:LEU:HD12	1:E:218:SER:H	1.63	0.62
2:D:102:MET:HE2	2:D:103:GLU:HG2	1.81	0.62
2:B:2:LEU:HD22	2:B:109:ASP:OD2	2.00	0.62
1:C:95:GLU:OE1	1:C:99:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:ILE:HD12	2:F:142:HIS:O	2.00	0.61
2:B:9:PHE:HB2	2:F:121:ARG:NE	2.15	0.61
2:B:107:THR:CA	2:B:110:LEU:HD22	2.27	0.61
1:C:93:VAL:HG21	1:C:224:HIS:HD2	1.65	0.61
1:E:31:GLU:CD	1:E:33:VAL:H	2.09	0.60
1:E:153:PRO:O	1:E:155:MET:HG3	2.01	0.60
2:F:66:ILE:HD12	2:F:66:ILE:C	2.26	0.60
1:E:164:LYS:HD3	3:E:401:NAG:H81	1.83	0.60
2:B:123:LYS:NZ	2:D:132:GLU:OE1	2.33	0.60
1:C:35:ARG:HD3	1:C:303:ARG:HG3	1.82	0.60
1:A:226:LEU:HD11	1:A:234:VAL:HG11	1.83	0.60
1:A:230:PRO:O	1:A:231:ASN:HB2	2.02	0.60
1:C:1:ASP:OD2	2:D:142:HIS:O	2.20	0.60
1:C:115:PHE:HB3	1:C:117:TYR:CE1	2.37	0.60
1:A:21:GLU:CD	1:A:24:VAL:HG11	2.27	0.59
1:C:7:HIS:HB3	2:D:115:MET:HE1	1.84	0.59
1:A:53:GLN:HG2	1:A:82:GLU:HG3	1.83	0.59
1:C:88:TYR:CD2	1:C:221:ILE:HD12	2.38	0.59
1:E:140:MET:HE1	1:E:170:VAL:O	2.03	0.59
1:A:7:HIS:HE1	1:A:314:VAL:HG22	1.66	0.59
1:C:210:ALA:C	1:C:211:ARG:HG3	2.27	0.59
2:D:55:LEU:HD22	2:D:99:LEU:HD21	1.85	0.59
2:F:2:LEU:O	2:F:4:GLY:N	2.36	0.58
2:B:158:ASP:OD1	2:B:160:ARG:HG2	2.04	0.58
1:C:117:TYR:HD1	1:C:157:LYS:HE3	1.69	0.58
2:B:2:LEU:O	2:B:4:GLY:N	2.36	0.57
2:F:17:LEU:HD11	2:F:36:ALA:HB2	1.85	0.57
1:A:213:GLN:HA	1:A:217:LEU:O	2.04	0.57
1:A:207:SER:O	1:A:207:SER:OG	2.22	0.57
1:E:79:GLU:HB2	1:E:259:GLN:HB3	1.86	0.57
1:A:256:MET:HE1	1:A:294:GLY:N	2.18	0.57
1:C:298:ARG:NH2	2:F:90:GLU:OE1	2.37	0.57
2:B:60:ASN:O	2:B:60:ASN:ND2	2.38	0.57
2:F:113:SER:O	2:F:117:LYS:HG3	2.04	0.57
2:B:17:LEU:HD11	2:B:36:ALA:HB2	1.85	0.56
1:A:232:ASP:OD1	1:A:233:THR:N	2.38	0.56
1:C:207:SER:O	1:C:207:SER:OG	2.21	0.56
1:A:153:PRO:O	1:A:155:MET:HG3	2.06	0.56
2:B:151:SER:HB2	2:B:157:TYR:HB2	1.87	0.56
1:C:169:ILE:N	1:C:169:ILE:HD12	2.20	0.56
1:C:169:ILE:HD11	1:C:228:LEU:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:GLU:HG2	2:F:138:PHE:CE2	2.40	0.56
1:C:173:ILE:HB	1:C:222:ASP:OD2	2.05	0.56
1:A:170:VAL:O	1:A:245:PRO:HB3	2.06	0.55
2:D:22:TYR:HD2	2:D:115:MET:HE3	1.70	0.55
2:F:159:HIS:C	2:F:159:HIS:CD2	2.85	0.55
1:C:173:ILE:HD11	1:C:193:VAL:HG21	1.88	0.55
1:E:191:LYS:HA	1:E:239:ASN:ND2	2.08	0.55
2:B:107:THR:O	2:B:110:LEU:CD2	2.55	0.55
1:C:33:VAL:HG22	1:C:285:PHE:HB2	1.89	0.55
1:E:63:PRO:HB2	1:E:65:GLN:HE22	1.72	0.54
1:E:207:SER:O	1:E:207:SER:OG	2.22	0.54
2:B:140:ILE:HD12	2:B:144:CYS:HB2	1.88	0.54
1:E:191:LYS:O	1:E:206:PRO:HD2	2.08	0.54
1:A:197:SER:HB3	1:A:234:VAL:HG12	1.90	0.54
1:C:169:ILE:CD1	1:C:228:LEU:HB2	2.37	0.54
2:B:55:LEU:HD22	2:B:99:LEU:HD21	1.90	0.54
1:A:298:ARG:NH2	2:D:90:GLU:OE1	2.41	0.54
2:D:2:LEU:O	2:D:4:GLY:N	2.38	0.54
1:E:106:GLY:HA2	1:E:255:SER:HB3	1.90	0.53
1:A:173:ILE:CD1	1:A:193:VAL:HG21	2.38	0.53
2:B:106:HIS:O	2:B:110:LEU:HD22	2.08	0.53
2:B:164:GLU:CD	2:B:164:GLU:H	2.16	0.53
1:C:169:ILE:HD11	1:C:228:LEU:HB2	1.90	0.53
1:C:1:ASP:CG	2:D:140:ILE:O	2.51	0.53
2:B:127:ARG:HG3	2:B:159:HIS:CG	2.44	0.53
2:D:50:GLY:HA3	1:E:20:THR:O	2.09	0.53
2:F:140:ILE:HD13	2:F:144:CYS:HB2	1.90	0.53
1:C:201:GLN:NE2	1:E:91:LYS:HB2	2.24	0.53
1:A:228:LEU:HD22	1:A:234:VAL:HG13	1.91	0.53
2:B:152:ILE:HG13	2:B:153:ARG:N	2.24	0.53
1:E:31:GLU:CD	1:E:32:THR:H	2.17	0.53
1:E:79:GLU:OE2	1:E:103:ARG:NE	2.37	0.53
1:A:222:ASP:HB3	1:E:201:GLN:OE1	2.08	0.52
1:C:87:CYS:O	1:C:215:ASN:ND2	2.42	0.52
1:C:121:ARG:HG2	1:C:123:ASN:OD1	2.09	0.52
2:F:160:ARG:HA	2:F:163:ARG:CB	2.40	0.52
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.92	0.52
1:A:211:ARG:HD2	1:A:220:ARG:CG	2.33	0.52
2:B:66:ILE:HD12	2:B:66:ILE:C	2.35	0.52
1:E:164:LYS:NZ	3:E:401:NAG:H81	2.24	0.52
2:F:167:MET:O	2:F:170:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ILE:C	2:F:66:ILE:CD1	2.83	0.51
1:E:228:LEU:HD22	1:E:234:VAL:HB	1.91	0.51
1:A:10:VAL:HG12	1:A:11:SER:H	1.75	0.51
2:B:123:LYS:HB2	2:B:138:PHE:CZ	2.46	0.51
1:C:147:THR:HG22	1:C:150:ALA:HB2	1.93	0.51
1:A:47:ARG:NH1	1:A:75:ASP:OD1	2.44	0.50
1:A:191:LYS:HB2	1:A:206:PRO:HG3	1.94	0.50
2:F:45:ILE:O	2:F:49:THR:HG23	2.12	0.50
1:E:3:ILE:CG2	2:F:138:PHE:HB2	2.40	0.50
1:A:203:SER:HB3	1:C:207:SER:HB2	1.94	0.50
1:E:44:LYS:HE3	1:E:269:GLU:HB2	1.92	0.50
1:E:172:GLY:HA3	1:E:243:ILE:CD1	2.41	0.50
1:C:65:GLN:O	1:C:68:GLN:NE2	2.45	0.50
2:D:127:ARG:HG3	2:D:159:HIS:CG	2.47	0.50
1:E:164:LYS:HZ3	3:E:401:NAG:C8	2.24	0.50
2:F:2:LEU:C	2:F:4:GLY:H	2.19	0.50
1:A:3:ILE:HD12	2:B:152:ILE:HD11	1.94	0.49
1:C:47:ARG:NH1	1:C:75:ASP:OD1	2.45	0.49
2:B:4:GLY:HA2	2:F:117:LYS:HD2	1.94	0.49
2:B:26:HIS:CD2	2:B:153:ARG:HH12	2.22	0.49
1:C:163:ARG:HD3	1:C:250:PHE:CZ	2.47	0.49
1:C:113:MET:HE1	1:C:245:PRO:HG2	1.94	0.49
1:C:191:LYS:HB2	1:C:206:PRO:HG3	1.94	0.49
1:C:175:HIS:HB3	1:C:211:ARG:HH22	1.77	0.49
1:C:192:LEU:H	1:C:239:ASN:ND2	2.11	0.49
1:A:126:THR:C	1:A:134:SER:HB2	2.37	0.49
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.47	0.49
1:C:170:VAL:O	1:C:245:PRO:HB3	2.12	0.49
2:F:55:LEU:HD22	2:F:99:LEU:HD21	1.94	0.49
1:A:89:PRO:HB3	1:A:214:VAL:HG23	1.94	0.49
1:A:156:THR:O	1:A:157:LYS:NZ	2.46	0.49
1:A:140:MET:HE1	1:A:170:VAL:O	2.12	0.49
1:A:314:VAL:HG23	2:B:13:GLY:H	1.78	0.49
1:E:256:MET:HE3	1:E:256:MET:HB2	1.72	0.49
2:F:168:GLN:O	2:F:168:GLN:HG2	2.11	0.49
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.95	0.48
1:C:156:THR:HG21	1:E:210:ALA:HB3	1.95	0.48
1:C:204:PHE:HE2	1:C:224:HIS:CD2	2.31	0.48
2:D:148:CYS:O	2:D:151:SER:OG	2.22	0.48
1:E:88:TYR:CD2	1:E:221:ILE:HD12	2.48	0.48
1:C:3:ILE:HD11	2:D:24:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ASP:OD1	1:E:233:THR:N	2.46	0.48
1:E:163:ARG:HD3	1:E:250:PHE:CZ	2.48	0.48
2:B:2:LEU:C	2:B:4:GLY:H	2.21	0.48
1:E:164:LYS:HZ2	3:E:401:NAG:H83	1.79	0.48
1:A:90:GLY:HA2	1:E:201:GLN:NE2	2.28	0.48
1:E:173:ILE:HB	1:E:222:ASP:OD2	2.14	0.48
2:B:125:GLN:HE22	2:B:155:ASN:HA	1.79	0.47
1:C:88:TYR:CZ	1:C:217:LEU:HD23	2.49	0.47
1:C:228:LEU:CD1	1:C:232:ASP:HB3	2.44	0.47
2:F:96:ALA:O	2:F:100:ILE:HD12	2.14	0.47
2:F:163:ARG:O	2:F:167:MET:HG2	2.14	0.47
2:B:18:ILE:O	2:B:18:ILE:HG22	2.14	0.47
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.95	0.47
2:D:128:GLU:O	2:D:170:ARG:NH1	2.47	0.47
1:E:164:LYS:HZ2	3:E:401:NAG:C8	2.27	0.47
1:E:291:ARG:HH21	2:F:67:ASP:HB3	1.77	0.47
1:A:86:VAL:HG22	1:A:88:TYR:O	2.13	0.47
1:A:256:MET:HE3	2:B:62:GLN:OE1	2.15	0.47
1:E:35:ARG:NH1	1:E:303:ARG:O	2.42	0.47
1:E:47:ARG:NH1	1:E:75:ASP:OD1	2.46	0.47
1:E:139:GLU:OE1	1:E:247:ARG:HD3	2.13	0.47
1:E:164:LYS:O	1:E:164:LYS:HG3	2.14	0.47
1:A:52:GLY:O	1:A:80:ARG:HB2	2.14	0.47
1:A:71:GLU:OE1	1:A:110:LYS:N	2.43	0.47
2:D:55:LEU:HD11	2:D:103:GLU:OE1	2.14	0.47
1:E:155:MET:HE3	1:E:157:LYS:HE3	1.97	0.47
2:B:134:GLY:O	2:F:121:ARG:NH1	2.48	0.47
1:C:117:TYR:CD2	1:C:120:ILE:HD11	2.50	0.47
1:E:1:ASP:O	2:F:140:ILE:HG13	2.15	0.47
2:F:25:ARG:HE	2:F:34:THR:CG2	2.28	0.47
1:C:160:LYS:HG3	1:C:232:ASP:O	2.15	0.47
1:C:191:LYS:O	1:C:206:PRO:HD2	2.15	0.46
1:E:217:LEU:HG	1:E:219:GLY:H	1.80	0.46
1:C:117:TYR:HB2	1:C:120:ILE:HD11	1.97	0.46
1:C:207:SER:O	1:C:211:ARG:NH2	2.48	0.46
1:C:204:PHE:CE2	1:C:224:HIS:CD2	3.04	0.46
1:A:35:ARG:NH1	1:A:303:ARG:O	2.49	0.46
2:B:37:ASP:OD1	2:B:39:LYS:HG2	2.15	0.46
1:C:60:ILE:HG22	1:C:170:VAL:HG11	1.98	0.46
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.15	0.46
1:C:139:GLU:OE1	1:C:247:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LEU:H	1:C:239:ASN:CG	2.24	0.46
1:A:44:LYS:HE3	1:A:269:GLU:HB2	1.97	0.46
2:D:2:LEU:C	2:D:4:GLY:H	2.22	0.46
2:F:120:GLU:O	2:F:124:ARG:HG3	2.16	0.46
2:F:159:HIS:CE1	2:F:163:ARG:HH11	2.33	0.46
1:E:113:MET:HE1	1:E:169:ILE:HG23	1.98	0.45
2:D:164:GLU:H	2:D:164:GLU:CD	2.24	0.45
1:E:149:ASN:HD22	1:E:184:LYS:HA	1.81	0.45
1:A:121:ARG:HG2	1:A:146:ASN:HA	1.99	0.45
2:B:161:LYS:O	2:B:164:GLU:OE2	2.35	0.45
2:F:154:ASN:CG	2:F:154:ASN:O	2.59	0.45
1:A:191:LYS:O	1:A:206:PRO:HD2	2.17	0.45
2:B:115:MET:HE3	2:B:115:MET:HA	1.99	0.45
2:D:123:LYS:HB2	2:D:138:PHE:CZ	2.52	0.45
1:E:105:SER:HB2	1:E:251:LEU:HB3	1.99	0.45
1:E:295:LYS:HE2	2:F:60:ASN:ND2	2.31	0.45
1:A:172:GLY:O	1:A:173:ILE:HD13	2.16	0.45
1:A:192:LEU:H	1:A:239:ASN:CG	2.25	0.45
2:B:129:ASN:ND2	2:B:157:TYR:OH	2.50	0.45
2:B:131:GLU:OE2	2:F:127:ARG:HB3	2.17	0.45
1:C:44:LYS:HE2	1:C:269:GLU:HB2	1.98	0.45
1:C:145:SER:HB3	1:C:150:ALA:HB3	1.99	0.45
2:D:114:GLU:HA	2:D:117:LYS:HD3	1.99	0.45
2:F:123:LYS:HB2	2:F:138:PHE:CE2	2.52	0.45
1:A:198:SER:O	1:C:91:LYS:NZ	2.49	0.45
1:C:115:PHE:HB3	1:C:117:TYR:CZ	2.52	0.45
2:B:75:LYS:HD2	1:E:101:ILE:HD11	1.99	0.45
1:E:149:ASN:ND2	1:E:184:LYS:HA	2.30	0.45
2:F:51:LYS:NZ	2:F:107:THR:OG1	2.42	0.45
1:A:108:ILE:O	1:A:252:ARG:NH1	2.49	0.45
2:B:25:ARG:HE	2:B:34:THR:HG21	1.82	0.45
1:C:191:LYS:HD3	1:C:239:ASN:HD21	1.80	0.45
2:D:120:GLU:O	2:D:124:ARG:HG3	2.18	0.44
1:E:170:VAL:O	1:E:245:PRO:HB3	2.17	0.44
2:F:121:ARG:HD2	2:F:121:ARG:HA	1.61	0.44
1:C:171:TRP:CH2	1:C:226:LEU:HD23	2.52	0.44
1:C:212:PRO:O	1:C:220:ARG:NH2	2.41	0.44
1:E:167:ALA:HB2	1:E:250:PHE:CZ	2.52	0.44
1:A:211:ARG:HA	1:E:235:THR:HB	1.98	0.44
1:C:93:VAL:HG21	1:C:224:HIS:CD2	2.49	0.44
1:E:164:LYS:HZ3	3:E:401:NAG:H81	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LYS:HE3	2:D:58:LYS:HB3	1.73	0.44
1:E:63:PRO:HB2	1:E:65:GLN:NE2	2.30	0.44
2:F:16:GLY:O	2:F:18:ILE:HD12	2.17	0.44
1:A:126:THR:O	1:A:134:SER:HB2	2.17	0.44
2:B:134:GLY:O	2:F:121:ARG:CZ	2.66	0.44
1:C:117:TYR:CD1	1:C:157:LYS:HE3	2.49	0.44
2:D:72:GLU:OE2	2:D:75:LYS:HE2	2.17	0.44
1:A:207:SER:HB2	1:E:203:SER:HB3	2.00	0.44
2:F:28:ASN:ND2	2:F:146:ASP:OD2	2.45	0.44
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.52	0.44
1:A:228:LEU:HD12	1:A:229:ASN:H	1.83	0.44
2:F:129:ASN:OD1	2:F:129:ASN:N	2.48	0.44
1:A:1:ASP:OD2	2:B:143:LYS:HD3	2.18	0.44
2:F:129:ASN:OD1	2:F:159:HIS:CD2	2.71	0.44
1:A:121:ARG:HG3	1:A:144:LEU:HB2	1.98	0.43
1:E:88:TYR:CE1	1:E:217:LEU:HD23	2.53	0.43
2:B:125:GLN:NE2	2:B:155:ASN:HA	2.33	0.43
1:C:169:ILE:HD11	1:C:228:LEU:HB3	1.99	0.43
2:F:66:ILE:HD13	2:F:81:ILE:HD13	2.01	0.43
2:B:25:ARG:HE	2:B:34:THR:CG2	2.30	0.43
2:B:131:GLU:OE2	2:F:127:ARG:NE	2.51	0.43
1:C:153:PRO:O	1:C:155:MET:HG3	2.18	0.43
2:F:47:GLN:OE1	2:F:110:LEU:HD11	2.19	0.43
1:A:197:SER:HA	1:A:234:VAL:HA	2.00	0.43
1:A:209:GLY:O	1:A:211:ARG:NH2	2.51	0.43
1:C:8:HIS:HE1	1:C:311:MET:HE3	1.83	0.43
2:D:133:ASP:CG	2:D:137:CYS:H	2.26	0.43
1:E:218:SER:OG	1:E:218:SER:O	2.37	0.43
1:A:158:SER:OG	1:A:235:THR:HG23	2.18	0.43
1:A:197:SER:CB	1:A:234:VAL:HG12	2.48	0.43
2:B:164:GLU:HA	2:B:167:MET:SD	2.59	0.43
1:C:193:VAL:HG22	1:C:204:PHE:HB2	2.00	0.43
1:C:203:SER:HB3	1:E:207:SER:HB2	2.01	0.43
2:F:119:TYR:OH	2:F:132:GLU:HB3	2.19	0.43
1:C:1:ASP:OD2	2:D:140:ILE:O	2.37	0.43
2:B:148:CYS:O	2:B:151:SER:OG	2.35	0.43
1:C:2:LYS:HB2	1:C:2:LYS:HE3	1.94	0.43
1:C:8:HIS:CE1	1:C:311:MET:HE3	2.54	0.43
1:E:90:GLY:HA3	1:E:221:ILE:O	2.19	0.43
1:C:291:ARG:HH21	2:D:67:ASP:HB3	1.83	0.43
1:E:8:HIS:CE1	1:E:311:MET:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLY:C	1:C:91:LYS:HG2	2.44	0.42
1:C:286:GLN:O	1:C:299:TYR:HA	2.19	0.42
1:E:31:GLU:CD	1:E:32:THR:N	2.75	0.42
2:B:140:ILE:HD12	2:B:144:CYS:CB	2.49	0.42
1:E:32:THR:HG22	1:E:305:LEU:O	2.20	0.42
2:D:52:LEU:HD12	2:D:52:LEU:HA	1.92	0.42
1:A:63:PRO:HB2	1:A:65:GLN:OE1	2.19	0.42
1:C:10:VAL:HG22	1:C:11:SER:N	2.35	0.42
1:C:169:ILE:HD12	1:C:169:ILE:H	1.84	0.42
1:C:228:LEU:HD11	1:C:232:ASP:HB3	2.02	0.42
1:E:8:HIS:HE1	1:E:311:MET:HE3	1.85	0.42
1:E:173:ILE:HD11	1:E:193:VAL:HG21	2.02	0.42
2:B:25:ARG:HG3	2:B:34:THR:CG2	2.50	0.42
2:B:10:ILE:N	2:B:10:ILE:HD12	2.35	0.42
2:D:141:PHE:CD1	2:D:170:ARG:HD2	2.55	0.42
1:A:90:GLY:HA2	1:E:201:GLN:HE22	1.85	0.42
2:B:66:ILE:C	2:B:66:ILE:CD1	2.93	0.42
1:C:218:SER:O	1:C:218:SER:OG	2.37	0.42
2:D:141:PHE:HD1	2:D:170:ARG:HD2	1.85	0.41
1:E:156:THR:HA	1:E:236:PHE:O	2.20	0.41
1:E:183:THR:HA	1:E:187:GLY:O	2.20	0.41
1:C:288:ILE:HG22	1:C:289:ASP:HB2	2.02	0.41
2:D:25:ARG:HG3	2:D:33:GLY:O	2.20	0.41
1:C:10:VAL:HG22	1:C:11:SER:H	1.85	0.41
1:C:191:LYS:HB2	1:C:206:PRO:CG	2.50	0.41
2:D:121:ARG:NH1	2:F:9:PHE:HB2	2.36	0.41
2:F:148:CYS:O	2:F:151:SER:OG	2.35	0.41
1:C:175:HIS:HB3	1:C:211:ARG:NH2	2.35	0.41
2:F:25:ARG:HE	2:F:34:THR:HG21	1.85	0.41
2:B:131:GLU:OE1	2:F:163:ARG:NH1	2.51	0.41
2:B:152:ILE:HG21	2:B:152:ILE:HD13	1.63	0.41
1:E:121:ARG:NH2	1:E:145:SER:O	2.54	0.41
2:F:56:ILE:HD12	2:F:56:ILE:N	2.36	0.41
1:A:298:ARG:HG2	2:B:92:TRP:CE2	2.56	0.41
1:C:21:GLU:CG	1:C:24:VAL:HG23	2.51	0.41
2:D:121:ARG:HH11	2:F:9:PHE:HB2	1.85	0.41
1:E:52:GLY:O	1:E:80:ARG:HB2	2.21	0.41
1:E:171:TRP:CH2	1:E:195:VAL:HG11	2.56	0.41
2:F:119:TYR:O	2:F:122:VAL:HG22	2.21	0.41
2:F:122:VAL:HG23	2:F:138:PHE:CE1	2.56	0.41
1:A:10:VAL:HG12	1:A:11:SER:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:VAL:O	2:B:126:LEU:HG	2.20	0.41
2:D:122:VAL:HG23	2:D:138:PHE:CE1	2.56	0.41
2:F:161:LYS:HE2	2:F:162:TYR:CZ	2.55	0.41
1:C:232:ASP:OD2	1:C:233:THR:N	2.54	0.40
2:F:52:LEU:HD12	2:F:52:LEU:HA	1.93	0.40
2:B:66:ILE:HD13	2:B:81:ILE:HD13	2.03	0.40
1:C:173:ILE:CD1	1:C:193:VAL:HG21	2.51	0.40
1:A:33:VAL:HG22	1:A:285:PHE:HB2	2.04	0.40
2:F:117:LYS:O	2:F:121:ARG:HB2	2.22	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	314/321 (98%)	293 (93%)	19 (6%)	2 (1%)	21	45
1	C	314/321 (98%)	294 (94%)	18 (6%)	2 (1%)	21	45
1	E	314/321 (98%)	293 (93%)	18 (6%)	3 (1%)	12	32
2	B	169/221 (76%)	153 (90%)	13 (8%)	3 (2%)	6	19
2	D	169/221 (76%)	153 (90%)	13 (8%)	3 (2%)	6	19
2	F	169/221 (76%)	153 (90%)	13 (8%)	3 (2%)	6	19
All	All	1449/1626 (89%)	1339 (92%)	94 (6%)	16 (1%)	11	29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	PHE
2	B	12	ASN
2	D	12	ASN

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Mol	Chain	Res	Type
2	F	12	ASN
2	F	127	ARG
1	A	197	SER
1	C	197	SER
2	D	3	PHE
1	E	197	SER
1	E	231	ASN
2	F	3	PHE
2	D	127	ARG
1	A	315	PRO
2	B	127	ARG
1	E	315	PRO
1	C	315	PRO

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	267/271 (98%)	266 (100%)	1 (0%)	84	92
1	C	267/271 (98%)	266 (100%)	1 (0%)	84	92
1	E	267/271 (98%)	264 (99%)	3 (1%)	65	80
2	B	145/189 (77%)	143 (99%)	2 (1%)	59	77
2	D	145/189 (77%)	145 (100%)	0	100	100
2	F	145/189 (77%)	145 (100%)	0	100	100
All	All	1236/1380 (90%)	1229 (99%)	7 (1%)	78	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
2	B	117	LYS
2	B	151	SER
1	C	11	SER
1	E	11	SER

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Mol	Chain	Res	Type
1	E	256	MET
1	E	280	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	94	ASN
1	A	149	ASN
1	A	182	GLN
1	A	190	ASN
1	A	215	ASN
2	B	26	HIS
2	B	60	ASN
2	B	61	GLN
2	B	125	GLN
1	C	8	HIS
1	C	65	GLN
1	C	182	GLN
1	C	224	HIS
1	C	239	ASN
2	D	125	GLN
1	E	65	GLN
1	E	94	ASN
1	E	149	ASN
1	E	182	GLN
1	E	190	ASN
1	E	201	GLN
1	E	213	GLN
1	E	259	GLN
2	F	26	HIS
2	F	53	ASN
2	F	60	ASN
2	F	76	GLN
2	F	159	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	C	401	1	14,14,15	0.29	0	17,19,21	1.23	3 (17%)
3	NAG	E	401	1	14,14,15	0.96	1 (7%)	17,19,21	2.54	6 (35%)
3	NAG	D	301	2	14,14,15	0.44	0	17,19,21	0.66	1 (5%)
3	NAG	F	301	2	14,14,15	0.39	0	17,19,21	0.62	0
3	NAG	B	301	2	14,14,15	0.47	0	17,19,21	0.73	1 (5%)
3	NAG	A	401	1	14,14,15	2.09	2 (14%)	17,19,21	2.50	3 (17%)

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	C	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	1	-	3/6/23/26	0/1/1/1
3	NAG	D	301	2	-	1/6/23/26	0/1/1/1
3	NAG	F	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAG	C1-C2	7.09	1.62	1.52
3	A	401	NAG	O5-C1	2.89	1.48	1.43
3	E	401	NAG	O5-C1	2.67	1.48	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	NAG	C1-O5-C5	7.99	122.90	112.19
3	A	401	NAG	C1-O5-C5	6.80	121.30	112.19
3	A	401	NAG	C1-C2-N2	6.38	120.49	110.43
3	E	401	NAG	C1-C2-N2	3.51	115.96	110.43
3	E	401	NAG	C3-C4-C5	2.80	115.32	110.23
3	C	401	NAG	C2-N2-C7	2.58	126.36	122.90
3	E	401	NAG	O4-C4-C5	2.55	115.59	109.32
3	A	401	NAG	C4-C3-C2	-2.49	107.36	111.02
3	C	401	NAG	C1-C2-N2	2.45	114.29	110.43
3	C	401	NAG	C1-O5-C5	2.42	115.44	112.19
3	B	301	NAG	C1-O5-C5	2.42	115.43	112.19
3	D	301	NAG	C1-O5-C5	2.18	115.11	112.19
3	E	401	NAG	C4-C3-C2	-2.17	107.84	111.02
3	E	401	NAG	O3-C3-C4	2.05	115.20	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAG	C1-C2-N2-C7
3	C	401	NAG	C1-C2-N2-C7
3	E	401	NAG	O5-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	B	301	NAG	C4-C5-C6-O6
3	D	301	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	E	401	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	NAG	8	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	316/321 (98%)	-0.30	11 (3%)	47 40	42, 80, 122, 150	1 (0%)
1	C	316/321 (98%)	-0.34	6 (1%)	66 58	45, 79, 119, 149	1 (0%)
1	E	316/321 (98%)	-0.40	4 (1%)	75 69	43, 79, 123, 151	1 (0%)
2	B	171/221 (77%)	-0.19	7 (4%)	41 34	41, 99, 139, 149	0
2	D	171/221 (77%)	-0.35	1 (0%)	85 82	42, 100, 140, 156	0
2	F	171/221 (77%)	-0.52	2 (1%)	76 71	40, 101, 139, 149	0
All	All	1461/1626 (89%)	-0.35	31 (2%)	63 55	40, 87, 134, 156	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	23	GLY	9.4
2	B	24	PHE	7.8
1	C	281	SER	4.8
1	A	149	ASN	4.4
2	B	21	TRP	4.3
1	E	295	LYS	3.8
2	F	60	ASN	3.6
1	A	73	SER	3.5
1	A	124	GLY	3.5
1	E	84	SER	3.3
2	B	35	ALA	3.2
1	C	282	ASN	3.0
2	F	1	GLY	2.9
1	A	143	LEU	2.9
2	D	55	LEU	2.7
1	E	137	TYR	2.6
1	C	72	PHE	2.5
1	A	188	SER	2.4
1	A	292	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	92	PHE	2.3
1	C	189	GLY	2.3
1	C	198	SER	2.2
1	E	86	VAL	2.2
2	B	154	ASN	2.1
1	A	190	ASN	2.1
1	A	306	LEU	2.1
1	C	144	LEU	2.1
2	B	9	PHE	2.1
1	A	32	THR	2.0
2	B	5	ALA	2.0
1	A	273	TYR	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	401	14/15	0.92	0.10	138,158,163,169	0
3	NAG	D	301	14/15	0.92	0.12	79,100,123,142	0
3	NAG	A	401	14/15	0.94	0.08	124,154,169,169	0
3	NAG	E	401	14/15	0.94	0.10	112,158,164,165	0
3	NAG	F	301	14/15	0.95	0.15	81,107,124,128	0
3	NAG	B	301	14/15	0.97	0.07	84,107,127,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.