Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:44 am BST

PDB ID	:	6N4F
Title	:	The crystal structure of hemagglutinin from A/canine/IL/11613/2015 (H3N2) influenza virus.
Authors	:	Yang, H.; Stevesn, J.
Deposited on	:	2018-11-19
Resolution	:	3.01 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 following versions of software and data (see references ①) were used in the production of this report:

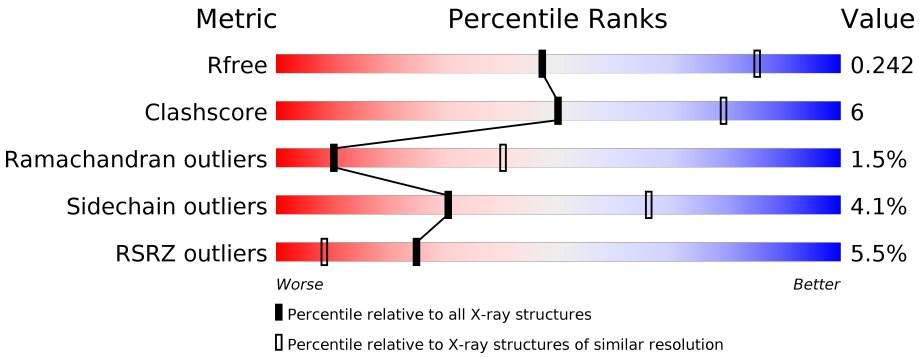
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	334	2% 78% 16% • 5%
1	C	334	2% 77% 17% • 5%
1	E	334	% 79% 15% • 5%
1	G	334	2% 78% 17% • 5%
2	B	182	10% 77% 16% • 5%
2	D	182	12% 78% 15% • 5%

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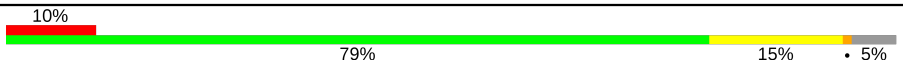
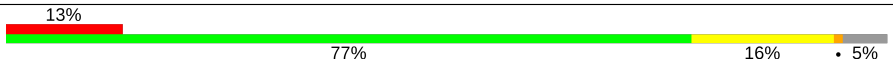
Mol	Chain	Length	Quality of chain
2	F	182	
2	H	182	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15352 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	317	Total	C	N	O	S	0	0	0
			2442	1526	434	468	14			
1	C	317	Total	C	N	O	S	0	0	0
			2442	1526	434	468	14			
1	E	317	Total	C	N	O	S	0	0	0
			2442	1526	434	468	14			
1	G	317	Total	C	N	O	S	0	0	0
			2442	1526	434	468	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	expression tag	UNP A0A218KIQ1
A	-3	ASP	-	expression tag	UNP A0A218KIQ1
A	-2	LEU	-	expression tag	UNP A0A218KIQ1
A	-1	GLY	-	expression tag	UNP A0A218KIQ1
A	0	SER	-	expression tag	UNP A0A218KIQ1
C	-4	ALA	-	expression tag	UNP A0A218KIQ1
C	-3	ASP	-	expression tag	UNP A0A218KIQ1
C	-2	LEU	-	expression tag	UNP A0A218KIQ1
C	-1	GLY	-	expression tag	UNP A0A218KIQ1
C	0	SER	-	expression tag	UNP A0A218KIQ1
E	-4	ALA	-	expression tag	UNP A0A218KIQ1
E	-3	ASP	-	expression tag	UNP A0A218KIQ1
E	-2	LEU	-	expression tag	UNP A0A218KIQ1
E	-1	GLY	-	expression tag	UNP A0A218KIQ1
E	0	SER	-	expression tag	UNP A0A218KIQ1
G	-4	ALA	-	expression tag	UNP A0A218KIQ1
G	-3	ASP	-	expression tag	UNP A0A218KIQ1
G	-2	LEU	-	expression tag	UNP A0A218KIQ1
G	-1	GLY	-	expression tag	UNP A0A218KIQ1
G	0	SER	-	expression tag	UNP A0A218KIQ1

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1396	863	248	279	6			
2	D	172	Total	C	N	O	S	0	0	0
			1396	863	248	279	6			
2	F	172	Total	C	N	O	S	0	0	0
			1396	863	248	279	6			
2	H	172	Total	C	N	O	S	0	0	0
			1396	863	248	279	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A2U5FPI7
B	176	GLY	-	expression tag	UNP A0A2U5FPI7
B	177	ARG	-	expression tag	UNP A0A2U5FPI7
B	178	LEU	-	expression tag	UNP A0A2U5FPI7
B	179	VAL	-	expression tag	UNP A0A2U5FPI7
B	180	PRO	-	expression tag	UNP A0A2U5FPI7
B	181	ARG	-	expression tag	UNP A0A2U5FPI7
B	182	GLY	-	expression tag	UNP A0A2U5FPI7
D	175	SER	-	expression tag	UNP A0A2U5FPI7
D	176	GLY	-	expression tag	UNP A0A2U5FPI7
D	177	ARG	-	expression tag	UNP A0A2U5FPI7
D	178	LEU	-	expression tag	UNP A0A2U5FPI7
D	179	VAL	-	expression tag	UNP A0A2U5FPI7
D	180	PRO	-	expression tag	UNP A0A2U5FPI7
D	181	ARG	-	expression tag	UNP A0A2U5FPI7
D	182	GLY	-	expression tag	UNP A0A2U5FPI7
F	175	SER	-	expression tag	UNP A0A2U5FPI7
F	176	GLY	-	expression tag	UNP A0A2U5FPI7
F	177	ARG	-	expression tag	UNP A0A2U5FPI7
F	178	LEU	-	expression tag	UNP A0A2U5FPI7
F	179	VAL	-	expression tag	UNP A0A2U5FPI7
F	180	PRO	-	expression tag	UNP A0A2U5FPI7
F	181	ARG	-	expression tag	UNP A0A2U5FPI7
F	182	GLY	-	expression tag	UNP A0A2U5FPI7
H	175	SER	-	expression tag	UNP A0A2U5FPI7
H	176	GLY	-	expression tag	UNP A0A2U5FPI7
H	177	ARG	-	expression tag	UNP A0A2U5FPI7
H	178	LEU	-	expression tag	UNP A0A2U5FPI7
H	179	VAL	-	expression tag	UNP A0A2U5FPI7
H	180	PRO	-	expression tag	UNP A0A2U5FPI7

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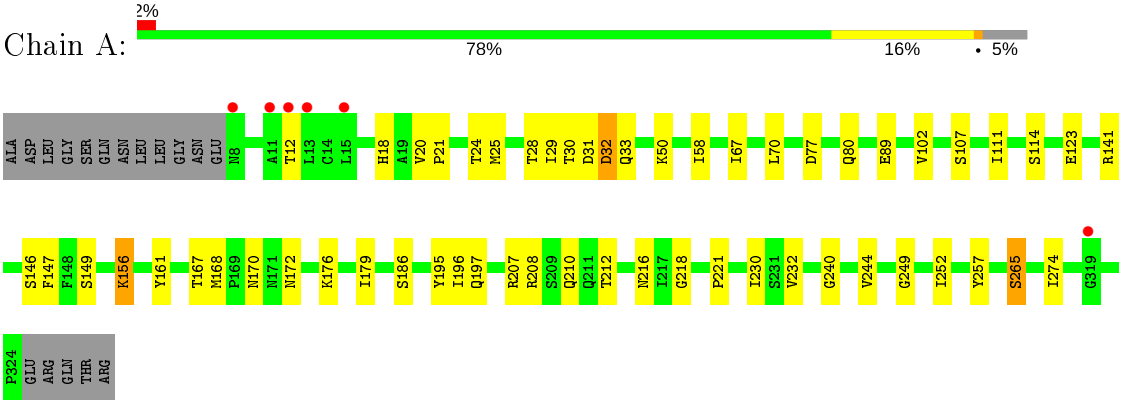
Chain	Residue	Modelled	Actual	Comment	Reference
H	181	ARG	-	expression tag	UNP A0A2U5FPI7
H	182	GLY	-	expression tag	UNP A0A2U5FPI7

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

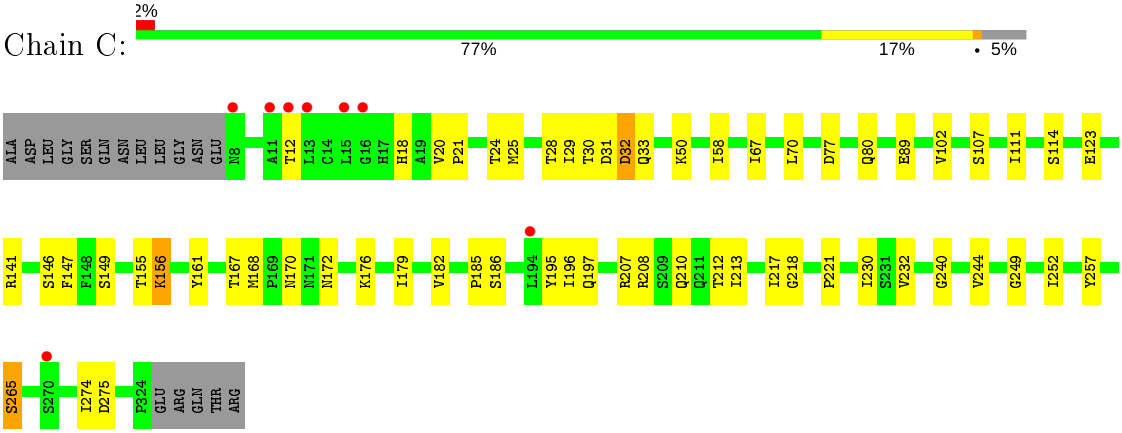
- Molecule 1: Hemagglutinin HA1

Chain A:



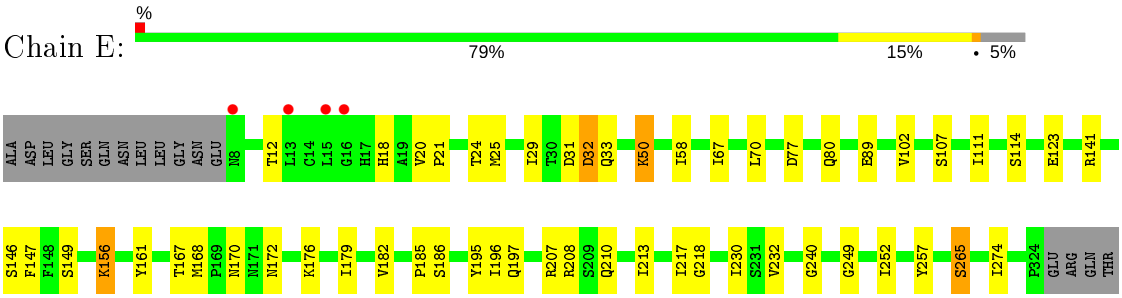
- Molecule 1: Hemagglutinin HA1

Chain C:



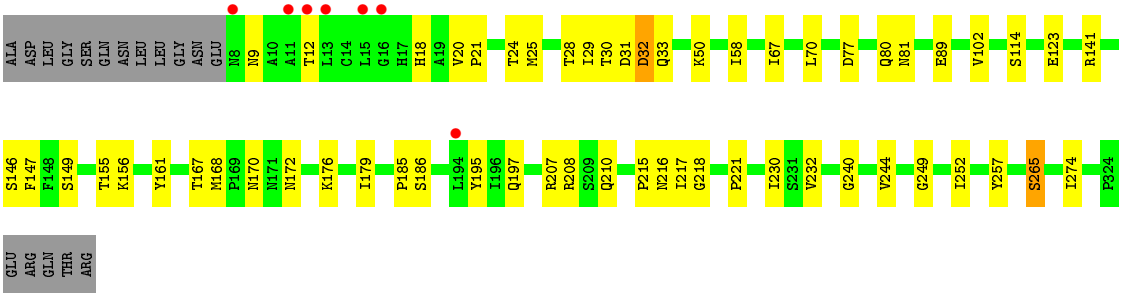
- Molecule 1: Hemagglutinin HA1

Chain E:



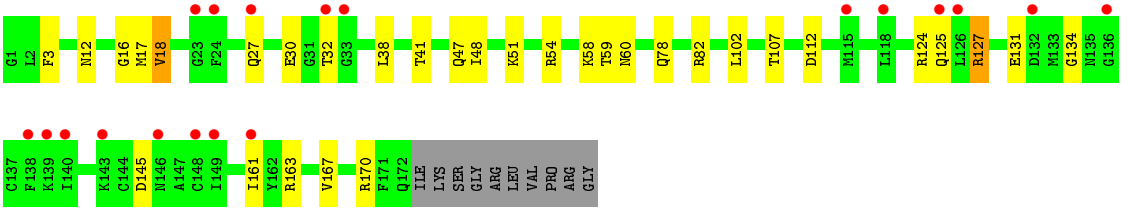
• Molecule 1: Hemagglutinin HA1

Chain G:



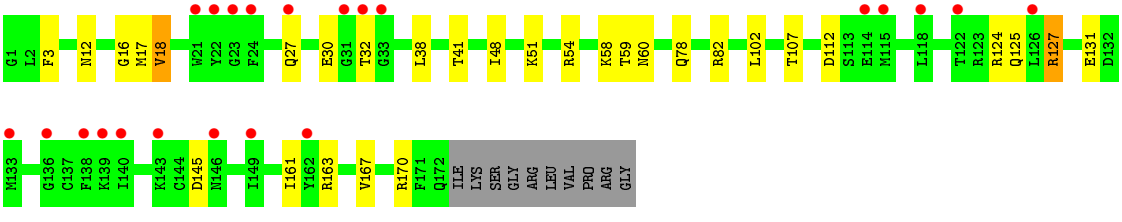
• Molecule 2: Hemagglutinin HA2

Chain B:



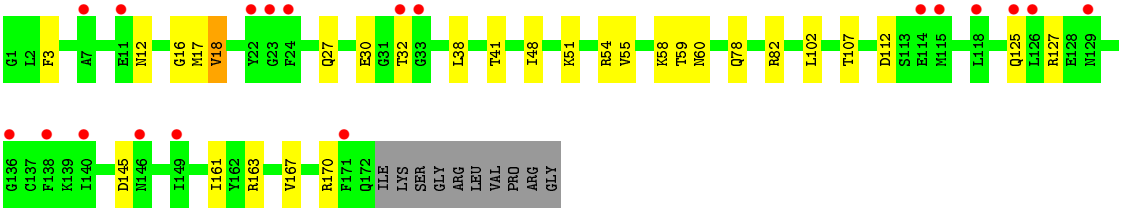
• Molecule 2: Hemagglutinin HA2

Chain D:



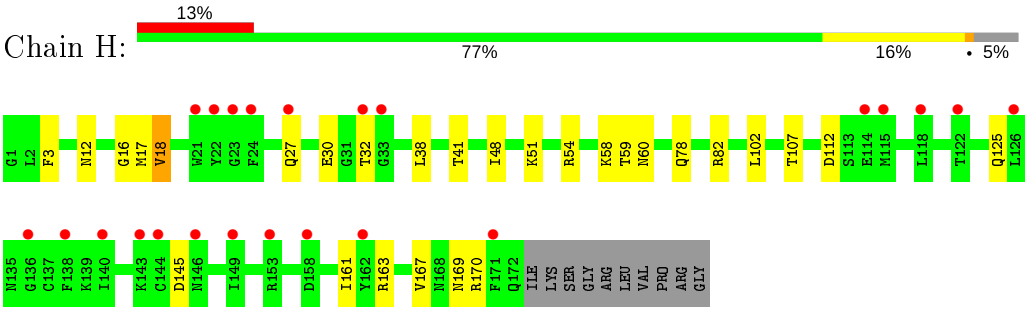
• Molecule 2: Hemagglutinin HA2

Chain F:



• Molecule 2: Hemagglutinin HA2

Chain H:


13%
77%
16%
• 5%
G1 L2 F3 N12 G16 M17 V18 W21 Y22 G23 F24 Q27 E30 G31 T32 G33 L38 T41 I48 K51 R54 K58 T59 N60 Q78 R82 L102 T107 D112 S113 E114 M115 L118 T122 Q125 L126 R127 E131 G134
N135 G136 C137 F138 K139 I140 K143 C144 D145 N146 I149 R153 D158 I161 Y162 R163 V167 N168 N169 R170 F171 Q172 ILE LYS SER GLY ARG LEU VAL PRO ARG GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	241.15Å 241.15Å 147.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.01 45.61 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-3.01) 98.6 (45.61-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.213 , 0.242 0.215 , 0.242	Depositor DCC
R_{free} test set	3188 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	84.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.009 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.009 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.005 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.428 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.417 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.428 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.010 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15352	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.60	0/2497	0.79	0/3402
1	C	0.59	0/2497	0.79	0/3402
1	E	0.59	0/2497	0.78	0/3402
1	G	0.59	0/2497	0.79	0/3402
2	B	0.57	0/1419	0.69	0/1908
2	D	0.56	0/1419	0.69	0/1908
2	F	0.56	0/1419	0.69	0/1908
2	H	0.56	0/1419	0.69	0/1908
All	All	0.58	0/15664	0.75	0/21240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2442	0	2389	35	0
1	C	2442	0	2389	35	0
1	E	2442	0	2389	27	1
1	G	2442	0	2389	33	0
2	B	1396	0	1314	22	0
2	D	1396	0	1314	21	0
2	F	1396	0	1314	13	1
2	H	1396	0	1314	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15352	0	14812	174	1

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 6.

All (174) 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)
2:B:163:ARG:O	2:B:167:VAL:HG23	1.79	0.83
2:H:163:ARG:O	2:H:167:VAL:HG23	1.79	0.83
2:D:163:ARG:O	2:D:167:VAL:HG23	1.79	0.81
2:F:163:ARG:O	2:F:167:VAL:HG23	1.79	0.81
2:B:78:GLN:OE1	2:B:82:ARG:NH1	2.21	0.73
2:D:78:GLN:OE1	2:D:82:ARG:NH1	2.22	0.73
2:H:78:GLN:OE1	2:H:82:ARG:NH1	2.22	0.72
1:A:32:ASP:OD1	2:D:54:ARG:NH1	2.21	0.72
2:F:78:GLN:OE1	2:F:82:ARG:NH1	2.22	0.72
1:C:32:ASP:OD1	2:H:54:ARG:NH1	2.25	0.70
2:B:54:ARG:NH1	1:G:32:ASP:OD1	2.25	0.70
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.76	0.67
2:H:48:ILE:HD11	2:H:107:THR:HG23	1.75	0.67
2:D:48:ILE:HD11	2:D:107:THR:HG23	1.75	0.67
2:F:16:GLY:O	2:F:18:VAL:HG23	1.95	0.67
2:H:16:GLY:O	2:H:18:VAL:HG23	1.95	0.67
2:F:48:ILE:HD11	2:F:107:THR:HG23	1.75	0.66
2:D:51:LYS:NZ	2:D:107:THR:OG1	2.28	0.66
2:B:16:GLY:O	2:B:18:VAL:HG23	1.95	0.66
2:D:16:GLY:O	2:D:18:VAL:HG23	1.96	0.66
2:F:51:LYS:NZ	2:F:107:THR:OG1	2.28	0.66
1:E:70:LEU:HD21	1:E:179:ILE:CD1	2.28	0.64
1:A:70:LEU:HD21	1:A:179:ILE:CD1	2.27	0.64
2:B:127:ARG:NH2	2:H:131:GLU:OE1	2.30	0.64
2:B:51:LYS:NZ	2:B:107:THR:OG1	2.29	0.64
2:H:51:LYS:NZ	2:H:107:THR:OG1	2.28	0.63
1:C:70:LEU:HD21	1:C:179:ILE:CD1	2.28	0.63
1:G:70:LEU:HD21	1:G:179:ILE:CD1	2.28	0.62
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.00	0.62
2:H:30:GLU:OE2	2:H:145:ASP:HB2	2.00	0.62
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.00	0.61
2:F:30:GLU:OE2	2:F:145:ASP:HB2	2.00	0.61
2:F:16:GLY:O	2:F:18:VAL:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:GLY:O	2:H:18:VAL:N	2.37	0.58
2:B:16:GLY:O	2:B:18:VAL:N	2.37	0.58
2:D:16:GLY:O	2:D:18:VAL:N	2.37	0.58
1:C:70:LEU:HD21	1:C:179:ILE:HD11	1.87	0.56
1:A:170:ASN:OD1	1:A:172:ASN:HB2	2.06	0.56
1:G:77:ASP:OD2	1:G:141:ARG:NH1	2.39	0.55
1:C:170:ASN:OD1	1:C:172:ASN:HB2	2.06	0.55
1:C:30:THR:O	2:H:54:ARG:NH2	2.39	0.55
1:E:170:ASN:OD1	1:E:172:ASN:HB2	2.06	0.55
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.39	0.55
1:E:70:LEU:HD21	1:E:179:ILE:HD11	1.88	0.55
1:G:170:ASN:OD1	1:G:172:ASN:HB2	2.07	0.54
2:B:54:ARG:NH2	1:G:30:THR:O	2.41	0.54
1:G:70:LEU:HD21	1:G:179:ILE:HD11	1.88	0.54
1:C:30:THR:C	2:H:54:ARG:NH2	2.61	0.54
1:A:70:LEU:HD21	1:A:179:ILE:HD11	1.87	0.54
1:A:30:THR:C	2:D:54:ARG:NH2	2.62	0.54
2:D:131:GLU:OE1	2:H:127:ARG:NH2	2.39	0.54
1:A:30:THR:O	2:D:54:ARG:NH2	2.41	0.53
1:A:25:MET:HE3	1:A:33:GLN:HB3	1.90	0.53
2:B:54:ARG:NH2	1:G:30:THR:C	2.62	0.53
2:D:18:VAL:O	2:D:18:VAL:HG12	2.09	0.53
1:C:195:TYR:O	1:C:197:GLN:N	2.40	0.52
2:B:18:VAL:O	2:B:18:VAL:HG12	2.09	0.52
2:F:18:VAL:HG12	2:F:18:VAL:O	2.09	0.52
1:A:195:TYR:O	1:A:197:GLN:N	2.40	0.52
2:H:18:VAL:O	2:H:18:VAL:HG12	2.09	0.52
1:E:77:ASP:OD2	1:E:141:ARG:NH1	2.39	0.51
1:C:221:PRO:HG3	1:G:244:VAL:HG23	1.93	0.51
1:A:28:THR:O	2:D:54:ARG:HD2	2.10	0.50
1:E:186:SER:HA	1:E:218:GLY:O	2.12	0.50
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.94	0.50
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.94	0.50
1:E:195:TYR:O	1:E:197:GLN:N	2.40	0.49
1:C:28:THR:O	2:H:54:ARG:HD2	2.13	0.49
1:C:77:ASP:OD2	1:C:141:ARG:NH1	2.38	0.49
1:A:186:SER:HA	1:A:218:GLY:O	2.12	0.49
2:B:54:ARG:HD2	1:G:28:THR:O	2.13	0.49
1:G:186:SER:HA	1:G:218:GLY:O	2.13	0.48
1:A:146:SER:OG	1:A:147:PHE:N	2.46	0.48
2:B:131:GLU:OE1	2:D:127:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG23	1:G:221:PRO:HG3	1.94	0.48
1:G:146:SER:OG	1:G:147:PHE:N	2.46	0.48
1:E:146:SER:OG	1:E:147:PHE:N	2.46	0.48
1:A:221:PRO:HG3	1:C:244:VAL:HG23	1.95	0.47
2:B:48:ILE:HA	2:B:51:LYS:HG2	1.96	0.47
1:C:146:SER:OG	1:C:147:PHE:N	2.45	0.47
1:C:186:SER:HA	1:C:218:GLY:O	2.13	0.47
2:H:48:ILE:HA	2:H:51:LYS:HG2	1.97	0.47
1:A:70:LEU:HD21	1:A:179:ILE:HD13	1.95	0.47
1:E:176:LYS:HE2	1:E:257:TYR:CE2	2.49	0.47
1:G:195:TYR:O	1:G:197:GLN:N	2.40	0.47
2:F:48:ILE:HA	2:F:51:LYS:HG2	1.97	0.47
1:G:176:LYS:HE2	1:G:257:TYR:CE2	2.50	0.47
2:D:48:ILE:HA	2:D:51:LYS:HG2	1.97	0.47
1:G:58:ILE:HG21	1:G:274:ILE:HD12	1.97	0.47
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.96	0.47
1:E:58:ILE:HG21	1:E:274:ILE:HD12	1.97	0.47
2:D:27:GLN:HG2	2:D:32:THR:HG22	1.97	0.46
1:A:58:ILE:HG21	1:A:274:ILE:HD12	1.97	0.46
1:C:25:MET:HE3	1:C:33:GLN:HB3	1.98	0.46
2:B:27:GLN:HG2	2:B:32:THR:HG22	1.97	0.46
1:C:176:LYS:HE2	1:C:257:TYR:CE2	2.51	0.46
1:G:70:LEU:HD21	1:G:179:ILE:HD13	1.96	0.46
2:H:27:GLN:HG2	2:H:32:THR:HG22	1.97	0.46
1:A:102:VAL:HG22	1:A:232:VAL:HB	1.99	0.45
1:C:58:ILE:HG21	1:C:274:ILE:HD12	1.98	0.45
1:E:230:ILE:HD13	1:E:252:ILE:HD13	1.99	0.45
1:E:102:VAL:HG22	1:E:232:VAL:HB	1.98	0.45
2:F:27:GLN:HG2	2:F:32:THR:HG22	1.97	0.45
1:A:176:LYS:HE2	1:A:257:TYR:CE2	2.51	0.45
1:G:102:VAL:HG22	1:G:232:VAL:HB	1.98	0.45
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.98	0.45
2:B:124:ARG:HD3	2:H:134:GLY:HA2	1.99	0.45
1:G:29:ILE:HD11	2:H:102:LEU:HD23	1.98	0.45
2:H:3:PHE:HB2	2:H:112:ASP:OD1	2.17	0.45
1:C:102:VAL:HG22	1:C:232:VAL:HB	1.99	0.44
1:E:70:LEU:HD21	1:E:179:ILE:HD13	1.96	0.44
1:C:114:SER:HA	1:C:265:SER:O	2.18	0.44
1:G:230:ILE:HD13	1:G:252:ILE:HD13	1.99	0.44
2:F:3:PHE:HB2	2:F:112:ASP:OD1	2.18	0.44
2:D:3:PHE:HB2	2:D:112:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HD13	1:A:111:ILE:HG21	1.77	0.44
1:C:230:ILE:HD13	1:C:252:ILE:HD13	2.00	0.44
1:E:114:SER:HA	1:E:265:SER:O	2.18	0.44
1:C:70:LEU:HD21	1:C:179:ILE:HD13	1.96	0.43
1:C:20:VAL:HB	1:C:21:PRO:HD2	2.00	0.43
1:G:24:THR:HG22	1:G:25:MET:N	2.34	0.43
1:A:207:ARG:NH2	1:A:240:GLY:O	2.51	0.43
1:A:77:ASP:O	1:A:80:GLN:HG3	2.19	0.43
2:B:134:GLY:HA2	2:D:124:ARG:HD3	1.99	0.43
1:A:212:THR:HG21	1:G:216:ASN:HB3	2.01	0.43
1:C:32:ASP:N	2:H:54:ARG:NH1	2.66	0.43
2:B:3:PHE:HB2	2:B:112:ASP:OD1	2.18	0.43
1:E:24:THR:HG22	1:E:25:MET:N	2.34	0.43
1:E:67:ILE:O	1:E:70:LEU:HB3	2.19	0.43
1:A:20:VAL:HB	1:A:21:PRO:HD2	2.01	0.42
1:C:77:ASP:O	1:C:80:GLN:HG3	2.19	0.42
1:A:28:THR:O	2:D:54:ARG:CD	2.67	0.42
1:A:32:ASP:N	2:D:54:ARG:NH1	2.67	0.42
1:C:24:THR:HG22	1:C:25:MET:N	2.34	0.42
1:E:207:ARG:NH2	1:E:240:GLY:O	2.51	0.42
1:A:67:ILE:O	1:A:70:LEU:HB3	2.20	0.42
1:G:77:ASP:O	1:G:80:GLN:HG3	2.20	0.42
1:E:77:ASP:O	1:E:80:GLN:HG3	2.19	0.42
1:A:230:ILE:HD13	1:A:252:ILE:HD13	2.00	0.42
1:C:123:GLU:OE1	1:C:168:MET:HG2	2.20	0.42
1:G:25:MET:HE3	1:G:33:GLN:HB3	2.02	0.42
1:G:67:ILE:O	1:G:70:LEU:HB3	2.19	0.42
1:A:123:GLU:OE1	1:A:168:MET:HG2	2.20	0.42
1:C:107:SER:O	1:C:111:ILE:HG23	2.20	0.42
1:G:123:GLU:OE1	1:G:168:MET:HG2	2.20	0.42
1:G:207:ARG:NH2	1:G:240:GLY:O	2.52	0.42
1:C:207:ARG:NH2	1:C:240:GLY:O	2.53	0.41
1:A:161:TYR:CE2	1:A:249:GLY:HA2	2.55	0.41
1:C:67:ILE:O	1:C:70:LEU:HB3	2.19	0.41
1:G:114:SER:HA	1:G:265:SER:O	2.20	0.41
1:A:114:SER:HA	1:A:265:SER:O	2.20	0.41
1:A:24:THR:HG22	1:A:25:MET:N	2.35	0.41
1:E:123:GLU:OE1	1:E:168:MET:HG2	2.19	0.41
1:E:185:PRO:O	1:E:217:ILE:HA	2.20	0.41
1:G:20:VAL:HB	1:G:21:PRO:HD2	2.01	0.41
1:E:107:SER:O	1:E:111:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:PRO:O	1:G:217:ILE:HA	2.21	0.41
1:C:156:LYS:HD3	1:C:196:ILE:HD11	2.03	0.41
2:B:54:ARG:CD	1:G:28:THR:O	2.68	0.41
1:A:107:SER:O	1:A:111:ILE:HG23	2.21	0.41
1:E:20:VAL:HB	1:E:21:PRO:HD2	2.01	0.41
1:C:161:TYR:CE2	1:C:249:GLY:HA2	2.56	0.41
1:C:275:ASP:OD1	1:E:50:LYS:HE3	2.20	0.41
2:F:55:VAL:HG12	2:F:55:VAL:O	2.21	0.41
1:G:161:TYR:CE2	1:G:249:GLY:HA2	2.55	0.41
2:B:47:GLN:HG2	1:G:30:THR:HB	2.03	0.41
1:C:185:PRO:O	1:C:217:ILE:HA	2.22	0.40
1:E:25:MET:HE3	1:E:33:GLN:HB3	2.03	0.40
1:E:182:VAL:HG21	1:E:213:ILE:HG21	2.04	0.40
1:E:161:TYR:CE2	1:E:249:GLY:HA2	2.57	0.40
1:A:156:LYS:HD3	1:A:196:ILE:HD11	2.03	0.40
1:C:182:VAL:HG21	1:C:213:ILE:HG21	2.04	0.40
1:E:156:LYS:HD3	1:E:196:ILE:HD11	2.03	0.40
1:G:9:ASN:O	2:H:169:ASN:ND2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ASP:OD1	2:F:54:ARG:NH1[2_455]	2.18	0.02

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	315/334 (94%)	286 (91%)	29 (9%)	0	100	100
1	C	315/334 (94%)	284 (90%)	31 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	315/334 (94%)	285 (90%)	30 (10%)	0	100 100
1	G	315/334 (94%)	285 (90%)	28 (9%)	2 (1%)	25 62
2	B	170/182 (93%)	150 (88%)	13 (8%)	7 (4%)	3 15
2	D	170/182 (93%)	150 (88%)	13 (8%)	7 (4%)	3 15
2	F	170/182 (93%)	150 (88%)	13 (8%)	7 (4%)	3 15
2	H	170/182 (93%)	150 (88%)	13 (8%)	7 (4%)	3 15
All	All	1940/2064 (94%)	1740 (90%)	170 (9%)	30 (2%)	10 40

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	MET
2	D	17	MET
2	F	17	MET
2	H	17	MET
2	B	59	THR
2	B	170	ARG
2	D	59	THR
2	D	170	ARG
2	F	59	THR
2	F	170	ARG
2	H	59	THR
2	H	170	ARG
2	B	58	LYS
2	D	58	LYS
2	F	58	LYS
2	H	58	LYS
2	B	127	ARG
2	D	127	ARG
2	F	127	ARG
1	G	81	ASN
2	H	127	ARG
1	G	215	PRO
2	B	161	ILE
2	D	161	ILE
2	F	18	VAL
2	F	161	ILE
2	H	161	ILE
2	B	18	VAL
2	D	18	VAL

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Mol	Chain	Res	Type
2	H	18	VAL

5.3.2 Protein sidechains (i)

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	276/290 (95%)	264 (96%)	12 (4%)	29	64
1	C	276/290 (95%)	263 (95%)	13 (5%)	26	61
1	E	276/290 (95%)	264 (96%)	12 (4%)	29	64
1	G	276/290 (95%)	263 (95%)	13 (5%)	26	61
2	B	147/155 (95%)	142 (97%)	5 (3%)	37	72
2	D	147/155 (95%)	142 (97%)	5 (3%)	37	72
2	F	147/155 (95%)	142 (97%)	5 (3%)	37	72
2	H	147/155 (95%)	142 (97%)	5 (3%)	37	72
All	All	1692/1780 (95%)	1622 (96%)	70 (4%)	30	66

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	18	HIS
1	A	31	ASP
1	A	32	ASP
1	A	50	LYS
1	A	89	GLU
1	A	149	SER
1	A	156	LYS
1	A	167	THR
1	A	208	ARG
1	A	210	GLN
1	A	265	SER
2	B	12	ASN
2	B	38	LEU

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Mol	Chain	Res	Type
2	B	41	THR
2	B	60	ASN
2	B	125	GLN
1	C	12	THR
1	C	18	HIS
1	C	31	ASP
1	C	32	ASP
1	C	50	LYS
1	C	89	GLU
1	C	149	SER
1	C	155	THR
1	C	156	LYS
1	C	167	THR
1	C	208	ARG
1	C	210	GLN
1	C	265	SER
2	D	12	ASN
2	D	38	LEU
2	D	41	THR
2	D	60	ASN
2	D	125	GLN
1	E	12	THR
1	E	18	HIS
1	E	31	ASP
1	E	32	ASP
1	E	50	LYS
1	E	89	GLU
1	E	149	SER
1	E	156	LYS
1	E	167	THR
1	E	208	ARG
1	E	210	GLN
1	E	265	SER
2	F	12	ASN
2	F	38	LEU
2	F	41	THR
2	F	60	ASN
2	F	125	GLN
1	G	12	THR
1	G	18	HIS
1	G	31	ASP
1	G	32	ASP

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Mol	Chain	Res	Type
1	G	50	LYS
1	G	89	GLU
1	G	149	SER
1	G	155	THR
1	G	156	LYS
1	G	167	THR
1	G	208	ARG
1	G	210	GLN
1	G	265	SER
2	H	12	ASN
2	H	38	LEU
2	H	41	THR
2	H	60	ASN
2	H	125	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	197	GLN
1	A	216	ASN
2	B	60	ASN
2	B	116	ASN
1	C	8	ASN
1	C	75	HIS
1	C	197	GLN
1	C	216	ASN
2	D	60	ASN
2	D	116	ASN
1	E	8	ASN
1	E	75	HIS
1	E	197	GLN
1	E	216	ASN
2	F	60	ASN
2	F	116	ASN
1	G	8	ASN
1	G	75	HIS
1	G	197	GLN
1	G	216	ASN
2	H	60	ASN
2	H	116	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	317/334 (94%)	0.04	6 (1%)	66	37	57, 84, 132, 199	0
1	C	317/334 (94%)	0.06	8 (2%)	57	28	57, 84, 132, 197	0
1	E	317/334 (94%)	0.05	4 (1%)	77	51	59, 86, 132, 189	0
1	G	317/334 (94%)	0.07	7 (2%)	62	32	59, 85, 135, 199	0
2	B	172/182 (94%)	0.47	19 (11%)	5	2	61, 135, 185, 202	0
2	D	172/182 (94%)	0.56	22 (12%)	3	1	59, 137, 186, 212	0
2	F	172/182 (94%)	0.51	19 (11%)	5	2	57, 137, 184, 203	0
2	H	172/182 (94%)	0.56	23 (13%)	3	1	55, 136, 191, 208	0
All	All	1956/2064 (94%)	0.22	108 (5%)	25	8	55, 92, 173, 212	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	15	LEU	6.9
2	B	138	PHE	6.8
2	H	138	PHE	6.7
2	D	136	GLY	6.6
2	D	138	PHE	5.9
1	E	15	LEU	5.8
1	G	13	LEU	5.8
2	B	126	LEU	5.7
2	H	23	GLY	5.7
2	F	126	LEU	5.6
2	F	24	PHE	5.5
1	C	16	GLY	5.5
1	C	15	LEU	5.3
2	H	24	PHE	5.3
1	A	15	LEU	5.2
1	G	16	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	138	PHE	4.9
2	H	146	ASN	4.7
2	D	23	GLY	4.7
1	E	8	ASN	4.6
2	B	24	PHE	4.6
2	F	23	GLY	4.6
2	D	146	ASN	4.5
2	H	33	GLY	4.5
2	H	143	LYS	4.5
2	H	149	ILE	4.4
2	D	32	THR	4.3
2	H	126	LEU	4.3
1	A	11	ALA	4.3
2	B	140	ILE	4.2
1	E	13	LEU	4.2
2	D	126	LEU	4.2
1	E	16	GLY	4.2
2	D	140	ILE	4.0
2	B	149	ILE	3.9
2	B	146	ASN	3.9
1	C	13	LEU	3.9
2	F	146	ASN	3.8
2	D	118	LEU	3.8
2	D	149	ILE	3.8
2	B	143	LYS	3.7
2	D	24	PHE	3.7
2	H	118	LEU	3.6
1	C	8	ASN	3.6
2	F	140	ILE	3.6
2	B	32	THR	3.5
1	A	12	THR	3.4
2	H	140	ILE	3.4
2	H	22	TYR	3.4
2	D	22	TYR	3.3
2	B	23	GLY	3.3
2	H	32	THR	3.2
1	A	13	LEU	3.1
1	G	12	THR	3.1
2	F	149	ILE	3.0
2	F	11	GLU	3.0
1	A	8	ASN	3.0
2	D	115	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	171	PHE	3.0
2	D	33	GLY	2.9
2	F	114	GLU	2.9
2	H	136	GLY	2.9
2	D	122	THR	2.9
2	F	33	GLY	2.9
2	B	33	GLY	2.8
2	B	136	GLY	2.8
1	A	319	GLY	2.8
2	D	21	TRP	2.7
1	G	11	ALA	2.7
1	C	11	ALA	2.7
2	H	114	GLU	2.7
1	G	8	ASN	2.7
2	F	32	THR	2.6
2	H	115	MET	2.6
2	H	158	ASP	2.6
2	F	118	LEU	2.6
2	D	139	LYS	2.6
2	F	136	GLY	2.6
2	H	144	CYS	2.6
2	D	114	GLU	2.5
2	B	118	LEU	2.5
2	H	21	TRP	2.5
2	D	31	GLY	2.5
2	B	139	LYS	2.5
2	B	132	ASP	2.5
2	B	148	CYS	2.5
2	B	161	ILE	2.4
2	D	162	TYR	2.4
1	C	270	SER	2.4
2	F	115	MET	2.3
2	F	129	ASN	2.3
1	C	194	LEU	2.3
2	H	171	PHE	2.3
2	H	162	TYR	2.3
1	C	12	THR	2.3
2	F	7	ALA	2.2
2	B	115	MET	2.2
2	D	133	MET	2.2
2	F	125	GLN	2.2
2	D	143	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	27	GLN	2.2
2	H	27	GLN	2.2
2	H	122	THR	2.2
2	B	27	GLN	2.1
2	B	125	GLN	2.1
2	F	22	TYR	2.0
1	G	194	LEU	2.0
2	H	153	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.