



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:43 AM BST

PDB ID : 3QQO
Title : Crystal structure of HA2 R106H mutant of H2 hemagglutinin, acidic pH form
Authors : Xu, R.; Wilson, I.A.
Deposited on : 2011-02-15
Resolution : 2.90 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

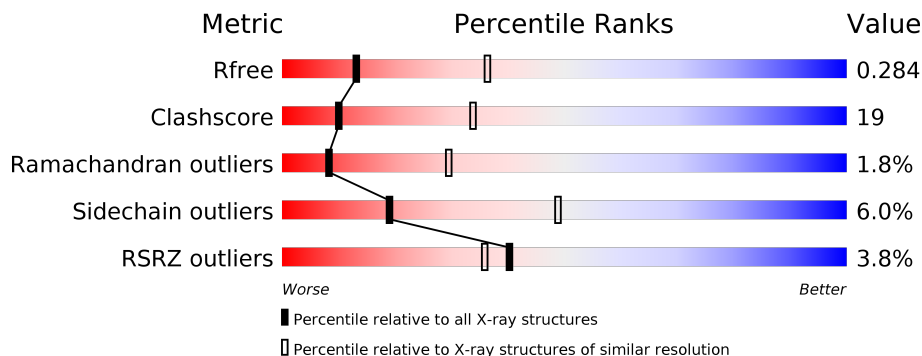
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	0% (Poor fit) 61% (0 outliers), 36% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
1	C	327	2% (Poor fit) 55% (0 outliers), 40% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
1	E	327	6% (Poor fit) 55% (0 outliers), 40% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
2	B	174	6% (Poor fit) 70% (0 outliers), 27% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
2	D	174	3% (Poor fit) 66% (0 outliers), 28% (1 outlier), 6% (2 outliers), 0% (3+ outliers)
2	F	174	6% (Poor fit) 59% (0 outliers), 34% (1 outlier), 6% (2 outliers), 0% (3+ outliers)

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11864 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
			Total	C	N	O	S			
1	A	322	2520	1584	437	484	15	0	1	0
1	C	322	2520	1584	437	484	15	0	1	0
1	E	322	2520	1584	437	484	15	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP C7S226
C	9	PRO	-	expression tag	UNP C7S226
E	9	PRO	-	expression tag	UNP C7S226

- Molecule 2 is a protein called Hemagglutinin.

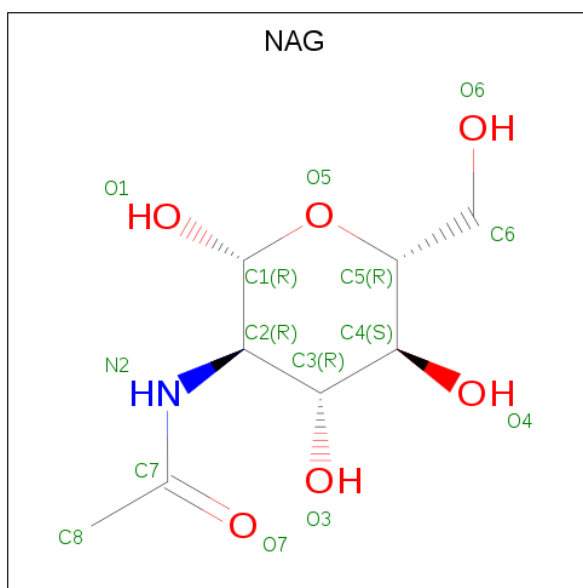
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1402	876	238	279	9	0	1	0
2	D	172	1402	876	238	279	9	0	1	0
2	F	172	1402	876	238	279	9	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	HIS	ARG	engineered mutation	UNP C7S226
D	106	HIS	ARG	engineered mutation	UNP C7S226
F	106	HIS	ARG	engineered mutation	UNP C7S226

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



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	C	1	Total	C	N	O	0	0
			14	8	1	5		

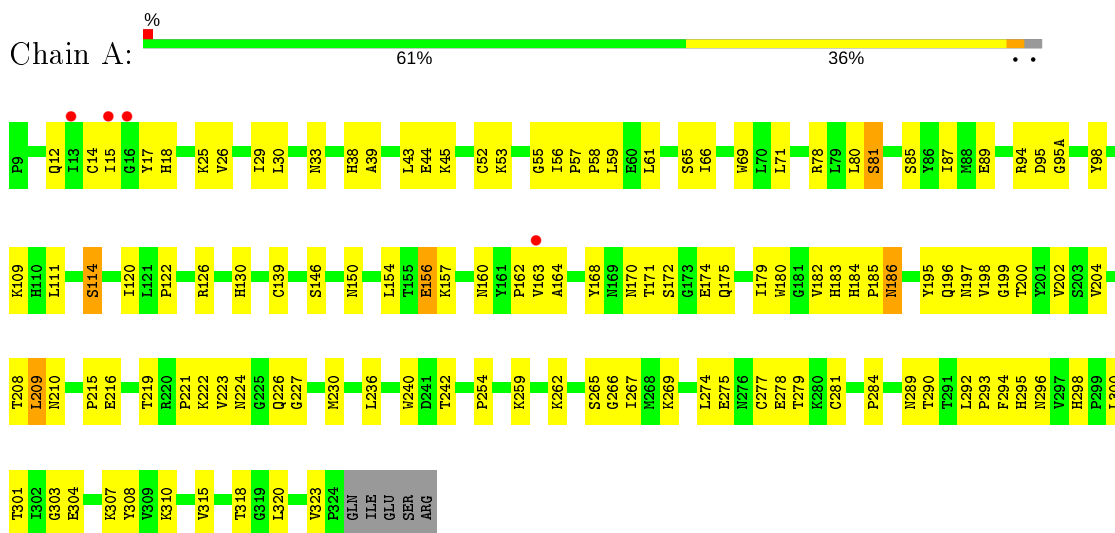
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	3	Total	O	0	0
			3	3		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		
4	E	4	Total	O	0	0
			4	4		
4	F	5	Total	O	0	0
			5	5		

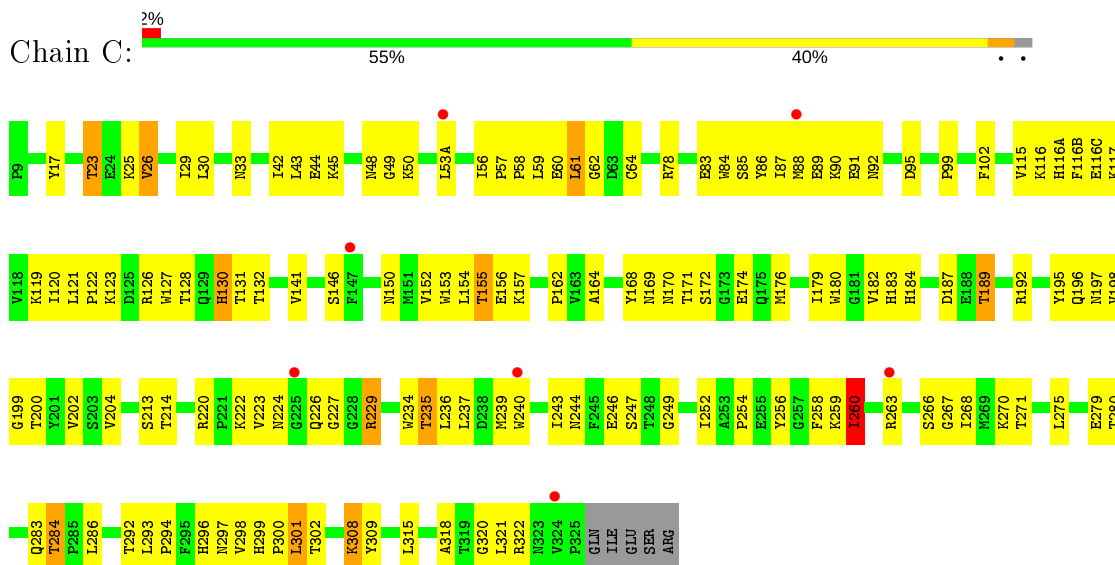
3 Residue-property plots [i](#)

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

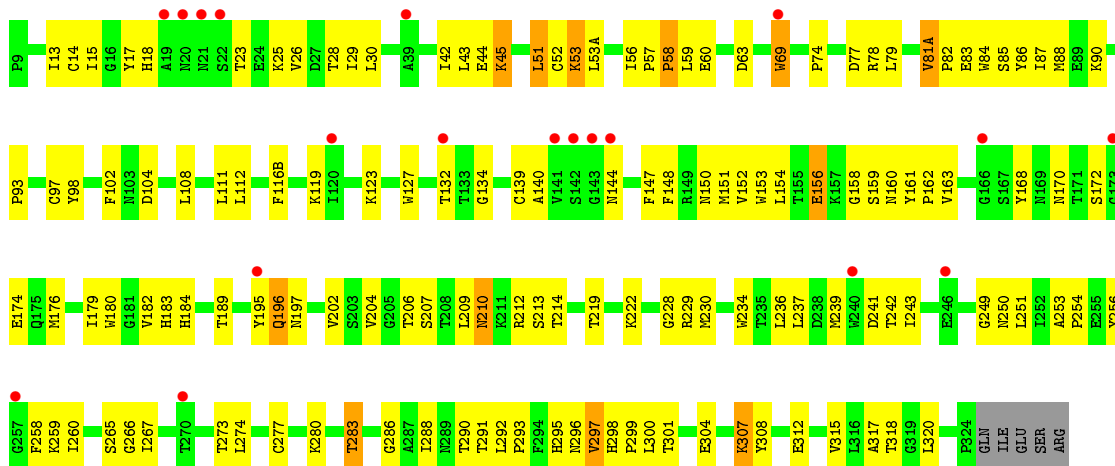


- Molecule 1: Hemagglutinin

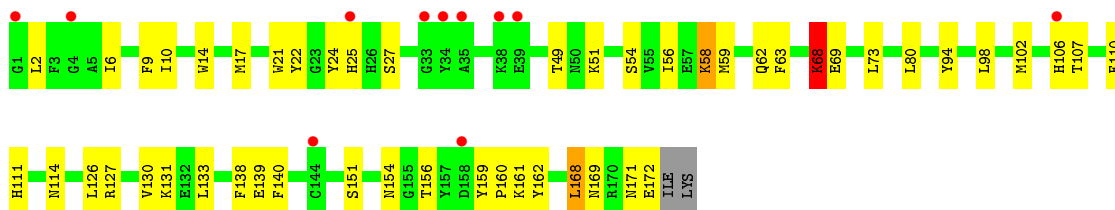


- Molecule 1: Hemagglutinin

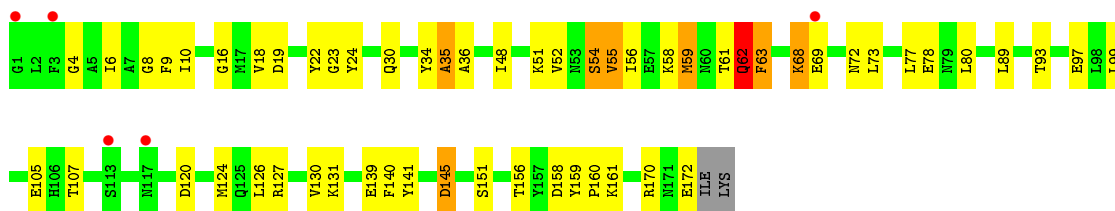




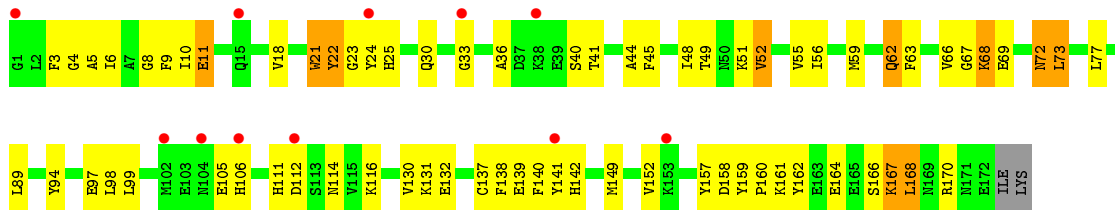
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.00Å 240.12Å 70.33Å 90.00° 116.52° 90.00°	Depositor
Resolution (Å)	43.44 – 2.90 43.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.1 (43.44-2.90) 88.0 (43.44-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.222 , 0.290 0.217 , 0.284	Depositor DCC
R_{free} test set	1994 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.030 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11864	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/2583	0.49	0/3506
1	C	0.28	0/2583	0.48	0/3506
1	E	0.26	0/2583	0.46	0/3506
2	B	0.26	0/1435	0.40	0/1928
2	D	0.28	0/1435	0.43	0/1928
2	F	0.27	0/1435	0.42	0/1928
All	All	0.28	0/12054	0.46	0/16302

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 [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	2520	0	2470	97	0
1	C	2520	0	2471	123	0
1	E	2520	0	2472	125	0
2	B	1402	0	1300	43	0
2	D	1402	0	1300	50	0
2	F	1402	0	1300	61	0
3	A	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	13	0	0
4	A	28	0	0	1	0
4	B	3	0	0	1	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
4	E	4	0	0	0	0
4	F	5	0	0	0	0
All	All	11864	0	11352	440	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 19.

All (440) 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:E:148:PHE:HB2	1:E:151:MET:HB2	1.47	0.94
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.32	0.93
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.51	0.91
1:E:56:ILE:HD12	1:E:57:PRO:HD2	1.50	0.91
1:C:229:ARG:HH11	1:C:229:ARG:CG	1.85	0.88
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.52	0.88
1:A:172:SER:HB2	1:A:259:LYS:HD3	1.55	0.86
1:E:298:HIS:HE1	1:E:300:LEU:HD12	1.41	0.85
1:E:26:VAL:HG21	1:E:317:ALA:HB2	1.61	0.81
1:A:18:HIS:HB2	2:B:21:TRP:HA	1.65	0.79
1:C:59:LEU:HD22	1:C:61:LEU:HD23	1.66	0.77
1:A:198:VAL:HG12	1:A:199:GLY:H	1.50	0.76
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.01	0.76
2:F:152:VAL:HG22	2:F:157:TYR:HD1	1.51	0.76
1:C:56:ILE:HD12	1:C:57:PRO:HD2	1.67	0.75
1:A:56:ILE:HD12	1:A:57:PRO:HD2	1.69	0.75
1:C:116:LYS:HD2	1:C:263:ARG:HE	1.52	0.74
1:A:122:PRO:O	1:A:126:ARG:HG2	1.87	0.74
1:A:168:TYR:CE2	1:A:170:ASN:HA	2.25	0.71
1:A:87:ILE:HB	1:A:267:ILE:HG13	1.72	0.71
2:B:68:LYS:O	2:B:69:GLU:HB2	1.90	0.71
1:E:17:TYR:CE2	2:F:6:ILE:HA	2.26	0.70
1:E:119:LYS:HA	1:E:256:TYR:HA	1.70	0.70
1:A:14:CYS:HB2	2:B:25:HIS:HB3	1.72	0.70
1:C:122:PRO:HB2	1:C:126:ARG:HG2	1.73	0.69
2:B:69:GLU:HA	4:B:175:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:MET:HG2	2:F:94:TYR:CE1	2.28	0.69
1:C:229:ARG:NH1	1:C:229:ARG:HG3	2.05	0.69
1:A:78:ARG:HA	1:A:78:ARG:NE	2.08	0.68
2:B:127:ARG:HH12	2:F:131:LYS:NZ	1.90	0.68
1:A:186:ASN:ND2	1:A:219:THR:HA	2.09	0.68
1:A:56:ILE:HG23	1:A:85:SER:HB3	1.76	0.68
1:A:59:LEU:HD21	1:A:61:LEU:HD21	1.75	0.68
1:E:307:LYS:HE3	2:F:59:MET:HE1	1.75	0.67
1:E:78:ARG:NE	1:E:78:ARG:HA	2.08	0.67
1:C:220:ARG:HD2	1:C:227:GLY:O	1.93	0.67
1:A:29:ILE:HG22	1:A:30:LEU:HD12	1.77	0.67
1:C:180:TRP:CZ3	1:C:235:THR:HG22	2.30	0.67
1:E:127:TRP:CD1	1:E:154:LEU:HD11	2.30	0.67
1:E:170:ASN:HD22	1:E:239:MET:HA	1.59	0.66
1:C:56:ILE:HG12	1:C:83:GLU:HG2	1.78	0.66
1:E:293:PRO:HG3	2:F:56:ILE:HA	1.78	0.66
1:E:170:ASN:ND2	1:E:239:MET:HA	2.10	0.65
2:F:152:VAL:HG22	2:F:157:TYR:CD1	2.29	0.65
1:C:182:VAL:HG12	1:C:202:VAL:HG21	1.79	0.65
1:C:180:TRP:HZ3	1:C:235:THR:HG22	1.62	0.64
2:D:141:TYR:CE2	2:D:170:ARG:HG3	2.32	0.64
1:E:18:HIS:HB2	2:F:21:TRP:O	1.97	0.64
1:C:59:LEU:CD2	1:C:61:LEU:HD23	2.27	0.64
2:D:51:LYS:O	2:D:55:VAL:HG12	1.97	0.64
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.79	0.64
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.32	0.63
1:C:91:GLU:HG3	1:C:92:ASN:OD1	1.98	0.63
2:D:93:THR:O	2:D:97:GLU:HG2	1.98	0.63
1:E:172:SER:HB2	1:E:259:LYS:HD3	1.79	0.63
1:C:168:TYR:CE2	1:C:170:ASN:HA	2.33	0.62
1:C:182:VAL:HG23	1:C:184:HIS:HE2	1.63	0.62
1:A:111:LEU:HD12	1:A:262:LYS:HD3	1.82	0.62
2:D:130:VAL:HG12	2:D:140:PHE:HA	1.81	0.62
1:C:237:LEU:HD22	1:C:243:ILE:HB	1.83	0.61
1:C:275:LEU:C	1:C:275:LEU:HD23	2.20	0.61
1:C:294:PRO:HD3	2:D:56:ILE:HG12	1.82	0.61
1:A:12:GLN:NE2	2:B:133:LEU:HD11	2.15	0.61
1:A:98:TYR:CD2	1:A:230:MET:HG3	2.36	0.61
1:E:28:THR:HB	2:F:105:GLU:OE2	2.00	0.61
1:C:120:ILE:HG22	1:C:168:TYR:CE1	2.36	0.61
1:E:51:LEU:HD23	1:E:51:LEU:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ILE:HD11	1:E:112:LEU:O	2.00	0.61
1:C:59:LEU:HD22	1:C:61:LEU:CD2	2.31	0.61
1:A:120:ILE:HG22	1:A:168:TYR:CE1	2.36	0.61
1:A:284:PRO:HD3	1:A:300:LEU:O	2.00	0.61
2:F:68:LYS:O	2:F:69:GLU:HB2	2.00	0.61
1:C:26:VAL:HG11	1:C:318:ALA:HB2	1.82	0.60
1:C:182:VAL:HG23	1:C:184:HIS:NE2	2.17	0.60
1:A:195:TYR:O	1:A:196:GLN:HB2	2.02	0.60
1:E:209:LEU:HD12	1:E:210:ASN:H	1.64	0.60
1:A:274:LEU:HD23	1:A:275:GLU:O	2.02	0.60
1:A:52:CYS:HB3	1:A:277:CYS:O	2.01	0.60
1:E:78:ARG:HE	1:E:78:ARG:HA	1.67	0.60
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.37	0.59
2:B:2:LEU:HG	2:B:2:LEU:O	2.02	0.59
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.37	0.59
1:E:168:TYR:O	1:E:242:THR:HA	2.01	0.59
1:E:156:GLU:HG3	1:E:196:GLN:HG3	1.85	0.59
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.38	0.59
1:E:180:TRP:CH2	1:E:209:LEU:HD21	2.37	0.59
1:A:61:LEU:HD11	1:A:66:ILE:HD13	1.85	0.58
1:A:307:LYS:HG2	2:B:59:MET:HE1	1.85	0.58
1:C:171:THR:HA	1:C:240:TRP:CZ3	2.38	0.58
1:A:29:ILE:HG21	2:D:51:LYS:HE2	1.84	0.58
1:E:298:HIS:CE1	1:E:300:LEU:HD12	2.31	0.58
1:E:59:LEU:HD22	1:E:84:TRP:CE3	2.39	0.58
1:A:168:TYR:HE2	1:A:170:ASN:HA	1.69	0.58
1:E:59:LEU:HD22	1:E:84:TRP:CD2	2.38	0.58
1:C:29:ILE:HG21	2:F:51:LYS:HE2	1.86	0.58
1:E:74:PRO:HA	1:E:77:ASP:OD1	2.04	0.58
1:C:229:ARG:NH2	1:E:207:SER:HA	2.19	0.57
1:E:249:GLY:O	1:E:250:ASN:HB2	2.03	0.57
1:C:123:LYS:O	1:C:132:THR:HG21	2.04	0.57
1:C:299:HIS:ND1	1:C:300:PRO:HD2	2.19	0.57
1:E:295:HIS:CE1	1:E:308:TYR:HD1	2.22	0.57
1:A:53:LYS:HD2	1:A:55:GLY:O	2.05	0.57
1:C:58:PRO:HD2	1:C:275:LEU:CD1	2.34	0.57
1:E:228:GLY:O	1:E:229:ARG:HG3	2.05	0.57
1:C:294:PRO:HG3	2:D:56:ILE:HA	1.87	0.57
2:D:54:SER:O	2:D:58:LYS:HB2	2.05	0.57
1:C:229:ARG:NH1	1:C:229:ARG:CG	2.56	0.56
1:A:293:PRO:HB2	1:A:294:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:O	1:E:292:LEU:HB3	2.05	0.56
1:C:172:SER:HB2	1:C:259:LYS:HD3	1.85	0.56
2:B:51:LYS:HE2	1:E:29:ILE:HG21	1.86	0.56
1:E:229:ARG:CG	1:E:229:ARG:HH11	2.19	0.56
1:E:280:LYS:HG2	1:E:304:GLU:OE2	2.05	0.56
1:C:59:LEU:HD23	1:C:60:GLU:N	2.21	0.56
1:A:39:ALA:HA	1:A:318:THR:HG23	1.88	0.56
1:C:49:GLY:HA2	1:C:286:LEU:O	2.05	0.56
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.40	0.56
1:C:220:ARG:HD3	1:C:229:ARG:NE	2.20	0.55
1:A:265:SER:OG	1:A:266:GLY:N	2.38	0.55
1:A:278:GLU:HG3	1:A:279:THR:N	2.21	0.55
1:A:310:LYS:HD3	1:A:310:LYS:O	2.06	0.55
1:C:123:LYS:HE2	1:C:132:THR:O	2.04	0.55
1:E:170:ASN:HB2	1:E:237:LEU:HD23	1.88	0.55
1:A:53:LYS:HG2	1:A:57:PRO:HB3	1.89	0.55
1:C:222:LYS:N	1:C:222:LYS:HD2	2.21	0.55
1:A:198:VAL:HG12	1:A:199:GLY:N	2.18	0.54
1:A:58:PRO:HD2	1:A:274:LEU:HD12	1.88	0.54
1:C:182:VAL:CG2	1:C:184:HIS:HE2	2.19	0.54
2:F:25:HIS:HA	2:F:33:GLY:O	2.08	0.54
1:C:123:LYS:HG3	1:C:152:VAL:HG13	1.89	0.54
1:E:13:ILE:HG23	1:E:13:ILE:O	2.07	0.54
1:E:182:VAL:HG11	1:E:213:SER:HB2	1.88	0.54
1:C:164:ALA:O	1:C:246:GLU:HA	2.08	0.54
1:E:182:VAL:HG12	1:E:202:VAL:HG21	1.89	0.54
1:C:220:ARG:HD3	1:C:229:ARG:CD	2.37	0.54
1:A:130:HIS:CE1	1:A:164:ALA:HB2	2.43	0.53
2:D:120:ASP:O	2:D:124:MET:HG3	2.08	0.53
1:E:58:PRO:HD2	1:E:274:LEU:HD12	1.89	0.53
1:E:293:PRO:HB3	2:F:59:MET:HG3	1.90	0.53
1:E:127:TRP:HB2	1:E:132:THR:HG21	1.91	0.53
1:A:29:ILE:CG2	2:D:51:LYS:HE2	2.39	0.53
1:A:175:GLN:OE1	1:A:236:LEU:HD23	2.08	0.53
1:C:30:LEU:HD12	2:D:105:GLU:CD	2.30	0.52
1:A:186:ASN:OD1	1:A:227:GLY:HA3	2.09	0.52
2:B:98:LEU:HD23	2:D:99:LEU:HD11	1.92	0.52
1:A:320:LEU:HB3	2:B:111:HIS:CG	2.44	0.52
1:A:80:LEU:HD12	1:A:81:SER:H	1.73	0.52
1:C:42:ILE:HA	1:C:293:LEU:HD22	1.91	0.52
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:PRO:O	1:E:84:TRP:HB2	2.10	0.52
2:F:130:VAL:HG12	2:F:140:PHE:HA	1.91	0.52
1:C:223:VAL:HG21	1:E:207:SER:HB3	1.91	0.52
1:C:85:SER:O	1:C:86:TYR:HB3	2.08	0.52
1:C:87:ILE:HB	1:C:268:ILE:HG13	1.92	0.52
1:C:127:TRP:CD1	1:C:154:LEU:HD11	2.45	0.52
1:E:51:LEU:HD23	1:E:51:LEU:H	1.74	0.52
1:E:58:PRO:HD2	1:E:274:LEU:CD1	2.39	0.52
1:A:223:VAL:O	1:A:224:ASN:HB2	2.09	0.52
1:A:15:ILE:O	2:B:10:ILE:HD13	2.10	0.52
1:C:48:ASN:O	1:C:50:LYS:HG3	2.09	0.52
2:B:172:GLU:HA	2:B:172:GLU:OE2	2.10	0.52
1:A:293:PRO:HB3	2:B:59:MET:HG3	1.92	0.52
1:E:26:VAL:HG12	1:E:315:VAL:HG12	1.91	0.52
2:D:73:LEU:HD21	1:E:104:ASP:OD2	2.10	0.51
1:E:229:ARG:HH11	1:E:229:ARG:HG2	1.73	0.51
1:C:26:VAL:HG21	1:C:318:ALA:HB2	1.92	0.51
2:D:19:ASP:OD1	2:D:19:ASP:N	2.42	0.51
1:E:243:ILE:HG23	1:E:243:ILE:O	2.10	0.51
1:C:283:GLN:NE2	1:C:284:THR:O	2.42	0.51
2:D:16:GLY:HA3	2:D:34:TYR:CE2	2.45	0.51
1:A:224:ASN:O	1:A:226:GLN:HG2	2.11	0.51
1:E:274:LEU:HD23	1:E:274:LEU:C	2.30	0.51
2:F:23:GLY:CA	2:F:36:ALA:HA	2.34	0.51
1:E:108:LEU:HD13	1:E:234:TRP:CD2	2.46	0.51
1:E:172:SER:OG	1:E:259:LYS:HG2	2.10	0.51
1:A:98:TYR:CE2	1:A:230:MET:HG3	2.46	0.51
1:A:293:PRO:HG3	2:B:56:ILE:HA	1.92	0.51
1:C:309:TYR:HD2	2:D:89:LEU:HD13	1.76	0.51
2:D:16:GLY:O	2:D:18:VAL:HG13	2.11	0.51
2:D:30:GLN:HE22	2:D:145:ASP:HB2	1.76	0.51
1:E:58:PRO:CD	1:E:274:LEU:HD12	2.42	0.50
2:B:102:MET:O	2:B:106[B]:HIS:ND1	2.44	0.50
2:B:107:THR:O	2:B:110:PHE:HB3	2.10	0.50
1:C:183:HIS:HD2	1:C:184:HIS:N	2.09	0.50
1:C:220:ARG:HD3	1:C:229:ARG:HD2	1.92	0.50
1:A:182:VAL:HB	1:A:202:VAL:HG21	1.93	0.50
1:E:108:LEU:HD22	1:E:234:TRP:CD1	2.46	0.50
1:A:274:LEU:HD23	1:A:275:GLU:N	2.27	0.50
1:E:69:TRP:HD1	1:E:79:LEU:HD12	1.76	0.50
2:F:142:HIS:CD2	2:F:162:TYR:CD1	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:GLY:O	2:F:8:GLY:HA3	2.11	0.50
1:A:168:TYR:O	1:A:242:THR:HA	2.11	0.50
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.93	0.50
1:E:174:GLU:OE2	1:E:259:LYS:HB3	2.12	0.50
1:C:172:SER:HB2	1:C:259:LYS:CD	2.42	0.50
1:E:98:TYR:CD2	1:E:230:MET:HG3	2.47	0.49
1:E:45:LYS:HB3	1:E:296:ASN:OD1	2.12	0.49
1:E:320:LEU:HB3	2:F:111:HIS:CD2	2.47	0.49
1:A:284:PRO:HG2	1:A:298:HIS:CE1	2.47	0.49
1:E:56:ILE:HD11	1:E:83:GLU:O	2.12	0.49
2:F:22:TYR:HE2	2:F:40:SER:O	1.95	0.49
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.48	0.49
1:C:42:ILE:C	1:C:293:LEU:HD13	2.33	0.49
2:D:131:LYS:HB3	2:D:139:GLU:HB3	1.94	0.49
2:B:151:SER:HA	2:B:154:ASN:OD1	2.13	0.49
1:E:134:GLY:O	1:E:153:TRP:CE3	2.66	0.49
1:C:309:TYR:CD2	2:D:89:LEU:HD13	2.48	0.49
1:A:200:THR:OG1	1:A:215:PRO:HG2	2.12	0.48
1:C:182:VAL:HG23	1:C:184:HIS:CD2	2.48	0.48
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.47	0.48
1:C:89:GLU:O	1:C:270:LYS:HA	2.13	0.48
1:E:183:HIS:CD2	1:E:184:HIS:N	2.81	0.48
2:F:164:GLU:HA	2:F:167:LYS:HG2	1.95	0.48
1:A:66:ILE:HG13	1:A:109:LYS:HD2	1.95	0.48
1:C:266:SER:OG	1:C:267:GLY:N	2.45	0.48
1:A:184:HIS:HB3	1:A:216:GLU:O	2.13	0.48
1:C:174:GLU:HA	1:C:239:MET:SD	2.53	0.48
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.49	0.48
2:F:48:ILE:O	2:F:52:VAL:HG13	2.13	0.48
1:C:42:ILE:O	1:C:293:LEU:HB3	2.13	0.48
1:C:43:LEU:HB2	1:C:315:LEU:HB2	1.95	0.48
1:E:168:TYR:CE2	1:E:170:ASN:HA	2.48	0.48
1:A:95(A):GLY:HA3	4:A:348:HOH:O	2.12	0.48
2:D:63:PHE:C	2:D:63:PHE:CD2	2.87	0.48
1:C:127:TRP:HB2	1:C:132:THR:HG21	1.96	0.48
1:A:25:LYS:HD3	1:A:33:ASN:OD1	2.13	0.48
2:D:30:GLN:HE21	2:D:145:ASP:HB2	1.75	0.48
1:C:308:LYS:HD3	2:D:59:MET:HE1	1.96	0.48
1:A:26:VAL:HG12	1:A:315:VAL:HG12	1.96	0.48
2:D:158:ASP:O	2:D:161:LYS:HB3	2.13	0.48
1:C:45:LYS:HB3	1:C:297:ASN:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:THR:HG21	1:C:249:GLY:HA3	1.94	0.47
1:A:44:GLU:HG2	1:A:290:THR:HG21	1.96	0.47
1:A:78:ARG:NE	1:A:78:ARG:CA	2.75	0.47
1:E:14:CYS:HA	2:F:137:CYS:HA	1.97	0.47
1:E:116(B):PHE:HD1	1:E:260:ILE:HG13	1.79	0.47
1:E:318:THR:HB	2:F:48:ILE:HG21	1.95	0.47
1:C:59:LEU:HD12	1:C:84:TRP:CZ2	2.50	0.47
1:C:179:ILE:O	1:C:254:PRO:HG3	2.15	0.47
1:C:23:THR:O	1:C:25:LYS:HG3	2.15	0.47
1:C:116(A):HIS:CD2	1:C:116(B):PHE:H	2.33	0.47
1:C:195:TYR:O	1:C:196:GLN:HB2	2.14	0.47
1:E:29:ILE:HG22	1:E:30:LEU:HD12	1.97	0.47
2:F:44:ALA:HB2	2:F:114:ASN:HD22	1.79	0.47
1:C:119:LYS:HA	1:C:256:TYR:CD1	2.49	0.47
1:C:64:CYS:SG	1:C:95:ASP:HB2	2.55	0.47
2:D:68:LYS:O	2:D:69:GLU:HB2	2.14	0.46
1:A:59:LEU:CD2	1:A:61:LEU:HD21	2.44	0.46
1:E:237:LEU:HD11	1:E:241:ASP:HB3	1.97	0.46
1:E:267:ILE:N	1:E:267:ILE:HD12	2.30	0.46
1:C:184:HIS:HB3	1:C:220:ARG:NH2	2.30	0.46
2:F:66:VAL:HG12	2:F:67:GLY:N	2.30	0.46
1:A:186:ASN:C	1:A:186:ASN:HD22	2.18	0.46
2:B:14:TRP:HE3	2:B:17:MET:HE2	1.80	0.46
1:C:234:TRP:HZ3	1:C:236:LEU:HD13	1.79	0.46
1:E:195:TYR:O	1:E:197:ASN:N	2.49	0.46
2:F:6:ILE:N	2:F:112:ASP:OD1	2.48	0.46
2:F:167:LYS:HA	2:F:170:ARG:NH1	2.30	0.46
1:A:71:LEU:O	1:A:150:ASN:HB2	2.15	0.46
1:C:182:VAL:HG11	1:C:213:SER:HB2	1.98	0.46
1:C:153:TRP:HZ2	1:C:183:HIS:ND1	2.13	0.46
1:E:150:ASN:ND2	1:E:256:TYR:CD2	2.84	0.46
2:B:58:LYS:HG2	2:F:97:GLU:HB3	1.97	0.46
1:C:30:LEU:HD11	2:F:106[A]:HIS:CE1	2.51	0.46
2:D:77:LEU:O	2:D:78:GLU:C	2.53	0.46
1:E:206:THR:OG1	1:E:207:SER:N	2.48	0.46
2:F:158:ASP:OD2	2:F:161:LYS:HB2	2.15	0.46
1:C:117:LYS:HE3	1:C:117:LYS:HB2	1.74	0.46
1:E:44:GLU:N	1:E:292:LEU:HD12	2.31	0.46
1:E:58:PRO:HG3	1:E:86:TYR:CE2	2.51	0.46
1:E:56:ILE:HG23	1:E:85:SER:HB3	1.98	0.46
2:B:22:TYR:CE2	2:B:114:ASN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:O	1:C:121:LEU:HD23	2.15	0.45
1:C:153:TRP:HZ2	1:C:183:HIS:CE1	2.33	0.45
2:F:158:ASP:HB3	2:F:161:LYS:HE2	1.98	0.45
2:F:44:ALA:HB2	2:F:114:ASN:ND2	2.32	0.45
1:C:279:GLU:CG	1:C:280:THR:N	2.78	0.45
1:E:265:SER:OG	1:E:266:GLY:N	2.50	0.45
1:A:58:PRO:HD2	1:A:274:LEU:CD1	2.45	0.45
1:A:303:GLY:HA2	2:B:63:PHE:CD1	2.51	0.45
1:C:127:TRP:HB2	1:C:132:THR:CG2	2.46	0.45
1:C:183:HIS:CD2	1:C:184:HIS:N	2.85	0.45
1:C:78:ARG:HG3	1:C:78:ARG:O	2.15	0.45
1:C:153:TRP:CZ2	1:C:183:HIS:ND1	2.82	0.45
1:E:60:GLU:OE2	1:E:273:THR:HG22	2.16	0.45
1:A:293:PRO:HB2	1:A:294:PHE:CE2	2.51	0.45
2:B:68:LYS:HA	2:B:68:LYS:HD2	1.70	0.45
2:D:9:PHE:CD1	2:D:9:PHE:C	2.89	0.45
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.52	0.45
1:A:89:GLU:O	1:A:269:LYS:HA	2.16	0.45
1:C:141:VAL:HG23	1:C:146:SER:HB3	1.98	0.45
1:C:279:GLU:HG3	1:C:280:THR:N	2.32	0.45
1:C:62:GLY:O	1:C:90:LYS:HG3	2.17	0.45
1:E:18:HIS:N	2:F:21:TRP:O	2.50	0.45
2:D:77:LEU:HD11	2:F:77:LEU:HD21	1.99	0.45
1:C:279:GLU:CD	1:C:280:THR:H	2.20	0.45
1:E:108:LEU:HB2	1:E:234:TRP:CE2	2.52	0.45
1:E:23:THR:O	1:E:25:LYS:HG3	2.17	0.45
1:E:63:ASP:HA	1:E:90:LYS:HD2	1.99	0.45
1:E:229:ARG:CG	1:E:229:ARG:NH1	2.76	0.45
1:E:308:TYR:O	2:F:89:LEU:HD12	2.16	0.45
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.98	0.44
1:E:15:ILE:CD1	2:F:24:TYR:HD1	2.30	0.44
1:E:237:LEU:CD1	1:E:241:ASP:HB3	2.47	0.44
1:E:51:LEU:HD12	1:E:88:MET:CE	2.48	0.44
1:E:58:PRO:HG3	1:E:86:TYR:CZ	2.53	0.44
2:F:73:LEU:HD12	2:F:73:LEU:HA	1.83	0.44
1:E:307:LYS:CE	2:F:59:MET:HE1	2.45	0.44
1:E:179:ILE:O	1:E:254:PRO:HB3	2.16	0.44
1:E:78:ARG:CA	1:E:78:ARG:NE	2.80	0.44
1:E:158:GLY:C	1:E:160:ASN:N	2.71	0.44
1:E:111:LEU:HD21	1:E:236:LEU:HD21	1.98	0.44
2:F:98:LEU:O	2:F:99:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.53	0.44
1:C:301:LEU:N	1:C:301:LEU:HD23	2.32	0.44
2:D:34:TYR:O	2:D:35:ALA:HB2	2.17	0.44
1:C:279:GLU:O	1:C:280:THR:HB	2.18	0.44
1:E:170:ASN:HD22	1:E:239:MET:CA	2.28	0.44
1:E:63:ASP:O	1:E:93:PRO:HB3	2.18	0.44
1:C:198:VAL:CG1	1:C:199:GLY:N	2.80	0.44
1:E:98:TYR:N	1:E:139:CYS:SG	2.91	0.44
1:A:56:ILE:CD1	1:A:57:PRO:HD2	2.44	0.44
2:B:130:VAL:HG12	2:B:140:PHE:HA	1.99	0.43
1:C:53(A):LEU:HB3	1:C:85:SER:OG	2.18	0.43
1:E:170:ASN:OD1	1:E:176:MET:HE3	2.18	0.43
2:F:132:GLU:HA	2:F:138:PHE:HD1	1.83	0.43
2:F:21:TRP:HZ3	2:F:45:PHE:CA	2.31	0.43
2:D:151:SER:HB2	2:D:156:THR:O	2.18	0.43
1:E:183:HIS:CD2	1:E:184:HIS:H	2.36	0.43
1:A:156:GLU:HG2	1:A:157:LYS:N	2.33	0.43
1:E:123:LYS:HE2	1:E:132:THR:O	2.18	0.43
2:D:126:LEU:O	2:D:127:ARG:HB2	2.19	0.43
2:B:94:TYR:CE1	2:D:59:MET:HG2	2.52	0.43
1:E:127:TRP:HD1	1:E:152:VAL:HG11	1.83	0.43
1:E:53(A):LEU:C	1:E:53(A):LEU:HD23	2.38	0.43
1:A:281:CYS:HB2	1:A:304:GLU:O	2.17	0.43
1:C:183:HIS:C	1:C:183:HIS:CD2	2.91	0.43
1:C:224:ASN:O	1:C:226:GLN:HG2	2.18	0.43
2:D:30:GLN:HE21	2:D:145:ASP:CB	2.31	0.43
1:C:294:PRO:HB3	2:D:59:MET:HG3	2.00	0.43
1:E:81(A):VAL:HA	1:E:82:PRO:HD3	1.79	0.43
2:F:10:ILE:O	2:F:11:GLU:C	2.57	0.43
1:A:274:LEU:HD23	1:A:274:LEU:C	2.39	0.43
2:D:131:LYS:HD3	2:D:139:GLU:OE1	2.18	0.43
1:A:45:LYS:HB3	1:A:296:ASN:OD1	2.18	0.43
1:E:288:ILE:HD11	1:E:297:VAL:HG21	2.01	0.43
1:A:12:GLN:HA	2:B:138:PHE:O	2.19	0.43
1:A:44:GLU:CA	1:A:292:LEU:HD12	2.49	0.43
1:C:17:TYR:CE2	2:D:6:ILE:HA	2.54	0.43
1:C:318:ALA:O	2:D:107:THR:HG21	2.19	0.43
1:C:17:TYR:CD2	2:D:6:ILE:HG12	2.53	0.43
1:E:78:ARG:CA	1:E:78:ARG:HE	2.30	0.43
2:B:127:ARG:HH12	2:F:131:LYS:HZ1	1.64	0.42
1:C:153:TRP:HZ2	1:C:183:HIS:HD1	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:PHE:O	2:D:63:PHE:HD2	2.02	0.42
1:E:283:THR:HG23	1:E:286:GLY:O	2.19	0.42
1:E:18:HIS:O	1:E:320:LEU:HD11	2.19	0.42
2:F:140:PHE:HD1	2:F:142:HIS:CE1	2.36	0.42
1:A:139:CYS:O	1:A:146:SER:HB3	2.19	0.42
1:A:80:LEU:HD12	1:A:81:SER:N	2.34	0.42
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.54	0.42
1:C:187:ASP:CG	1:C:189:THR:HG23	2.39	0.42
1:E:42:ILE:C	1:E:292:LEU:HD13	2.40	0.42
2:F:141:TYR:CB	2:F:166:SER:HB3	2.50	0.42
1:E:304:GLU:HG3	2:F:63:PHE:HB2	2.00	0.42
1:E:43:LEU:HD23	1:E:312:GLU:O	2.18	0.42
1:A:17:TYR:HE1	1:A:323:VAL:CG2	2.32	0.42
1:C:130:HIS:HB3	1:C:155:THR:O	2.19	0.42
1:C:321:LEU:HD13	2:D:6:ILE:HD13	2.02	0.42
2:F:159:TYR:HB3	2:F:160:PRO:HD3	2.02	0.42
1:A:183:HIS:O	1:A:185:PRO:HD3	2.19	0.42
1:A:296:ASN:HA	1:A:308:TYR:CE1	2.54	0.42
1:A:43:LEU:HD12	1:A:295:HIS:HA	2.02	0.42
2:B:126:LEU:O	2:B:127:ARG:HB2	2.19	0.42
2:B:127:ARG:HH12	2:F:131:LYS:HZ3	1.64	0.42
1:E:127:TRP:HB2	1:E:132:THR:CG2	2.49	0.42
1:A:179:ILE:O	1:A:254:PRO:HB3	2.19	0.42
1:A:44:GLU:N	1:A:292:LEU:HD12	2.35	0.42
1:C:176:MET:HA	1:C:258:PHE:O	2.20	0.42
1:C:99:PRO:O	1:C:229:ARG:HA	2.19	0.42
1:E:108:LEU:HD13	1:E:234:TRP:CE2	2.55	0.42
1:E:53:LYS:HD2	1:E:57:PRO:HD3	2.01	0.42
1:A:174:GLU:HG3	1:A:259:LYS:HB3	2.01	0.42
2:B:161:LYS:HD2	2:B:162:TYR:CE2	2.55	0.42
2:F:166:SER:C	2:F:168:LEU:N	2.73	0.42
2:B:151:SER:HB2	2:B:156:THR:O	2.20	0.41
2:D:61:THR:O	2:D:62:GLN:CB	2.68	0.41
1:E:298:HIS:HA	1:E:299:PRO:HD3	1.94	0.41
2:F:3:PHE:O	2:F:116:LYS:HD2	2.20	0.41
1:A:18:HIS:CB	2:B:21:TRP:HA	2.44	0.41
1:C:58:PRO:HD2	1:C:275:LEU:HD12	2.02	0.41
1:E:158:GLY:C	1:E:160:ASN:H	2.23	0.41
2:F:142:HIS:HB3	2:F:166:SER:OG	2.20	0.41
1:A:221:PRO:HD3	1:C:244:ASN:HD22	1.84	0.41
2:F:170:ARG:HB2	2:F:170:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ARG:HD3	1:C:196:GLN:O	2.21	0.41
1:C:229:ARG:HH21	1:E:207:SER:HA	1.83	0.41
1:E:290:THR:OG1	1:E:292:LEU:HG	2.20	0.41
2:F:149:MET:O	2:F:152:VAL:HB	2.21	0.41
1:A:94:ARG:HD2	1:A:95:ASP:OD2	2.20	0.41
1:C:127:TRP:CE2	1:C:154:LEU:HD21	2.56	0.41
2:B:106[B]:HIS:CD2	2:F:106[B]:HIS:HE2	2.37	0.41
2:D:172:GLU:OE2	2:D:172:GLU:HA	2.21	0.41
1:A:186:ASN:HD21	1:A:219:THR:HA	1.84	0.41
1:A:65:SER:O	1:A:66:ILE:C	2.59	0.41
2:D:4:GLY:O	2:D:8:GLY:HA3	2.21	0.41
1:E:127:TRP:CD1	1:E:152:VAL:HG11	2.56	0.41
1:A:114:SER:HB3	1:A:265:SER:HB3	2.03	0.41
2:B:131:LYS:HB2	2:B:139:GLU:HB3	2.02	0.41
1:C:202:VAL:HA	1:C:247:SER:HB2	2.01	0.41
1:E:140:ALA:HB1	1:E:144:ASN:O	2.20	0.41
2:F:131:LYS:HB3	2:F:139:GLU:HB3	2.03	0.41
2:F:159:TYR:N	2:F:160:PRO:CD	2.83	0.41
1:A:66:ILE:O	1:A:69:TRP:HB3	2.20	0.41
1:C:321:LEU:HD12	1:C:322:ARG:O	2.21	0.41
1:E:162:PRO:O	1:E:163:VAL:C	2.59	0.41
1:C:235:THR:OG1	1:C:236:LEU:N	2.53	0.41
2:D:48:ILE:CD1	2:D:107:THR:HG23	2.51	0.41
1:E:251:LEU:HD11	1:E:253:ALA:HA	2.03	0.41
1:A:171:THR:HA	1:A:240:TRP:CZ3	2.56	0.41
1:A:38:HIS:HB3	1:A:318:THR:OG1	2.21	0.41
1:C:44:GLU:N	1:C:293:LEU:HD12	2.36	0.41
2:F:72:ASN:OD1	2:F:72:ASN:N	2.53	0.41
2:B:73:LEU:HD12	2:B:73:LEU:HA	1.80	0.40
1:C:156:GLU:HG2	1:C:157:LYS:N	2.36	0.40
1:C:25:LYS:HD2	1:C:33:ASN:ND2	2.36	0.40
2:F:9:PHE:CD1	2:F:10:ILE:HG13	2.56	0.40
1:A:209:LEU:HG	1:A:210:ASN:N	2.35	0.40
1:A:242:THR:OG1	3:A:331:NAG:H82	2.21	0.40
1:A:14:CYS:O	2:B:24:TYR:HA	2.21	0.40
2:B:49:THR:HG22	2:B:49:THR:O	2.21	0.40
1:C:88:MET:HE3	1:C:271:THR:HG21	2.04	0.40
1:E:156:GLU:HG3	1:E:196:GLN:CG	2.49	0.40
1:E:52:CYS:HB3	1:E:277:CYS:C	2.41	0.40
1:C:308:LYS:N	1:C:308:LYS:HD3	2.37	0.40
1:A:160:ASN:O	1:A:162:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LYS:NZ	1:C:150:ASN:HD21	2.19	0.40
1:C:260:ILE:O	1:C:260:ILE:HG23	2.21	0.40
2:D:63:PHE:O	2:D:63:PHE:CD2	2.75	0.40
1:E:176:MET:HA	1:E:258:PHE:O	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	321/327 (98%)	283 (88%)	38 (12%)	0	100	100
1	C	321/327 (98%)	270 (84%)	45 (14%)	6 (2%)	8	28
1	E	321/327 (98%)	276 (86%)	39 (12%)	6 (2%)	8	28
2	B	171/174 (98%)	137 (80%)	30 (18%)	4 (2%)	6	23
2	D	171/174 (98%)	142 (83%)	24 (14%)	5 (3%)	4	18
2	F	171/174 (98%)	139 (81%)	27 (16%)	5 (3%)	4	18
All	All	1476/1503 (98%)	1247 (84%)	203 (14%)	26 (2%)	8	29

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	68	LYS
2	D	63	PHE
2	D	68	LYS
1	E	297	VAL
2	F	68	LYS
2	D	35	ALA
2	D	62	GLN
2	D	145	ASP

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Mol	Chain	Res	Type
1	E	58	PRO
1	E	210	ASN
2	B	62	GLN
2	B	168	LEU
1	C	301	LEU
1	E	53	LYS
1	E	159	SER
2	F	11	GLU
2	B	171	ASN
1	C	162	PRO
1	C	298	VAL
1	E	69	TRP
1	C	116(C)	GLU
2	F	5	ALA
2	F	62	GLN
1	C	260	ILE
1	C	320	GLY
2	F	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	284/288 (99%)	272 (96%)	12 (4%)	30	63
1	C	284/288 (99%)	263 (93%)	21 (7%)	13	38
1	E	284/288 (99%)	267 (94%)	17 (6%)	19	49
2	B	150/151 (99%)	143 (95%)	7 (5%)	26	59
2	D	150/151 (99%)	141 (94%)	9 (6%)	19	49
2	F	150/151 (99%)	138 (92%)	12 (8%)	12	33
All	All	1302/1317 (99%)	1224 (94%)	78 (6%)	19	49

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	114	SER
1	A	154	LEU
1	A	156	GLU
1	A	163	VAL
1	A	186	ASN
1	A	197	ASN
1	A	208	THR
1	A	209	LEU
1	A	222	LYS
1	A	289	ASN
1	A	301	THR
2	B	27	SER
2	B	54	SER
2	B	58	LYS
2	B	68	LYS
2	B	80	LEU
2	B	168	LEU
2	B	169	ASN
1	C	23	THR
1	C	26	VAL
1	C	61	LEU
1	C	102	PHE
1	C	115	VAL
1	C	128	THR
1	C	130	HIS
1	C	131	THR
1	C	155	THR
1	C	169	ASN
1	C	189	THR
1	C	197	ASN
1	C	214	THR
1	C	229	ARG
1	C	235	THR
1	C	260	ILE
1	C	284	THR
1	C	292	THR
1	C	296	HIS
1	C	302	THR
1	C	308	LYS
2	D	22	TYR
2	D	24	TYR
2	D	52	VAL

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Mol	Chain	Res	Type
2	D	54	SER
2	D	55	VAL
2	D	59	MET
2	D	62	GLN
2	D	72	ASN
2	D	80	LEU
1	E	45	LYS
1	E	51	LEU
1	E	81(A)	VAL
1	E	97	CYS
1	E	102	PHE
1	E	147	PHE
1	E	156	GLU
1	E	189	THR
1	E	196	GLN
1	E	212	ARG
1	E	214	THR
1	E	219	THR
1	E	222	LYS
1	E	283	THR
1	E	291	THR
1	E	301	THR
1	E	307	LYS
2	F	21	TRP
2	F	22	TYR
2	F	30	GLN
2	F	41	THR
2	F	49	THR
2	F	52	VAL
2	F	55	VAL
2	F	62	GLN
2	F	72	ASN
2	F	73	LEU
2	F	167	LYS
2	F	168	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	C	33	ASN
1	C	150	ASN

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Mol	Chain	Res	Type
1	C	169	ASN
1	C	244	ASN
2	D	26	HIS
2	D	30	GLN
1	E	18	HIS
1	E	210	ASN
1	E	250	ASN
1	E	298	HIS
2	F	114	ASN
2	F	142	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	331	1	14,14,15	0.40	0	17,19,21	1.43	2 (11%)
3	NAG	C	331	1	14,14,15	0.59	0	17,19,21	0.68	0
3	NAG	A	330	1	14,14,15	0.54	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	331	1	-	2/6/23/26	0/1/1/1
3	NAG	C	331	1	-	1/6/23/26	0/1/1/1
3	NAG	A	330	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	331	NAG	C1-O5-C5	4.14	117.81	112.19
3	A	331	NAG	C4-C3-C2	-2.96	106.69	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	330	NAG	C8-C7-N2-C2
3	A	330	NAG	O7-C7-N2-C2
3	A	331	NAG	C4-C5-C6-O6
3	A	331	NAG	O5-C5-C6-O6
3	C	331	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	331	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data 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, 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	322/327 (98%)	-0.26	4 (1%) 79 79	36, 64, 101, 168	0
1	C	322/327 (98%)	0.04	7 (2%) 62 59	45, 83, 135, 178	0
1	E	322/327 (98%)	0.18	19 (5%) 22 18	49, 101, 159, 201	0
2	B	172/174 (98%)	0.35	11 (6%) 19 15	37, 88, 157, 190	0
2	D	172/174 (98%)	-0.09	5 (2%) 51 47	42, 68, 106, 138	0
2	F	172/174 (98%)	0.37	11 (6%) 19 15	45, 91, 148, 210	0
All	All	1482/1503 (98%)	0.07	57 (3%) 40 36	36, 81, 140, 210	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	21	ASN	6.1
2	B	25	HIS	5.1
2	F	1	GLY	5.0
2	F	106[A]	HIS	4.6
1	E	142	SER	4.3
2	B	35	ALA	4.3
2	F	24	TYR	4.2
2	B	1	GLY	4.1
2	F	15	GLN	3.8
2	D	3	PHE	3.3
2	B	34	TYR	3.3
1	E	141	VAL	3.2
1	E	195	TYR	3.2
1	E	39	ALA	3.2
2	F	33	GLY	3.1
1	E	270	THR	3.1
1	E	257	GLY	3.1
1	E	20	ASN	3.1
2	B	144	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	225	GLY	3.0
1	A	15	ILE	3.0
1	E	173	GLY	3.0
1	E	143	GLY	2.9
2	D	113	SER	2.7
1	C	147	PHE	2.7
1	A	16	GLY	2.7
2	F	153	LYS	2.6
1	E	144	ASN	2.6
2	B	33	GLY	2.6
1	C	324	VAL	2.5
2	F	38	LYS	2.5
1	C	263	ARG	2.5
2	B	4	GLY	2.5
1	A	13	ILE	2.5
1	E	240	TRP	2.4
2	D	1	GLY	2.4
2	B	39	GLU	2.3
2	D	69	GLU	2.3
2	F	112	ASP	2.3
1	E	22	SER	2.3
2	B	106[A]	HIS	2.3
1	E	246	GLU	2.3
2	B	158	ASP	2.2
2	D	117	ASN	2.2
1	C	240	TRP	2.2
2	F	104	ASN	2.2
2	F	102	MET	2.2
1	E	166	GLY	2.2
1	C	53(A)	LEU	2.2
1	E	69	TRP	2.2
2	B	38	LYS	2.1
1	E	19	ALA	2.1
1	E	132	THR	2.1
1	E	120	ILE	2.1
1	A	163	VAL	2.0
2	F	141	TYR	2.0
1	C	88	MET	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 monosaccharides 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(\AA^2)	Q<0.9
3	NAG	A	330	14/15	0.80	0.29	172,180,193,194	0
3	NAG	C	331	14/15	0.86	0.32	129,137,152,153	0
3	NAG	A	331	14/15	0.88	0.15	85,99,125,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.