



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 10:09 AM BST

PDB ID : 5K9O
Title : Crystal structure of multidonor HV1-18+HD3-9 class broadly neutralizing Influenza A antibody 31.b.09 in complex with Hemagglutinin H1 A/California/04/2009
Authors : Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2016-06-01
Resolution : 3.39 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

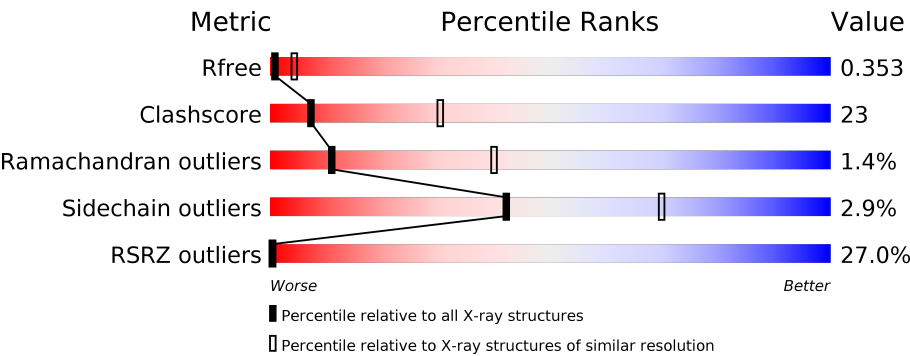
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	227	<div><div>40%</div><div><div></div><div></div><div></div><div></div></div><div>74%</div><div>19%</div><div>• •</div></div>
1	H	227	<div><div>38%</div><div><div></div><div></div><div></div><div></div></div><div>71%</div><div>22%</div><div>• •</div></div>
2	B	219	<div><div>44%</div><div><div></div><div></div><div></div><div></div></div><div>69%</div><div>23%</div><div>• •</div></div>
2	L	219	<div><div>39%</div><div><div></div><div></div><div></div><div></div></div><div>75%</div><div>20%</div><div>• •</div></div>
3	F	505	<div><div>18%</div><div><div></div><div></div><div></div><div></div></div><div>78%</div><div>11%</div><div>• • 8%</div></div>
3	I	505	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>76%</div><div>15%</div><div>• 8%</div></div>

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Mol	Chain	Length	Quality of chain
4	C	3	 <div>33% 67%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	2	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14056 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 31.b.09 Heavy Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1655	1043	277	327	8			
1	H	221	Total	C	N	O	S	0	0	0
			1661	1046	280	327	8			

- Molecule 2 is a protein called 31.b.09 Light Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1654	1036	281	331	6			
2	L	217	Total	C	N	O	S	0	0	0
			1684	1055	285	337	7			

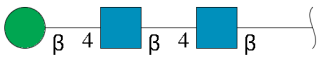
- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	467	Total	C	N	O	S	0	0	0
			3685	2329	628	711	17			
3	I	466	Total	C	N	O	S	0	0	0
			3678	2317	629	715	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	506	SER	-	expression tag	UNP C3W5S1
F	507	GLY	-	expression tag	UNP C3W5S1
I	506	SER	-	expression tag	UNP C3W5S1
I	507	GLY	-	expression tag	UNP C3W5S1

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

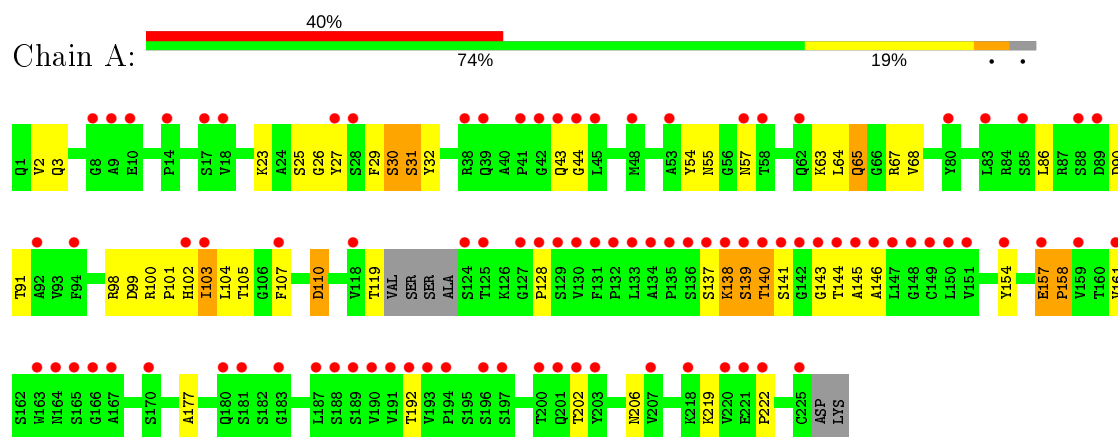


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

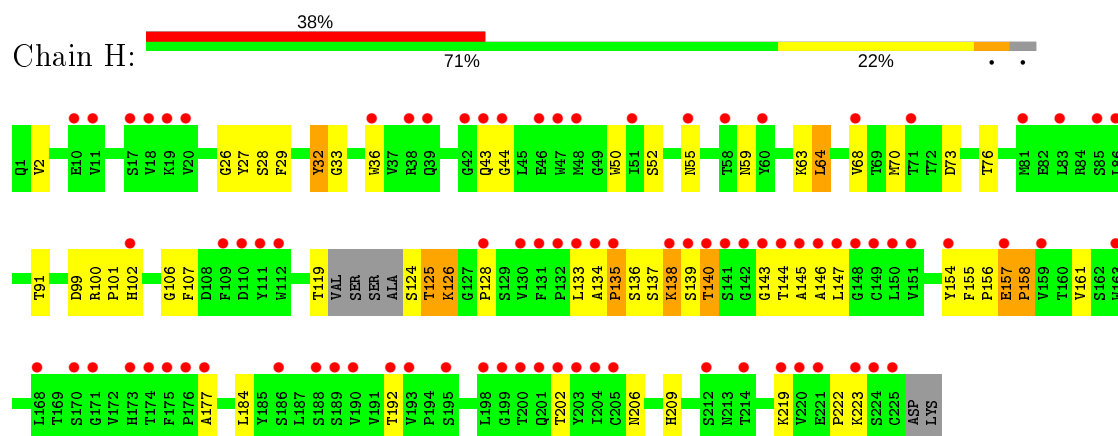
3 Residue-property plots [i](#)

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.

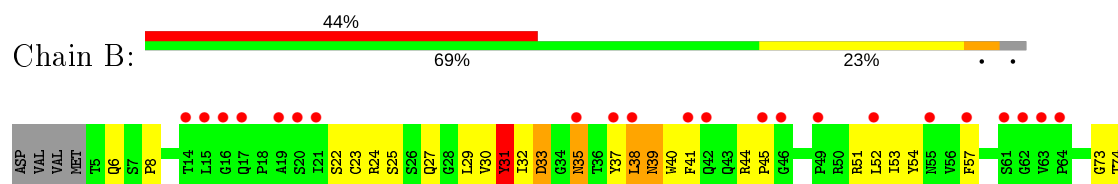
• Molecule 1: 31.b.09 Heavy Fv

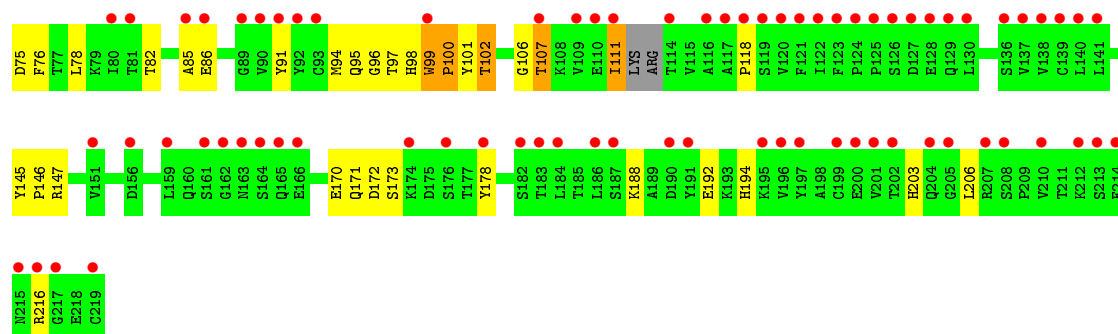


• Molecule 1: 31.b.09 Heavy Fv

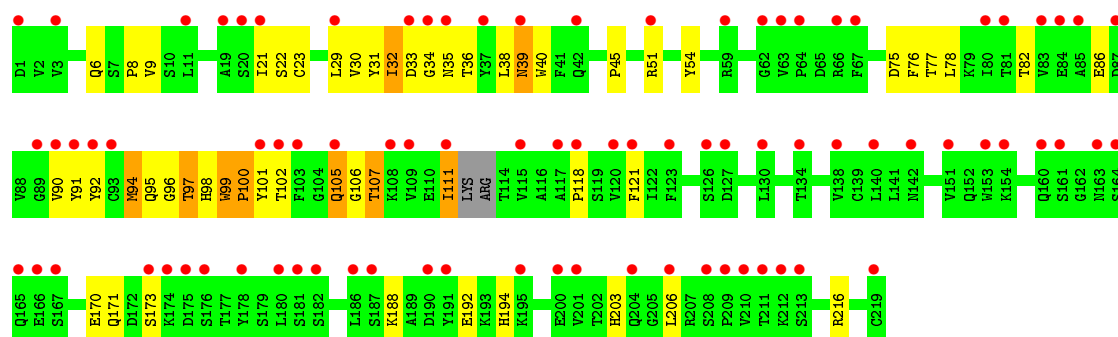
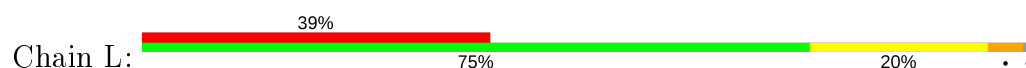


• Molecule 2: 31.b.09 Light Fv

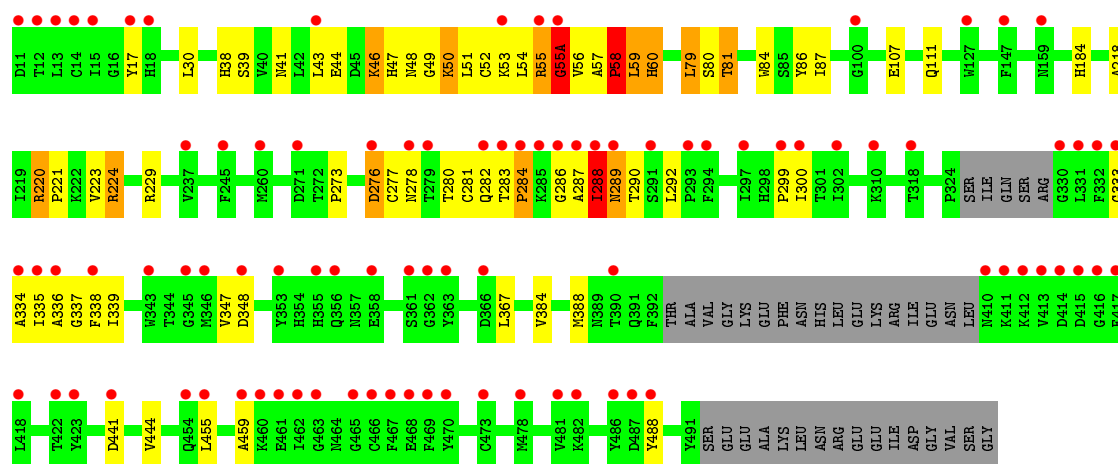
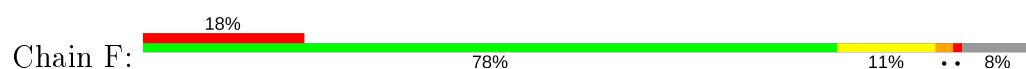




• Molecule 2: 31.b.09 Light Fv



• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	208.65Å 208.65Å 252.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.97 – 3.39 46.57 – 3.39	Depositor EDS
% Data completeness (in resolution range)	63.8 (38.97-3.39) 63.8 (46.57-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.291 , 0.346 0.304 , 0.353	Depositor DCC
R_{free} test set	1432 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	102.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 160.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	14056	wwPDB-VP
Average B, all atoms (Å ²)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

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: BMA, 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	0.31	0/1695	0.55	3/2308 (0.1%)
1	H	0.32	0/1701	0.59	3/2315 (0.1%)
2	B	0.33	1/1692 (0.1%)	0.58	2/2299 (0.1%)
2	L	0.28	0/1722	0.54	0/2340
3	F	0.32	0/3774	0.69	5/5117 (0.1%)
3	I	0.28	0/3765	0.49	0/5104
All	All	0.30	1/14349 (0.0%)	0.59	13/19483 (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
3	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	PRO	N-CD	5.08	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	55(A)	GLY	C-N-CA	-25.34	58.34	121.70
3	F	55(A)	GLY	CA-C-N	-19.58	74.12	117.20
1	H	134	ALA	C-N-CD	-11.96	94.30	120.60
3	F	55(A)	GLY	O-C-N	6.33	132.83	122.70
3	F	57	ALA	C-N-CD	6.33	141.69	128.40
3	F	220	ARG	C-N-CD	5.88	140.75	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	158	PRO	CA-N-CD	-5.83	103.33	111.50
2	B	99	TRP	C-N-CD	5.82	140.61	128.40
1	A	158	PRO	CA-N-CD	-5.67	103.56	111.50
1	A	157	GLU	C-N-CD	5.37	139.68	128.40
1	H	157	GLU	C-N-CD	5.30	139.53	128.40
1	A	110	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	39	ASN	N-CA-CB	-5.04	101.53	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	55(A)	GLY	Mainchain

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	1655	0	1611	76	0
1	H	1661	0	1621	119	0
2	B	1654	0	1584	120	0
2	L	1684	0	1621	111	0
3	F	3685	0	3557	139	0
3	I	3678	0	3546	104	0
4	C	39	0	34	0	0
All	All	14056	0	13574	622	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 23.

All (622) 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)
3:F:59:LEU:CD2	3:F:81:THR:HA	1.24	1.65
1:A:107:PHE:CZ	2:B:99:TRP:CH2	1.76	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:SER:CA	1:H:155:PHE:HE1	1.05	1.59
1:A:107:PHE:CE2	2:B:99:TRP:CZ3	1.90	1.57
1:H:124:SER:HA	1:H:155:PHE:CE1	0.98	1.51
1:A:107:PHE:CE2	2:B:99:TRP:CH2	1.93	1.50
2:B:57:PHE:HB2	3:F:289:ASN:ND2	1.19	1.47
1:H:124:SER:CA	1:H:155:PHE:CE1	1.84	1.43
3:F:54:LEU:O	3:F:56:VAL:CG2	1.71	1.38
2:L:8:PRO:O	2:L:107:THR:CG2	1.74	1.34
1:A:110:ASP:OD1	2:B:51:ARG:NH1	1.56	1.34
2:L:39:ASN:H	2:L:94:MET:CG	1.43	1.32
2:B:95:GLN:HG2	2:B:101:TYR:CA	1.51	1.31
1:A:107:PHE:HE2	2:B:99:TRP:CZ3	1.34	1.31
1:A:102:HIS:NE2	3:F:347:VAL:O	1.66	1.29
3:F:280:THR:OG1	3:F:288:ILE:HD11	1.17	1.29
2:B:57:PHE:CB	3:F:289:ASN:ND2	1.95	1.29
3:I:51:LEU:CD2	3:I:272:THR:OG1	1.83	1.26
3:F:59:LEU:CD2	3:F:81:THR:CA	2.13	1.25
2:B:95:GLN:CG	2:B:101:TYR:HA	1.64	1.25
2:L:39:ASN:N	2:L:94:MET:HG2	1.53	1.23
3:I:51:LEU:HD22	3:I:272:THR:OG1	1.34	1.22
2:L:91:TYR:O	2:L:106:GLY:HA2	1.36	1.21
2:B:57:PHE:CB	3:F:289:ASN:HD21	1.53	1.20
3:F:280:THR:OG1	3:F:288:ILE:CD1	1.90	1.19
1:A:141:SER:OG	1:A:144:THR:O	1.59	1.18
1:A:139:SER:O	1:A:141:SER:N	1.76	1.18
2:L:6:GLN:HE22	2:L:106:GLY:N	1.40	1.17
1:H:106:GLY:HA3	2:L:35:ASN:HD21	1.08	1.17
3:F:221:PRO:O	3:F:229:ARG:NH2	1.77	1.16
1:H:126:LYS:HE3	1:H:184:LEU:HD21	1.19	1.15
3:F:54:LEU:O	3:F:56:VAL:HG21	1.32	1.15
3:I:496:LYS:HB3	3:I:497:LEU:HB2	1.23	1.15
1:H:100:ARG:NH1	2:L:99:TRP:HH2	0.91	1.13
3:F:282:GLN:HB2	3:F:288:ILE:HG13	1.23	1.13
1:H:126:LYS:HD3	1:H:184:LEU:CD2	1.80	1.11
1:H:100:ARG:NH1	2:L:99:TRP:CH2	1.77	1.09
3:F:55(A):GLY:O	3:F:56:VAL:HG22	1.37	1.09
2:B:98:HIS:HB3	2:B:100:PRO:HD2	1.30	1.09
3:F:59:LEU:HD22	3:F:81:THR:CA	1.79	1.08
3:F:55(A):GLY:O	3:F:56:VAL:CG2	1.84	1.07
3:F:59:LEU:HD21	3:F:81:THR:HA	1.33	1.07
2:L:38:LEU:HB2	2:L:94:MET:HG3	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:SER:HA	1:H:155:PHE:CD1	1.89	1.06
2:B:39:ASN:HB3	2:B:54:TYR:HA	1.40	1.04
1:A:30:SER:OG	1:A:101:PRO:HG3	1.58	1.04
1:A:107:PHE:HZ	2:B:99:TRP:CH2	1.28	1.03
3:F:48:ASN:HB3	3:F:51:LEU:HD13	1.34	1.03
1:H:135:PRO:HG2	1:H:147:LEU:HB3	1.39	1.03
2:L:39:ASN:H	2:L:94:MET:HG2	0.87	1.02
3:I:224:ARG:HH21	3:I:224:ARG:HB2	1.22	1.02
2:B:44:ARG:NH2	2:B:86:GLU:OE2	1.91	1.01
1:H:106:GLY:CA	2:L:35:ASN:HD21	1.72	1.01
1:A:107:PHE:CZ	2:B:99:TRP:HH2	1.36	1.01
1:H:126:LYS:CE	1:H:184:LEU:HD21	1.90	1.00
2:B:37:TYR:HD1	2:B:76:PHE:CE2	1.74	1.00
3:I:496:LYS:HG2	3:I:497:LEU:CD1	1.93	0.99
2:L:90:VAL:CG1	2:L:106:GLY:O	2.10	0.99
2:B:44:ARG:HH22	2:B:86:GLU:CD	1.66	0.99
3:F:54:LEU:O	3:F:56:VAL:HG23	1.62	0.99
2:L:8:PRO:O	2:L:107:THR:HG21	0.82	0.98
1:A:107:PHE:HZ	2:B:99:TRP:CZ2	1.82	0.98
2:B:32:ILE:HG21	3:F:38:HIS:HB3	1.45	0.98
3:F:280:THR:HG1	3:F:288:ILE:HD11	1.23	0.98
3:F:287:ALA:HA	3:F:288:ILE:HG22	1.42	0.98
1:A:157:GLU:CG	1:A:158:PRO:HA	1.94	0.97
1:H:126:LYS:HE3	1:H:184:LEU:CD2	1.94	0.97
1:H:55:ASN:ND2	3:I:348:ASP:OD1	1.97	0.97
2:L:91:TYR:O	2:L:106:GLY:CA	2.13	0.97
1:H:36:TRP:CD1	1:H:70:MET:CE	2.47	0.97
2:L:90:VAL:HG13	2:L:106:GLY:O	1.64	0.97
3:I:496:LYS:HG2	3:I:497:LEU:HD12	1.46	0.97
2:B:37:TYR:CD1	2:B:76:PHE:CE2	2.39	0.96
3:I:496:LYS:HG3	3:I:497:LEU:HA	1.48	0.96
3:F:59:LEU:HD21	3:F:81:THR:CA	1.90	0.96
2:L:6:GLN:NE2	2:L:106:GLY:N	2.13	0.95
2:B:44:ARG:NH2	2:B:86:GLU:HG2	1.81	0.95
3:I:492:SER:OG	3:I:494:GLU:HG2	1.65	0.95
2:B:29:LEU:HB2	2:B:97:THR:HG21	1.46	0.95
2:L:9:VAL:C	2:L:107:THR:HG22	1.86	0.95
2:L:9:VAL:HA	2:L:107:THR:CG2	1.97	0.94
3:F:49:GLY:H	3:F:284:PRO:HG2	1.29	0.94
2:L:6:GLN:NE2	2:L:106:GLY:H	1.66	0.94
2:L:32:ILE:HG22	2:L:33:ASP:H	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:SER:CB	1:H:155:PHE:HE1	1.80	0.93
2:B:44:ARG:NH2	2:B:86:GLU:CG	2.30	0.93
1:H:126:LYS:HD3	1:H:184:LEU:HD22	1.50	0.93
2:B:95:GLN:HG2	2:B:101:TYR:HA	0.93	0.93
2:L:6:GLN:HE22	2:L:106:GLY:H	1.15	0.92
3:I:51:LEU:HD22	3:I:272:THR:HG1	1.24	0.92
1:H:126:LYS:CD	1:H:184:LEU:CD2	2.47	0.91
2:B:98:HIS:HB3	2:B:100:PRO:CD	2.00	0.91
1:H:126:LYS:CE	1:H:184:LEU:CD2	2.48	0.91
3:F:286:GLY:C	3:F:288:ILE:CG2	2.39	0.91
2:B:75:ASP:O	2:B:76:PHE:CD1	2.23	0.90
3:F:288:ILE:H	3:F:290:THR:HG23	1.33	0.90
3:F:218:ALA:O	3:F:220:ARG:NH2	2.03	0.90
1:H:124:SER:C	1:H:155:PHE:CE1	2.45	0.90
1:H:140:THR:HG21	1:H:146:ALA:N	1.87	0.90
3:F:338:PHE:CD2	3:F:339:ILE:N	2.41	0.89
2:L:92:TYR:CE1	2:L:106:GLY:HA3	2.07	0.89
2:L:98:HIS:CD2	2:L:100:PRO:HD2	2.08	0.89
1:H:36:TRP:CD1	1:H:70:MET:HE1	2.07	0.88
2:L:9:VAL:CA	2:L:107:THR:HG22	2.03	0.88
3:F:282:GLN:HB2	3:F:288:ILE:CG1	2.04	0.88
3:I:496:LYS:CG	3:I:497:LEU:HA	2.04	0.88
2:B:95:GLN:OE1	2:B:101:TYR:O	1.89	0.87
1:H:125:THR:N	1:H:155:PHE:HD1	1.71	0.87
1:H:126:LYS:HD3	1:H:155:PHE:HB3	1.57	0.87
1:H:126:LYS:CD	1:H:155:PHE:HB3	2.04	0.87
1:A:157:GLU:OE2	1:A:177:ALA:CB	2.22	0.86
3:I:224:ARG:HH21	3:I:224:ARG:CB	1.88	0.86
3:F:55:ARG:C	3:F:56:VAL:HG23	1.95	0.86
2:L:8:PRO:C	2:L:107:THR:HG21	1.94	0.86
1:A:65:GLN:O	1:A:65:GLN:NE2	2.09	0.85
1:A:139:SER:O	1:A:141:SER:O	1.93	0.85
3:I:496:LYS:HB3	3:I:497:LEU:CB	2.05	0.84
2:L:194:HIS:O	2:L:216:ARG:NH1	2.09	0.84
3:I:45:ASP:HB3	3:I:296:ASN:ND2	1.91	0.84
2:B:38:LEU:HB3	2:B:94:MET:CB	2.08	0.83
3:F:59:LEU:HD22	3:F:81:THR:HA	0.85	0.83
1:H:140:THR:CB	1:H:145:ALA:HA	2.08	0.83
1:H:136:SER:O	1:H:139:SER:N	2.12	0.83
1:A:107:PHE:CE2	2:B:99:TRP:HZ3	1.53	0.83
3:F:46:LYS:NZ	3:F:287:ALA:O	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:GLY:HA3	2:L:35:ASN:ND2	1.93	0.82
2:B:194:HIS:O	2:B:216:ARG:NH1	2.13	0.82
2:B:57:PHE:CG	3:F:289:ASN:ND2	2.47	0.82
1:A:157:GLU:OE2	1:A:177:ALA:HB1	1.80	0.82
2:B:57:PHE:HB2	3:F:289:ASN:HD21	0.70	0.82
1:H:124:SER:CA	1:H:155:PHE:CD1	2.57	0.82
3:I:97:CYS:O	3:I:224:ARG:HD2	1.79	0.82
3:I:51:LEU:HD23	3:I:272:THR:OG1	1.78	0.81
1:H:126:LYS:CD	1:H:184:LEU:HD22	2.08	0.81
1:H:106:GLY:CA	2:L:35:ASN:ND2	2.43	0.81
1:H:140:THR:HG21	1:H:146:ALA:H	1.46	0.81
1:H:135:PRO:CG	1:H:147:LEU:HB3	2.09	0.81
1:H:136:SER:HB2	1:H:223:LYS:HB2	1.63	0.81
3:F:287:ALA:CA	3:F:288:ILE:HG22	2.11	0.81
3:F:59:LEU:O	3:F:60:HIS:C	2.19	0.81
2:B:44:ARG:NH2	2:B:86:GLU:CD	2.32	0.80
3:F:58:PRO:HB3	3:F:84:TRP:CG	2.17	0.80
2:B:37:TYR:OH	2:B:74:THR:HA	1.80	0.80
3:I:320:LEU:HD12	3:I:440:HIS:HB3	1.63	0.79
2:B:8:PRO:O	2:B:107:THR:HG23	1.81	0.79
2:L:39:ASN:N	2:L:94:MET:CG	2.24	0.79
2:L:39:ASN:N	2:L:94:MET:SD	2.54	0.79
3:F:287:ALA:HB1	3:F:289:ASN:HB3	1.65	0.79
2:B:32:ILE:CG2	3:F:38:HIS:HB3	2.11	0.78
2:B:38:LEU:HB3	2:B:94:MET:HB3	1.66	0.78
1:A:54:TYR:N	1:A:55:ASN:HA	1.98	0.78
2:B:39:ASN:O	2:B:94:MET:HG3	1.84	0.78
2:L:32:ILE:HG22	2:L:33:ASP:N	1.98	0.78
2:L:9:VAL:HA	2:L:107:THR:HG22	1.62	0.78
3:I:357:ASN:ND2	3:I:475:ASN:OD1	2.11	0.78
2:L:95:GLN:HG3	2:L:101:TYR:HA	1.65	0.78
3:F:280:THR:CB	3:F:288:ILE:HD11	2.14	0.78
2:L:9:VAL:CA	2:L:107:THR:CG2	2.60	0.77
3:F:58:PRO:CG	3:F:87:ILE:HA	2.15	0.77
1:H:124:SER:HA	1:H:155:PHE:CZ	2.06	0.77
1:A:157:GLU:HG2	1:A:158:PRO:HA	1.63	0.77
3:F:455:LEU:HD13	3:F:459:ALA:HB3	1.64	0.77
2:B:95:GLN:CG	2:B:101:TYR:CA	2.30	0.77
2:B:29:LEU:HB2	2:B:97:THR:CG2	2.16	0.76
3:F:55:ARG:O	3:F:56:VAL:N	2.17	0.76
1:H:124:SER:C	1:H:155:PHE:CD1	2.58	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:48:ASN:OD1	3:F:51:LEU:HD21	1.85	0.76
2:L:92:TYR:CD1	2:L:106:GLY:HA3	2.20	0.76
1:H:125:THR:N	1:H:155:PHE:CD1	2.54	0.76
1:H:33:GLY:N	1:H:100:ARG:O	2.18	0.76
1:H:64:LEU:N	1:H:64:LEU:HD22	2.01	0.76
2:L:32:ILE:HD12	2:L:32:ILE:N	2.01	0.75
2:B:24:ARG:CB	2:B:75:ASP:OD2	2.34	0.75
3:I:47:HIS:CG	3:I:48:ASN:H	2.04	0.75
1:A:64:LEU:N	1:A:64:LEU:HD22	2.02	0.75
1:A:102:HIS:CE1	3:F:347:VAL:O	2.40	0.75
2:L:9:VAL:O	2:L:107:THR:HG22	1.86	0.75
3:F:58:PRO:HG3	3:F:87:ILE:HA	1.69	0.74
3:F:55:ARG:HB2	3:F:278:ASN:OD1	1.86	0.74
1:H:36:TRP:CD1	1:H:70:MET:HE3	2.22	0.74
2:L:95:GLN:HB2	2:L:101:TYR:CD2	2.24	0.73
2:B:91:TYR:O	2:B:106:GLY:CA	2.36	0.73
1:H:140:THR:HB	1:H:145:ALA:HA	1.69	0.73
2:L:38:LEU:CB	2:L:94:MET:HG3	2.15	0.73
2:L:33:ASP:O	2:L:35:ASN:N	2.22	0.73
3:F:282:GLN:CB	3:F:288:ILE:HG13	2.14	0.73
1:H:124:SER:C	1:H:155:PHE:HE1	1.86	0.72
1:A:30:SER:HB3	1:A:98:ARG:HH21	1.52	0.72
3:F:286:GLY:C	3:F:288:ILE:HG22	2.08	0.72
1:H:138:LYS:C	1:H:138:LYS:HD2	2.09	0.72
3:F:59:LEU:O	3:F:60:HIS:O	2.07	0.72
2:L:95:GLN:HG2	2:L:96:GLY:N	2.04	0.72
1:H:43:GLN:HG3	1:H:44:GLY:H	1.52	0.72
2:B:24:ARG:HB2	2:B:75:ASP:OD2	1.87	0.72
2:B:39:ASN:O	2:B:94:MET:CG	2.38	0.71
1:A:65:GLN:HE21	1:A:65:GLN:C	1.94	0.71
3:F:44:GLU:HG3	3:F:292:LEU:HD22	1.72	0.71
1:H:124:SER:O	1:H:125:THR:HG23	1.91	0.71
1:A:107:PHE:CE2	2:B:99:TRP:HH2	1.60	0.71
3:F:54:LEU:C	3:F:56:VAL:CG2	2.59	0.71
3:F:286:GLY:O	3:F:288:ILE:CG2	2.39	0.70
3:I:41:ASN:ND2	3:I:314:LEU:O	2.24	0.70
1:A:30:SER:OG	1:A:32:TYR:O	2.09	0.70
2:L:90:VAL:HG12	2:L:106:GLY:O	1.91	0.70
3:I:496:LYS:HG2	3:I:497:LEU:HD13	1.73	0.70
3:F:276:ASP:OD1	3:F:276:ASP:N	2.25	0.69
3:I:272:THR:HG21	3:I:285:LYS:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:48:ASN:CB	3:F:51:LEU:HD13	2.17	0.69
3:F:48:ASN:HB3	3:F:51:LEU:CD1	2.15	0.69
1:H:136:SER:CB	1:H:223:LYS:HB2	2.23	0.69
1:A:32:TYR:HB2	1:A:101:PRO:HB3	1.74	0.69
3:I:492:SER:CB	3:I:494:GLU:HG2	2.22	0.69
3:F:287:ALA:N	3:F:288:ILE:HB	2.07	0.69
3:F:54:LEU:HB3	3:F:56:VAL:HG21	1.73	0.69
2:L:98:HIS:HD2	2:L:99:TRP:H	1.39	0.69
3:F:287:ALA:CA	3:F:289:ASN:HB3	2.23	0.68
3:F:58:PRO:HB3	3:F:84:TRP:CB	2.23	0.68
2:L:92:TYR:CD1	2:L:106:GLY:CA	2.76	0.68
3:F:286:GLY:C	3:F:288:ILE:HG21	2.11	0.68
1:H:126:LYS:CD	1:H:184:LEU:HD21	2.18	0.68
2:L:9:VAL:HA	2:L:107:THR:HG23	1.75	0.68
3:F:54:LEU:C	3:F:56:VAL:HG21	2.14	0.68
1:H:63:LYS:HB2	1:H:64:LEU:HD22	1.76	0.68
3:I:296:ASN:N	3:I:296:ASN:HD22	1.91	0.68
1:H:135:PRO:HG2	1:H:147:LEU:CB	2.22	0.68
1:H:102:HIS:CD2	3:I:347:VAL:HG23	2.29	0.68
1:H:140:THR:HG22	2:L:121:PHE:CE2	2.30	0.68
3:I:45:ASP:HB3	3:I:296:ASN:HD21	1.59	0.67
3:F:286:GLY:O	3:F:288:ILE:HG22	1.94	0.67
3:I:455:LEU:HD13	3:I:459:ALA:HB3	1.76	0.67
2:B:38:LEU:HB3	2:B:94:MET:HB2	1.74	0.67
3:F:58:PRO:HG3	3:F:87:ILE:HG22	1.75	0.67
2:L:22:SER:HB2	2:L:76:PHE:CE1	2.29	0.67
2:B:91:TYR:O	2:B:106:GLY:HA2	1.94	0.67
2:L:98:HIS:CD2	2:L:99:TRP:H	2.13	0.67
3:I:50:LYS:HB3	3:I:275:HIS:HD2	1.59	0.67
2:B:98:HIS:O	2:B:101:TYR:CE1	2.49	0.66
2:L:38:LEU:HB2	2:L:94:MET:CG	2.19	0.66
2:B:98:HIS:O	2:B:101:TYR:CD1	2.48	0.66
3:F:79:LEU:HD12	3:F:81:THR:HB	1.77	0.66
1:H:126:LYS:O	1:H:209:HIS:CE1	2.49	0.66
1:A:107:PHE:CZ	2:B:99:TRP:CZ3	2.43	0.65
3:F:55:ARG:CG	3:F:55(A):GLY:H	2.10	0.65
2:L:99:TRP:HA	2:L:99:TRP:CE3	2.31	0.65
1:A:157:GLU:OE1	1:A:177:ALA:HB3	1.97	0.65
3:F:287:ALA:CB	3:F:289:ASN:HB3	2.26	0.65
3:I:282:GLN:NE2	3:I:282:GLN:HA	2.11	0.65
2:L:39:ASN:OD1	2:L:94:MET:SD	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB2	1:A:32:TYR:CE2	2.31	0.65
3:I:492:SER:OG	3:I:494:GLU:CG	2.41	0.65
1:A:157:GLU:HG3	1:A:158:PRO:HA	1.77	0.65
2:B:98:HIS:CB	2:B:100:PRO:HD2	2.17	0.65
2:B:45:PRO:CG	2:B:170:GLU:HG3	2.26	0.65
3:F:49:GLY:N	3:F:284:PRO:HG2	2.09	0.65
2:L:95:GLN:HG3	2:L:101:TYR:CG	2.32	0.65
1:A:102:HIS:CE1	1:A:104:LEU:HB3	2.32	0.64
2:B:37:TYR:CD1	2:B:76:PHE:CD2	2.85	0.64
3:F:17:TYR:HE1	3:F:444:VAL:HG21	1.62	0.64
1:A:86:LEU:HD12	1:A:90:ASP:HB3	1.78	0.64
3:F:287:ALA:C	3:F:289:ASN:HB3	2.18	0.64
2:B:75:ASP:O	2:B:76:PHE:HD1	1.80	0.64
2:B:118:PRO:HD2	2:B:206:LEU:HD11	1.79	0.64
3:F:224:ARG:NH1	3:F:224:ARG:HG3	2.12	0.64
1:H:100:ARG:HD3	1:H:107:PHE:CD1	2.33	0.64
1:A:64:LEU:HD12	1:A:67:ARG:HH21	1.63	0.63
2:L:95:GLN:CG	2:L:101:TYR:HA	2.28	0.63
2:L:38:LEU:H	2:L:94:MET:CG	2.11	0.63
1:A:30:SER:HB3	1:A:98:ARG:NH2	2.13	0.63
3:F:17:TYR:CE1	3:F:444:VAL:HG21	2.33	0.63
3:I:90:THR:HG22	3:I:91:SER:H	1.63	0.63
1:A:139:SER:O	1:A:141:SER:C	2.37	0.63
3:F:59:LEU:HD21	3:F:81:THR:N	2.13	0.63
3:I:496:LYS:CB	3:I:497:LEU:HB2	2.16	0.63
2:B:6:GLN:HE22	2:B:106:GLY:HA2	1.64	0.62
3:F:55:ARG:HG2	3:F:55(A):GLY:H	1.62	0.62
3:I:497:LEU:O	3:I:497:LEU:HG	1.99	0.62
2:L:22:SER:HA	2:L:76:PHE:O	1.98	0.62
2:B:40:TRP:O	2:B:52:LEU:HD12	2.00	0.62
1:H:125:THR:HA	1:H:155:PHE:O	2.00	0.62
1:H:126:LYS:N	1:H:155:PHE:O	2.33	0.61
3:I:50:LYS:HB3	3:I:275:HIS:CD2	2.36	0.61
3:I:268:ILE:HD11	3:I:302:ILE:HD12	1.80	0.61
3:I:224:ARG:NH2	3:I:224:ARG:HB2	2.05	0.61
3:F:287:ALA:HA	3:F:288:ILE:CG2	2.25	0.61
1:H:157:GLU:HB3	1:H:158:PRO:HA	1.81	0.61
3:I:97:CYS:O	3:I:224:ARG:CD	2.49	0.61
3:I:52:CYS:SG	3:I:277:CYS:N	2.65	0.61
2:L:118:PRO:HD2	2:L:206:LEU:HD11	1.81	0.61
3:F:287:ALA:HB1	3:F:289:ASN:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:HG3	1:A:44:GLY:H	1.65	0.60
1:H:126:LYS:CG	1:H:155:PHE:HB3	2.31	0.60
1:A:157:GLU:CD	1:A:177:ALA:CB	2.70	0.60
2:L:29:LEU:HD21	2:L:96:GLY:HA2	1.82	0.60
2:B:74:THR:O	2:B:74:THR:HG23	2.01	0.60
3:F:46:LYS:HE3	3:F:283:THR:HG23	1.83	0.60
2:B:98:HIS:HB3	2:B:100:PRO:CG	2.32	0.59
1:A:102:HIS:CD2	3:F:347:VAL:O	2.52	0.59
1:A:31:SER:HB2	1:A:32:TYR:CZ	2.37	0.59
3:I:51:LEU:CD2	3:I:272:THR:HG1	1.91	0.59
2:B:203:HIS:HB3	2:B:206:LEU:HD13	1.83	0.59
2:L:91:TYR:O	2:L:106:GLY:C	2.41	0.59
1:A:29:PHE:CE2	1:A:31:SER:HA	2.37	0.59
3:I:50:LYS:HD3	3:I:275:HIS:NE2	2.17	0.59
2:B:32:ILE:HG21	3:F:38:HIS:CB	2.28	0.59
2:L:38:LEU:H	2:L:94:MET:HG3	1.67	0.59
2:B:27:GLN:NE2	2:B:98:HIS:NE2	2.50	0.59
3:F:59:LEU:CD2	3:F:81:THR:CB	2.80	0.59
3:F:184:HIS:HB3	3:F:220:ARG:NH1	2.17	0.58
2:B:40:TRP:O	2:B:52:LEU:HB2	2.03	0.58
3:F:335:ILE:O	3:F:336:ALA:HB3	2.03	0.58
1:H:156:PRO:O	1:H:209:HIS:NE2	2.31	0.58
3:F:224:ARG:HG3	3:F:224:ARG:HH11	1.68	0.58
1:H:140:THR:CG2	1:H:145:ALA:HA	2.32	0.58
3:I:51:LEU:HD13	3:I:286:GLY:H	1.68	0.58
1:A:107:PHE:HE1	2:B:31:TYR:CE1	2.21	0.58
2:L:35:ASN:O	2:L:36:THR:OG1	2.21	0.58
3:I:385:ILE:O	3:I:388:MET:HG3	2.04	0.58
3:F:58:PRO:CD	3:F:87:ILE:HA	2.33	0.58
3:I:224:ARG:HH21	3:I:224:ARG:CG	2.14	0.58
1:H:140:THR:HG21	1:H:145:ALA:HA	1.86	0.57
2:L:39:ASN:ND2	2:L:51:ARG:HG3	2.19	0.57
3:F:224:ARG:CG	3:F:224:ARG:HH11	2.15	0.57
3:I:320:LEU:HD23	3:I:321:ARG:N	2.19	0.57
3:F:54:LEU:C	3:F:56:VAL:HG23	2.22	0.57
3:I:62:GLY:O	3:I:63:LYS:HB3	2.04	0.57
3:F:43:LEU:N	3:F:292:LEU:HD23	2.20	0.57
1:H:73:ASP:HB3	1:H:76:THR:HG22	1.87	0.57
3:I:282:GLN:HE21	3:I:282:GLN:CA	2.17	0.57
3:I:47:HIS:CG	3:I:48:ASN:N	2.72	0.57
2:B:24:ARG:HB3	2:B:75:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:55:ARG:HH21	3:F:55:ARG:CG	2.18	0.57
1:H:135:PRO:CD	1:H:147:LEU:HB3	2.34	0.56
3:F:286:GLY:O	3:F:288:ILE:HG21	2.05	0.56
3:F:48:ASN:CB	3:F:51:LEU:CD1	2.80	0.56
2:L:95:GLN:HG2	2:L:96:GLY:H	1.68	0.56
2:L:98:HIS:CD2	2:L:99:TRP:N	2.73	0.56
1:H:124:SER:CB	1:H:155:PHE:CE1	2.67	0.56
1:H:36:TRP:NE1	1:H:70:MET:HE1	2.20	0.56
1:A:140:THR:HG21	1:A:146:ALA:H	1.69	0.56
2:B:41:PHE:CZ	2:B:94:MET:SD	2.98	0.56
2:B:44:ARG:CZ	2:B:86:GLU:CG	2.84	0.56
3:F:50:LYS:HG3	3:F:273:PRO:O	2.06	0.56
1:H:126:LYS:CE	1:H:184:LEU:HD22	2.27	0.56
3:I:296:ASN:HD22	3:I:296:ASN:H	1.54	0.56
2:L:38:LEU:N	2:L:94:MET:CG	2.68	0.56
3:I:295:GLN:HB3	3:I:306:PRO:HG2	1.88	0.56
1:H:32:TYR:CD1	1:H:32:TYR:N	2.73	0.56
3:I:51:LEU:HD12	3:I:282:GLN:OE1	2.06	0.56
2:L:23:CYS:O	2:L:75:ASP:HA	2.06	0.56
1:H:126:LYS:HD3	1:H:155:PHE:CB	2.32	0.56
1:H:27:TYR:HA	1:H:28:SER:OG	2.06	0.56
1:H:106:GLY:HA2	2:L:35:ASN:ND2	2.19	0.56
3:I:220:ARG:HB3	3:I:221:PRO:HD2	1.86	0.55
1:A:63:LYS:HB2	1:A:64:LEU:HD22	1.87	0.55
2:B:32:ILE:N	2:B:32:ILE:HD12	2.21	0.55
3:F:58:PRO:HD3	3:F:86:TYR:O	2.05	0.55
2:B:57:PHE:HB2	3:F:289:ASN:HD22	1.53	0.55
2:L:45:PRO:CG	2:L:170:GLU:HG3	2.37	0.55
3:I:496:LYS:CB	3:I:497:LEU:CA	2.84	0.55
2:L:38:LEU:CB	2:L:94:MET:CG	2.82	0.55
1:A:107:PHE:HE2	2:B:99:TRP:HZ3	0.96	0.55
3:F:287:ALA:CA	3:F:289:ASN:CB	2.85	0.55
1:H:33:GLY:H	1:H:100:ARG:C	2.09	0.55
1:A:138:LYS:HB3	1:A:138:LYS:NZ	2.22	0.54
3:F:59:LEU:HD23	3:F:81:THR:HG23	1.88	0.54
1:H:59:ASN:ND2	2:L:99:TRP:NE1	2.56	0.54
1:A:157:GLU:HG2	1:A:158:PRO:CA	2.36	0.54
2:L:32:ILE:CG2	2:L:33:ASP:H	2.10	0.54
2:B:45:PRO:HG2	2:B:170:GLU:HG3	1.89	0.54
1:H:128:PRO:HB3	1:H:154:TYR:HB3	1.89	0.54
1:H:64:LEU:O	1:H:68:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:LEU:N	2:L:94:MET:HG2	2.22	0.54
1:A:107:PHE:HE2	2:B:99:TRP:CH2	1.65	0.54
2:L:96:GLY:O	2:L:98:HIS:N	2.41	0.54
2:B:95:GLN:HB3	2:B:101:TYR:CB	2.37	0.53
3:F:338:PHE:CG	3:F:339:ILE:N	2.75	0.53
2:L:188:LYS:O	2:L:192:GLU:HG2	2.08	0.53
2:L:203:HIS:HB3	2:L:206:LEU:HD13	1.89	0.53
2:B:86:GLU:HA	2:B:173:SER:HA	1.90	0.53
2:B:39:ASN:CB	2:B:53:ILE:O	2.56	0.53
3:F:280:THR:CA	3:F:288:ILE:HD11	2.38	0.53
1:A:138:LYS:HB3	1:A:138:LYS:HZ2	1.73	0.53
2:B:44:ARG:CZ	2:B:86:GLU:OE2	2.54	0.53
2:L:99:TRP:N	2:L:100:PRO:HD2	2.24	0.53
2:B:31:TYR:C	2:B:32:ILE:HD12	2.29	0.53
3:F:52:CYS:SG	3:F:277:CYS:N	2.81	0.53
2:L:6:GLN:NE2	2:L:105:GLN:N	2.57	0.53
1:A:128:PRO:HB3	1:A:154:TYR:HB3	1.91	0.53
3:F:184:HIS:HB3	3:F:220:ARG:HH12	1.73	0.52
1:H:126:LYS:CG	1:H:155:PHE:N	2.72	0.52
3:I:496:LYS:HZ2	3:I:497:LEU:HD13	1.74	0.52
3:I:323:ILE:O	3:I:342:GLY:N	2.41	0.52
2:B:6:GLN:NE2	2:B:106:GLY:HA2	2.21	0.52
3:F:48:ASN:OD1	3:F:51:LEU:CD2	2.55	0.52
3:I:90:THR:O	3:I:92:SER:OG	2.19	0.52
2:L:8:PRO:C	2:L:107:THR:CG2	2.67	0.52
2:L:32:ILE:CD1	2:L:32:ILE:N	2.73	0.52
2:B:32:ILE:CD1	2:B:32:ILE:N	2.73	0.52
1:H:157:GLU:CB	1:H:158:PRO:HA	2.39	0.52
3:F:287:ALA:N	3:F:288:ILE:HG22	2.24	0.52
3:I:282:GLN:HE21	3:I:282:GLN:HA	1.75	0.52
1:H:140:THR:CG2	1:H:146:ALA:H	2.19	0.52
3:I:496:LYS:NZ	3:I:497:LEU:CD1	2.73	0.52
3:F:287:ALA:N	3:F:288:ILE:CG2	2.73	0.52
2:L:99:TRP:O	2:L:101:TYR:N	2.43	0.51
1:H:126:LYS:HG3	1:H:155:PHE:N	2.25	0.51
1:H:157:GLU:OE2	1:H:177:ALA:HB3	2.10	0.51
1:A:23:LYS:HE3	1:A:25:SER:HB3	1.91	0.51
2:B:147:ARG:HB2	2:B:178:TYR:CE2	2.46	0.51
1:H:50:TRP:CZ2	1:H:52:SER:HB2	2.46	0.51
2:L:31:TYR:C	2:L:32:ILE:HD12	2.31	0.51
1:H:43:GLN:HG3	1:H:44:GLY:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:TRP:HD1	1:H:70:MET:HE3	1.75	0.51
2:B:101:TYR:O	2:B:102:THR:OG1	2.28	0.51
3:I:282:GLN:NE2	3:I:282:GLN:CA	2.73	0.51
1:A:102:HIS:O	1:A:103:ILE:HG22	2.11	0.51
3:F:287:ALA:N	3:F:288:ILE:CB	2.73	0.51
3:F:55:ARG:CG	3:F:55(A):GLY:N	2.73	0.51
3:I:206:SER:OG	3:I:241:ASP:OD2	2.28	0.51
3:I:496:LYS:CB	3:I:497:LEU:HA	2.41	0.51
1:H:100:ARG:HD2	1:H:102:HIS:O	2.12	0.50
3:I:224:ARG:NH2	3:I:224:ARG:CG	2.73	0.50
3:F:384:VAL:O	3:F:388:MET:HG2	2.12	0.50
2:L:38:LEU:CA	2:L:94:MET:CG	2.89	0.50
1:A:64:LEU:O	1:A:68:VAL:HG22	2.12	0.50
1:H:126:LYS:CB	1:H:126:LYS:NZ	2.73	0.50
2:L:95:GLN:HB2	2:L:101:TYR:HD2	1.74	0.50
1:A:107:PHE:HE1	2:B:31:TYR:HE1	1.59	0.50
1:H:135:PRO:CG	1:H:147:LEU:CB	2.85	0.50
1:A:138:LYS:CB	1:A:138:LYS:NZ	2.73	0.50
3:F:333:GLY:O	3:F:337:GLY:HA3	2.11	0.50
2:L:95:GLN:NE2	2:L:97:THR:O	2.44	0.50
1:H:126:LYS:CB	1:H:126:LYS:HZ3	2.24	0.50
3:I:40:VAL:HG12	2:L:33:ASP:HA	1.92	0.50
2:B:188:LYS:O	2:B:192:GLU:HG2	2.11	0.50
2:B:8:PRO:O	2:B:107:THR:CG2	2.56	0.50
2:B:96:GLY:O	2:B:98:HIS:N	2.40	0.49
3:F:287:ALA:CA	3:F:288:ILE:CG2	2.86	0.49
3:I:47:HIS:ND1	3:I:48:ASN:N	2.60	0.49
1:A:64:LEU:N	1:A:64:LEU:CD2	2.73	0.49
1:H:36:TRP:HD1	1:H:70:MET:CE	2.15	0.49
2:B:99:TRP:HZ3	2:B:101:TYR:HH	1.54	0.49
1:H:33:GLY:CA	1:H:100:ARG:O	2.60	0.49
1:H:33:GLY:HA3	1:H:100:ARG:O	2.12	0.49
2:B:33:ASP:OD2	3:F:39:SER:O	2.29	0.49
3:F:338:PHE:C	3:F:338:PHE:CD2	2.85	0.49
3:I:47:HIS:ND1	3:I:49:GLY:N	2.58	0.49
2:B:30:VAL:O	2:B:31:TYR:CB	2.60	0.49
3:I:296:ASN:N	3:I:296:ASN:ND2	2.59	0.49
3:I:471:HIS:HB3	3:I:493:GLU:OE1	2.13	0.49
2:B:91:TYR:O	2:B:106:GLY:HA3	2.13	0.48
2:B:95:GLN:HB3	2:B:101:TYR:HB3	1.94	0.48
3:F:220:ARG:HG3	3:F:229:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:PRO:HD2	2:B:206:LEU:CD1	2.41	0.48
3:F:334:ALA:HA	3:F:338:PHE:CE1	2.48	0.48
3:F:58:PRO:CG	3:F:87:ILE:HG22	2.41	0.48
2:B:23:CYS:O	2:B:76:PHE:N	2.46	0.48
2:L:86:GLU:HA	2:L:173:SER:HB2	1.95	0.48
3:F:287:ALA:HA	3:F:289:ASN:HB2	1.95	0.48
3:I:496:LYS:HZ3	3:I:497:LEU:CD1	2.25	0.48
1:A:91:THR:HG23	1:A:119:THR:HA	1.95	0.48
3:F:51:LEU:HG	3:F:53:LYS:HE3	1.95	0.48
2:B:35:ASN:C	2:B:35:ASN:HD22	2.17	0.48
3:F:55:ARG:CG	3:F:55:ARG:NH2	2.76	0.48
1:H:27:TYR:HB3	1:H:29:PHE:HB2	1.95	0.48
3:I:297:ILE:HG22	3:I:298:HIS:CD2	2.48	0.48
2:L:76:PHE:CD2	2:L:77:THR:HB	2.49	0.48
1:H:140:THR:HG22	2:L:121:PHE:CD2	2.49	0.48
3:I:492:SER:HB2	3:I:494:GLU:HG2	1.95	0.48
3:F:287:ALA:HA	3:F:289:ASN:CB	2.44	0.47
1:H:133:LEU:O	1:H:135:PRO:HD3	2.13	0.47
2:L:118:PRO:HD2	2:L:206:LEU:CD1	2.43	0.47
1:A:139:SER:O	1:A:141:SER:CA	2.59	0.47
2:B:41:PHE:CE2	2:B:94:MET:SD	3.07	0.47
2:L:95:GLN:CB	2:L:101:TYR:CD2	2.95	0.47
1:H:135:PRO:HD2	1:H:147:LEU:HB3	1.97	0.47
3:I:44:GLU:HB2	3:I:292:LEU:HD23	1.97	0.47
3:I:462:ILE:HD11	3:I:468:GLU:HB2	1.96	0.47
2:L:38:LEU:N	2:L:94:MET:HG3	2.29	0.47
2:L:6:GLN:HE21	2:L:105:GLN:H	1.62	0.47
3:I:63:LYS:HG3	3:I:63:LYS:O	2.14	0.47
2:L:38:LEU:C	2:L:94:MET:HG2	2.27	0.47
1:A:107:PHE:CE1	2:B:31:TYR:HE1	2.32	0.47
1:H:135:PRO:CD	1:H:147:LEU:CB	2.92	0.47
1:H:136:SER:O	1:H:139:SER:CA	2.62	0.47
3:I:79:LEU:HD23	3:I:117:ARG:HD3	1.97	0.47
2:L:111:ILE:HG13	2:L:171:GLN:CD	2.35	0.47
3:I:179:LEU:O	3:I:254:PRO:HB3	2.14	0.47
3:I:281:CYS:O	3:I:302:ILE:O	2.33	0.47
2:L:99:TRP:HA	2:L:99:TRP:HE3	1.76	0.47
1:H:140:THR:HG22	2:L:121:PHE:HE2	1.78	0.47
3:I:47:HIS:CE1	3:I:286:GLY:HA3	2.50	0.47
2:L:30:VAL:HG23	2:L:31:TYR:H	1.80	0.47
1:A:139:SER:C	1:A:141:SER:N	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB2	1:A:32:TYR:CD2	2.49	0.47
2:B:97:THR:OG1	2:B:98:HIS:N	2.48	0.46
3:F:79:LEU:HG	3:F:80:SER:O	2.16	0.46
3:I:50:LYS:O	3:I:51:LEU:C	2.52	0.46
1:A:161:VAL:HA	1:A:206:ASN:O	2.16	0.46
3:F:287:ALA:CA	3:F:288:ILE:CB	2.93	0.46
1:A:143:GLY:O	1:A:144:THR:OG1	2.29	0.46
1:A:157:GLU:CD	1:A:177:ALA:HB3	2.36	0.46
2:B:96:GLY:O	2:B:97:THR:OG1	2.25	0.46
1:H:161:VAL:HA	1:H:206:ASN:O	2.14	0.46
3:I:282:GLN:NE2	3:I:287:ALA:HB2	2.31	0.46
2:L:30:VAL:HG23	2:L:31:TYR:N	2.31	0.46
1:H:59:ASN:ND2	2:L:99:TRP:HE1	2.14	0.46
2:L:38:LEU:CA	2:L:94:MET:HG2	2.45	0.46
2:B:98:HIS:HB3	2:B:100:PRO:HG2	1.97	0.46
3:I:195:TYR:O	3:I:197:ASN:N	2.48	0.46
3:I:79:LEU:CD2	3:I:117:ARG:HD3	2.46	0.46
2:B:44:ARG:NH1	2:B:86:GLU:OE2	2.49	0.45
1:H:100:ARG:HD3	1:H:107:PHE:HD1	1.81	0.45
3:I:496:LYS:CB	3:I:497:LEU:CB	2.85	0.45
1:H:126:LYS:HG2	1:H:155:PHE:N	2.31	0.45
1:H:64:LEU:N	1:H:64:LEU:CD2	2.73	0.45
2:L:6:GLN:HE21	2:L:105:GLN:N	2.13	0.45
2:L:95:GLN:HG3	2:L:101:TYR:CA	2.42	0.45
2:B:57:PHE:CD1	3:F:289:ASN:ND2	2.84	0.45
1:A:157:GLU:OE1	1:A:177:ALA:CB	2.64	0.45
2:B:99:TRP:N	2:B:100:PRO:HD2	2.32	0.45
1:H:135:PRO:CG	1:H:147:LEU:CA	2.95	0.45
2:B:75:ASP:C	2:B:76:PHE:CD1	2.89	0.45
2:B:40:TRP:HE3	2:B:78:LEU:CD2	2.29	0.45
2:B:98:HIS:O	2:B:101:TYR:HE1	1.99	0.45
3:F:58:PRO:HB3	3:F:84:TRP:HB2	1.99	0.45
2:B:98:HIS:O	2:B:101:TYR:HD1	1.97	0.45
1:H:140:THR:HG21	1:H:145:ALA:CA	2.47	0.45
2:B:40:TRP:CZ3	2:B:78:LEU:HB3	2.51	0.45
3:F:455:LEU:O	3:F:455:LEU:HD12	2.17	0.45
3:F:55:ARG:O	3:F:56:VAL:HG23	2.16	0.45
2:L:45:PRO:HG2	2:L:170:GLU:HG3	1.97	0.45
1:A:140:THR:HB	1:A:145:ALA:HA	1.98	0.44
2:B:75:ASP:C	2:B:76:PHE:HD1	2.20	0.44
1:H:140:THR:HG21	1:H:145:ALA:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:HG23	1:A:219:LYS:HE2	1.99	0.44
2:B:38:LEU:HD13	2:B:38:LEU:HA	1.78	0.44
3:I:47:HIS:O	3:I:48:ASN:HB2	2.17	0.44
2:B:73:GLY:O	2:B:75:ASP:N	2.43	0.44
1:H:2:VAL:HG12	1:H:26:GLY:O	2.17	0.44
1:A:29:PHE:CZ	1:A:30:SER:O	2.70	0.44
2:B:85:ALA:HB1	2:B:172:ASP:O	2.18	0.44
3:F:284:PRO:HA	3:F:286:GLY:H	1.82	0.44
3:I:50:LYS:CB	3:I:275:HIS:CD2	3.01	0.44
1:H:100:ARG:HD3	1:H:107:PHE:CE1	2.52	0.44
2:L:77:THR:OG1	2:L:78:LEU:N	2.51	0.44
1:A:29:PHE:CE2	1:A:30:SER:O	2.70	0.44
2:B:111:ILE:C	2:B:171:GLN:HE22	2.22	0.43
3:F:48:ASN:HA	3:F:51:LEU:HD11	2.00	0.43
3:I:268:ILE:HD11	3:I:302:ILE:CD1	2.46	0.43
3:I:496:LYS:NZ	3:I:497:LEU:HD13	2.32	0.43
1:A:57:ASN:HB2	3:F:367:LEU:HD22	2.00	0.43
3:F:281:CYS:SG	3:F:282:GLN:N	2.91	0.43
2:L:32:ILE:CG2	2:L:33:ASP:N	2.69	0.43
1:A:26:GLY:HA2	1:A:27:TYR:HA	1.58	0.43
3:F:58:PRO:HG3	3:F:87:ILE:CG2	2.46	0.43
3:F:288:ILE:N	3:F:289:ASN:C	2.72	0.43
3:I:305:CYS:HB3	3:I:306:PRO:HD2	2.01	0.43
1:A:140:THR:HG21	1:A:146:ALA:N	2.34	0.43
1:H:32:TYR:HD1	1:H:32:TYR:N	2.15	0.43
3:I:455:LEU:HD12	3:I:455:LEU:O	2.19	0.43
3:I:47:HIS:HE1	3:I:49:GLY:O	2.01	0.43
2:L:38:LEU:O	2:L:54:TYR:HA	2.19	0.43
1:A:102:HIS:HB3	1:A:105:THR:HG22	2.01	0.43
3:F:54:LEU:HA	3:F:54:LEU:HD12	1.86	0.43
3:F:55(A):GLY:N	3:F:56:VAL:HG23	2.33	0.43
1:H:137:SER:HB3	1:H:140:THR:H	1.84	0.43
3:F:50:LYS:HE3	3:F:273:PRO:HB2	2.01	0.43
1:H:202:THR:HG23	1:H:219:LYS:HE2	2.00	0.42
3:I:288:ILE:HD12	3:I:290:THR:H	1.84	0.42
2:B:25:SER:HG	2:B:74:THR:HG1	0.93	0.42
3:I:63:LYS:O	3:I:64:CYS:SG	2.77	0.42
2:L:40:TRP:CG	2:L:78:LEU:HD22	2.55	0.42
3:F:334:ALA:HB3	3:F:441:ASP:OD1	2.19	0.42
1:H:126:LYS:HG2	1:H:155:PHE:HB3	1.98	0.42
1:H:2:VAL:HA	1:H:26:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:GLY:O	1:H:144:THR:OG1	2.31	0.42
1:H:63:LYS:HB2	1:H:64:LEU:CD2	2.47	0.42
2:B:39:ASN:HB2	2:B:53:ILE:O	2.19	0.42
2:B:40:TRP:HE3	2:B:78:LEU:HD23	1.84	0.42
1:A:2:VAL:O	1:A:3:GLN:HG3	2.20	0.42
1:H:145:ALA:O	1:H:192:THR:HA	2.19	0.42
2:B:86:GLU:N	2:B:173:SER:O	2.53	0.42
3:I:320:LEU:HD23	3:I:321:ARG:H	1.84	0.42
2:B:35:ASN:ND2	2:B:35:ASN:C	2.73	0.41
3:F:59:LEU:HD21	3:F:81:THR:H	1.82	0.41
1:H:158:PRO:HD2	1:H:158:PRO:O	2.20	0.41
3:I:290:THR:OG1	3:I:306:PRO:HD3	2.20	0.41
3:I:26:VAL:HG21	3:I:317:ALA:HB2	2.02	0.41
3:I:41:ASN:OD1	3:I:43:LEU:O	2.38	0.41
3:I:60:HIS:HA	3:I:88:VAL:HG23	2.01	0.41
2:B:99:TRP:N	2:B:100:PRO:CD	2.84	0.41
3:F:280:THR:OG1	3:F:288:ILE:HD13	2.04	0.41
3:F:41:ASN:HB3	3:F:292:LEU:HD21	2.03	0.41
1:A:145:ALA:O	1:A:192:THR:HA	2.21	0.41
1:H:33:GLY:O	1:H:99:ASP:N	2.46	0.41
3:I:60:HIS:HA	3:I:88:VAL:CG2	2.51	0.41
2:B:29:LEU:HD11	2:B:37:TYR:CD2	2.55	0.41
3:F:223:VAL:HB	3:F:229:ARG:NH1	2.34	0.41
1:H:135:PRO:HD2	1:H:147:LEU:CB	2.51	0.41
3:I:496:LYS:CG	3:I:497:LEU:CA	2.86	0.41
2:L:99:TRP:O	2:L:100:PRO:C	2.59	0.41
2:B:145:TYR:CG	2:B:146:PRO:HA	2.56	0.41
3:I:90:THR:HG22	3:I:91:SER:N	2.33	0.41
2:B:39:ASN:CB	2:B:54:TYR:HA	2.28	0.41
1:H:138:LYS:O	1:H:138:LYS:HD2	2.21	0.41
1:H:91:THR:CG2	1:H:119:THR:HA	2.50	0.41
3:I:99:PRO:HB2	3:I:229:ARG:HD3	2.03	0.41
3:I:496:LYS:HB3	3:I:497:LEU:CA	2.46	0.41
2:L:38:LEU:CA	2:L:94:MET:HG3	2.50	0.41
1:A:99:ASP:OD1	1:A:100:ARG:N	2.48	0.40
3:F:107:GLU:O	3:F:111:GLN:HG2	2.21	0.40
2:L:6:GLN:HE22	2:L:106:GLY:CA	2.25	0.40
2:L:21:ILE:O	2:L:77:THR:HA	2.21	0.40
3:I:70:ILE:O	3:I:150:ASN:ND2	2.53	0.40
3:F:50:LYS:HD2	3:F:273:PRO:HG2	2.04	0.40
3:I:47:HIS:CE1	3:I:49:GLY:O	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:299:PRO:HB2	3:F:300:ILE:HD12	2.03	0.40
3:F:30:LEU:HD21	3:I:434:GLU:HG3	2.02	0.40
1:H:157:GLU:OE2	1:H:177:ALA:CB	2.69	0.40
3:I:186:SER:HB3	3:I:227:GLU:HB3	2.04	0.40
2:L:111:ILE:C	2:L:171:GLN:HE22	2.24	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	217/227 (96%)	196 (90%)	18 (8%)	3 (1%)	11	40
1	H	217/227 (96%)	193 (89%)	21 (10%)	3 (1%)	11	40
2	B	209/219 (95%)	187 (90%)	19 (9%)	3 (1%)	11	40
2	L	213/219 (97%)	186 (87%)	20 (9%)	7 (3%)	4	24
3	F	461/505 (91%)	422 (92%)	33 (7%)	6 (1%)	12	42
3	I	460/505 (91%)	426 (93%)	32 (7%)	2 (0%)	34	68
All	All	1777/1902 (93%)	1610 (91%)	143 (8%)	24 (1%)	11	40

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	THR
2	B	82	THR
3	F	60	HIS
3	F	288	ILE
2	L	34	GLY
2	L	39	ASN
2	L	82	THR

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Mol	Chain	Res	Type
3	F	50	LYS
3	F	81	THR
2	L	32	ILE
2	B	31	TYR
2	B	102	THR
1	H	101	PRO
3	I	81	THR
2	L	97	THR
1	A	222	PRO
3	F	58	PRO
1	H	135	PRO
1	H	222	PRO
3	I	48	ASN
2	L	100	PRO
2	L	102	THR
1	A	103	ILE
3	F	284	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	186/192 (97%)	180 (97%)	6 (3%)	39	68
1	H	187/192 (97%)	181 (97%)	6 (3%)	39	68
2	B	188/194 (97%)	181 (96%)	7 (4%)	34	63
2	L	192/194 (99%)	187 (97%)	5 (3%)	46	72
3	F	407/440 (92%)	395 (97%)	12 (3%)	42	70
3	I	408/440 (93%)	398 (98%)	10 (2%)	47	73
All	All	1568/1652 (95%)	1522 (97%)	46 (3%)	42	70

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER

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Mol	Chain	Res	Type
1	A	31	SER
1	A	65	GLN
1	A	137	SER
1	A	138	LYS
1	A	139	SER
2	B	22	SER
2	B	31	TYR
2	B	33	ASP
2	B	35	ASN
2	B	38	LEU
2	B	107	THR
2	B	111	ILE
3	F	46	LYS
3	F	47	HIS
3	F	55	ARG
3	F	58	PRO
3	F	59	LEU
3	F	79	LEU
3	F	224	ARG
3	F	276	ASP
3	F	288	ILE
3	F	289	ASN
3	F	348	ASP
3	F	488	TYR
1	H	32	TYR
1	H	64	LEU
1	H	125	THR
1	H	126	LYS
1	H	138	LYS
1	H	140	THR
3	I	41	ASN
3	I	46	LYS
3	I	51	LEU
3	I	52	CYS
3	I	208	ARG
3	I	224	ARG
3	I	282	GLN
3	I	288	ILE
3	I	296	ASN
3	I	496	LYS
2	L	94	MET
2	L	99	TRP

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Mol	Chain	Res	Type
2	L	105	GLN
2	L	107	THR
2	L	111	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	GLN
2	B	35	ASN
2	B	95	GLN
3	F	289	ASN
1	H	59	ASN
3	I	41	ASN
3	I	275	HIS
3	I	296	ASN
3	I	298	HIS
2	L	6	GLN
2	L	35	ASN
2	L	39	ASN
2	L	95	GLN
2	L	98	HIS

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 ⓘ

3 monosaccharides 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	$\# Z > 2$
4	NAG	C	1	3,4	14,14,15	0.94	1 (7%)	17,19,21	1.18	1 (5%)
4	NAG	C	2	4	14,14,15	0.26	0	17,19,21	0.69	0
4	BMA	C	3	4	11,11,12	0.68	0	15,15,17	0.96	1 (6%)

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
4	NAG	C	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	3.26	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	4.63	118.47	112.19
4	C	3	BMA	C1-O5-C5	2.16	115.12	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	221/227 (97%)	2.24	91 (41%) 0 0	110, 280, 411, 476	0
1	H	221/227 (97%)	1.77	86 (38%) 0 0	146, 249, 355, 409	3 (1%)
2	B	213/219 (97%)	2.55	96 (45%) 0 0	164, 287, 364, 434	2 (0%)
2	L	217/219 (99%)	1.89	85 (39%) 0 0	143, 256, 349, 411	3 (1%)
3	F	467/505 (92%)	1.13	92 (19%) 1 1	54, 156, 288, 362	9 (1%)
3	I	466/505 (92%)	0.66	38 (8%) 11 14	47, 123, 238, 322	10 (2%)
All	All	1805/1902 (94%)	1.48	488 (27%) 0 0	47, 210, 352, 476	27 (1%)

All (488) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	334	ALA	15.9
1	A	130	VAL	14.2
1	A	134	ALA	13.4
2	B	138	VAL	12.9
1	A	147	LEU	12.8
1	A	148	GLY	12.8
1	A	128	PRO	12.6
1	A	28	SER	12.0
2	B	191	TYR	11.9
1	A	220	VAL	11.7
2	B	215	ASN	10.9
2	B	124	PRO	10.8
2	B	199	CYS	10.5
2	B	190	ASP	10.4
2	B	111	ILE	10.4
2	B	123	PHE	10.3
2	B	121	PHE	10.1
2	L	219	CYS	9.9
2	B	127	ASP	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	9.1
2	B	139	CYS	9.0
2	B	204	GLN	8.9
3	F	289	ASN	8.6
2	L	201	VAL	8.5
2	L	210	VAL	8.5
1	H	220	VAL	8.4
3	F	12	THR	8.4
3	F	467	PHE	8.3
2	B	201	VAL	8.3
1	A	135	PRO	8.1
2	B	122	ILE	8.0
2	B	136	SER	7.9
1	H	10	GLU	7.9
1	A	166	GLY	7.9
2	L	111	ILE	7.8
1	A	27	TYR	7.6
1	A	149	CYS	7.5
2	L	102	THR	7.5
1	A	200	THR	7.5
1	A	137	SER	7.4
2	B	128	GLU	7.4
2	B	219	CYS	7.4
2	B	151	VAL	7.4
2	B	114	THR	7.3
1	A	136	SER	7.2
2	B	117	ALA	7.2
2	B	217	GLY	7.1
1	A	189	SER	7.1
1	A	203	TYR	7.0
1	A	132	PRO	7.0
1	H	139	SER	6.8
3	F	333	GLY	6.8
3	F	335	ILE	6.8
2	L	121	PHE	6.8
1	H	128	PRO	6.7
2	B	214	PHE	6.7
2	B	120	VAL	6.7
3	F	486	TYR	6.6
1	A	181	SER	6.6
1	A	202	THR	6.5
1	A	194	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
2	L	176	SER	6.5
1	A	125	THR	6.3
1	A	192	THR	6.3
1	A	142	GLY	6.2
2	B	20	SER	6.2
3	F	338	PHE	6.2
1	A	146	ALA	6.1
3	I	330	GLY	6.1
1	H	39	GLN	6.1
3	F	468	GLU	6.1
3	F	15	ILE	6.0
2	L	213	SER	6.0
2	B	137	VAL	6.0
1	H	223	LYS	5.9
1	H	134	ALA	5.9
1	H	171	GLY	5.8
1	H	221	GLU	5.8
1	H	225	CYS	5.8
3	I	326	ILE	5.8
2	L	186	LEU	5.8
3	I	391	GLN	5.7
2	L	165	GLN	5.7
2	B	17	GLN	5.7
2	B	99	TRP	5.7
2	B	80	ILE	5.6
2	B	208	SER	5.6
2	L	140	LEU	5.5
2	L	173	SER	5.5
1	A	141	SER	5.5
1	H	48	MET	5.5
1	H	140	THR	5.5
1	A	127	GLY	5.4
3	F	55(A)	GLY	5.4
3	F	336	ALA	5.4
3	I	328	SER	5.4
1	A	10	GLU	5.3
1	A	41	PRO	5.3
3	F	356	GLN	5.3
1	H	163	TRP	5.3
3	F	390	THR	5.2
2	L	175	ASP	5.2
1	H	11	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
3	F	13	LEU	5.2
3	F	470	TYR	5.1
1	H	203	TYR	5.1
1	A	167	ALA	5.1
3	F	330	GLY	5.1
3	F	412	LYS	5.0
1	H	148	GLY	5.0
1	H	141	SER	4.9
3	F	469	PHE	4.9
1	H	144	THR	4.9
2	B	90	VAL	4.9
2	B	186	LEU	4.9
2	L	204	GLN	4.9
3	F	11	ASP	4.9
3	F	455	LEU	4.9
1	H	17	SER	4.9
2	B	37	TYR	4.9
3	I	327	GLN	4.8
2	B	156	ASP	4.8
2	L	164	SER	4.8
3	F	465	GLY	4.8
1	A	154	TYR	4.8
2	L	109	VAL	4.8
1	H	201	GLN	4.8
1	H	142	GLY	4.7
3	I	348	ASP	4.7
1	A	88	SER	4.6
2	B	107	THR	4.6
2	B	210	VAL	4.6
1	A	44	GLY	4.6
1	H	44	GLY	4.6
3	I	290	THR	4.6
1	H	192	THR	4.5
2	L	85	ALA	4.5
2	B	126	SER	4.5
3	F	361	SER	4.5
2	L	11	LEU	4.5
1	A	225	CYS	4.5
1	H	159	VAL	4.5
2	L	115	VAL	4.5
2	L	37	TYR	4.4
2	L	103	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	118	PRO	4.4
2	L	130	LEU	4.4
2	L	187	SER	4.4
2	L	161	SER	4.3
1	A	140	THR	4.3
1	A	188	SER	4.3
2	B	164	SER	4.3
3	F	282	GLN	4.3
2	B	166	GLU	4.3
1	A	124	SER	4.3
3	I	340	GLU	4.3
2	B	125	PRO	4.3
1	H	43	GLN	4.3
2	L	3	VAL	4.3
3	F	294	PHE	4.2
3	F	413	VAL	4.2
2	L	20	SER	4.2
1	A	131	PHE	4.2
1	H	224	SER	4.2
2	L	138	VAL	4.2
1	H	133	LEU	4.2
2	L	105	GLN	4.2
1	H	199	GLY	4.2
3	F	17	TYR	4.1
1	H	214	THR	4.1
1	H	200	THR	4.1
3	F	460	LYS	4.1
3	F	345	GLY	4.1
2	L	134	THR	4.1
2	L	174	LYS	4.1
3	I	279	THR	4.1
3	F	293	PRO	4.0
2	L	1	ASP	4.0
2	L	206	LEU	4.0
2	B	21	ILE	4.0
3	F	14	CYS	4.0
1	A	43	GLN	4.0
2	B	195	LYS	4.0
3	F	55	ARG	4.0
1	H	170	SER	4.0
3	F	291	SER	3.9
1	A	163	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
3	F	355	HIS	3.8
1	A	150	LEU	3.8
1	A	159	VAL	3.8
1	A	193	VAL	3.8
2	B	63	VAL	3.8
2	L	151	VAL	3.8
2	B	162	GLY	3.8
2	L	117	ALA	3.8
1	A	139	SER	3.8
3	F	127	TRP	3.8
3	F	487	ASP	3.7
3	F	358	GLU	3.7
2	B	140	LEU	3.7
3	F	417	PHE	3.7
2	B	91	TYR	3.7
2	L	92	TYR	3.7
2	L	108	LYS	3.7
2	B	46	GLY	3.6
2	L	181	SER	3.6
1	H	18	VAL	3.6
2	B	109	VAL	3.6
1	H	186	SER	3.6
2	B	187	SER	3.6
2	B	41	PHE	3.6
3	F	478	MET	3.6
2	L	120	VAL	3.6
1	H	176	PRO	3.6
2	L	191	TYR	3.6
2	L	87	ASP	3.5
3	I	346	MET	3.5
3	F	332	PHE	3.5
2	L	142	ASN	3.5
3	F	276	ASP	3.5
2	L	67	PHE	3.5
1	H	149	CYS	3.5
2	B	165	GLN	3.4
3	F	288	ILE	3.4
3	I	417	PHE	3.4
1	H	83	LEU	3.4
1	H	151	VAL	3.4
1	H	190	VAL	3.4
2	B	92	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
2	L	33	ASP	3.4
3	I	329	ARG	3.4
1	H	175	PHE	3.4
2	L	123	PHE	3.4
3	I	467	PHE	3.3
1	A	83	LEU	3.3
3	F	462	ILE	3.3
3	I	225	ASP	3.3
1	A	191	VAL	3.3
1	A	201	GLN	3.3
3	F	416	GLY	3.3
1	H	189	SER	3.2
1	A	190	VAL	3.2
2	B	57	PHE	3.2
1	H	138	LYS	3.2
2	B	62	GLY	3.2
2	L	21	ILE	3.2
1	H	195	SER	3.2
2	B	184	LEU	3.2
1	H	145	ALA	3.2
1	H	193	VAL	3.2
1	A	8	GLY	3.2
1	A	42	GLY	3.2
1	A	170	SER	3.2
2	L	167	SER	3.2
1	A	92	ALA	3.1
1	A	207	VAL	3.1
3	F	366	ASP	3.1
3	F	418	LEU	3.1
3	F	310	LYS	3.1
3	F	159	ASN	3.1
1	A	165	SER	3.1
2	B	52	LEU	3.1
1	H	58	THR	3.1
3	F	343	TRP	3.1
2	B	212	LYS	3.0
3	F	278	ASN	3.0
3	F	466	CYS	3.0
1	A	196	SER	3.0
2	B	61	SER	3.0
2	L	42	GLN	3.0
3	F	346	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	66	ARG	3.0
3	F	481	VAL	3.0
2	L	34	GLY	3.0
3	F	363	TYR	3.0
2	L	208	SER	3.0
3	I	325	SER	3.0
2	B	161	SER	3.0
1	A	144	THR	3.0
1	H	143	GLY	3.0
2	L	91	TYR	3.0
2	L	190	ASP	3.0
1	H	198	LEU	3.0
2	B	15	LEU	3.0
3	F	43	LEU	3.0
1	A	222	PRO	3.0
2	B	163	ASN	2.9
2	B	38	LEU	2.9
1	H	154	TYR	2.9
2	L	93	CYS	2.9
2	L	195	LYS	2.9
2	B	202	THR	2.9
2	B	45	PRO	2.9
3	F	459	ALA	2.9
1	A	48	MET	2.9
2	L	211	THR	2.9
1	H	38	ARG	2.9
3	F	461	GLU	2.9
3	F	283	THR	2.9
1	H	110	ASP	2.9
3	I	245	PHE	2.9
3	F	482	LYS	2.9
3	I	415	ASP	2.9
3	F	422	THR	2.9
1	H	177	ALA	2.9
2	B	216	ARG	2.8
3	F	362	GLY	2.8
1	A	9	ALA	2.8
2	L	64	PRO	2.8
2	L	83	VAL	2.8
3	I	350	TRP	2.8
2	B	174	LYS	2.8
2	B	213	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	218	LYS	2.8
1	H	204	ILE	2.8
1	A	221	GLU	2.8
3	F	410	ASN	2.8
2	L	62	GLY	2.8
3	I	15	ILE	2.7
3	F	287	ALA	2.7
1	H	130	VAL	2.7
2	B	182	SER	2.7
1	H	60	TYR	2.7
1	H	146	ALA	2.7
1	H	111	TYR	2.7
1	A	118	VAL	2.7
2	B	35	ASN	2.7
2	B	49	PRO	2.7
3	F	284	PRO	2.7
1	A	17	SER	2.7
2	B	85	ALA	2.7
1	H	68	VAL	2.7
2	B	16	GLY	2.7
2	B	176	SER	2.7
3	F	53	LYS	2.7
3	F	285	LYS	2.7
3	F	348	ASP	2.6
3	I	338	PHE	2.6
1	A	164	ASN	2.6
1	A	38	ARG	2.6
1	A	183	GLY	2.6
3	F	415	ASP	2.6
3	I	48	ASN	2.6
2	L	166	GLU	2.6
1	A	85	SER	2.6
2	B	14	THR	2.6
1	H	42	GLY	2.6
3	F	286	GLY	2.6
1	H	51	ILE	2.6
2	L	29	LEU	2.6
3	I	448	TYR	2.6
2	B	197	TYR	2.6
2	L	212	LYS	2.6
2	B	119	SER	2.6
1	H	55	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	463	GLY	2.5
3	F	297	ILE	2.5
2	L	81	THR	2.5
3	F	318	THR	2.5
1	A	180	GLN	2.5
1	A	102	HIS	2.5
2	B	89	GLY	2.5
1	A	57	ASN	2.5
3	I	353	TYR	2.5
2	L	80	ILE	2.5
1	A	145	ALA	2.5
3	I	416	GLY	2.5
1	H	147	LEU	2.5
2	L	59	ARG	2.5
1	H	19	LYS	2.5
1	A	157	GLU	2.5
1	A	107	PHE	2.5
1	A	62	GLN	2.5
1	H	102	HIS	2.5
3	F	147	PHE	2.5
2	B	141	LEU	2.5
2	L	178	TYR	2.5
1	H	132	PRO	2.5
1	H	212	SER	2.5
1	H	86	LEU	2.5
1	A	58	THR	2.4
3	F	271	ASP	2.4
1	A	129	SER	2.4
2	B	178	TYR	2.4
2	B	110	GLU	2.4
2	L	209	PRO	2.4
1	H	219	LYS	2.4
2	L	126	SER	2.4
3	F	353	TYR	2.4
2	B	86	GLU	2.4
3	F	279	THR	2.4
3	F	237	VAL	2.4
1	H	131	PHE	2.4
3	I	297	ILE	2.4
2	B	207	ARG	2.4
1	H	135	PRO	2.4
3	I	176	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	153	TRP	2.4
3	F	441	ASP	2.4
1	A	80	TYR	2.4
1	H	81	MET	2.4
3	F	260	MET	2.4
2	L	51	ARG	2.4
2	L	19	ALA	2.4
2	L	35	ASN	2.4
1	H	150	LEU	2.4
1	A	151	VAL	2.4
2	L	182	SER	2.4
3	F	454	GLN	2.4
3	I	492	SER	2.4
1	A	187	LEU	2.4
1	H	20	VAL	2.3
1	H	112	TRP	2.3
2	B	42	GLN	2.3
3	F	299	PRO	2.3
3	I	288	ILE	2.3
2	B	93	CYS	2.3
1	H	174	THR	2.3
3	I	485	THR	2.3
1	H	168	LEU	2.3
2	L	180	LEU	2.3
3	I	101	ASP	2.3
1	A	103	ILE	2.3
3	F	414	ASP	2.3
2	L	154	LYS	2.3
1	H	173	HIS	2.3
2	L	101	TYR	2.3
2	L	127	ASP	2.3
3	F	300	ILE	2.3
3	F	411	LYS	2.3
2	B	196	VAL	2.3
3	F	423	TYR	2.3
3	I	345	GLY	2.2
2	B	205	GLY	2.2
1	A	14	PRO	2.2
1	A	94	PHE	2.2
2	B	19	ALA	2.2
2	L	160	GLN	2.2
3	F	18	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	245	PHE	2.2
1	A	197	SER	2.2
1	A	45	LEU	2.2
1	H	202	THR	2.2
1	H	85	SER	2.2
3	I	311	SER	2.2
2	B	116	ALA	2.2
2	L	84	GLU	2.2
1	H	109	PHE	2.2
1	A	138	LYS	2.2
3	I	49	GLY	2.2
2	L	200	GLU	2.2
1	H	157	GLU	2.2
2	L	63	VAL	2.2
3	F	488	TYR	2.1
2	L	90	VAL	2.1
3	F	302	ILE	2.1
3	F	473	CYS	2.1
1	A	39	GLN	2.1
2	B	200	GLU	2.1
1	A	53	ALA	2.1
1	H	36	TRP	2.1
2	B	183	THR	2.1
1	A	161	VAL	2.1
2	B	129	GLN	2.1
1	H	47	TRP	2.1
2	L	89	GLY	2.1
2	B	81	THR	2.1
1	H	205	CYS	2.1
1	A	143	GLY	2.1
1	H	71	THR	2.1
2	B	130	LEU	2.1
3	I	427	LEU	2.1
1	H	46	GLU	2.1
3	F	331	LEU	2.1
2	L	39	ASN	2.1
3	F	100	GLY	2.1
3	I	440	HIS	2.1
2	B	55	ASN	2.0
2	L	163	ASN	2.0
3	I	41	ASN	2.0
2	B	159	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	299	PRO	2.0
3	I	432	GLU	2.0
1	A	18	VAL	2.0
2	B	64	PRO	2.0
2	L	118	PRO	2.0
1	A	89	ASP	2.0
1	H	188	SER	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](#)

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(Å ²)	Q<0.9
4	BMA	C	3	11/12	0.47	0.39	247,256,270,274	0
4	NAG	C	2	14/15	0.49	0.62	250,259,274,277	0
4	NAG	C	1	14/15	0.59	0.30	212,224,243,250	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.