



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2017 – 02:00 PM EDT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

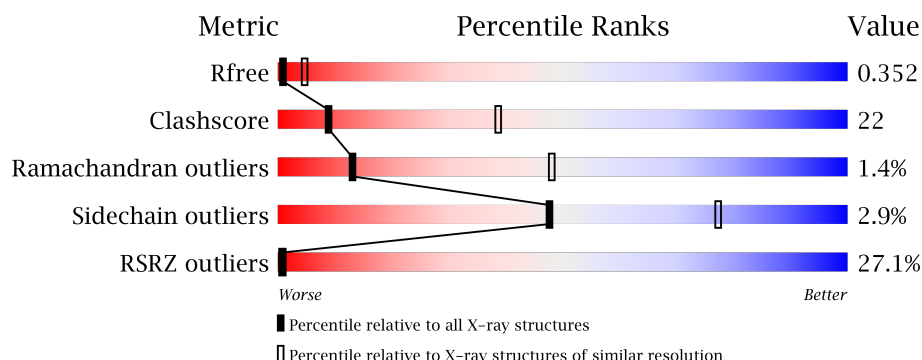
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1241 (3.46-3.30)
Clashscore	112137	1319 (3.46-3.30)
Ramachandran outliers	110173	1298 (3.46-3.30)
Sidechain outliers	110143	1297 (3.46-3.30)
RSRZ outliers	101464	1251 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	<div> <div>41%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>
1	H	227	<div> <div>38%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• •</div> </div> </div>
2	B	219	<div> <div>44%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• •</div> </div> </div>
2	L	219	<div> <div>39%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
3	F	505	<div> <div>18%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>• • 8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	I	505	<div><div></div><div>8%</div><div>76%</div><div>15%</div><div>•</div><div>8%</div></div>

## 2 Entry composition

There are 5 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:

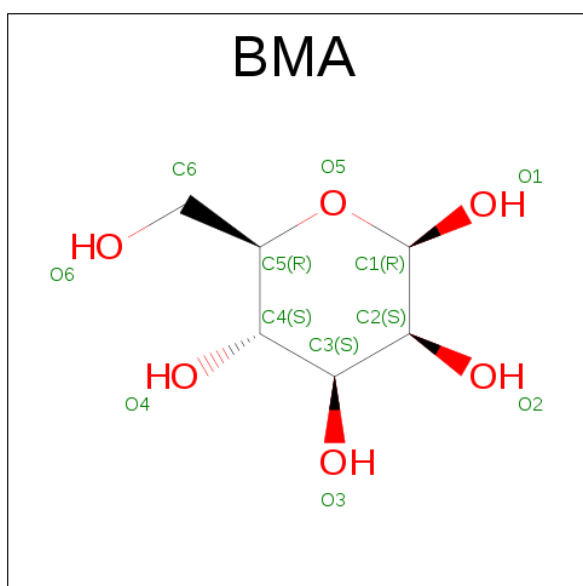
Chain	Residue	Modelled	Actual	Comment	Reference
F	506	SER	-	expression tag	UNP C3W5S1
F	507	GLY	-	expression tag	UNP C3W5S1
I	506	SER	-	expression tag	UNP C3W5S1
I	507	GLY	-	expression tag	UNP C3W5S1

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

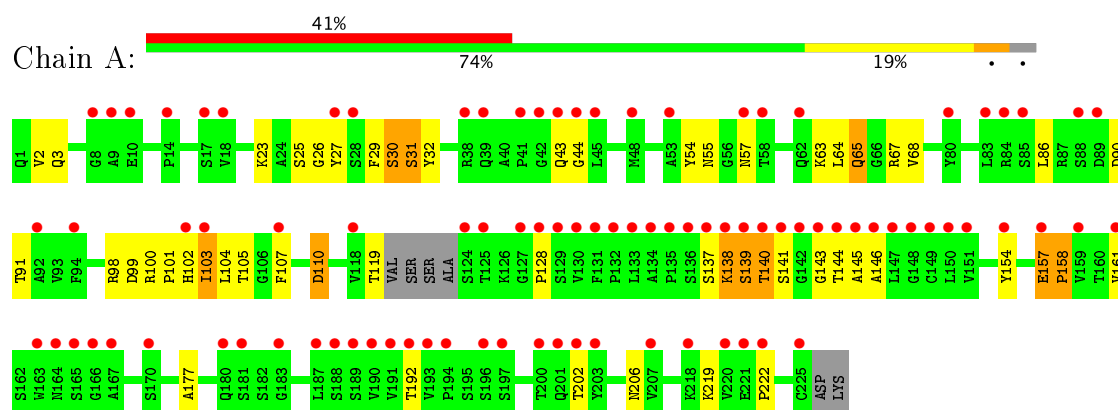


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			11	6	5		

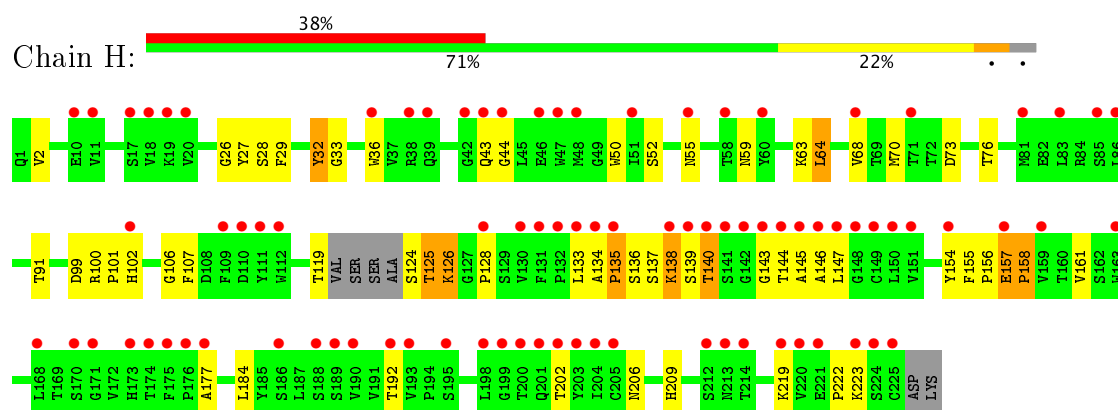
### 3 Residue-property plots [i](#)

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

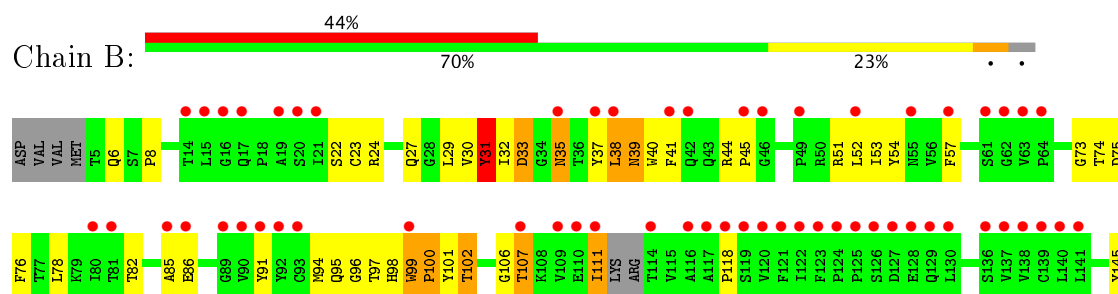
#### • Molecule 1: 31.b.09 Heavy Fv

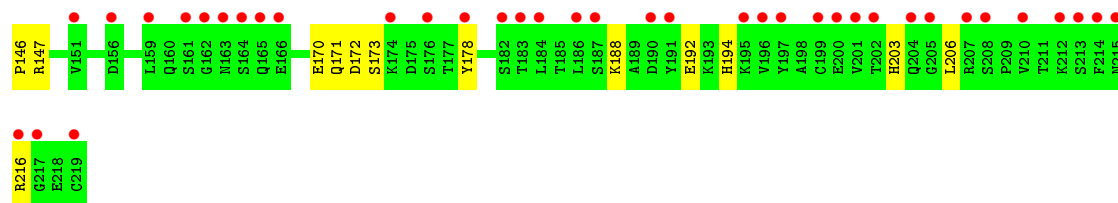


#### • Molecule 1: 31.b.09 Heavy Fv

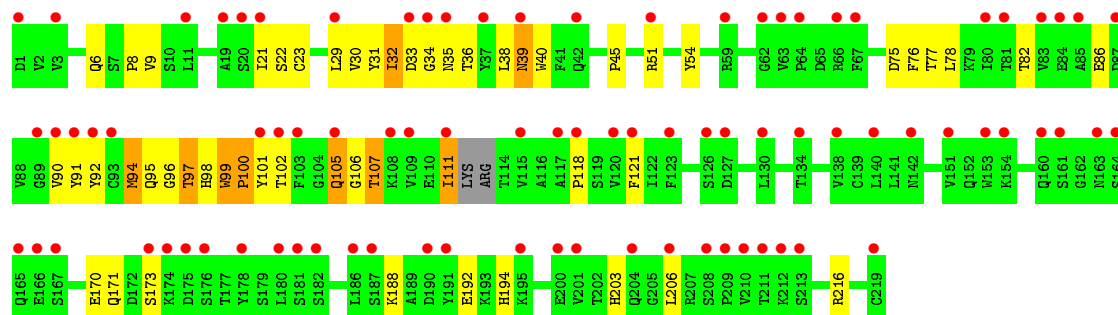
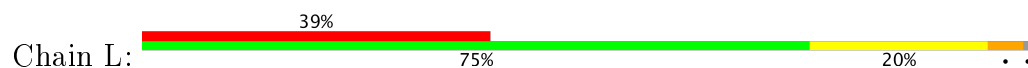


#### • Molecule 2: 31.b.09 Light Fv

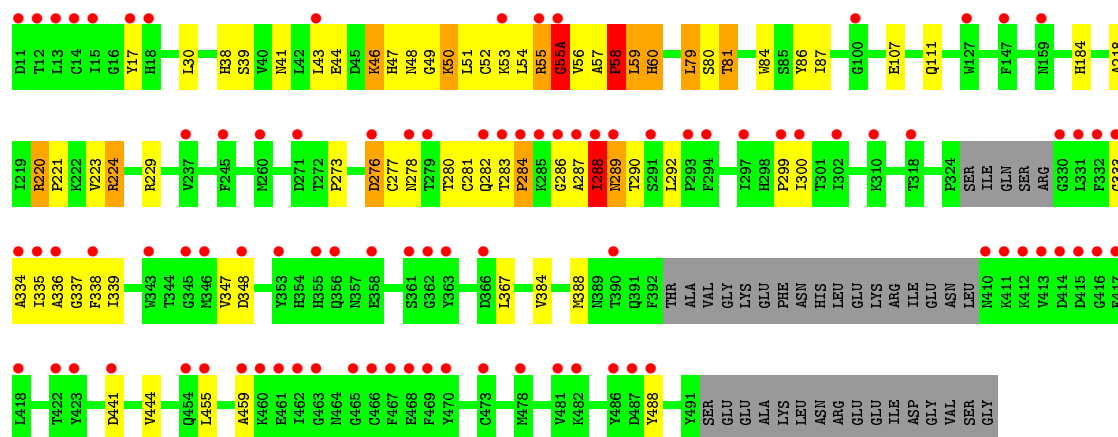
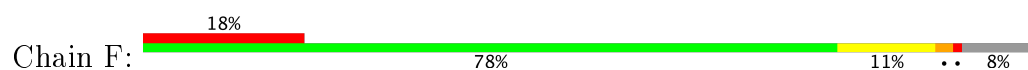




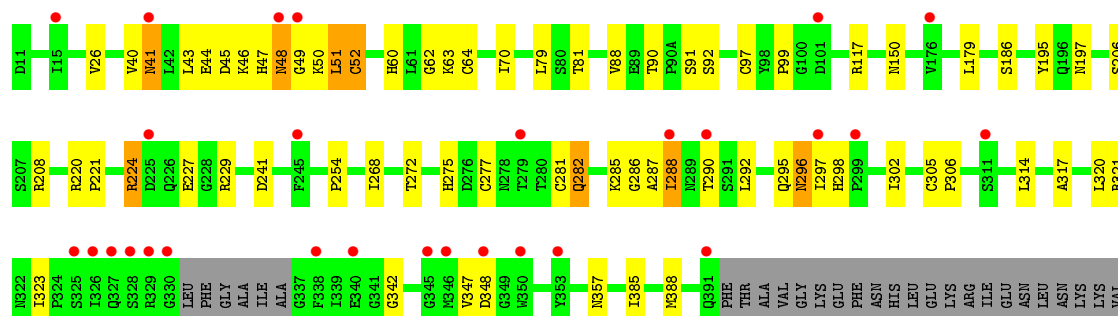
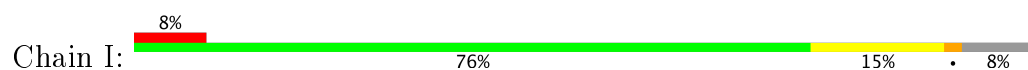
• Molecule 2: 31.b.09 Light Fv

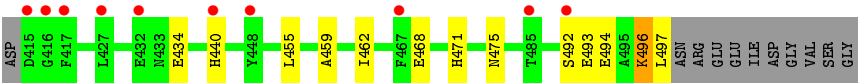


• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.291 , 0.346 0.302 , 0.352	Depositor DCC
$R_{free}$ test set	1430 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 160.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	119	0
2	L	1684	0	1621	111	0
3	F	3685	0	3557	139	0
3	I	3678	0	3546	104	0
4	I	28	0	24	0	0
5	I	11	0	10	0	0
All	All	14056	0	13574	621	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 22.

All (621) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PHE:CZ	2:B:99:TRP:CH2	1.76	1.64
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
2:B:57:PHE:CB	3:F:289:ASN:ND2	1.95	1.29
3:F:280:THR:OG1	3:F:288:ILE:HD11	1.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:LEU:HB2	2:L:94:MET:HG3	1.37	1.06
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:32:ILE:HG22	2:L:33:ASP:H	1.31	0.94
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:46:LYS:NZ	3:F:287:ALA:O	2.12	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:SER:C	1:H:155:PHE:CD1	2.58	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:272:THR:HG21	3:I:285:LYS:HG3	1.74	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:ASN:OD1	2:L:94:MET:SD	2.54	0.65
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:38:LEU:H	2:L:94:MET:CG	2.11	0.63
2:L:95:GLN:CG	2:L:101:TYR:HA	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:287:ALA:HB1	3:F:289:ASN:CB	2.30	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ARG:HB3	2:B:75:ASP:OD2	2.04	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:LEU:O	1:H:68:VAL:HG22	2.08	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:GLN:HG3	1:H:44:GLY:N	2.24	0.51
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:95:GLN:HB3	2:B:101:TYR:HB3	1.94	0.48
2:B:91:TYR:O	2:B:106:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:220:ARG:HG3	3:F:229:ARG:HG3	1.94	0.48
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
3:I:492:SER:HB2	3:I:494:GLU:HG2	1.95	0.48
1:H:140:THR:HG22	2:L:121:PHE:CD2	2.49	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:6:GLN:HE21	2:L:105:GLN:H	1.62	0.47
2:L:38:LEU:N	2:L:94:MET:HG3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:SER:C	1:A:141:SER:N	2.57	0.47
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:40:TRP:HE3	2:B:78:LEU:CD2	2.29	0.45
2:B:75:ASP:C	2:B:76:PHE:CD1	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:THR:HG21	1:H:145:ALA:C	2.38	0.44
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
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:40:TRP:HE3	2:B:78:LEU:HD23	1.84	0.42
2:B:39:ASN:HB2	2:B:53:ILE:O	2.19	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:91:THR:CG2	1:H:119:THR:HA	2.50	0.41
1:H:138:LYS:O	1:H:138:LYS:HD2	2.21	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%)	13	48
1	H	217/227 (96%)	193 (89%)	21 (10%)	3 (1%)	13	48
2	B	209/219 (95%)	187 (90%)	19 (9%)	3 (1%)	13	48
2	L	213/219 (97%)	186 (87%)	20 (9%)	7 (3%)	4	30
3	F	461/505 (91%)	422 (92%)	33 (7%)	6 (1%)	14	50
3	I	460/505 (91%)	426 (93%)	32 (7%)	2 (0%)	38	75
All	All	1777/1902 (93%)	1610 (91%)	143 (8%)	24 (1%)	13	48

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%)	44	76
1	H	187/192 (97%)	181 (97%)	6 (3%)	44	76
2	B	188/194 (97%)	181 (96%)	7 (4%)	39	72
2	L	192/194 (99%)	187 (97%)	5 (3%)	51	79
3	F	407/440 (92%)	395 (97%)	12 (3%)	48	77
3	I	408/440 (93%)	398 (98%)	10 (2%)	53	80
All	All	1568/1652 (95%)	1522 (97%)	46 (3%)	48	77

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 [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
4	NAG	I	601	3,4	14,14,15	0.92	1 (7%)	15,19,21	1.25	1 (6%)
4	NAG	I	602	5,4	14,14,15	0.25	0	15,19,21	0.75	0
5	BMA	I	603	4	11,11,12	0.68	0	13,15,17	0.99	1 (7%)

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	I	601	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	602	5,4	-	0/6/23/26	0/1/1/1
5	BMA	I	603	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	I	601	NAG	O5-C1	3.18	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	603	BMA	C1-O5-C5	2.14	115.12	112.17
4	I	601	NAG	C1-O5-C5	4.57	118.47	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	221/227 (97%)	2.24	92 (41%) 0 0	110, 280, 411, 476	0
1	H	221/227 (97%)	1.77	87 (39%) 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%)	1.12	92 (19%) 1 1	54, 156, 288, 362	9 (1%)
3	I	466/505 (92%)	0.66	38 (8%) 12 14	47, 123, 238, 322	10 (2%)
All	All	1805/1902 (94%)	1.48	490 (27%) 1 1	47, 210, 352, 476	27 (1%)

All (490) 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	12.7
1	A	28	SER	11.9
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	123	PHE	10.4
2	B	111	ILE	10.4
2	B	121	PHE	10.1
2	L	219	CYS	9.9
1	A	133	LEU	9.1

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Mol	Chain	Res	Type	RSRZ
2	B	127	ASP	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
3	F	12	THR	8.4
1	H	220	VAL	8.4
3	F	467	PHE	8.3
2	B	201	VAL	8.3
1	A	135	PRO	8.1
2	B	122	ILE	7.9
2	B	136	SER	7.9
1	A	166	GLY	7.9
1	H	10	GLU	7.9
2	L	111	ILE	7.7
1	A	149	CYS	7.6
1	A	27	TYR	7.5
2	L	102	THR	7.5
1	A	200	THR	7.5
2	B	219	CYS	7.4
1	A	137	SER	7.4
2	B	128	GLU	7.4
2	B	151	VAL	7.4
1	A	136	SER	7.2
2	B	114	THR	7.2
2	B	217	GLY	7.2
2	B	117	ALA	7.2
1	A	189	SER	7.1
1	A	203	TYR	6.9
1	A	132	PRO	6.9
3	F	333	GLY	6.9
1	H	139	SER	6.8
2	L	121	PHE	6.8
3	F	335	ILE	6.8
1	H	128	PRO	6.8
2	B	120	VAL	6.7
2	B	214	PHE	6.6
1	A	181	SER	6.6
1	A	202	THR	6.6
3	F	486	TYR	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	6.2
2	B	20	SER	6.2
1	A	142	GLY	6.2
3	F	338	PHE	6.2
1	A	146	ALA	6.1
1	H	39	GLN	6.1
3	I	330	GLY	6.1
3	F	468	GLU	6.0
3	F	15	ILE	6.0
2	L	213	SER	6.0
2	B	137	VAL	5.9
1	H	223	LYS	5.9
1	H	134	ALA	5.9
1	H	221	GLU	5.8
1	H	171	GLY	5.8
1	H	225	CYS	5.8
3	I	326	ILE	5.8
2	L	186	LEU	5.7
3	I	391	GLN	5.7
2	B	17	GLN	5.7
2	B	80	ILE	5.6
2	B	99	TRP	5.6
2	L	165	GLN	5.6
2	B	208	SER	5.6
2	L	140	LEU	5.5
1	A	141	SER	5.5
2	L	173	SER	5.5
1	H	140	THR	5.5
1	H	48	MET	5.4
1	A	127	GLY	5.4
3	F	55(A)	GLY	5.4
3	I	328	SER	5.4
1	A	10	GLU	5.4
3	F	336	ALA	5.4
1	A	41	PRO	5.3
1	H	163	TRP	5.3
1	H	11	VAL	5.3
3	F	356	GLN	5.3
3	F	390	THR	5.2
2	L	175	ASP	5.2

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

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Mol	Chain	Res	Type	RSRZ
2	L	187	SER	4.4
2	B	118	PRO	4.4
2	L	130	LEU	4.4
2	L	161	SER	4.3
1	A	140	THR	4.3
2	B	164	SER	4.3
2	B	166	GLU	4.3
3	F	282	GLN	4.3
1	A	188	SER	4.3
3	I	340	GLU	4.3
1	A	124	SER	4.3
2	B	125	PRO	4.3
1	H	43	GLN	4.3
2	L	3	VAL	4.3
3	F	294	PHE	4.3
2	L	20	SER	4.2
3	F	413	VAL	4.2
1	A	131	PHE	4.2
1	H	224	SER	4.2
2	L	105	GLN	4.2
2	L	138	VAL	4.2
1	H	133	LEU	4.2
1	H	199	GLY	4.2
3	F	17	TYR	4.1
1	H	200	THR	4.1
2	L	174	LYS	4.1
1	H	214	THR	4.1
3	F	460	LYS	4.1
2	L	134	THR	4.1
3	F	345	GLY	4.1
3	I	279	THR	4.1
3	F	293	PRO	4.0
2	L	206	LEU	4.0
2	B	21	ILE	4.0
2	L	1	ASP	4.0
3	F	14	CYS	4.0
2	B	195	LYS	4.0
1	A	43	GLN	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	193	VAL	3.8
2	B	63	VAL	3.8
1	A	159	VAL	3.8
2	L	151	VAL	3.8
1	A	139	SER	3.8
2	L	117	ALA	3.8
2	B	162	GLY	3.8
3	F	487	ASP	3.7
3	F	127	TRP	3.7
2	B	140	LEU	3.7
3	F	358	GLU	3.7
3	F	417	PHE	3.7
2	L	108	LYS	3.7
2	B	91	TYR	3.7
2	L	92	TYR	3.7
2	L	181	SER	3.6
2	B	46	GLY	3.6
1	H	18	VAL	3.6
2	B	109	VAL	3.6
3	F	478	MET	3.6
1	H	186	SER	3.6
2	B	41	PHE	3.6
2	B	187	SER	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	67	PHE	3.5
2	L	142	ASN	3.5
1	H	149	CYS	3.5
3	F	276	ASP	3.5
3	I	417	PHE	3.5
2	B	165	GLN	3.4
3	F	288	ILE	3.4
1	H	190	VAL	3.4
1	H	83	LEU	3.4
1	H	151	VAL	3.4
1	H	175	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
3	I	329	ARG	3.4
2	L	33	ASP	3.4
2	B	92	TYR	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	F	416	GLY	3.3
3	I	225	ASP	3.3
1	A	191	VAL	3.3
1	A	201	GLN	3.3
1	H	189	SER	3.3
1	A	190	VAL	3.3
2	B	62	GLY	3.2
1	H	138	LYS	3.2
2	L	21	ILE	3.2
2	B	57	PHE	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
2	L	167	SER	3.2
1	A	170	SER	3.2
1	A	8	GLY	3.1
1	A	92	ALA	3.1
1	A	42	GLY	3.1
1	A	207	VAL	3.1
3	F	366	ASP	3.1
3	F	310	LYS	3.1
2	B	52	LEU	3.1
3	F	418	LEU	3.1
1	A	165	SER	3.1
3	F	159	ASN	3.1
1	H	58	THR	3.1
3	F	343	TRP	3.1
3	F	466	CYS	3.1
3	F	278	ASN	3.0
2	B	212	LYS	3.0
1	A	196	SER	3.0
2	L	42	GLN	3.0
2	B	61	SER	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	363	TYR	3.0
3	F	481	VAL	3.0
2	L	34	GLY	3.0
1	H	143	GLY	3.0
2	B	161	SER	3.0
2	L	91	TYR	3.0
2	L	208	SER	3.0
3	F	43	LEU	3.0
3	I	325	SER	3.0
1	A	144	THR	3.0
1	H	198	LEU	3.0
2	L	190	ASP	3.0
2	B	163	ASN	3.0
1	A	222	PRO	2.9
2	B	15	LEU	2.9
1	H	154	TYR	2.9
2	L	93	CYS	2.9
2	B	38	LEU	2.9
3	F	459	ALA	2.9
2	B	202	THR	2.9
2	B	45	PRO	2.9
1	H	110	ASP	2.9
2	L	195	LYS	2.9
2	L	211	THR	2.9
3	F	283	THR	2.9
3	F	461	GLU	2.9
1	A	48	MET	2.9
1	H	38	ARG	2.9
3	I	415	ASP	2.9
3	I	245	PHE	2.9
3	F	422	THR	2.9
1	H	177	ALA	2.9
3	F	482	LYS	2.9
2	L	64	PRO	2.8
2	B	216	ARG	2.8
1	A	9	ALA	2.8
3	F	362	GLY	2.8
2	L	83	VAL	2.8
2	B	174	LYS	2.8
3	I	350	TRP	2.8
2	B	213	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLU	2.8
3	F	410	ASN	2.8
2	L	62	GLY	2.8
1	A	218	LYS	2.8
1	H	204	ILE	2.8
3	F	287	ALA	2.8
3	I	15	ILE	2.7
1	H	146	ALA	2.7
1	H	60	TYR	2.7
1	H	130	VAL	2.7
1	H	111	TYR	2.7
2	B	182	SER	2.7
2	B	16	GLY	2.7
1	A	17	SER	2.7
2	B	35	ASN	2.7
2	B	49	PRO	2.7
3	F	284	PRO	2.7
2	B	85	ALA	2.7
2	B	176	SER	2.7
1	A	118	VAL	2.7
3	F	53	LYS	2.6
3	F	348	ASP	2.6
1	H	68	VAL	2.6
3	F	285	LYS	2.6
3	I	338	PHE	2.6
1	A	164	ASN	2.6
1	A	38	ARG	2.6
3	I	48	ASN	2.6
1	A	183	GLY	2.6
2	L	166	GLU	2.6
3	F	415	ASP	2.6
2	B	14	THR	2.6
1	H	51	ILE	2.6
1	A	85	SER	2.6
1	H	42	GLY	2.6
3	F	286	GLY	2.6
2	L	29	LEU	2.6
2	B	197	TYR	2.6
3	I	448	TYR	2.6
2	L	212	LYS	2.6
2	B	119	SER	2.6
3	F	318	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	89	GLY	2.5
3	I	416	GLY	2.5
3	F	297	ILE	2.5
1	A	57	ASN	2.5
1	H	55	ASN	2.5
1	A	180	GLN	2.5
3	I	353	TYR	2.5
3	F	463	GLY	2.5
1	A	102	HIS	2.5
2	L	80	ILE	2.5
1	A	145	ALA	2.5
2	L	81	THR	2.5
1	H	147	LEU	2.5
2	L	59	ARG	2.5
1	A	157	GLU	2.5
1	H	19	LYS	2.5
1	A	62	GLN	2.5
1	H	132	PRO	2.5
1	H	86	LEU	2.5
2	L	178	TYR	2.5
1	A	107	PHE	2.5
3	F	147	PHE	2.5
1	H	102	HIS	2.5
2	B	141	LEU	2.5
1	H	212	SER	2.5
2	L	209	PRO	2.4
2	B	86	GLU	2.4
1	A	129	SER	2.4
2	B	178	TYR	2.4
1	A	58	THR	2.4
3	F	271	ASP	2.4
2	L	126	SER	2.4
1	H	219	LYS	2.4
1	H	131	PHE	2.4
3	F	353	TYR	2.4
2	B	110	GLU	2.4
3	F	279	THR	2.4
2	B	207	ARG	2.4
3	F	237	VAL	2.4
1	H	135	PRO	2.4
2	L	153	TRP	2.4
1	A	80	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	297	ILE	2.4
3	I	176	VAL	2.4
3	F	441	ASP	2.4
3	I	492	SER	2.4
2	L	51	ARG	2.4
2	L	35	ASN	2.4
1	H	150	LEU	2.4
2	L	182	SER	2.4
3	F	260	MET	2.4
3	F	299	PRO	2.4
1	A	187	LEU	2.4
1	H	112	TRP	2.3
1	H	81	MET	2.3
2	B	42	GLN	2.3
1	A	151	VAL	2.3
1	H	20	VAL	2.3
3	F	454	GLN	2.3
2	L	19	ALA	2.3
3	I	288	ILE	2.3
2	B	93	CYS	2.3
1	H	174	THR	2.3
1	H	168	LEU	2.3
3	I	485	THR	2.3
1	A	103	ILE	2.3
2	L	180	LEU	2.3
3	I	101	ASP	2.3
2	L	154	LYS	2.3
3	F	411	LYS	2.3
2	L	127	ASP	2.3
3	F	414	ASP	2.3
1	H	173	HIS	2.3
2	B	19	ALA	2.3
2	B	196	VAL	2.3
2	L	101	TYR	2.3
3	F	423	TYR	2.3
3	F	300	ILE	2.2
1	A	14	PRO	2.2
1	A	94	PHE	2.2
2	B	205	GLY	2.2
2	L	160	GLN	2.2
1	A	197	SER	2.2
3	F	18	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	345	GLY	2.2
3	F	245	PHE	2.2
1	A	45	LEU	2.2
1	H	202	THR	2.2
1	A	138	LYS	2.2
1	H	85	SER	2.2
3	I	311	SER	2.2
2	B	116	ALA	2.2
1	H	109	PHE	2.2
2	L	84	GLU	2.2
3	I	49	GLY	2.2
1	H	157	GLU	2.2
3	F	302	ILE	2.2
2	L	90	VAL	2.1
2	L	200	GLU	2.1
3	F	473	CYS	2.1
3	F	488	TYR	2.1
1	A	161	VAL	2.1
2	L	63	VAL	2.1
1	A	53	ALA	2.1
2	B	200	GLU	2.1
1	H	36	TRP	2.1
2	B	183	THR	2.1
2	B	129	GLN	2.1
1	A	143	GLY	2.1
1	H	47	TRP	2.1
1	H	205	CYS	2.1
1	A	39	GLN	2.1
2	B	81	THR	2.1
2	L	89	GLY	2.1
2	L	39	ASN	2.1
2	B	130	LEU	2.1
3	F	331	LEU	2.1
3	I	427	LEU	2.1
1	H	71	THR	2.1
1	H	46	GLU	2.1
2	B	159	LEU	2.1
3	F	100	GLY	2.1
3	I	440	HIS	2.1
1	A	18	VAL	2.0
2	L	163	ASN	2.0
3	I	41	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	299	PRO	2.0
2	B	55	ASN	2.0
3	I	432	GLU	2.0
1	H	188	SER	2.0
2	L	118	PRO	2.0
1	A	89	ASP	2.0
2	B	64	PRO	2.0
1	H	213	ASN	2.0
1	A	84	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	I	602	14/15	0.50	0.61	-	250,259,274,277	0
4	NAG	I	601	14/15	0.59	0.30	-	212,224,243,250	0
5	BMA	I	603	11/12	0.47	0.39	-	247,256,270,274	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.