



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1NB5  
Title : Crystal structure of stefin A in complex with cathepsin H  
Authors : Jenko, S.; Dolenc, I.; Guncar, G.; Dobersek, A.; Podobnik, M.; Turk, D.  
Deposited on : 2002-12-02  
Resolution : 2.40 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

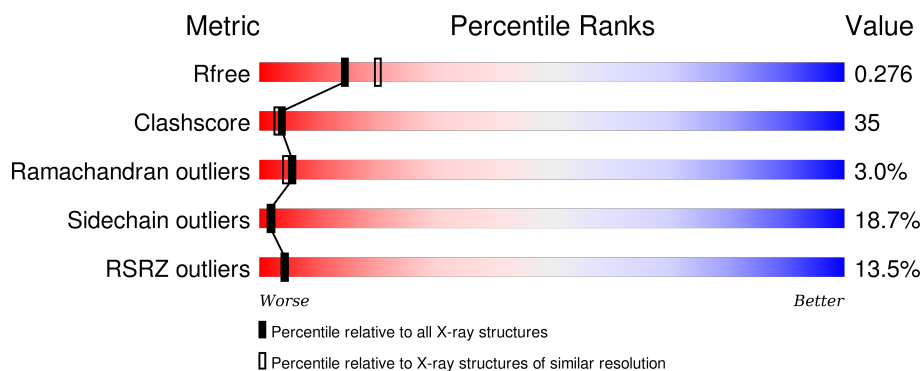
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	220	<div> <div>9%</div> <div>45%</div> <div>43%</div> <div>12%</div> </div>
1	B	220	<div> <div>10%</div> <div>43%</div> <div>46%</div> <div>10%</div> </div>
1	C	220	<div> <div>11%</div> <div>46%</div> <div>44%</div> <div>10%</div> </div>
1	D	220	<div> <div>7%</div> <div>47%</div> <div>44%</div> <div>9%</div> </div>
2	P	8	<div> <div>75%</div> <div>50%</div> <div>25%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
2	R	8	<div><div></div><div>50%</div><div></div><div>50%</div><div>38%</div><div>13%</div></div>
2	S	8	<div><div></div><div>50%</div><div></div><div>25%</div><div>38%</div><div>38%</div></div>
2	T	8	<div><div></div><div>38%</div><div></div><div>63%</div><div>38%</div></div>
3	I	98	<div><div></div><div>16%</div><div></div><div>51%</div><div>41%</div><div>8%</div></div>
3	J	98	<div><div></div><div>20%</div><div></div><div>36%</div><div>51%</div><div>12%</div></div>
3	K	98	<div><div></div><div>18%</div><div></div><div>46%</div><div>49%</div><div>5%</div></div>
3	L	98	<div><div></div><div>22%</div><div></div><div>40%</div><div>45%</div><div>15%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10312 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 Cathepsin H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	60	0	0
			1706	1085	283	322	16			
1	B	220	Total	C	N	O	S	70	0	0
			1706	1085	283	322	16			
1	C	220	Total	C	N	O	S	71	0	0
			1706	1085	283	322	16			
1	D	220	Total	C	N	O	S	63	0	0
			1706	1085	283	322	16			

- Molecule 2 is a protein called Cathepsin H MINI CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	S	8	0	0
			58	32	10	15	1			
2	R	8	Total	C	N	O	S	15	0	0
			58	32	10	15	1			
2	S	8	Total	C	N	O	S	13	0	0
			58	32	10	15	1			
2	T	8	Total	C	N	O	S	17	0	0
			58	32	10	15	1			

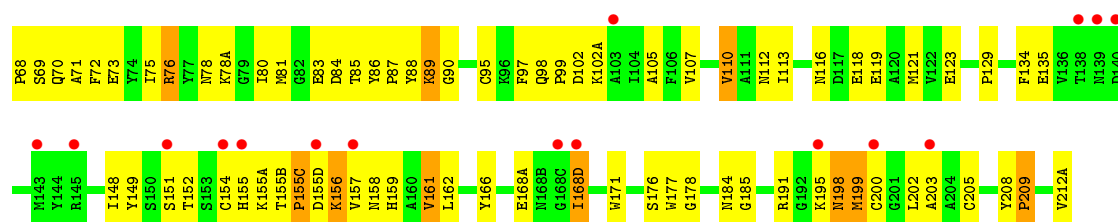
- Molecule 3 is a protein called STEFIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	98	Total	C	N	O	S	41	0	0
			775	492	126	155	2			
3	J	98	Total	C	N	O	S	39	0	0
			775	492	126	155	2			
3	K	98	Total	C	N	O	S	64	0	0
			775	492	126	155	2			
3	L	98	Total	C	N	O	S	62	0	0
			775	492	126	155	2			

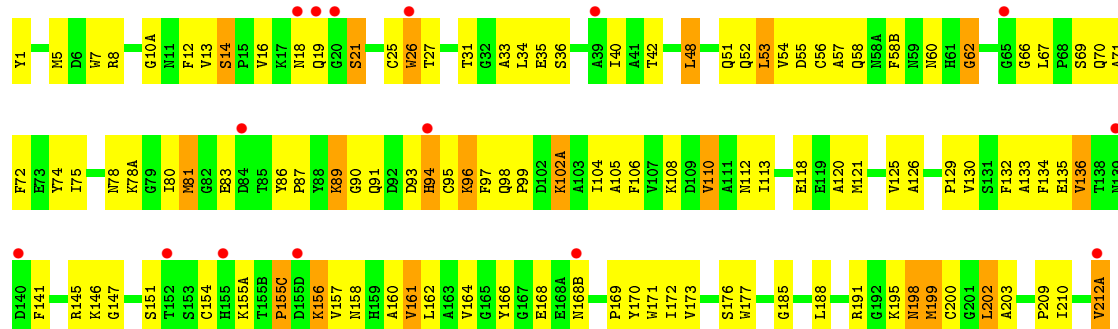
- Molecule 4 is a polymer of unknown type called SUGAR (NAG-NAG-BMA).

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

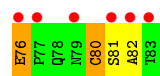




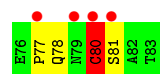
• Molecule 1: Cathepsin H



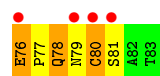
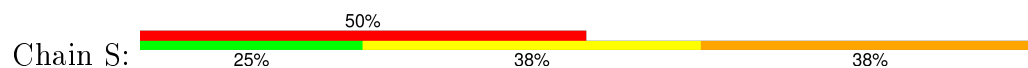
• Molecule 2: Cathepsin H MINI CHAIN



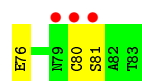
• Molecule 2: Cathepsin H MINI CHAIN



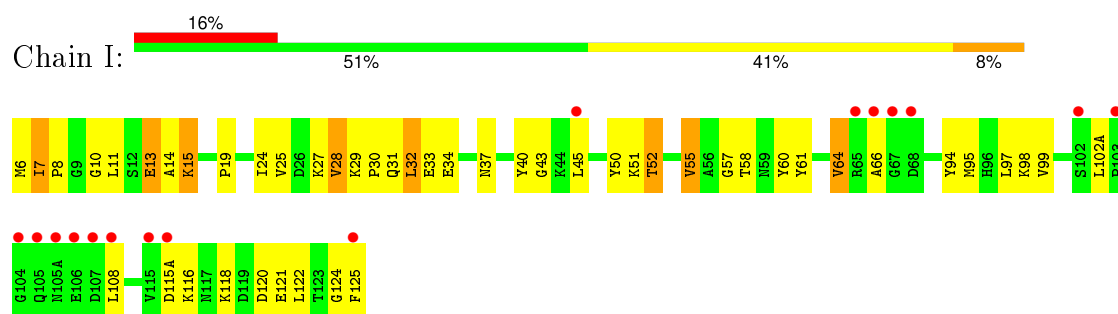
• Molecule 2: Cathepsin H MINI CHAIN



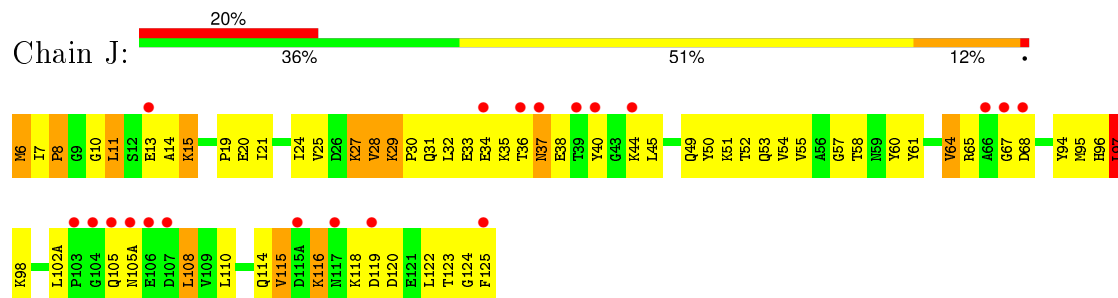
• Molecule 2: Cathepsin H MINI CHAIN



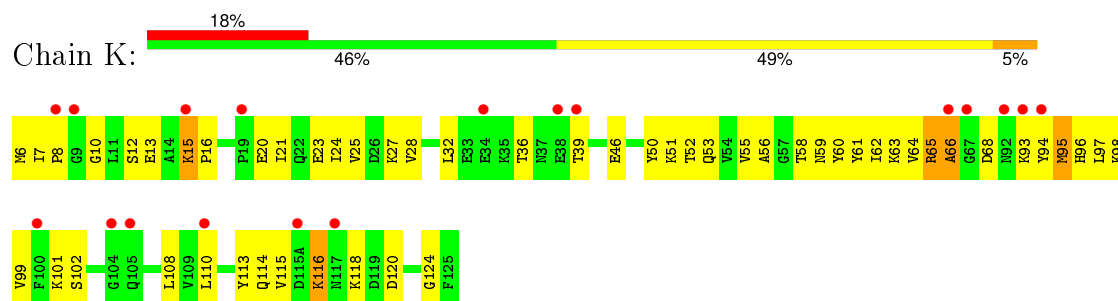
• Molecule 3: STEFIN A



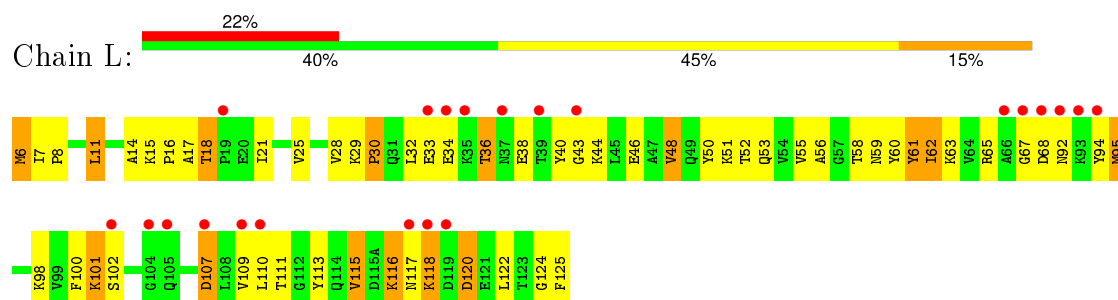
• Molecule 3: STEFIN A



• Molecule 3: STEFIN A



• Molecule 3: STEFIN A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.63Å 97.58Å 162.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 87.9 (10.00-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	MAIN	Depositor
R, $R_{free}$	0.235 , 0.274 0.267 , 0.276	Depositor DCC
$R_{free}$ test set	2550 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 80.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	7 of 55861 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.69 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6402e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.50	0/1753	0.75	1/2377 (0.0%)
1	B	0.51	0/1753	0.83	5/2377 (0.2%)
1	C	0.50	0/1753	0.72	0/2377
1	D	0.51	2/1753 (0.1%)	0.74	0/2377
2	P	0.40	0/58	0.88	0/77
2	R	0.34	0/58	0.77	0/77
2	S	0.56	0/58	0.82	0/77
2	T	0.46	0/58	0.74	0/77
3	I	0.52	0/788	0.81	1/1062 (0.1%)
3	J	0.61	0/788	0.88	3/1062 (0.3%)
3	K	0.50	0/788	0.77	0/1062
3	L	0.48	0/788	0.77	0/1062
All	All	0.51	2/10396 (0.0%)	0.78	10/14064 (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	K	0	1
3	L	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	212(A)	VAL	C-OXT	5.82	1.34	1.23
1	D	25	CYS	CB-SG	-5.68	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155(C)	PRO	N-CA-C	9.65	137.19	112.10
1	B	58(A)	ASN	N-CA-C	8.54	134.05	111.00
3	J	36	THR	N-CA-C	6.97	129.83	111.00
3	J	11	LEU	CA-CB-CG	6.44	130.11	115.30
3	J	97	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	127	TYR	N-CA-C	5.55	125.98	111.00
1	B	155(B)	THR	N-CA-C	5.49	125.81	111.00
1	B	155(D)	ASP	N-CA-C	5.30	125.31	111.00
3	I	11	LEU	N-CA-C	-5.12	97.17	111.00
1	B	58(A)	ASN	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	113	TYR	Sidechain
3	L	113	TYR	Sidechain

## 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	1706	0	1622	130	1
1	B	1706	0	1622	125	2
1	C	1706	0	1622	99	2
1	D	1706	0	1622	107	0
2	P	58	0	47	24	0
2	R	58	0	47	10	0
2	S	58	0	47	6	0
2	T	58	0	47	6	0
3	I	775	0	777	76	0
3	J	775	0	777	64	7
3	K	775	0	777	44	1
3	L	775	0	777	41	7
4	A	39	0	34	9	0
4	B	39	0	34	11	0
4	C	39	0	34	2	0
4	D	39	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10312	0	9920	667	10

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 35.

All (667) 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:I:45:LEU:HD22	3:I:64:VAL:CG1	1.23	1.64
3:I:45:LEU:CD2	3:I:66:ALA:HB2	1.32	1.56
3:I:45:LEU:CD2	3:I:64:VAL:CG1	1.86	1.50
1:B:8:ARG:NH2	1:B:172:ILE:HG21	1.62	1.11
2:S:81:SER:HA	3:K:7:ILE:HG12	1.26	1.11
3:I:45:LEU:HD21	3:I:66:ALA:HB2	1.18	1.10
3:I:45:LEU:CD2	3:I:64:VAL:HG12	1.80	1.10
3:I:45:LEU:CD2	3:I:66:ALA:CB	2.29	1.10
3:I:45:LEU:CD2	3:I:64:VAL:HG11	1.64	1.08
3:I:45:LEU:HD23	3:I:66:ALA:HB2	1.27	1.08
3:L:94:TYR:HB2	3:L:116:LYS:O	1.57	1.04
3:I:24:ILE:HG12	3:I:108:LEU:HD21	1.35	1.03
1:D:19:GLN:HG2	1:D:176:SER:O	1.59	1.02
3:J:37:ASN:N	3:J:37:ASN:HD22	1.56	1.02
3:I:45:LEU:HD23	3:I:64:VAL:CG1	1.88	1.01
1:D:125:VAL:HG21	1:D:171:TRP:HZ3	1.29	0.98
1:A:72:PHE:CZ	1:A:209:PRO:HD3	1.99	0.97
1:B:72:PHE:CZ	1:B:209:PRO:HD3	1.98	0.97
3:I:45:LEU:CD2	3:I:64:VAL:HG13	1.93	0.95
1:B:8:ARG:HH21	1:B:172:ILE:HG21	1.28	0.94
1:C:152:THR:HG21	1:D:212(A):VAL:OXT	1.65	0.94
3:J:37:ASN:H	3:J:37:ASN:HD22	0.94	0.93
1:A:49:ALA:HB2	1:A:82:GLY:O	1.68	0.93
3:I:45:LEU:CG	3:I:66:ALA:HB2	1.99	0.92
3:J:24:ILE:HG23	3:J:108:LEU:CD2	2.00	0.92
3:L:61:TYR:CE2	3:L:124:GLY:HA2	2.07	0.89
3:I:24:ILE:HG23	3:I:108:LEU:HD23	1.53	0.89
1:D:135:GLU:HB2	1:D:156:LYS:O	1.73	0.89
1:C:19:GLN:HB3	1:C:28:PHE:CE1	2.08	0.88
3:I:45:LEU:HD23	3:I:64:VAL:HG13	1.53	0.88
1:D:19:GLN:NE2	1:D:177:TRP:HE1	1.73	0.87
3:J:29:LYS:HG3	3:J:45:LEU:HD12	1.57	0.86
3:J:24:ILE:HG23	3:J:108:LEU:HD23	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ALA:O	1:C:60:ASN:HB2	1.76	0.85
1:A:81:MET:HE2	1:A:98:GLN:H	1.39	0.85
3:I:24:ILE:HG23	3:I:108:LEU:CD2	2.06	0.85
3:I:24:ILE:HG12	3:I:108:LEU:CD2	2.07	0.84
1:A:70:GLN:NE2	2:P:81:SER:CB	2.39	0.84
1:A:121:MET:SD	1:A:203:ALA:HB2	2.17	0.84
1:B:7:TRP:CD1	1:B:129:PRO:HG3	2.13	0.83
1:A:70:GLN:HG2	4:A:214:NAG:H81	1.60	0.83
4:B:213:NAG:C6	2:R:78:GLN:H	1.91	0.83
3:J:94:TYR:HB2	3:J:116:LYS:O	1.78	0.83
3:I:61:TYR:HE2	3:I:124:GLY:HA2	1.44	0.83
1:B:51:GLN:HE21	1:B:89:LYS:H	1.27	0.83
1:B:77:TYR:HE1	4:B:215:BMA:H3	1.44	0.82
3:J:108:LEU:HD12	3:J:108:LEU:H	1.45	0.82
3:K:94:TYR:HB2	3:K:116:LYS:O	1.80	0.82
3:I:45:LEU:HD21	3:I:66:ALA:CB	2.02	0.82
1:B:199:MET:O	1:B:202:LEU:HD13	1.79	0.81
4:B:213:NAG:H62	2:R:78:GLN:H	1.43	0.81
3:I:61:TYR:CE2	3:I:124:GLY:HA2	2.15	0.81
1:A:58(B):PHE:CE1	1:A:74:TYR:HA	2.15	0.81
1:B:49:ALA:HB2	1:B:82:GLY:O	1.81	0.80
3:L:36:THR:HG21	3:L:40:TYR:OH	1.80	0.80
1:A:52:GLN:HE22	1:A:80:ILE:HA	1.46	0.80
1:A:67:LEU:CB	2:P:81:SER:OG	2.29	0.80
1:B:49:ALA:HA	1:B:83:GLU:HG3	1.62	0.79
1:D:19:GLN:NE2	1:D:177:TRP:NE1	2.29	0.79
1:A:53:LEU:H	1:A:53:LEU:HD22	1.45	0.79
1:B:121:MET:SD	1:B:203:ALA:HB2	2.21	0.79
3:L:61:TYR:HE2	3:L:124:GLY:HA2	1.47	0.79
3:I:45:LEU:HG	3:I:66:ALA:CB	2.13	0.79
1:D:135:GLU:CB	1:D:156:LYS:O	2.32	0.78
1:D:113:ILE:HD13	1:D:121:MET:HA	1.64	0.78
3:J:37:ASN:N	3:J:37:ASN:ND2	2.32	0.78
1:D:57:ALA:O	1:D:60:ASN:HB2	1.83	0.78
1:B:52:GLN:HE22	1:B:80:ILE:HA	1.48	0.77
3:J:11:LEU:HD23	3:J:53:GLN:HB2	1.65	0.77
1:B:58(B):PHE:CE1	1:B:74:TYR:HA	2.19	0.76
4:A:213:NAG:O7	2:P:76:GLU:N	2.18	0.76
3:I:45:LEU:CG	3:I:66:ALA:CB	2.63	0.76
1:A:70:GLN:NE2	2:P:81:SER:HB3	2.01	0.76
1:A:70:GLN:NE2	2:P:81:SER:HB2	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HB2	2:P:81:SER:OG	1.86	0.75
1:B:58(B):PHE:CE2	4:B:215:BMA:H62	2.22	0.75
3:K:66:ALA:HB3	3:K:93:LYS:HB2	1.69	0.74
3:L:94:TYR:CB	3:L:116:LYS:O	2.34	0.74
1:D:125:VAL:HG21	1:D:171:TRP:CZ3	2.20	0.74
1:B:189:ILE:HD13	1:B:202:LEU:HD11	1.68	0.74
1:B:50:GLU:HA	1:B:53:LEU:HD23	1.69	0.74
1:B:51:GLN:NE2	1:B:89:LYS:H	1.85	0.74
1:A:139:ASN:HA	1:A:142:LEU:HD12	1.70	0.74
1:A:51:GLN:HE21	1:A:89:LYS:H	1.36	0.73
3:J:33:GLU:HG2	3:J:38:GLU:O	1.87	0.73
3:K:28:VAL:CG2	3:K:110:LEU:HB2	2.19	0.73
1:C:64:GLN:O	3:K:10:GLY:HA2	1.88	0.73
1:A:70:GLN:HG2	4:A:214:NAG:C8	2.19	0.73
1:C:27:THR:HG23	1:C:53:LEU:HB2	1.71	0.73
2:T:81:SER:HA	3:L:7:ILE:HG12	1.70	0.73
3:I:45:LEU:HD23	3:I:66:ALA:CB	2.08	0.73
1:D:52:GLN:HE22	1:D:80:ILE:HA	1.53	0.73
1:A:70:GLN:CG	4:A:214:NAG:H81	2.19	0.72
1:A:8:ARG:HH21	1:A:172:ILE:HG21	1.54	0.72
3:L:21:ILE:HG23	3:L:62:ILE:HD13	1.71	0.72
3:J:37:ASN:ND2	3:J:37:ASN:H	1.78	0.72
3:L:17:ALA:HB2	3:L:48:VAL:O	1.87	0.72
3:I:94:TYR:CE2	3:I:118:LYS:HB2	2.24	0.72
1:C:1:TYR:CE1	1:C:123:GLU:HG3	2.25	0.71
1:A:70:GLN:CD	2:P:81:SER:CB	2.58	0.71
1:C:155(D):ASP:O	3:K:6:MET:HB3	1.91	0.70
3:I:45:LEU:HG	3:I:66:ALA:HB1	1.73	0.70
1:A:58(B):PHE:CD1	1:A:74:TYR:HA	2.26	0.70
3:J:14:ALA:HB2	3:J:51:LYS:HE2	1.71	0.70
1:B:157:VAL:HG21	2:R:80:CYS:SG	2.32	0.70
1:C:16:VAL:HG11	1:C:185:GLY:HA3	1.72	0.70
1:B:81:MET:CE	1:B:97:PHE:HA	2.21	0.70
1:D:67:LEU:HB2	2:T:81:SER:HB2	1.72	0.70
1:A:70:GLN:HE22	2:P:81:SER:HB3	1.56	0.69
1:C:17:LYS:NZ	1:C:47:SER:OG	2.25	0.69
1:C:205:CYS:HB2	2:S:78:GLN:HG2	1.74	0.69
3:J:31:GLN:O	3:J:34:GLU:HG2	1.91	0.69
1:D:19:GLN:NE2	1:D:177:TRP:CD1	2.59	0.69
1:A:121:MET:SD	1:A:203:ALA:CB	2.81	0.69
3:K:15:LYS:HZ2	3:K:50:TYR:HE2	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD12	1:B:46:LEU:H	1.57	0.69
1:D:53:LEU:HD11	1:D:80:ILE:HD12	1.74	0.68
1:D:58:GLN:HA	1:D:60:ASN:O	1.92	0.68
3:I:32:LEU:HD13	3:I:40:TYR:CZ	2.28	0.68
1:C:70:GLN:HG2	4:C:214:NAG:H81	1.75	0.68
3:I:45:LEU:HD22	3:I:64:VAL:HG11	0.68	0.68
2:P:82:ALA:H	3:I:7:ILE:HG13	1.58	0.68
1:B:81:MET:HE1	1:B:98:GLN:H	1.57	0.68
2:P:81:SER:HA	3:I:7:ILE:HG12	1.76	0.68
1:B:70:GLN:HE22	2:R:81:SER:CB	2.06	0.68
1:C:51:GLN:HG2	1:C:88:TYR:HA	1.77	0.67
1:B:108:LYS:HB3	1:B:210:ILE:HG22	1.77	0.67
1:A:24:SER:O	1:A:28:PHE:HD1	1.78	0.67
4:B:213:NAG:H62	2:R:77:PRO:HA	1.77	0.66
1:A:53:LEU:N	1:A:53:LEU:HD22	2.10	0.66
3:J:20:GLU:O	3:J:24:ILE:HG13	1.96	0.66
1:D:158:ASN:HB3	3:L:6:MET:HE2	1.77	0.66
3:K:20:GLU:HG3	1:D:98:GLN:NE2	2.11	0.66
3:L:117:ASN:O	3:L:120:ASP:HB2	1.95	0.66
1:A:52:GLN:NE2	1:A:80:ILE:HA	2.11	0.66
1:C:58(B):PHE:O	1:C:70:GLN:HG2	1.95	0.66
3:J:24:ILE:HG23	3:J:108:LEU:HD22	1.77	0.65
1:B:18:ASN:ND2	1:B:20:GLY:H	1.93	0.65
2:S:81:SER:HA	3:K:7:ILE:CG1	2.17	0.65
1:B:71:ALA:O	1:B:75:ILE:HG13	1.97	0.65
1:C:199:MET:O	1:C:202:LEU:HB2	1.96	0.65
1:A:73:GLU:HG3	4:A:213:NAG:O4	1.96	0.65
1:D:81:MET:CE	1:D:97:PHE:HA	2.27	0.65
1:A:171:TRP:CD1	1:A:202:LEU:HD21	2.32	0.65
1:D:198:ASN:ND2	1:D:203:ALA:H	1.93	0.64
1:A:18:ASN:HB3	1:A:177:TRP:C	2.18	0.64
1:C:71:ALA:O	1:C:75:ILE:HG13	1.97	0.64
3:I:94:TYR:HB2	3:I:116:LYS:O	1.96	0.64
1:D:132:PHE:CE2	1:D:161:VAL:HG23	2.33	0.64
3:K:96:HIS:HB2	3:K:114:GLN:HB2	1.79	0.64
1:C:8:ARG:HG2	1:C:13:VAL:HB	1.79	0.64
1:D:70:GLN:NE2	2:T:81:SER:HB3	2.13	0.64
3:I:24:ILE:O	3:I:28:VAL:HB	1.97	0.64
3:J:31:GLN:O	3:J:35:LYS:HD2	1.98	0.63
1:D:135:GLU:HG3	1:D:156:LYS:O	1.97	0.63
1:D:21:SER:O	3:L:55:VAL:HG11	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:30:PRO:O	3:L:34:GLU:HG3	1.98	0.63
3:I:94:TYR:CZ	3:I:118:LYS:HB2	2.33	0.63
1:B:18:ASN:HD22	1:B:20:GLY:H	1.45	0.63
3:I:31:GLN:HA	3:I:34:GLU:OE1	1.99	0.63
3:L:11:LEU:HD11	3:L:124:GLY:N	2.14	0.62
1:C:81:MET:HE1	1:C:86:TYR:HD2	1.64	0.62
3:L:59:ASN:HB3	3:L:61:TYR:HE1	1.65	0.62
1:A:33:ALA:HB1	1:A:209:PRO:HD2	1.82	0.62
3:L:36:THR:HG23	3:L:38:GLU:H	1.65	0.62
3:J:61:TYR:CE2	3:J:124:GLY:HA2	2.35	0.62
1:A:31:THR:HG21	1:A:50:GLU:HG3	1.81	0.62
1:B:58(B):PHE:CD1	1:B:74:TYR:HA	2.35	0.62
3:L:98:LYS:HB2	3:L:125:PHE:CZ	2.34	0.62
4:A:213:NAG:H2	2:P:76:GLU:O	1.99	0.61
3:L:29:LYS:HB3	3:L:30:PRO:HD3	1.81	0.61
1:B:44:LYS:HE3	1:B:46:LEU:HB3	1.82	0.61
1:B:27:THR:HB	1:B:50:GLU:HB3	1.82	0.61
1:D:108:LYS:HB3	1:D:210:ILE:HG22	1.82	0.61
3:I:15:LYS:HD3	3:I:50:TYR:CZ	2.34	0.61
3:K:65:ARG:HG3	3:K:94:TYR:CE1	2.36	0.61
1:A:8:ARG:HG2	1:A:13:VAL:HG21	1.82	0.61
3:K:61:TYR:CE2	3:K:124:GLY:HA2	2.35	0.61
1:A:94:HIS:O	1:A:96:LYS:NZ	2.33	0.61
3:L:36:THR:HG21	3:L:40:TYR:HH	1.66	0.61
3:L:21:ILE:HG13	3:L:50:TYR:CD1	2.36	0.61
3:J:32:LEU:HD23	3:J:32:LEU:C	2.20	0.61
3:J:24:ILE:O	3:J:28:VAL:HB	2.00	0.60
3:J:32:LEU:HD11	3:J:95:MET:CE	2.31	0.60
1:A:132:PHE:CE2	1:A:163:ALA:HB2	2.35	0.60
3:L:18:THR:CG2	3:L:21:ILE:HG12	2.30	0.60
1:C:51:GLN:HE21	1:C:90:GLY:H	1.47	0.60
1:C:52:GLN:HE22	1:C:80:ILE:HA	1.66	0.60
1:D:71:ALA:O	1:D:75:ILE:HG13	2.01	0.60
1:C:198:ASN:HD21	1:C:203:ALA:H	1.50	0.60
3:I:24:ILE:CG1	3:I:108:LEU:HD21	2.23	0.60
1:D:72:PHE:CZ	1:D:209:PRO:HD3	2.36	0.60
1:C:35:GLU:HB3	1:C:48:LEU:HD22	1.84	0.59
1:A:67:LEU:HB3	2:P:81:SER:OG	2.01	0.59
3:K:94:TYR:CE2	3:K:118:LYS:HB2	2.36	0.59
3:J:32:LEU:HD22	3:J:40:TYR:CE2	2.37	0.59
1:B:8:ARG:NH2	1:B:172:ILE:CG2	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:HG21	1:B:50:GLU:HG3	1.84	0.59
1:A:190:GLU:HB3	1:A:199:MET:HG3	1.85	0.59
3:K:50:TYR:HD2	3:K:51:LYS:O	1.85	0.59
1:C:52:GLN:NE2	1:C:80:ILE:HA	2.18	0.59
1:C:49:ALA:HB1	1:C:86:TYR:HB3	1.84	0.59
1:A:70:GLN:HE22	2:P:81:SER:CB	2.14	0.59
1:B:81:MET:HE1	1:B:97:PHE:HD1	1.67	0.59
1:B:48:LEU:HA	1:B:82:GLY:HA2	1.85	0.58
1:C:21:SER:HA	3:K:55:VAL:HG21	1.85	0.58
3:L:94:TYR:CZ	3:L:118:LYS:HB2	2.38	0.58
1:A:7:TRP:CD1	1:A:129:PRO:HG3	2.39	0.58
1:D:195:LYS:HD2	1:D:195:LYS:O	2.03	0.58
1:D:51:GLN:HE22	1:D:91:GLN:H	1.52	0.58
1:A:19:GLN:HG2	1:A:176:SER:O	2.02	0.58
1:A:5:MET:HB2	1:A:166:TYR:CZ	2.38	0.58
1:D:19:GLN:HG3	3:L:56:ALA:HB2	1.86	0.58
1:A:168(A):GLU:O	1:A:168(D):ILE:HG13	2.04	0.58
3:I:25:VAL:HG21	3:I:64:VAL:CG2	2.34	0.58
1:C:54:VAL:HG12	1:C:55:ASP:OD1	2.04	0.58
1:D:54:VAL:HG12	1:D:55:ASP:OD1	2.03	0.58
1:D:93:ASP:HB3	1:D:96:LYS:NZ	2.19	0.58
1:D:151:SER:HB3	1:D:154:CYS:SG	2.43	0.57
1:C:41:ALA:HB1	1:C:212(A):VAL:HG21	1.85	0.57
1:D:171:TRP:NE1	1:D:191:ARG:HG3	2.19	0.57
3:K:96:HIS:CE1	3:K:116:LYS:HD3	2.40	0.57
3:K:46:GLU:O	3:K:64:VAL:HA	2.04	0.57
3:I:32:LEU:HD13	3:I:40:TYR:CE2	2.39	0.57
1:B:67:LEU:HD12	1:B:68:PRO:HD2	1.85	0.57
1:C:72:PHE:CD1	1:C:209:PRO:HB3	2.40	0.57
1:C:81:MET:HG2	1:C:102(A):LYS:C	2.24	0.57
1:A:58(B):PHE:O	1:A:70:GLN:HB3	2.03	0.57
3:I:14:ALA:HB2	3:I:51:LYS:CE	2.35	0.57
1:C:55:ASP:C	1:C:56:CYS:SG	2.83	0.57
1:D:198:ASN:HD21	1:D:203:ALA:H	1.52	0.57
1:A:70:GLN:CD	2:P:81:SER:HB3	2.24	0.57
1:A:51:GLN:NE2	1:A:89:LYS:H	2.02	0.57
1:D:147:GLY:O	1:D:188:LEU:HB2	2.05	0.57
1:A:26:TRP:CD2	1:A:66:GLY:HA3	2.40	0.57
3:L:59:ASN:HB3	3:L:61:TYR:CE1	2.39	0.56
1:D:135:GLU:CG	1:D:156:LYS:O	2.53	0.56
1:A:31:THR:O	1:A:35:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:PHE:HA	1:C:31:THR:OG1	2.05	0.56
1:D:58(B):PHE:HD2	4:D:214:NAG:O7	1.87	0.56
1:A:8:ARG:HH21	1:A:172:ILE:CG2	2.16	0.56
1:B:81:MET:HE3	1:B:97:PHE:HA	1.87	0.56
1:C:51:GLN:NE2	1:C:90:GLY:H	2.04	0.56
1:A:26:TRP:HZ3	1:A:62:GLY:O	1.87	0.56
1:D:7:TRP:O	1:D:12:PHE:HB2	2.04	0.56
1:A:76:ARG:HD2	1:A:77:TYR:CE1	2.40	0.56
1:C:113:ILE:HD13	1:C:121:MET:HA	1.87	0.56
1:D:81:MET:HB3	1:D:102(A):LYS:O	2.05	0.56
1:C:157:VAL:HG21	2:S:80:CYS:SG	2.46	0.56
3:I:108:LEU:HD12	3:I:108:LEU:H	1.70	0.56
1:D:121:MET:O	1:D:125:VAL:HG23	2.06	0.56
1:C:73:GLU:OE2	4:C:213:NAG:H3	2.06	0.56
1:D:8:ARG:HG2	1:D:13:VAL:HG21	1.87	0.56
1:A:70:GLN:OE1	2:P:81:SER:CB	2.54	0.56
1:D:169:PRO:HB2	1:D:191:ARG:HE	1.71	0.55
3:J:96:HIS:ND1	3:J:116:LYS:HD3	2.21	0.55
1:B:8:ARG:HH21	1:B:172:ILE:CG2	2.12	0.55
1:A:53:LEU:CD2	1:A:53:LEU:H	2.18	0.55
3:J:11:LEU:CD2	3:J:53:GLN:HB2	2.33	0.55
3:I:94:TYR:O	3:I:116:LYS:HB2	2.05	0.55
1:C:166:TYR:HB2	1:C:191:ARG:HE	1.70	0.55
3:J:45:LEU:HD22	3:J:64:VAL:CG1	2.35	0.55
1:C:72:PHE:CZ	1:C:209:PRO:HD3	2.42	0.55
1:C:16:VAL:HG21	1:C:184:ASN:O	2.07	0.55
3:K:64:VAL:HG23	3:K:95:MET:HB3	1.88	0.55
3:J:114:GLN:HB2	3:J:116:LYS:HD2	1.88	0.55
3:J:29:LYS:HG3	3:J:45:LEU:CD1	2.32	0.55
1:B:132:PHE:CE2	1:B:163:ALA:HB2	2.42	0.55
3:I:99:VAL:HG11	3:I:108:LEU:HB3	1.89	0.54
3:K:12:SER:OG	3:K:15:LYS:HE3	2.07	0.54
1:C:27:THR:HG23	1:C:53:LEU:CB	2.36	0.54
3:J:49:GLN:HE21	3:J:122:LEU:HD12	1.73	0.54
1:B:52:GLN:NE2	1:B:80:ILE:HG13	2.23	0.54
2:P:82:ALA:H	3:I:7:ILE:CG1	2.20	0.54
1:A:22:CYS:HB2	1:A:90:GLY:O	2.08	0.54
1:B:53:LEU:HD11	1:B:75:ILE:HD11	1.88	0.54
2:S:76:GLU:HB2	2:S:77:PRO:HD2	1.90	0.54
3:I:55:VAL:C	3:I:57:GLY:H	2.10	0.54
1:D:26:TRP:CD2	1:D:66:GLY:HA3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HB3	1:A:177:TRP:CA	2.38	0.53
1:A:26:TRP:CZ2	1:A:60:ASN:HB3	2.44	0.53
3:J:55:VAL:C	3:J:57:GLY:H	2.11	0.53
1:A:14:SER:O	1:A:174:LYS:NZ	2.39	0.53
1:B:121:MET:SD	1:B:203:ALA:CB	2.94	0.53
1:C:49:ALA:HA	1:C:83:GLU:HG3	1.90	0.53
3:J:27:LYS:HZ2	3:J:108:LEU:CD1	2.22	0.53
1:A:70:GLN:OE1	2:P:81:SER:HB3	2.07	0.53
1:B:18:ASN:HD22	1:B:18:ASN:C	2.11	0.53
1:A:18:ASN:CB	1:A:177:TRP:HA	2.38	0.53
1:B:70:GLN:NE2	2:R:81:SER:CB	2.72	0.52
1:A:142:LEU:HD22	3:I:102(A):LEU:CD2	2.39	0.52
1:A:19:GLN:NE2	1:A:25:CYS:HB3	2.24	0.52
1:D:51:GLN:NE2	1:D:90:GLY:N	2.56	0.52
1:A:61:HIS:HE1	2:P:82:ALA:O	1.92	0.52
1:B:183:MET:SD	1:B:188:LEU:HD13	2.49	0.52
1:A:18:ASN:HB3	1:A:177:TRP:HA	1.91	0.52
1:B:58(B):PHE:HD1	1:B:74:TYR:HB2	1.73	0.52
3:L:100:PHE:CG	3:L:101:LYS:N	2.77	0.52
1:D:199:MET:SD	1:D:200:CYS:N	2.83	0.52
3:I:24:ILE:CG2	3:I:108:LEU:HD23	2.32	0.52
3:J:45:LEU:HD22	3:J:64:VAL:HG11	1.91	0.52
1:A:64:GLN:O	3:I:10:GLY:HA2	2.09	0.52
1:B:18:ASN:HD22	1:B:19:GLN:N	2.08	0.52
3:L:14:ALA:HA	3:L:51:LYS:HG2	1.91	0.52
1:C:8:ARG:HG2	1:C:13:VAL:CB	2.39	0.52
3:K:27:LYS:HD3	3:K:108:LEU:HD12	1.91	0.52
1:A:50:GLU:HA	1:A:53:LEU:HD23	1.91	0.52
1:B:53:LEU:HD22	1:B:53:LEU:N	2.24	0.52
1:B:181:TRP:CZ3	1:B:187:PHE:HB3	2.45	0.52
1:B:171:TRP:O	1:B:188:LEU:HA	2.09	0.52
1:B:37:ALA:O	1:B:40:ILE:N	2.43	0.52
1:D:166:TYR:CD2	1:D:191:ARG:NH1	2.78	0.51
1:A:98:GLN:NE2	1:A:102(A):LYS:HD3	2.25	0.51
1:A:198:ASN:HD21	1:A:203:ALA:H	1.57	0.51
1:B:46:LEU:HD22	1:B:48:LEU:HD11	1.92	0.51
1:D:52:GLN:NE2	1:D:80:ILE:HA	2.23	0.51
1:B:16:VAL:HG11	1:B:185:GLY:HA3	1.91	0.51
1:D:81:MET:HE2	1:D:98:GLN:H	1.75	0.51
1:D:51:GLN:HG3	1:D:89:LYS:H	1.74	0.51
1:B:39:ALA:O	1:B:43:GLY:HA2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HB2	1:C:107:VAL:HG12	1.92	0.51
3:J:60:TYR:O	3:J:98:LYS:HA	2.10	0.51
3:K:53:GLN:HB3	3:K:59:ASN:HB2	1.90	0.51
1:A:31:THR:CG2	1:A:50:GLU:HG3	2.40	0.51
1:C:20:GLY:O	3:K:55:VAL:HB	2.10	0.51
1:A:183:MET:SD	1:A:188:LEU:HD13	2.50	0.51
3:J:32:LEU:HD11	3:J:95:MET:HE2	1.91	0.51
3:J:32:LEU:HD22	3:J:40:TYR:HE2	1.75	0.51
3:I:25:VAL:HG21	3:I:64:VAL:HG21	1.91	0.51
1:A:8:ARG:HD3	1:A:186:TYR:CE1	2.46	0.51
1:A:67:LEU:CD2	2:P:81:SER:OG	2.58	0.51
1:A:67:LEU:CD1	3:I:8:PRO:HG2	2.40	0.51
1:C:81:MET:CE	1:C:86:TYR:HD2	2.23	0.51
1:A:19:GLN:HE22	1:A:25:CYS:HB3	1.76	0.51
1:A:26:TRP:CZ3	1:A:65:GLY:O	2.64	0.51
1:A:78(A):LYS:HD3	1:A:78(A):LYS:N	2.26	0.51
3:I:52:THR:HG22	3:I:58:THR:HG22	1.92	0.51
1:B:69:SER:O	1:B:72:PHE:HB2	2.11	0.50
1:A:81:MET:CE	1:A:97:PHE:HA	2.41	0.50
1:B:77:TYR:CE1	4:B:215:BMA:H3	2.36	0.50
2:R:81:SER:HA	3:J:7:ILE:CD1	2.41	0.50
1:B:171:TRP:CD1	1:B:202:LEU:HD23	2.47	0.50
1:B:46:LEU:N	1:B:46:LEU:HD12	2.23	0.50
1:A:7:TRP:HB2	1:A:164:VAL:O	2.11	0.50
1:D:55:ASP:C	1:D:56:CYS:SG	2.89	0.50
1:D:136:VAL:HG22	1:D:141:PHE:CD2	2.47	0.50
1:C:18:ASN:HB2	1:C:178:GLY:CA	2.41	0.50
3:I:98:LYS:HB2	3:I:125:PHE:CE2	2.46	0.50
1:C:191:ARG:HG2	1:C:191:ARG:HH11	1.77	0.50
1:C:148:ILE:HG21	1:C:168(D):ILE:HD11	1.92	0.50
3:I:32:LEU:HD11	3:I:95:MET:CE	2.42	0.50
1:B:158:ASN:HA	3:J:8:PRO:HA	1.93	0.50
1:D:53:LEU:CD1	1:D:80:ILE:HD12	2.42	0.50
1:C:198:ASN:ND2	1:C:203:ALA:H	2.08	0.50
3:L:28:VAL:CG2	3:L:110:LEU:HB2	2.42	0.50
3:I:45:LEU:HA	3:I:66:ALA:HA	1.93	0.50
3:J:97:LEU:HD12	3:J:110:LEU:HD11	1.94	0.50
1:A:155(D):ASP:O	3:I:6:MET:HB3	2.12	0.49
2:T:80:CYS:O	3:L:7:ILE:HG12	2.12	0.49
1:C:158:ASN:HB3	3:K:6:MET:HE2	1.94	0.49
1:D:94:HIS:O	1:D:96:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:THR:OG1	1:B:140:ASP:HB3	2.11	0.49
1:C:55:ASP:O	1:C:56:CYS:SG	2.70	0.49
3:K:60:TYR:CE2	3:K:101:LYS:HD2	2.47	0.49
1:A:121:MET:O	1:A:125:VAL:HG23	2.13	0.49
3:L:18:THR:HG23	3:L:21:ILE:H	1.78	0.49
1:D:51:GLN:NE2	1:D:90:GLY:H	2.10	0.49
1:C:171:TRP:CE2	1:C:191:ARG:HD3	2.47	0.49
1:B:26:TRP:CE3	1:B:66:GLY:N	2.81	0.49
1:D:121:MET:HG2	1:D:130:VAL:HG11	1.94	0.49
1:D:5:MET:HB3	1:D:166:TYR:CE1	2.48	0.49
2:P:81:SER:HA	3:I:7:ILE:CG1	2.41	0.49
3:K:61:TYR:CZ	3:K:98:LYS:HD2	2.48	0.49
1:A:26:TRP:CZ3	1:A:62:GLY:O	2.65	0.49
1:A:33:ALA:HB1	1:A:209:PRO:CD	2.43	0.49
3:J:114:GLN:OE1	3:J:116:LYS:HE3	2.13	0.49
3:L:18:THR:HG22	3:L:21:ILE:HG12	1.95	0.49
3:I:25:VAL:O	3:I:28:VAL:HG12	2.13	0.49
3:L:11:LEU:N	3:L:11:LEU:HD23	2.28	0.49
3:K:116:LYS:HB3	3:K:120:ASP:OD2	2.13	0.49
1:D:55:ASP:O	1:D:95:CYS:HB2	2.13	0.49
1:A:132:PHE:HE2	1:A:163:ALA:HB2	1.76	0.48
1:C:48:LEU:HD11	1:C:105:ALA:HB2	1.94	0.48
1:D:35:GLU:HB3	1:D:48:LEU:HD22	1.94	0.48
3:I:25:VAL:HG11	3:I:64:VAL:HG21	1.96	0.48
1:A:171:TRP:HD1	1:A:202:LEU:HD21	1.78	0.48
3:J:32:LEU:HD11	3:J:95:MET:HE1	1.95	0.48
1:C:23:GLY:HA2	3:K:55:VAL:HG12	1.94	0.48
1:D:51:GLN:HE21	1:D:90:GLY:H	1.61	0.48
3:L:50:TYR:HB3	3:L:62:ILE:HG23	1.95	0.48
1:C:44:LYS:HE2	1:C:44:LYS:HB2	1.51	0.48
1:B:53:LEU:HD21	1:B:80:ILE:CD1	2.44	0.48
1:B:81:MET:HE1	1:B:97:PHE:CD1	2.46	0.48
1:B:181:TRP:CD1	3:J:102(A):LEU:HD13	2.47	0.48
1:B:24:SER:O	1:B:28:PHE:HD1	1.97	0.48
1:D:168(B):ASN:O	1:D:168(B):ASN:ND2	2.46	0.48
3:I:99:VAL:CG1	3:I:108:LEU:HB3	2.43	0.48
1:B:86:TYR:N	1:B:87:PRO:HD3	2.29	0.48
1:D:118:GLU:O	1:D:121:MET:HB2	2.14	0.48
3:I:13:GLU:HG3	3:I:14:ALA:H	1.78	0.48
3:J:49:GLN:HG2	3:J:50:TYR:N	2.27	0.48
1:C:134:PHE:HB2	1:C:200:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:O	1:B:116:ASN:HB2	2.13	0.48
1:D:7:TRP:CD1	1:D:129:PRO:HG3	2.49	0.48
1:B:21:SER:HA	3:J:55:VAL:HG21	1.96	0.48
1:C:148:ILE:HD11	1:C:168(A):GLU:HB3	1.94	0.48
1:B:94:HIS:O	1:B:96:LYS:HE3	2.13	0.48
1:B:8:ARG:HD3	1:B:186:TYR:OH	2.14	0.48
1:A:98:GLN:O	1:A:102(A):LYS:HB2	2.14	0.48
3:K:95:MET:HG3	3:K:114:GLN:O	2.14	0.48
1:A:181:TRP:CH2	1:A:187:PHE:HB3	2.49	0.48
1:D:5:MET:HG2	1:D:126:ALA:HA	1.95	0.47
1:A:58(B):PHE:CD1	1:A:74:TYR:CA	2.96	0.47
1:B:70:GLN:HG2	4:B:214:NAG:H81	1.96	0.47
1:C:30:THR:CG2	1:C:53:LEU:HD21	2.44	0.47
1:D:134:PHE:HB2	1:D:200:CYS:O	2.14	0.47
3:J:15:LYS:HD2	3:J:15:LYS:H	1.79	0.47
1:A:67:LEU:CB	2:P:81:SER:HG	2.26	0.47
1:B:77:TYR:CE1	4:B:215:BMA:H5	2.49	0.47
3:J:94:TYR:CZ	3:J:118:LYS:HG3	2.49	0.47
1:D:198:ASN:ND2	1:D:202:LEU:N	2.62	0.47
3:L:18:THR:HG23	3:L:21:ILE:HG12	1.97	0.47
3:J:32:LEU:HD23	3:J:32:LEU:O	2.14	0.47
1:B:181:TRP:CH2	1:B:187:PHE:HB3	2.48	0.47
3:J:27:LYS:NZ	3:J:108:LEU:CD1	2.76	0.47
1:B:58(B):PHE:HE1	1:B:74:TYR:HA	1.73	0.47
1:B:198:ASN:ND2	1:B:203:ALA:H	2.12	0.47
3:K:28:VAL:HG21	3:K:110:LEU:HB2	1.96	0.47
1:C:30:THR:HG21	1:C:53:LEU:HD21	1.96	0.47
1:C:51:GLN:CG	1:C:88:TYR:HA	2.43	0.47
1:D:110:VAL:HG22	1:D:112:ASN:OD1	2.14	0.47
1:B:34:LEU:O	1:B:38:VAL:HG23	2.15	0.47
1:C:78:ASN:O	1:C:78(A):LYS:HB2	2.15	0.47
3:I:24:ILE:HG23	3:I:108:LEU:HD22	1.93	0.47
1:A:58(B):PHE:CE2	4:A:215:BMA:H62	2.49	0.47
1:A:67:LEU:HD22	2:P:81:SER:OG	2.15	0.47
1:B:170:TYR:HA	1:B:191:ARG:H	1.79	0.47
1:C:58:GLN:HA	1:C:60:ASN:O	2.15	0.47
1:D:70:GLN:HG2	4:D:214:NAG:C8	2.45	0.47
1:C:155(D):ASP:O	3:K:6:MET:CB	2.62	0.47
3:J:31:GLN:C	3:J:34:GLU:HG2	2.35	0.47
1:A:190:GLU:HG2	1:A:195:LYS:HD2	1.97	0.47
1:B:73:GLU:OE1	1:B:110:VAL:HG11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASP:CB	1:B:210:ILE:HD12	2.45	0.47
1:C:33:ALA:N	1:C:162:LEU:HD11	2.30	0.47
1:B:53:LEU:HD22	1:B:53:LEU:H	1.79	0.46
1:A:141:PHE:HD1	1:A:149:TYR:CE2	2.33	0.46
1:D:8:ARG:O	1:D:10(A):GLY:O	2.33	0.46
1:C:31:THR:HG21	1:C:50:GLU:HG3	1.98	0.46
3:I:24:ILE:CG1	3:I:108:LEU:CD2	2.86	0.46
3:K:118:LYS:HG2	3:K:118:LYS:O	2.14	0.46
3:I:60:TYR:O	3:I:98:LYS:HA	2.15	0.46
1:D:1:TYR:HD1	1:D:1:TYR:H1	1.56	0.46
1:D:169:PRO:CB	1:D:191:ARG:HH21	2.29	0.46
1:B:33:ALA:HB1	1:B:209:PRO:HD2	1.96	0.46
1:C:158:ASN:HB3	3:K:6:MET:CE	2.46	0.46
1:B:58(B):PHE:CD1	1:B:74:TYR:CA	2.99	0.46
1:D:74:TYR:CE1	1:D:78:ASN:HB2	2.50	0.46
3:I:45:LEU:HD23	3:I:66:ALA:CA	2.46	0.46
1:C:70:GLN:NE2	2:S:81:SER:OG	2.49	0.46
3:I:14:ALA:HB2	3:I:51:LYS:HE3	1.98	0.46
3:L:60:TYR:HE2	3:L:101:LYS:HZ3	1.62	0.46
3:K:21:ILE:O	3:K:25:VAL:HG23	2.16	0.46
3:J:27:LYS:NZ	3:J:108:LEU:HD11	2.31	0.45
1:B:77:TYR:OH	4:B:214:NAG:H61	2.15	0.45
3:K:20:GLU:O	3:K:24:ILE:HG13	2.16	0.45
1:A:8:ARG:HD3	1:A:186:TYR:CZ	2.50	0.45
1:B:181:TRP:HD1	3:J:102(A):LEU:HD13	1.81	0.45
1:C:149:TYR:OH	1:C:151:SER:HB2	2.17	0.45
1:B:58(B):PHE:N	1:B:58(B):PHE:CD2	2.82	0.45
3:I:29:LYS:HB3	3:I:30:PRO:HD3	1.97	0.45
1:C:34:LEU:HD13	1:C:107:VAL:HG23	1.99	0.45
1:D:164:VAL:HG23	1:D:172:ILE:HG22	1.99	0.45
1:C:89:LYS:HA	1:C:89:LYS:HD2	1.56	0.45
1:B:109:ASP:HB2	1:B:210:ILE:HD12	1.97	0.45
1:B:67:LEU:HD12	1:B:68:PRO:CD	2.46	0.45
1:C:18:ASN:HB2	1:C:178:GLY:HA2	1.98	0.45
1:B:148:ILE:CD1	1:B:168(D):ILE:HB	2.46	0.45
3:J:55:VAL:O	3:J:57:GLY:N	2.46	0.45
3:J:11:LEU:CD2	3:J:53:GLN:HE21	2.29	0.45
1:A:132:PHE:O	1:A:160:ALA:HA	2.17	0.45
3:I:24:ILE:CG2	3:I:108:LEU:CD2	2.87	0.45
1:B:26:TRP:CE2	1:B:60:ASN:OD1	2.70	0.45
1:B:108:LYS:N	1:B:210:ILE:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:O	1:C:38:VAL:HG23	2.17	0.45
1:D:8:ARG:HG2	1:D:13:VAL:CG2	2.47	0.45
1:A:110:VAL:O	1:A:110:VAL:HG23	2.17	0.45
1:B:7:TRP:CD1	1:B:129:PRO:CG	2.94	0.44
1:C:118:GLU:O	1:C:121:MET:HB2	2.17	0.44
1:C:110:VAL:CG2	1:C:112:ASN:OD1	2.65	0.44
1:A:56:CYS:HA	1:A:58:GLN:OE1	2.17	0.44
1:A:118:GLU:O	1:A:122:VAL:HG23	2.17	0.44
3:I:45:LEU:HD21	3:I:64:VAL:HG12	1.89	0.44
1:C:151:SER:HB3	1:C:154:CYS:SG	2.57	0.44
1:A:167:GLY:O	1:A:191:ARG:NH2	2.51	0.44
1:A:59:ASN:O	1:A:61:HIS:CE1	2.69	0.44
1:D:52:GLN:NE2	1:D:81:MET:H	2.16	0.44
1:D:70:GLN:HE22	2:T:81:SER:HB3	1.78	0.44
1:D:81:MET:HE1	1:D:97:PHE:HA	1.98	0.44
1:B:26:TRP:CZ3	1:B:62:GLY:O	2.70	0.44
1:A:199:MET:HA	1:A:199:MET:CE	2.48	0.44
1:A:56:CYS:C	1:A:58:GLN:H	2.19	0.44
3:K:20:GLU:HG3	1:D:98:GLN:HE21	1.81	0.44
3:J:27:LYS:HZ2	3:J:108:LEU:HD11	1.83	0.44
1:D:70:GLN:HG2	4:D:214:NAG:H81	2.00	0.44
3:I:30:PRO:O	3:I:34:GLU:HG3	2.18	0.44
1:B:73:GLU:CD	1:B:110:VAL:HG11	2.38	0.44
1:A:72:PHE:HB3	1:A:110:VAL:HG12	1.98	0.44
3:J:10:GLY:O	3:J:53:GLN:HG3	2.17	0.44
1:A:138:THR:OG1	1:A:140:ASP:HB3	2.18	0.44
1:A:12:PHE:O	1:A:36:SER:OG	2.26	0.44
1:B:8:ARG:HD3	1:B:186:TYR:CZ	2.53	0.44
3:K:63:LYS:NZ	3:K:120:ASP:O	2.48	0.44
1:A:5:MET:CB	1:A:166:TYR:CE2	3.00	0.44
1:C:60:ASN:HD21	1:C:70:GLN:HB2	1.81	0.43
1:A:67:LEU:HB3	2:P:81:SER:HG	1.81	0.43
1:C:51:GLN:HB3	1:C:86:TYR:CE1	2.53	0.43
3:J:123:THR:O	3:J:125:PHE:CD1	2.71	0.43
3:K:7:ILE:CG2	3:K:8:PRO:N	2.80	0.43
2:T:81:SER:HA	3:L:7:ILE:CG1	2.43	0.43
3:J:49:GLN:NE2	3:J:122:LEU:HD12	2.33	0.43
3:J:55:VAL:C	3:J:57:GLY:N	2.71	0.43
1:B:60:ASN:OD1	1:B:66:GLY:HA3	2.19	0.43
1:C:61:HIS:O	1:C:62:GLY:C	2.57	0.43
1:C:26:TRP:CZ3	1:C:62:GLY:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:TRP:CG	1:D:66:GLY:HA3	2.53	0.43
1:D:66:GLY:O	3:L:8:PRO:HD2	2.18	0.43
1:B:26:TRP:CD2	1:B:66:GLY:HA3	2.53	0.43
3:J:21:ILE:HD13	3:J:21:ILE:HA	1.86	0.43
1:B:121:MET:O	1:B:125:VAL:HG23	2.19	0.43
1:A:5:MET:O	1:A:165:GLY:CA	2.66	0.43
1:C:73:GLU:CD	1:C:110:VAL:HG11	2.39	0.43
1:B:24:SER:HB3	1:B:28:PHE:HE1	1.84	0.43
3:L:52:THR:CG2	3:L:53:GLN:N	2.81	0.43
1:B:150:SER:HB2	1:B:199:MET:HE3	2.01	0.43
1:B:27:THR:HG22	1:B:53:LEU:HB2	2.01	0.43
1:C:27:THR:CG2	1:C:53:LEU:HB2	2.42	0.43
3:L:7:ILE:HG22	3:L:8:PRO:N	2.34	0.43
1:C:18:ASN:HA	1:C:176:SER:O	2.19	0.43
1:D:19:GLN:HE22	1:D:177:TRP:HE1	1.59	0.43
3:I:15:LYS:HE3	3:I:51:LYS:HA	1.99	0.43
1:B:77:TYR:H	1:B:77:TYR:HD2	1.66	0.43
3:L:63:LYS:HZ1	3:L:120:ASP:CB	2.32	0.43
3:K:60:TYR:HE2	3:K:101:LYS:HD2	1.82	0.43
1:D:33:ALA:N	1:D:162:LEU:CD1	2.82	0.43
3:I:14:ALA:HB2	3:I:51:LYS:HE2	2.00	0.43
1:B:29:SER:HB3	1:B:68:PRO:HG3	2.00	0.43
1:D:133:ALA:HA	1:D:160:ALA:HA	1.99	0.43
1:A:99:PRO:C	1:A:102(A):LYS:H	2.22	0.43
1:A:69:SER:HB2	4:A:213:NAG:H62	2.01	0.43
3:I:55:VAL:C	3:I:57:GLY:N	2.71	0.43
1:D:104:ILE:HG13	1:D:105:ALA:N	2.33	0.43
3:J:25:VAL:HG21	3:J:64:VAL:CG2	2.49	0.42
1:B:77:TYR:CE1	4:B:215:BMA:C1	3.02	0.42
1:B:31:THR:CG2	1:B:50:GLU:HG3	2.48	0.42
1:D:51:GLN:HE21	1:D:90:GLY:N	2.17	0.42
1:C:5:MET:HB3	1:C:166:TYR:CE2	2.54	0.42
1:A:71:ALA:O	1:A:75:ILE:HG13	2.19	0.42
1:A:67:LEU:HD13	3:I:8:PRO:HG2	2.01	0.42
1:B:77:TYR:N	1:B:77:TYR:CD2	2.86	0.42
1:B:118:GLU:HA	1:B:121:MET:HG3	2.01	0.42
1:C:98:GLN:CB	1:C:102(A):LYS:HD3	2.49	0.42
3:J:97:LEU:HD12	3:J:110:LEU:CD1	2.49	0.42
1:D:27:THR:O	1:D:31:THR:HG23	2.19	0.42
3:J:32:LEU:HD21	3:J:40:TYR:OH	2.19	0.42
1:A:77:TYR:N	1:A:77:TYR:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:108:LEU:N	3:I:108:LEU:HD12	2.34	0.42
3:J:11:LEU:HD23	3:J:53:GLN:HE21	1.84	0.42
1:A:7:TRP:CG	1:A:129:PRO:HG3	2.54	0.42
1:D:14:SER:OG	1:D:35:GLU:HG3	2.20	0.42
1:A:46:LEU:HD13	1:A:48:LEU:HD11	2.02	0.42
3:J:29:LYS:N	3:J:30:PRO:HD2	2.35	0.42
1:B:58(B):PHE:CD1	1:B:74:TYR:HB2	2.52	0.42
1:C:86:TYR:N	1:C:87:PRO:HD3	2.35	0.42
1:C:116:ASN:N	1:C:116:ASN:HD22	2.17	0.42
1:D:16:VAL:HG11	1:D:185:GLY:HA3	2.00	0.42
3:K:24:ILE:HG22	3:K:99:VAL:HG21	2.01	0.42
1:C:27:THR:CG2	1:C:53:LEU:HD22	2.49	0.42
2:R:80:CYS:O	3:J:6:MET:O	2.38	0.42
1:A:78(A):LYS:CD	1:A:78(A):LYS:N	2.83	0.42
1:B:198:ASN:HD21	1:B:203:ALA:H	1.67	0.42
1:D:58(B):PHE:CE1	1:D:74:TYR:HA	2.55	0.42
3:K:50:TYR:CD2	3:K:51:LYS:O	2.70	0.42
1:A:16:VAL:HG11	1:A:185:GLY:HA3	2.01	0.42
3:J:96:HIS:CE1	3:J:116:LYS:HD3	2.55	0.42
1:D:55:ASP:CG	1:D:93:ASP:HB2	2.40	0.42
1:D:113:ILE:HG23	1:D:120:ALA:HB3	2.02	0.42
1:A:18:ASN:HA	1:A:176:SER:O	2.20	0.42
1:C:68:PRO:O	1:C:72:PHE:CD2	2.72	0.42
1:C:110:VAL:HG22	1:C:112:ASN:OD1	2.19	0.42
1:D:86:TYR:N	1:D:87:PRO:HD3	2.34	0.42
1:C:177:TRP:CD1	3:K:56:ALA:HA	2.54	0.42
1:D:166:TYR:HD2	1:D:191:ARG:HH12	1.68	0.42
1:A:70:GLN:HA	4:A:214:NAG:O7	2.20	0.42
1:A:198:ASN:ND2	1:A:203:ALA:H	2.18	0.42
1:B:27:THR:CB	1:B:50:GLU:HB3	2.49	0.42
3:I:94:TYR:CZ	3:I:118:LYS:HG3	2.55	0.42
1:B:99:PRO:C	1:B:102(A):LYS:H	2.23	0.42
1:C:161:VAL:HB	1:C:162:LEU:H	1.75	0.42
1:A:51:GLN:O	1:A:54:VAL:HB	2.19	0.41
1:A:18:ASN:HB3	1:A:178:GLY:N	2.34	0.41
1:D:34:LEU:HD11	1:D:106:PHE:O	2.20	0.41
1:A:81:MET:HE2	1:A:98:GLN:N	2.21	0.41
1:C:81:MET:SD	1:C:102(A):LYS:HB3	2.60	0.41
1:C:20:GLY:C	1:C:22:CYS:H	2.24	0.41
1:D:55:ASP:OD2	1:D:93:ASP:HB2	2.21	0.41
1:D:134:PHE:HA	1:D:157:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:MET:CE	1:B:98:GLN:H	2.29	0.41
1:B:94:HIS:O	1:B:96:LYS:HG3	2.20	0.41
1:D:26:TRP:CZ3	1:D:62:GLY:O	2.73	0.41
3:L:62:ILE:C	3:L:122:LEU:HD21	2.41	0.41
1:B:81:MET:SD	1:B:102(A):LYS:HB3	2.61	0.41
1:C:81:MET:SD	1:C:102(A):LYS:CB	3.09	0.41
1:B:18:ASN:HD22	1:B:20:GLY:N	2.16	0.41
4:B:213:NAG:H62	2:R:78:GLN:N	2.22	0.41
1:B:112:ASN:HB3	2:R:78:GLN:NE2	2.35	0.41
3:I:50:TYR:HA	3:I:61:TYR:O	2.19	0.41
1:D:78:ASN:O	1:D:78(A):LYS:HB2	2.20	0.41
1:C:17:LYS:NZ	1:C:47:SER:HG	2.18	0.41
1:D:162:LEU:HD23	1:D:164:VAL:HG13	2.02	0.41
1:B:11:ASN:HD21	1:B:45:MET:HB2	1.86	0.41
1:D:113:ILE:HG21	1:D:121:MET:HG3	2.03	0.41
1:A:17:LYS:HG3	1:A:28:PHE:CE2	2.55	0.41
1:D:16:VAL:HG21	1:D:185:GLY:HA3	2.02	0.41
1:C:97:PHE:CZ	1:C:99:PRO:HA	2.56	0.41
1:B:128:ASN:HB3	1:B:208:TYR:HD2	1.86	0.41
1:D:18:ASN:OD1	1:D:177:TRP:C	2.59	0.41
1:A:58(B):PHE:CD1	1:A:74:TYR:HB2	2.56	0.41
1:B:77:TYR:C	1:B:78(A):LYS:H	2.24	0.41
1:B:49:ALA:CA	1:B:83:GLU:HG3	2.42	0.41
1:A:27:THR:OG1	1:A:50:GLU:HB3	2.21	0.41
3:K:24:ILE:O	3:K:28:VAL:HG12	2.21	0.41
1:A:199:MET:O	1:A:202:LEU:HB2	2.20	0.41
1:D:164:VAL:CG2	1:D:172:ILE:HG22	2.50	0.41
3:I:33:GLU:O	3:I:37:ASN:HA	2.20	0.41
1:A:42:THR:HG21	1:A:212(A):VAL:HG11	2.03	0.41
1:A:89:LYS:HA	1:A:89:LYS:HD3	1.89	0.41
1:B:8:ARG:HH22	1:B:172:ILE:HG21	1.70	0.40
1:C:67:LEU:CD1	3:K:8:PRO:HG2	2.51	0.40
3:L:61:TYR:N	3:L:61:TYR:CD1	2.90	0.40
1:B:118:GLU:O	1:B:121:MET:HB2	2.21	0.40
1:B:53:LEU:HD21	1:B:80:ILE:HD11	2.03	0.40
1:B:78:ASN:ND2	1:B:97:PHE:CE2	2.89	0.40
1:C:51:GLN:O	1:C:54:VAL:HB	2.20	0.40
1:C:55:ASP:O	1:C:95:CYS:HB2	2.21	0.40
1:D:93:ASP:HB3	1:D:96:LYS:HZ2	1.86	0.40
1:B:36:SER:O	1:B:39:ALA:HB3	2.21	0.40
3:I:52:THR:HG22	3:I:58:THR:CG2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TRP:CZ3	1:B:65:GLY:C	2.94	0.40
1:A:70:GLN:OE1	2:P:81:SER:OG	2.34	0.40
1:A:53:LEU:CD2	1:A:53:LEU:N	2.82	0.40
1:D:67:LEU:HA	1:D:67:LEU:HD12	1.88	0.40
1:A:5:MET:O	1:A:165:GLY:HA3	2.22	0.40
3:I:61:TYR:N	3:I:61:TYR:CD1	2.90	0.40
1:A:8:ARG:HG2	1:A:13:VAL:CG2	2.48	0.40
1:B:56:CYS:O	1:B:58:GLN:N	2.51	0.40
1:D:36:SER:O	1:D:40:ILE:HG13	2.21	0.40
1:A:57:ALA:HA	1:A:74:TYR:CD1	2.57	0.40
3:K:62:ILE:HG22	3:K:63:LYS:N	2.36	0.40
1:C:8:ARG:HG3	1:C:13:VAL:HG21	2.03	0.40
1:A:133:ALA:HA	1:A:160:ALA:HA	2.04	0.40
1:B:7:TRP:CG	1:B:129:PRO:HG3	2.56	0.40
3:J:13:GLU:HG3	3:J:14:ALA:H	1.86	0.40
1:D:170:TYR:CD1	1:D:188:LEU:HG	2.56	0.40
1:C:135:GLU:HG3	1:C:156:LYS:O	2.21	0.40
1:B:2:PRO:HB2	1:B:4:SER:O	2.21	0.40
3:L:95:MET:HB2	3:L:95:MET:HE2	1.90	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:119:ASP:OD2	3:L:107:ASP:CG[4_465]	1.37	0.83
3:J:119:ASP:OD1	3:L:107:ASP:OD2[4_465]	1.42	0.78
3:J:119:ASP:OD2	3:L:107:ASP:OD2[4_465]	1.47	0.73
3:J:119:ASP:CG	3:L:107:ASP:OD2[4_465]	1.54	0.66
1:A:84:ASP:O	3:L:115:VAL:CG2[4_455]	1.55	0.65
3:J:119:ASP:OD2	3:L:107:ASP:OD1[4_465]	1.59	0.61
1:B:127:TYR:OH	1:C:208:TYR:OH[3_655]	2.01	0.19
1:B:84:ASP:O	3:K:115:VAL:CG2[4_455]	2.10	0.10
3:J:119:ASP:CG	3:L:107:ASP:CG[4_465]	2.15	0.05
3:J:115:VAL:CG2	1:C:84:ASP:O[4_455]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	218/220 (99%)	191 (88%)	22 (10%)	5 (2%)	8	8
1	B	218/220 (99%)	184 (84%)	26 (12%)	8 (4%)	4	3
1	C	218/220 (99%)	182 (84%)	29 (13%)	7 (3%)	5	4
1	D	218/220 (99%)	190 (87%)	24 (11%)	4 (2%)	11	13
2	P	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
2	R	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
2	S	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
2	T	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
3	I	96/98 (98%)	79 (82%)	14 (15%)	3 (3%)	5	4
3	J	96/98 (98%)	83 (86%)	10 (10%)	3 (3%)	5	4
3	K	96/98 (98%)	82 (85%)	12 (12%)	2 (2%)	9	10
3	L	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	5	4
All	All	1280/1304 (98%)	1091 (85%)	151 (12%)	38 (3%)	5	4

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155(B)	THR
1	B	155(C)	PRO
1	D	155(C)	PRO
1	D	156	LYS
3	L	67	GLY
2	P	80	CYS
1	B	11	ASN
2	R	80	CYS
3	J	67	GLY
3	L	43	GLY
1	A	102	ASP
1	B	57	ALA

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Mol	Chain	Res	Type
1	B	58(B)	PHE
1	B	155(A)	LYS
1	B	190	GLU
3	J	105(A)	ASN
3	K	68	ASP
1	A	57	ALA
1	A	155(B)	THR
1	B	63	CYS
1	C	62	GLY
2	S	80	CYS
3	K	66	ALA
3	L	48	VAL
1	A	84	ASP
1	A	155(D)	ASP
3	J	120	ASP
1	C	19	GLN
1	C	58(B)	PHE
1	C	102	ASP
3	I	115(A)	ASP
1	C	155(C)	PRO
1	C	159	HIS
1	D	62	GLY
1	D	99	PRO
3	I	55	VAL
1	C	209	PRO
3	I	43	GLY

### 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	181/181 (100%)	146 (81%)	35 (19%)	2	2
1	B	181/181 (100%)	148 (82%)	33 (18%)	2	2
1	C	181/181 (100%)	152 (84%)	29 (16%)	3	3
1	D	181/181 (100%)	156 (86%)	25 (14%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	7/7 (100%)	5 (71%)	2 (29%)	0	0
2	R	7/7 (100%)	6 (86%)	1 (14%)	4	4
2	S	7/7 (100%)	4 (57%)	3 (43%)	0	0
2	T	7/7 (100%)	6 (86%)	1 (14%)	4	4
3	I	85/85 (100%)	72 (85%)	13 (15%)	3	4
3	J	85/85 (100%)	65 (76%)	20 (24%)	1	1
3	K	85/85 (100%)	71 (84%)	14 (16%)	3	3
3	L	85/85 (100%)	57 (67%)	28 (33%)	0	0
All	All	1092/1092 (100%)	888 (81%)	204 (19%)	2	2

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	15	PRO
1	A	17	LYS
1	A	21	SER
1	A	26	TRP
1	A	35	GLU
1	A	36	SER
1	A	46	LEU
1	A	52	GLN
1	A	56	CYS
1	A	59	ASN
1	A	64	GLN
1	A	78(A)	LYS
1	A	80	ILE
1	A	81	MET
1	A	83	GLU
1	A	86	TYR
1	A	94	HIS
1	A	96	LYS
1	A	99	PRO
1	A	102(A)	LYS
1	A	109	ASP
1	A	114	THR
1	A	126(A)	LEU
1	A	139	ASN
1	A	146	LYS

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Mol	Chain	Res	Type
1	A	155(A)	LYS
1	A	155(B)	THR
1	A	161	VAL
1	A	168(A)	GLU
1	A	168(D)	ILE
1	A	184	ASN
1	A	195	LYS
1	A	199	MET
1	A	212(A)	VAL
2	P	76	GLU
2	P	80	CYS
3	I	7	ILE
3	I	13	GLU
3	I	15	LYS
3	I	19	PRO
3	I	27	LYS
3	I	28	VAL
3	I	32	LEU
3	I	52	THR
3	I	64	VAL
3	I	97	LEU
3	I	120	ASP
3	I	121	GLU
3	I	122	LEU
1	B	18	ASN
1	B	19	GLN
1	B	21	SER
1	B	24	SER
1	B	26	TRP
1	B	36	SER
1	B	44	LYS
1	B	46	LEU
1	B	56	CYS
1	B	76	ARG
1	B	78(A)	LYS
1	B	81	MET
1	B	86	TYR
1	B	99	PRO
1	B	102(A)	LYS
1	B	109	ASP
1	B	110	VAL
1	B	126(A)	LEU

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Mol	Chain	Res	Type
1	B	129	PRO
1	B	139	ASN
1	B	143	MET
1	B	145	ARG
1	B	152	THR
1	B	155(B)	THR
1	B	155(D)	ASP
1	B	157	VAL
1	B	161	VAL
1	B	168	GLU
1	B	168(B)	ASN
1	B	184	ASN
1	B	202	LEU
1	B	212	LEU
1	B	212(A)	VAL
2	R	80	CYS
3	J	6	MET
3	J	8	PRO
3	J	15	LYS
3	J	19	PRO
3	J	27	LYS
3	J	28	VAL
3	J	29	LYS
3	J	37	ASN
3	J	44	LYS
3	J	52	THR
3	J	54	VAL
3	J	58	THR
3	J	64	VAL
3	J	65	ARG
3	J	68	ASP
3	J	97	LEU
3	J	105	GLN
3	J	108	LEU
3	J	115	VAL
3	J	116	LYS
1	C	1	TYR
1	C	17	LYS
1	C	22	CYS
1	C	24	SER
1	C	26	TRP
1	C	27	THR

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Mol	Chain	Res	Type
1	C	36	SER
1	C	44	LYS
1	C	46	LEU
1	C	48	LEU
1	C	52	GLN
1	C	55	ASP
1	C	69	SER
1	C	76	ARG
1	C	85	THR
1	C	89	LYS
1	C	110	VAL
1	C	119	GLU
1	C	129	PRO
1	C	155	HIS
1	C	155(A)	LYS
1	C	155(B)	THR
1	C	155(C)	PRO
1	C	156	LYS
1	C	161	VAL
1	C	168(D)	ILE
1	C	195	LYS
1	C	198	ASN
1	C	199	MET
2	S	76	GLU
2	S	78	GLN
2	S	79	ASN
3	K	13	GLU
3	K	15	LYS
3	K	16	PRO
3	K	23	GLU
3	K	32	LEU
3	K	36	THR
3	K	39	THR
3	K	52	THR
3	K	58	THR
3	K	65	ARG
3	K	95	MET
3	K	97	LEU
3	K	102	SER
3	K	116	LYS
1	D	14	SER
1	D	21	SER

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Mol	Chain	Res	Type
1	D	26	TRP
1	D	42	THR
1	D	48	LEU
1	D	53	LEU
1	D	69	SER
1	D	81	MET
1	D	83	GLU
1	D	89	LYS
1	D	94	HIS
1	D	96	LYS
1	D	102(A)	LYS
1	D	110	VAL
1	D	136	VAL
1	D	145	ARG
1	D	146	LYS
1	D	155(A)	LYS
1	D	155(C)	PRO
1	D	161	VAL
1	D	168	GLU
1	D	173	VAL
1	D	198	ASN
1	D	199	MET
1	D	202	LEU
2	T	76	GLU
3	L	6	MET
3	L	11	LEU
3	L	15	LYS
3	L	16	PRO
3	L	18	THR
3	L	25	VAL
3	L	30	PRO
3	L	32	LEU
3	L	33	GLU
3	L	36	THR
3	L	44	LYS
3	L	46	GLU
3	L	58	THR
3	L	61	TYR
3	L	62	ILE
3	L	65	ARG
3	L	68	ASP
3	L	92	ASN

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Mol	Chain	Res	Type
3	L	95	MET
3	L	101	LYS
3	L	102	SER
3	L	107	ASP
3	L	109	VAL
3	L	111	THR
3	L	115	VAL
3	L	116	LYS
3	L	118	LYS
3	L	120	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	51	GLN
1	A	52	GLN
1	A	61	HIS
1	A	64	GLN
1	A	78	ASN
1	A	98	GLN
1	A	116	ASN
1	A	180	GLN
1	A	198	ASN
1	B	11	ASN
1	B	18	ASN
1	B	19	GLN
1	B	51	GLN
1	B	52	GLN
1	B	60	ASN
1	B	70	GLN
1	B	116	ASN
1	B	198	ASN
3	J	37	ASN
3	J	49	GLN
1	C	51	GLN
1	C	52	GLN
1	C	70	GLN
1	C	116	ASN
1	C	158	ASN
1	C	198	ASN
1	D	51	GLN

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Mol	Chain	Res	Type
1	D	52	GLN
1	D	58(A)	ASN
1	D	59	ASN
1	D	60	ASN
1	D	61	HIS
1	D	78	ASN
1	D	98	GLN
1	D	184	ASN
1	D	198	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

12 carbohydrates 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	A	213	1,4	14,14,15	0.83	1 (7%)	15,19,21	1.00	1 (6%)
4	NAG	A	214	4	14,14,15	0.43	0	15,19,21	0.97	1 (6%)
4	BMA	A	215	4	11,11,12	0.80	0	14,15,17	1.55	2 (14%)
4	NAG	B	213	1,4	14,14,15	0.46	0	15,19,21	1.56	2 (13%)
4	NAG	B	214	4	14,14,15	0.56	0	15,19,21	1.21	1 (6%)
4	BMA	B	215	4	11,11,12	0.33	0	14,15,17	0.53	0
4	NAG	C	213	1,4	14,14,15	1.00	2 (14%)	15,19,21	0.89	1 (6%)
4	NAG	C	214	4	14,14,15	0.56	0	15,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	C	215	4	11,11,12	0.68	0	14,15,17	0.77	0
4	NAG	D	213	1,4	14,14,15	0.66	0	15,19,21	1.28	1 (6%)
4	NAG	D	214	4	14,14,15	0.56	0	15,19,21	0.94	1 (6%)
4	BMA	D	215	4	11,11,12	0.50	0	14,15,17	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	214	4	-	0/6/23/26	0/1/1/1
4	BMA	A	215	4	-	0/2/19/22	0/1/1/1
4	NAG	B	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	214	4	-	0/6/23/26	0/1/1/1
4	BMA	B	215	4	-	0/2/19/22	0/1/1/1
4	NAG	C	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	214	4	-	0/6/23/26	0/1/1/1
4	BMA	C	215	4	-	0/2/19/22	0/1/1/1
4	NAG	D	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	214	4	-	0/6/23/26	0/1/1/1
4	BMA	D	215	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	213	NAG	C4-C5	2.07	1.57	1.53
4	C	213	NAG	C4-C3	2.08	1.57	1.52
4	C	213	NAG	C4-C5	2.14	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	214	NAG	C2-N2-C7	-3.36	118.72	123.04
4	A	214	NAG	C2-N2-C7	-3.31	118.78	123.04
4	B	214	NAG	C2-N2-C7	-3.28	118.83	123.04
4	C	213	NAG	C2-N2-C7	-2.49	119.84	123.04
4	A	213	NAG	C2-N2-C7	-2.46	119.88	123.04
4	D	213	NAG	C3-C4-C5	2.62	114.76	110.20
4	A	215	BMA	C3-C4-C5	3.28	115.92	110.20
4	A	215	BMA	C2-C3-C4	3.41	116.83	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	213	NAG	C3-C4-C5	3.71	116.66	110.20
4	B	213	NAG	C1-O5-C5	3.83	117.11	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	213	NAG	4	0
4	A	214	NAG	4	0
4	A	215	BMA	1	0
4	B	213	NAG	4	0
4	B	214	NAG	2	0
4	B	215	BMA	5	0
4	C	213	NAG	1	0
4	C	214	NAG	1	0
4	D	214	NAG	3	0

## 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, 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	216/220 (98%)	0.74	20 (9%)	11 10	14, 36, 59, 79	13 (6%)
1	B	216/220 (98%)	0.73	21 (9%)	10 9	15, 35, 57, 67	15 (6%)
1	C	217/220 (98%)	0.89	24 (11%)	7 7	19, 36, 60, 78	16 (7%)
1	D	216/220 (98%)	0.85	15 (6%)	20 19	15, 37, 58, 75	14 (6%)
2	P	8/8 (100%)	3.51	6 (75%)	0 0	34, 52, 61, 65	2 (25%)
2	R	6/8 (75%)	2.50	4 (66%)	0 0	31, 53, 67, 69	1 (16%)
2	S	6/8 (75%)	2.72	4 (66%)	0 0	49, 64, 67, 68	0
2	T	6/8 (75%)	3.24	3 (50%)	0 0	42, 60, 69, 72	1 (16%)
3	I	98/98 (100%)	1.11	16 (16%)	2 2	16, 39, 59, 78	11 (11%)
3	J	98/98 (100%)	1.10	20 (20%)	1 1	17, 39, 64, 77	12 (12%)
3	K	96/98 (97%)	1.16	18 (18%)	2 1	18, 51, 67, 78	13 (13%)
3	L	96/98 (97%)	1.36	22 (22%)	1 1	21, 49, 68, 79	11 (11%)
All	All	1279/1304 (98%)	0.96	173 (13%)	4 4	14, 39, 64, 79	109 (8%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	66	ALA	11.7
3	I	105(A)	ASN	10.4
3	J	105(A)	ASN	9.8
2	P	82	ALA	9.8
1	B	155(D)	ASP	9.7
1	C	155(D)	ASP	9.4
2	T	81	SER	8.7
3	L	67	GLY	8.2
1	A	155(D)	ASP	7.5
1	D	155(D)	ASP	6.4
3	L	39	THR	6.4

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Mol	Chain	Res	Type	RSRZ
3	L	68	ASP	6.2
3	K	39	THR	6.2
3	J	67	GLY	5.8
3	I	104	GLY	5.7
1	A	153	SER	5.4
2	S	76	GLU	5.4
1	D	155	HIS	5.3
1	A	154	CYS	5.2
3	L	107	ASP	5.1
1	C	155	HIS	5.0
1	C	168(C)	GLY	4.9
1	D	139	ASN	4.7
1	D	18	ASN	4.7
3	L	34	GLU	4.6
3	J	36	THR	4.5
1	A	139	ASN	4.5
3	K	104	GLY	4.5
3	J	44	LYS	4.4
2	R	81	SER	4.4
1	C	139	ASN	4.3
3	L	19	PRO	4.3
1	D	20	GLY	4.2
3	I	107	ASP	4.2
2	P	83	THR	4.2
1	D	212(A)	VAL	4.0
3	J	37	ASN	4.0
3	L	92	ASN	4.0
3	J	105	GLN	3.9
1	C	21	SER	3.9
1	D	94	HIS	3.9
2	P	76	GLU	3.8
3	K	67	GLY	3.8
2	T	80	CYS	3.8
3	K	15	LYS	3.8
3	I	106	GLU	3.8
1	A	138	THR	3.7
1	B	58(A)	ASN	3.7
1	C	195	LYS	3.7
1	D	168(B)	ASN	3.7
1	B	153	SER	3.6
3	K	117	ASN	3.6
1	B	212(A)	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	L	37	ASN	3.6
3	L	104	GLY	3.6
3	L	33	GLU	3.6
3	K	105	GLN	3.5
1	A	168(A)	GLU	3.4
3	J	115(A)	ASP	3.4
3	K	66	ALA	3.3
3	I	103	PRO	3.3
3	L	105	GLN	3.2
2	R	79	ASN	3.2
2	T	79	ASN	3.2
1	A	152	THR	3.2
1	D	19	GLN	3.2
1	C	18	ASN	3.1
1	C	140	ASP	3.1
2	S	80	CYS	3.1
2	R	80	CYS	3.1
2	S	81	SER	3.1
1	B	58(B)	PHE	3.1
1	B	139	ASN	3.0
3	J	104	GLY	3.0
2	P	81	SER	3.0
3	L	35	LYS	3.0
1	C	1	TYR	3.0
1	C	19	GLN	3.0
1	C	203	ALA	3.0
2	P	79	ASN	2.9
1	C	54	VAL	2.9
3	I	115	VAL	2.9
1	C	20	GLY	2.9
1	B	154	CYS	2.9
1	C	143	MET	2.9
1	C	103	ALA	2.9
1	D	84	ASP	2.9
1	A	150	SER	2.9
3	I	115(A)	ASP	2.8
3	K	34	GLU	2.8
1	B	152	THR	2.8
1	C	154	CYS	2.8
1	A	45	MET	2.8
3	J	117	ASN	2.8
3	I	108	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	J	40	TYR	2.8
3	I	105	GLN	2.7
1	D	152	THR	2.7
1	D	65	GLY	2.7
3	J	34	GLU	2.7
1	B	168(D)	ILE	2.7
1	C	151	SER	2.7
1	C	157	VAL	2.7
3	J	103	PRO	2.7
3	L	94	TYR	2.7
1	D	26	TRP	2.6
3	I	68	ASP	2.6
3	I	125	PHE	2.6
1	B	26	TRP	2.6
1	D	39	ALA	2.6
3	K	100	PHE	2.6
1	A	179	PRO	2.6
1	B	168(B)	ASN	2.5
1	C	9	LYS	2.5
3	L	43	GLY	2.5
3	K	8	PRO	2.5
3	J	107	ASP	2.5
1	B	168(C)	GLY	2.5
3	J	125	PHE	2.5
3	I	67	GLY	2.5
1	D	140	ASP	2.5
3	L	118	LYS	2.5
3	J	106	GLU	2.4
2	R	77	PRO	2.4
3	K	115(A)	ASP	2.4
3	J	119	ASP	2.4
1	A	135	GLU	2.4
1	C	168(D)	ILE	2.4
3	J	68	ASP	2.4
1	A	69	SER	2.4
3	I	45	LEU	2.3
3	L	93	LYS	2.3
3	L	110	LEU	2.3
1	B	77	TYR	2.3
1	A	203	ALA	2.3
3	K	19	PRO	2.3
1	A	202	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	S	79	ASN	2.3
3	L	117	ASN	2.3
1	B	157	VAL	2.3
3	K	9	GLY	2.3
1	A	212(A)	VAL	2.3
1	C	145	ARG	2.3
1	A	82	GLY	2.2
2	P	77	PRO	2.2
1	B	206	ALA	2.2
1	B	138	THR	2.2
3	K	38	GLU	2.2
3	I	65	ARG	2.2
3	L	66	ALA	2.2
3	L	119	ASP	2.2
1	A	94	HIS	2.2
3	I	102	SER	2.2
3	J	66	ALA	2.2
1	C	200	CYS	2.2
1	A	151	SER	2.1
1	B	170	TYR	2.1
1	B	11	ASN	2.1
1	B	116	ASN	2.1
3	K	110	LEU	2.1
3	K	93	LYS	2.1
3	K	94	TYR	2.1
3	J	39	THR	2.1
3	L	102	SER	2.1
1	A	2	PRO	2.1
1	B	39	ALA	2.1
1	A	157	VAL	2.1
3	K	92	ASN	2.1
1	C	28	PHE	2.1
3	L	109	VAL	2.0
1	C	138	THR	2.0
1	B	168(A)	GLU	2.0
3	J	13	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. 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	C	214	14/15	0.84	0.20	0.58	21,39,47,49	0
4	NAG	A	213	14/15	0.81	0.27	0.18	43,50,69,70	0
4	NAG	B	213	14/15	0.82	0.22	-0.27	30,49,57,58	0
4	NAG	D	213	14/15	0.86	0.21	-0.39	21,32,53,54	0
4	NAG	C	213	14/15	0.89	0.17	-0.60	13,32,53,57	0
4	NAG	D	214	14/15	0.91	0.15	-0.91	28,41,49,54	0
4	NAG	B	214	14/15	0.86	0.16	-1.28	5,53,57,58	0
4	NAG	A	214	14/15	0.93	0.17	-1.29	22,50,65,68	0
4	BMA	B	215	11/12	0.83	0.22	-	40,52,61,70	0
4	BMA	D	215	11/12	0.66	0.21	-	42,54,65,69	0
4	BMA	C	215	11/12	0.70	0.26	-	36,49,63,67	0
4	BMA	A	215	11/12	0.53	0.34	-	43,61,65,68	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.