



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1NB3
Title : Crystal structure of stefin A in complex with cathepsin H: N-terminal residues of inhibitors can adapt to the active sites of endo-and exopeptidases
Authors : Jenko, S.; Dolenc, I.; Guncar, G.; Dobersek, A.; Podobnik, M.; Turk, D.
Deposited on : 2002-12-02
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

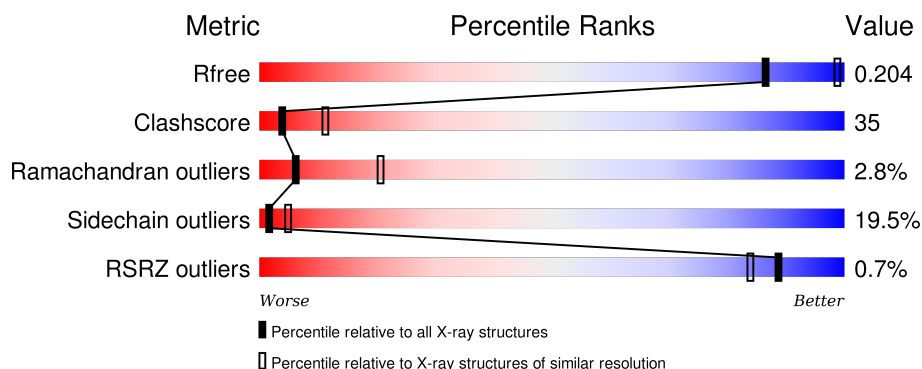
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>13%</div> <div>47%</div> <div>41%</div> <div>12%</div> </div>
1	B	220	<div> <div>37%</div> <div>48%</div> <div>14%</div> </div>
1	C	220	<div> <div>46%</div> <div>45%</div> <div>8%</div> </div>
1	D	220	<div> <div>40%</div> <div>51%</div> <div>9%</div> </div>
2	P	8	<div> <div>13%</div> <div>50%</div> <div>50%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	R	8	<div><div></div><div>25%</div><div>25%</div><div>63%</div><div>13%</div></div>
2	S	8	<div><div></div><div>13%</div><div>50%</div><div>25%</div><div>25%</div></div>
2	T	8	<div><div></div><div>50%</div><div>38%</div><div>13%</div></div>
3	I	98	<div><div></div><div>%</div><div>37%</div><div>53%</div><div>10%</div></div>
3	J	98	<div><div></div><div>42%</div><div>47%</div><div>11%</div></div>
3	K	98	<div><div></div><div>%</div><div>42%</div><div>47%</div><div>9%</div><div></div></div>
3	L	98	<div><div></div><div>%</div><div>44%</div><div>43%</div><div>13%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10855 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	43	0	0
			1706	1085	283	322	16			
1	B	220	Total	C	N	O	S	42	0	0
			1706	1085	283	322	16			
1	C	220	Total	C	N	O	S	43	0	0
			1706	1085	283	322	16			
1	D	220	Total	C	N	O	S	44	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	11	0	0
			58	32	10	15	1			
2	R	8	Total	C	N	O	S	11	0	0
			58	32	10	15	1			
2	S	8	Total	C	N	O	S	19	0	0
			58	32	10	15	1			
2	T	8	Total	C	N	O	S	23	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	42	0	0
			775	492	126	155	2			
3	J	98	Total	C	N	O	S	40	0	0
			775	492	126	155	2			
3	K	98	Total	C	N	O	S	50	0	0
			775	492	126	155	2			
3	L	98	Total	C	N	O	S	48	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 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total	O	0	0
			100	100		
5	B	78	Total	O	0	0
			78	78		
5	C	110	Total	O	0	0
			110	110		
5	D	94	Total	O	0	0
			94	94		
5	I	35	Total	O	0	0
			35	35		
5	J	43	Total	O	0	0
			43	43		
5	K	37	Total	O	0	0
			37	37		
5	L	39	Total	O	0	0
			39	39		
5	R	2	Total	O	0	0
			2	2		
5	S	2	Total	O	0	0
			2	2		
5	T	3	Total	O	0	0
			3	3		

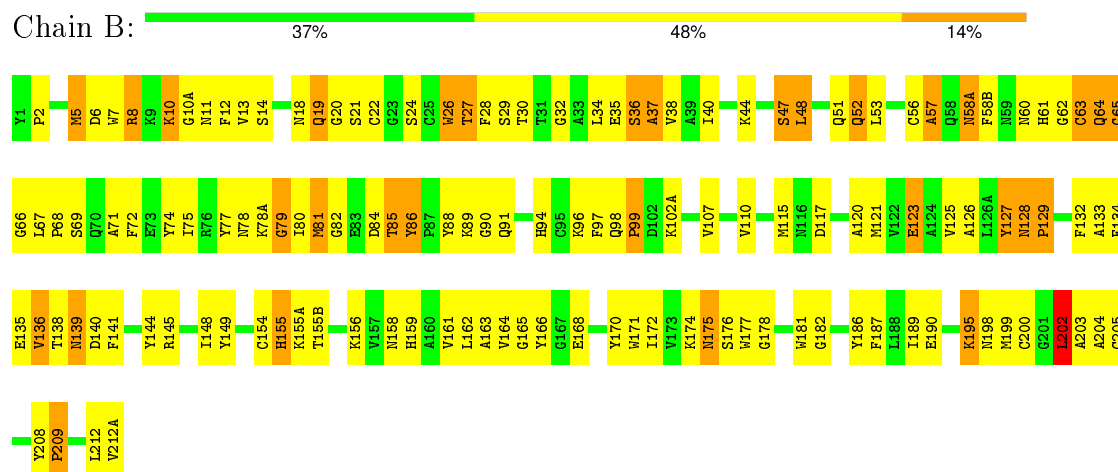
3 Residue-property plots

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

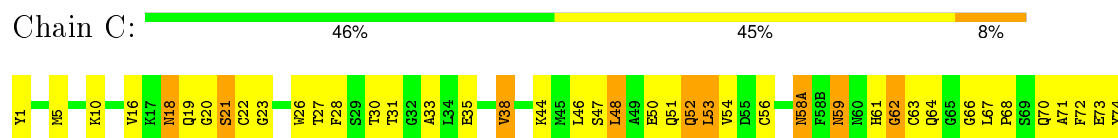
• Molecule 1: Cathepsin H

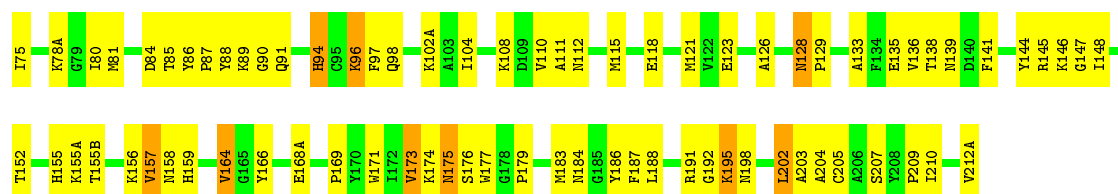


• Molecule 1: Cathepsin H

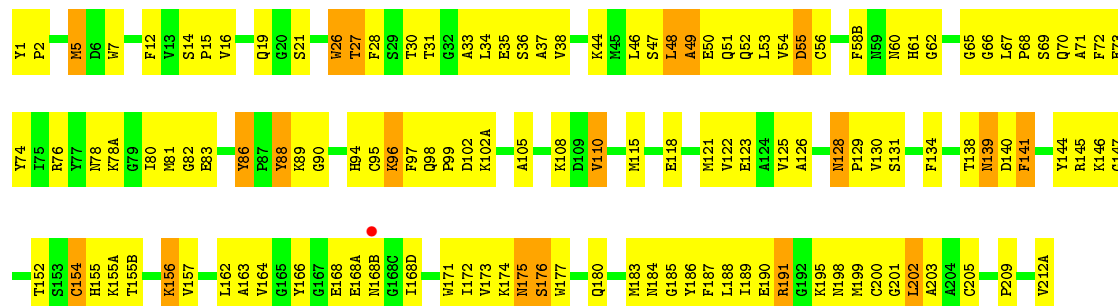


• Molecule 1: Cathepsin H





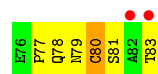
- Molecule 1: Cathepsin H



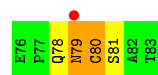
- Molecule 2: CATHEPSIN H MINI CHAIN



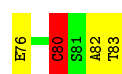
- Molecule 2: CATHEPSIN H MINI CHAIN



- Molecule 2: CATHEPSIN H MINI CHAIN



- Molecule 2: CATHEPSIN H MINI CHAIN

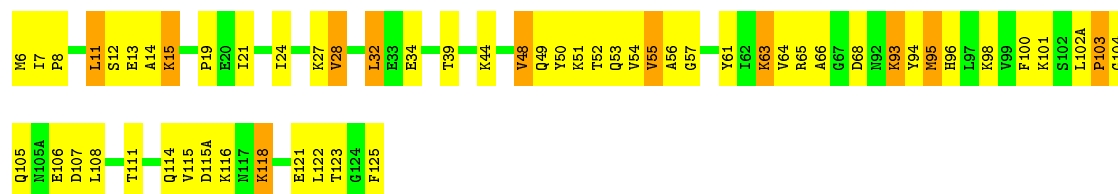


- Molecule 3: Stefin A

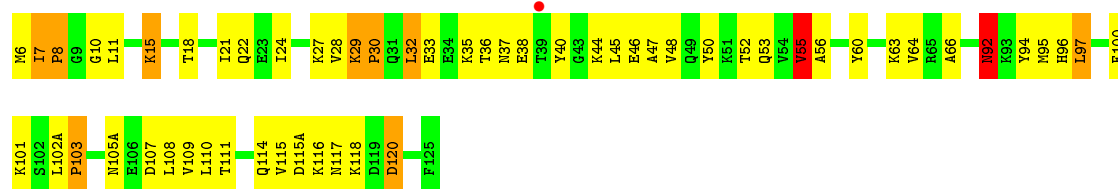
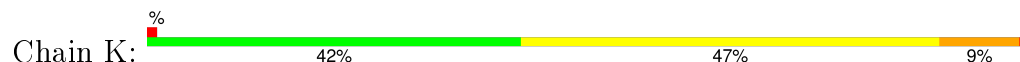




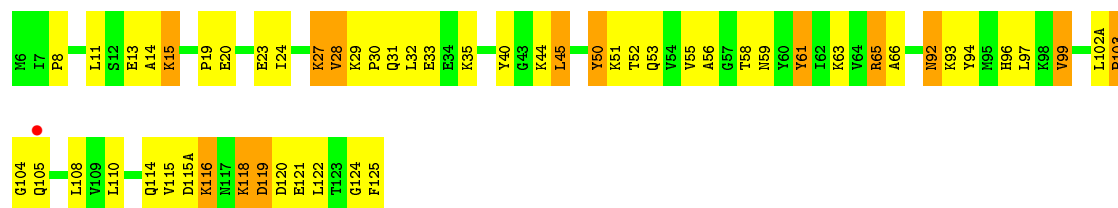
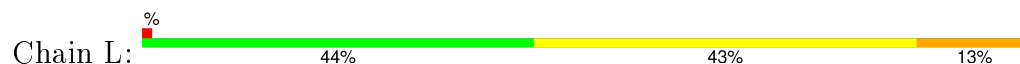
• Molecule 3: Stefin A



• Molecule 3: Stefin A



• Molecule 3: Stefin A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.58 Å 91.63 Å 161.24 Å 90.00° 93.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 90.8 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.227 , 0.246 0.201 , 0.204	Depositor DCC
R_{free} test set	1659 reflections (5.63%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 33744 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10855	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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	0.78	0/1753	0.94	1/2377 (0.0%)
1	B	0.78	0/1753	0.90	4/2377 (0.2%)
1	C	0.83	0/1753	0.89	0/2377
1	D	0.79	0/1753	0.92	1/2377 (0.0%)
2	P	0.66	0/58	1.05	0/77
2	R	0.76	0/58	1.11	0/77
2	S	0.62	0/58	0.99	0/77
2	T	0.57	0/58	0.76	0/77
3	I	0.77	0/788	0.94	1/1062 (0.1%)
3	J	0.78	0/788	0.93	1/1062 (0.1%)
3	K	0.81	0/788	0.88	0/1062
3	L	0.76	0/788	0.88	1/1062 (0.1%)
All	All	0.79	0/10396	0.91	9/14064 (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
1	A	0	1
1	C	0	1
1	D	0	1
3	I	0	1
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	11	LEU	CA-CB-CG	7.09	131.60	115.30
1	A	65	GLY	N-CA-C	5.76	127.50	113.10
1	D	191	ARG	NE-CZ-NH2	-5.51	117.54	120.30
3	L	45	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	127	TYR	N-CA-C	5.41	125.62	111.00
1	B	56	CYS	N-CA-C	5.37	125.50	111.00
3	I	67	GLY	N-CA-C	-5.19	100.14	113.10
1	B	79	GLY	N-CA-C	5.07	125.78	113.10
1	B	65	GLY	N-CA-C	5.01	125.63	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain
1	C	166	TYR	Sidechain
1	D	88	TYR	Sidechain
3	I	60	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	104	2
1	B	1706	0	1622	140	0
1	C	1706	0	1622	113	0
1	D	1706	0	1622	119	0
2	P	58	0	47	1	0
2	R	58	0	47	5	0
2	S	58	0	47	6	0
2	T	58	0	47	1	0
3	I	775	0	777	54	0
3	J	775	0	777	46	4
3	K	775	0	777	54	1
3	L	775	0	777	56	0
4	A	39	0	34	3	0
4	B	39	0	34	4	0
4	C	39	0	34	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	39	0	34	1	0
5	A	100	0	0	3	0
5	B	78	0	0	1	0
5	C	110	0	0	4	3
5	D	94	0	0	7	1
5	I	35	0	0	0	2
5	J	43	0	0	1	0
5	K	37	0	0	2	0
5	L	39	0	0	1	1
5	R	2	0	0	2	0
5	S	2	0	0	1	0
5	T	3	0	0	0	0
All	All	10855	0	9920	670	7

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 (670) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:MET:HE2	1:A:98:GLN:H	1.28	0.98
1:A:72:PHE:HB3	1:A:110:VAL:HG11	1.44	0.96
1:B:52:GLN:HE22	1:B:80:ILE:HA	1.31	0.96
3:I:31:GLN:HA	3:I:34:GLU:HG2	1.47	0.96
3:K:22:GLN:HE22	3:K:46:GLU:HA	1.32	0.93
1:A:156:LYS:HA	3:I:6:MET:HG3	1.51	0.91
1:B:175:ASN:HD22	1:B:176:SER:H	1.15	0.91
1:C:52:GLN:HE21	1:C:81:MET:HG2	1.35	0.90
3:L:51:LYS:HD2	3:L:122:LEU:HB2	1.50	0.90
1:A:81:MET:CE	1:A:98:GLN:H	1.83	0.90
1:D:14:SER:HB2	1:D:15:PRO:HD2	1.55	0.89
1:B:94:HIS:O	1:B:96:LYS:HE3	1.73	0.89
1:B:81:MET:HE2	1:B:98:GLN:H	1.42	0.84
3:K:45:LEU:HD23	3:K:66:ALA:HB2	1.59	0.84
1:C:81:MET:HE1	1:C:97:PHE:HA	1.61	0.82
1:C:146:LYS:HG3	1:C:183:MET:HG2	1.61	0.82
3:I:63:LYS:HB2	3:I:122:LEU:HD11	1.60	0.82
1:B:77:TYR:CE2	4:B:215:BMA:H3	2.16	0.81
1:B:121:MET:SD	1:B:203:ALA:HB2	2.21	0.80
1:C:73:GLU:OE2	4:C:213:NAG:H3	1.82	0.80
3:K:28:VAL:HG11	3:K:110:LEU:HD13	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:GLN:HE22	1:D:81:MET:HG3	1.47	0.79
3:J:103:PRO:HD3	5:J:522:HOH:O	1.83	0.79
1:B:158:ASN:HB3	3:J:6:MET:CE	2.13	0.78
1:D:81:MET:HE3	1:D:86:TYR:HD2	1.49	0.78
1:A:5:MET:HG2	1:A:126:ALA:HA	1.66	0.77
1:C:51:GLN:HG2	1:C:88:TYR:HA	1.66	0.77
1:B:51:GLN:HE21	1:B:90:GLY:H	1.32	0.76
1:D:67:LEU:HB3	1:D:70:GLN:HG3	1.67	0.76
3:J:94:TYR:OH	3:J:118:LYS:HG3	1.86	0.76
3:I:27:LYS:HE3	3:I:108:LEU:HD21	1.67	0.75
3:L:29:LYS:HG3	3:L:45:LEU:HD22	1.69	0.75
1:C:22:CYS:O	3:K:55:VAL:HG12	1.87	0.75
1:A:31:THR:O	1:A:35:GLU:HG3	1.87	0.74
1:B:175:ASN:ND2	1:B:176:SER:H	1.85	0.73
3:L:15:LYS:HD3	3:L:50:TYR:CE1	2.23	0.73
1:C:198:ASN:ND2	1:C:203:ALA:H	1.87	0.73
1:A:133:ALA:HA	1:A:159:HIS:O	1.88	0.73
1:D:162:LEU:O	1:D:173:VAL:HG13	1.89	0.73
1:D:121:MET:O	1:D:125:VAL:HG23	1.89	0.72
1:C:26:TRP:CH2	1:C:62:GLY:O	2.43	0.72
1:B:35:GLU:HB3	1:B:48:LEU:HD22	1.72	0.72
3:K:28:VAL:CG1	3:K:110:LEU:HD13	2.17	0.72
1:C:198:ASN:HD21	1:C:203:ALA:H	1.36	0.72
1:C:51:GLN:CG	1:C:88:TYR:HA	2.20	0.72
1:B:136:VAL:HG22	1:B:141:PHE:CD2	2.24	0.71
1:A:198:ASN:ND2	1:A:203:ALA:H	1.88	0.71
3:L:51:LYS:HD2	3:L:122:LEU:CB	2.20	0.71
1:C:52:GLN:NE2	1:C:81:MET:HG2	2.05	0.71
1:A:180:GLN:NE2	1:A:180:GLN:HA	2.06	0.71
3:I:48:VAL:HG21	3:I:65:ARG:HB2	1.73	0.71
1:A:125:VAL:HA	1:A:128:ASN:O	1.91	0.71
3:L:15:LYS:NZ	3:L:50:TYR:CE2	2.59	0.71
1:D:94:HIS:O	1:D:96:LYS:HE3	1.90	0.71
1:B:175:ASN:HD22	1:B:176:SER:N	1.88	0.70
3:L:94:TYR:HB2	3:L:116:LYS:O	1.90	0.70
1:D:51:GLN:NE2	1:D:90:GLY:H	1.90	0.70
1:B:81:MET:HE2	1:B:98:GLN:N	2.07	0.70
3:L:118:LYS:HG3	3:L:119:ASP:N	2.07	0.70
1:A:172:ILE:HA	1:A:188:LEU:CD1	2.22	0.70
1:A:72:PHE:CB	1:A:110:VAL:HG11	2.20	0.69
3:L:15:LYS:HE3	3:L:51:LYS:HA	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLU:OE2	5:D:281:HOH:O	2.10	0.69
1:D:51:GLN:HE22	1:D:90:GLY:H	1.39	0.69
1:C:121:MET:SD	5:C:306:HOH:O	2.51	0.69
1:C:28:PHE:CE2	1:C:50:GLU:HG2	2.28	0.69
1:C:70:GLN:HG2	4:C:214:NAG:H81	1.75	0.68
1:B:84:ASP:OD2	1:B:85:THR:HG23	1.94	0.68
1:C:81:MET:HB3	1:C:102(A):LYS:O	1.94	0.68
1:B:181:TRP:CH2	1:B:187:PHE:HB3	2.28	0.68
3:J:108:LEU:HD12	3:J:108:LEU:N	2.09	0.68
1:C:81:MET:CE	1:C:97:PHE:HA	2.24	0.68
3:L:114:GLN:HG2	3:L:116:LYS:HD3	1.75	0.68
1:B:189:ILE:CG2	1:B:202:LEU:HD21	2.24	0.67
1:A:119:GLU:HA	1:A:122:VAL:HG23	1.76	0.67
1:B:158:ASN:HB3	3:J:6:MET:HE1	1.75	0.67
1:B:198:ASN:HD21	1:B:203:ALA:H	1.41	0.67
1:B:115:MET:HG2	1:B:204:ALA:O	1.94	0.67
1:D:72:PHE:CZ	1:D:209:PRO:HD3	2.30	0.67
1:A:52:GLN:NE2	1:A:80:ILE:HA	2.11	0.66
1:B:199:MET:HG3	1:B:200:CYS:SG	2.35	0.66
1:A:77:TYR:H	1:A:77:TYR:HD1	1.43	0.66
3:K:15:LYS:NZ	3:K:50:TYR:CE2	2.60	0.66
3:L:33:GLU:HG2	3:L:40:TYR:HD2	1.60	0.66
3:K:27:LYS:HD2	3:K:108:LEU:HD22	1.76	0.66
1:A:26:TRP:HZ3	1:A:62:GLY:O	1.78	0.66
1:D:146:LYS:HB3	5:D:236:HOH:O	1.95	0.66
1:B:158:ASN:HB3	3:J:6:MET:HE3	1.76	0.66
1:D:52:GLN:NE2	1:D:81:MET:HG3	2.11	0.65
1:D:138:THR:HG21	1:D:154:CYS:HB2	1.77	0.65
1:A:179:PRO:O	1:A:184:ASN:HA	1.96	0.65
3:I:108:LEU:HD22	3:I:108:LEU:H	1.60	0.65
1:C:30:THR:HG23	1:C:72:PHE:CE1	2.31	0.65
3:J:55:VAL:C	3:J:57:GLY:H	1.99	0.65
3:K:22:GLN:NE2	3:K:47:ALA:H	1.94	0.65
3:L:29:LYS:HB3	3:L:30:PRO:HD3	1.79	0.65
3:I:114:GLN:OE1	3:I:116:LYS:HE3	1.96	0.65
1:B:189:ILE:HG23	1:B:202:LEU:HD21	1.79	0.65
1:B:26:TRP:CE2	1:B:27:THR:HG22	2.32	0.65
1:C:128:ASN:ND2	1:C:129:PRO:O	2.29	0.64
1:C:52:GLN:NE2	1:C:80:ILE:HA	2.12	0.64
1:D:19:GLN:HA	1:D:28:PHE:CE1	2.33	0.64
3:I:45:LEU:HD23	3:I:66:ALA:HB1	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:40:TYR:HB3	3:L:45:LEU:HD11	1.79	0.64
1:A:67:LEU:HD11	1:A:205:CYS:SG	2.37	0.64
1:A:119:GLU:HA	1:A:122:VAL:CG2	2.28	0.63
1:B:63:CYS:SG	1:B:91:GLN:HA	2.38	0.63
3:J:121:GLU:HG3	3:J:122:LEU:N	2.13	0.63
3:K:15:LYS:HB2	3:K:50:TYR:CE1	2.34	0.63
1:B:198:ASN:ND2	1:B:203:ALA:H	1.96	0.63
1:D:81:MET:HE3	1:D:86:TYR:CD2	2.33	0.63
3:L:96:HIS:HB2	3:L:114:GLN:HB3	1.78	0.63
1:A:118:GLU:O	1:A:122:VAL:HG23	1.99	0.63
1:B:120:ALA:O	1:B:123:GLU:HB3	1.99	0.62
1:A:52:GLN:HE21	1:A:81:MET:H	1.45	0.62
1:A:126:ALA:HB2	1:A:166:TYR:HE2	1.64	0.62
1:B:63:CYS:HB2	1:B:64:GLN:HE22	1.63	0.62
1:B:121:MET:SD	1:B:203:ALA:CB	2.88	0.62
3:I:96:HIS:CE1	3:I:116:LYS:HD2	2.35	0.62
1:A:52:GLN:HE22	1:A:80:ILE:HA	1.63	0.62
3:L:65:ARG:HE	3:L:92:ASN:ND2	1.98	0.62
1:B:81:MET:CE	1:B:97:PHE:HA	2.31	0.61
1:A:77:TYR:CD1	1:A:77:TYR:N	2.66	0.61
1:D:155:HIS:CE1	1:D:156:LYS:HD2	2.36	0.61
1:C:157:VAL:HG21	2:S:80:CYS:SG	2.40	0.61
3:J:94:TYR:CZ	3:J:118:LYS:HG3	2.36	0.61
1:C:26:TRP:HH2	1:C:62:GLY:O	1.84	0.61
1:A:72:PHE:HB3	1:A:110:VAL:CG1	2.24	0.61
1:B:63:CYS:HB2	1:B:64:GLN:NE2	2.16	0.61
3:K:15:LYS:NZ	3:K:50:TYR:HE2	1.95	0.60
3:L:61:TYR:N	3:L:61:TYR:CD1	2.70	0.60
3:J:12:SER:O	3:J:51:LYS:HG2	2.01	0.60
1:B:77:TYR:HE2	4:B:215:BMA:H3	1.64	0.60
1:A:81:MET:CE	1:A:97:PHE:HA	2.32	0.60
3:L:15:LYS:HD3	3:L:50:TYR:CZ	2.37	0.60
1:C:173:VAL:HB	1:C:187:PHE:CE2	2.37	0.60
1:D:26:TRP:HZ3	1:D:62:GLY:O	1.84	0.60
1:A:172:ILE:HA	1:A:188:LEU:HD13	1.83	0.60
1:B:37:ALA:O	1:B:40:ILE:HB	2.02	0.60
3:K:45:LEU:CD2	3:K:66:ALA:HB2	2.32	0.59
1:C:146:LYS:HG3	1:C:183:MET:CG	2.31	0.59
1:A:167:GLY:O	1:A:191:ARG:NH2	2.35	0.59
3:J:106:GLU:HG2	3:J:107:ASP:N	2.16	0.59
1:A:2:PRO:HB2	1:A:4:SER:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:TYR:CZ	1:C:123:GLU:HB2	2.37	0.59
3:I:45:LEU:HD23	3:I:66:ALA:CB	2.32	0.59
3:I:61:TYR:CE2	3:I:124:GLY:HA2	2.37	0.59
1:D:49:ALA:HB1	1:D:86:TYR:HB3	1.83	0.59
1:C:135:GLU:HG3	1:C:156:LYS:O	2.01	0.59
3:J:96:HIS:ND1	3:J:116:LYS:HD3	2.17	0.59
1:C:169:PRO:HB2	1:C:191:ARG:HB3	1.84	0.59
1:A:148:ILE:HD11	1:A:168(A):GLU:HB3	1.85	0.59
1:C:171:TRP:NE1	1:C:191:ARG:HG3	2.17	0.59
1:B:52:GLN:NE2	1:B:80:ILE:HA	2.11	0.59
1:B:149:TYR:HD2	1:B:189:ILE:HG13	1.67	0.58
1:B:12:PHE:CE2	1:B:40:ILE:HA	2.38	0.58
3:I:31:GLN:CA	3:I:34:GLU:HG2	2.29	0.58
1:B:69:SER:O	1:B:72:PHE:HB2	2.03	0.58
1:C:51:GLN:HE21	1:C:90:GLY:H	1.52	0.58
3:K:96:HIS:CE1	3:K:116:LYS:HD2	2.39	0.58
1:A:77:TYR:HD1	1:A:77:TYR:N	2.01	0.58
3:J:50:TYR:HA	3:J:61:TYR:O	2.04	0.58
3:L:19:PRO:O	3:L:23:GLU:HB2	2.03	0.58
1:B:190:GLU:HG2	1:B:195:LYS:HD3	1.85	0.58
1:B:8:ARG:HH21	1:B:172:ILE:HG21	1.69	0.58
1:B:71:ALA:O	1:B:75:ILE:HG13	2.04	0.58
1:A:22:CYS:HB2	1:A:90:GLY:O	2.03	0.58
1:A:49:ALA:HA	1:A:83:GLU:OE1	2.04	0.58
1:C:28:PHE:CD2	1:C:50:GLU:HG2	2.38	0.58
1:C:21:SER:HB3	3:K:100:PHE:CE2	2.39	0.57
3:L:31:GLN:O	3:L:35:LYS:HG3	2.03	0.57
1:D:198:ASN:HD21	1:D:203:ALA:HB3	1.70	0.57
3:J:98:LYS:HD3	3:J:111:THR:OG1	2.04	0.57
1:B:135:GLU:OE1	1:B:156:LYS:HB3	2.04	0.57
1:B:132:PHE:CE1	1:B:202:LEU:HD12	2.39	0.57
3:J:49:GLN:HB2	3:J:63:LYS:HB3	1.86	0.57
1:C:111:ALA:O	1:C:207:SER:HB2	2.04	0.57
3:I:94:TYR:CD2	3:I:94:TYR:N	2.73	0.57
1:D:130:VAL:HG12	1:D:163:ALA:HB3	1.86	0.57
1:A:56:CYS:HA	1:A:58:GLN:OE1	2.05	0.57
1:B:181:TRP:HH2	1:B:187:PHE:HB3	1.66	0.57
1:B:62:GLY:O	1:B:64:GLN:N	2.38	0.57
1:A:108:LYS:HG3	1:A:212:LEU:CD2	2.35	0.57
1:C:52:GLN:NE2	1:C:81:MET:N	2.53	0.57
1:B:51:GLN:NE2	1:B:90:GLY:H	2.01	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ASN:HD21	1:D:203:ALA:H	1.50	0.57
1:B:51:GLN:HE21	1:B:90:GLY:N	2.02	0.57
1:A:76:ARG:NE	1:A:77:TYR:HE1	2.03	0.57
1:C:48:LEU:HG	1:C:80:ILE:HG21	1.87	0.56
1:D:19:GLN:O	1:D:88:TYR:OH	2.22	0.56
1:A:34:LEU:HD23	1:A:48:LEU:HD23	1.88	0.56
3:I:102(A):LEU:O	3:I:104:GLY:N	2.37	0.56
1:D:144:TYR:OH	1:D:187:PHE:HA	2.04	0.56
1:A:198:ASN:HD21	1:A:203:ALA:H	1.52	0.56
3:I:65:ARG:HG3	3:I:94:TYR:CZ	2.40	0.56
3:J:96:HIS:CE1	3:J:116:LYS:HD3	2.40	0.56
1:C:71:ALA:O	1:C:74:TYR:HB3	2.05	0.56
1:C:123:GLU:O	1:C:126:ALA:HB3	2.05	0.56
3:K:94:TYR:HB2	3:K:116:LYS:O	2.05	0.56
3:K:30:PRO:HG3	5:K:337:HOH:O	2.03	0.56
1:D:51:GLN:NE2	1:D:89:LYS:H	2.03	0.56
1:C:176:SER:O	1:C:177:TRP:HD1	1.87	0.56
3:K:11:LEU:HD22	3:K:53:GLN:HB2	1.87	0.56
1:B:72:PHE:CZ	1:B:209:PRO:HD3	2.40	0.56
1:A:65:GLY:HA3	3:I:7:ILE:HD11	1.87	0.56
1:C:19:GLN:HA	1:C:28:PHE:CE1	2.39	0.56
3:L:27:LYS:HD3	3:L:108:LEU:HD12	1.87	0.56
1:B:174:LYS:HA	1:B:186:TYR:CD1	2.41	0.56
1:D:66:GLY:O	3:L:8:PRO:HD2	2.05	0.56
3:K:96:HIS:ND1	3:K:116:LYS:HD2	2.21	0.55
1:C:94:HIS:O	1:C:96:LYS:HE3	2.06	0.55
1:D:51:GLN:O	1:D:54:VAL:N	2.39	0.55
3:J:15:LYS:HD3	3:J:50:TYR:CZ	2.40	0.55
1:C:20:GLY:O	3:K:56:ALA:HB2	2.05	0.55
3:I:123:THR:O	3:I:125:PHE:HD2	1.89	0.55
1:D:123:GLU:O	1:D:126:ALA:HB3	2.07	0.55
3:K:15:LYS:HZ2	3:K:50:TYR:HE2	1.40	0.55
3:I:25:VAL:HG11	3:I:64:VAL:HG21	1.89	0.55
1:C:52:GLN:HE21	1:C:81:MET:H	1.54	0.55
1:D:81:MET:HE2	1:D:97:PHE:HA	1.86	0.55
3:I:25:VAL:HG23	3:I:62:ILE:HD13	1.88	0.55
3:J:55:VAL:C	3:J:57:GLY:N	2.60	0.55
1:B:37:ALA:O	1:B:40:ILE:N	2.39	0.55
1:B:10(A):GLY:O	1:B:12:PHE:N	2.40	0.55
1:B:65:GLY:HA3	3:J:7:ILE:HD11	1.89	0.55
3:J:48:VAL:HG12	3:J:63:LYS:HG2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:SER:O	1:B:28:PHE:HD1	1.89	0.55
1:D:58(B):PHE:CE1	1:D:74:TYR:HA	2.42	0.55
1:D:94:HIS:HB3	5:D:271:HOH:O	2.06	0.54
3:L:50:TYR:HE2	3:L:52:THR:HG23	1.72	0.54
1:D:26:TRP:HE1	1:D:71:ALA:HB2	1.71	0.54
1:C:112:ASN:HA	1:C:207:SER:HB3	1.90	0.54
1:B:58(B):PHE:CD1	1:B:74:TYR:HA	2.42	0.54
3:I:31:GLN:HA	3:I:34:GLU:CG	2.31	0.54
1:C:52:GLN:NE2	1:C:81:MET:H	2.06	0.54
3:K:107:ASP:O	3:K:109:VAL:HG23	2.06	0.54
3:L:61:TYR:CE2	3:L:124:GLY:HA2	2.42	0.54
1:C:148:ILE:HD11	1:C:168(A):GLU:HB3	1.90	0.54
1:A:81:MET:CE	1:A:98:GLN:N	2.63	0.54
3:L:66:ALA:O	3:L:93:LYS:HB3	2.08	0.54
1:B:51:GLN:NE2	1:B:90:GLY:N	2.56	0.54
1:A:35:GLU:HG2	1:A:48:LEU:HD13	1.88	0.54
1:A:114:THR:HG22	1:A:115:MET:N	2.23	0.54
1:D:48:LEU:HB3	1:D:80:ILE:HD13	1.89	0.54
1:D:47:SER:O	1:D:82:GLY:HA2	2.08	0.54
1:A:171:TRP:O	1:A:188:LEU:HA	2.08	0.54
1:D:55:ASP:O	1:D:95:CYS:HB2	2.08	0.54
1:B:26:TRP:HH2	1:B:62:GLY:N	2.06	0.54
1:B:127:TYR:HD2	1:B:208:TYR:HH	1.55	0.54
1:B:26:TRP:HH2	1:B:62:GLY:CA	2.20	0.53
1:B:138:THR:O	1:B:141:PHE:N	2.41	0.53
1:D:55:ASP:O	1:D:56:CYS:SG	2.67	0.53
3:K:18:THR:O	3:K:21:ILE:N	2.40	0.53
3:L:15:LYS:CE	3:L:51:LYS:HA	2.38	0.53
1:D:128:ASN:ND2	1:D:129:PRO:N	2.56	0.53
1:D:33:ALA:HB1	1:D:209:PRO:HD2	1.89	0.53
1:C:159:HIS:CE1	1:C:175:ASN:HD21	2.26	0.53
1:C:52:GLN:HE22	1:C:80:ILE:HA	1.73	0.53
1:D:60:ASN:HD21	1:D:70:GLN:HB2	1.72	0.53
1:A:108:LYS:HG3	1:A:212:LEU:HD23	1.91	0.53
1:D:55:ASP:C	1:D:56:CYS:SG	2.87	0.53
1:A:52:GLN:HE21	1:A:81:MET:HG3	1.72	0.53
1:B:26:TRP:O	1:B:29:SER:HB3	2.09	0.53
1:B:81:MET:HE2	1:B:97:PHE:HA	1.91	0.53
1:D:171:TRP:NE1	1:D:191:ARG:HG3	2.23	0.53
1:D:199:MET:O	1:D:202:LEU:HB2	2.09	0.53
1:C:33:ALA:HB3	1:C:72:PHE:HZ	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:63:LYS:HD3	3:J:96:HIS:NE2	2.24	0.53
1:C:35:GLU:HG3	1:C:48:LEU:HD22	1.90	0.53
1:A:48:LEU:HA	1:A:82:GLY:HA2	1.91	0.53
1:D:166:TYR:CD1	1:D:191:ARG:NH1	2.77	0.52
1:B:110:VAL:HG23	1:B:110:VAL:O	2.10	0.52
1:B:18:ASN:OD1	1:B:20:GLY:N	2.41	0.52
1:B:67:LEU:HD11	1:B:205:CYS:SG	2.50	0.52
1:D:19:GLN:HG2	3:L:56:ALA:HB2	1.91	0.52
1:D:30:THR:HG23	1:D:72:PHE:CE1	2.45	0.52
3:I:11:LEU:HD22	3:I:53:GLN:HB2	1.92	0.52
1:A:126:ALA:HB2	1:A:166:TYR:CE2	2.44	0.52
1:D:16:VAL:HG21	1:D:185:GLY:HA3	1.92	0.52
1:D:198:ASN:HD21	1:D:203:ALA:N	2.08	0.52
1:C:35:GLU:OE2	1:C:47:SER:HA	2.09	0.52
1:A:26:TRP:CZ3	1:A:62:GLY:O	2.61	0.52
2:S:81:SER:HA	3:K:7:ILE:HG22	1.91	0.52
1:A:212(A):VAL:HG23	1:A:212(A):VAL:OXT	2.10	0.52
1:D:31:THR:O	1:D:35:GLU:HG2	2.10	0.52
3:I:59:ASN:HB3	3:I:61:TYR:HE1	1.73	0.52
3:L:14:ALA:HA	3:L:51:LYS:HG2	1.91	0.52
3:I:10:GLY:O	3:I:53:GLN:HG3	2.10	0.52
1:A:132:PHE:O	1:A:161:VAL:N	2.40	0.52
1:C:108:LYS:HB3	1:C:210:ILE:HG22	1.91	0.52
3:L:63:LYS:HE3	3:L:118:LYS:O	2.10	0.52
1:B:190:GLU:CG	1:B:195:LYS:HD3	2.40	0.52
3:I:61:TYR:HE2	3:I:124:GLY:HA2	1.75	0.52
1:C:146:LYS:HG3	1:C:183:MET:SD	2.50	0.52
1:B:57:ALA:HA	1:B:74:TYR:CD1	2.45	0.52
1:A:132:PHE:CE1	1:A:202:LEU:HD12	2.45	0.52
1:B:128:ASN:ND2	1:B:129:PRO:O	2.44	0.51
3:J:7:ILE:HG13	3:J:8:PRO:O	2.11	0.51
1:C:179:PRO:O	1:C:184:ASN:HA	2.10	0.51
3:L:65:ARG:HG2	3:L:94:TYR:CZ	2.46	0.51
1:C:23:GLY:H	1:C:63:CYS:HB3	1.76	0.51
3:L:65:ARG:HD3	3:L:92:ASN:HA	1.91	0.51
1:B:72:PHE:HB3	1:B:110:VAL:HG12	1.93	0.51
3:K:95:MET:O	3:K:96:HIS:HD2	1.93	0.51
1:B:32:GLY:O	1:B:36:SER:HB2	2.11	0.51
1:D:2:PRO:O	1:D:166:TYR:CE1	2.64	0.51
1:C:115:MET:HG3	1:C:204:ALA:O	2.11	0.51
3:K:15:LYS:HB2	3:K:50:TYR:CZ	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:24:ILE:O	3:I:28:VAL:HB	2.11	0.51
3:L:15:LYS:HD2	3:L:50:TYR:O	2.11	0.51
3:K:18:THR:OG1	3:K:21:ILE:HG12	2.11	0.51
1:D:98:GLN:HG3	1:D:98:GLN:O	2.10	0.51
1:B:60:ASN:N	1:B:60:ASN:HD22	2.09	0.50
1:A:148:ILE:HA	1:A:188:LEU:O	2.11	0.50
3:I:45:LEU:CD2	3:I:66:ALA:CB	2.88	0.50
1:B:69:SER:HA	1:B:72:PHE:HD2	1.75	0.50
1:A:20:GLY:O	3:I:55:VAL:HB	2.11	0.50
1:D:174:LYS:HB2	1:D:186:TYR:CE1	2.45	0.50
1:A:34:LEU:HD23	1:A:48:LEU:CD2	2.40	0.50
3:I:12:SER:OG	3:I:15:LYS:HE3	2.11	0.50
3:L:14:ALA:O	3:L:15:LYS:HG3	2.11	0.50
1:B:26:TRP:CE2	1:B:60:ASN:OD1	2.64	0.50
1:C:136:VAL:HG22	1:C:141:PHE:CD2	2.46	0.50
1:D:198:ASN:HD21	1:D:203:ALA:CB	2.25	0.50
1:D:34:LEU:O	1:D:38:VAL:HG23	2.11	0.50
1:C:54:VAL:HG13	1:C:62:GLY:HA2	1.93	0.50
3:J:32:LEU:HD23	3:J:32:LEU:O	2.12	0.50
1:B:81:MET:HE3	1:B:86:TYR:CD2	2.45	0.50
1:D:78:ASN:O	1:D:78(A):LYS:HB2	2.12	0.50
1:B:132:PHE:CE2	1:B:163:ALA:HB2	2.46	0.50
1:D:180:GLN:HG2	5:D:256:HOH:O	2.11	0.50
1:A:69:SER:HB2	4:A:213:NAG:H62	1.92	0.50
1:D:138:THR:CG2	1:D:154:CYS:HB2	2.42	0.50
3:K:45:LEU:HD22	3:K:64:VAL:HG11	1.93	0.49
3:L:65:ARG:HH21	3:L:65:ARG:HB3	1.76	0.49
1:A:8:ARG:NH2	1:A:172:ILE:CG2	2.75	0.49
1:B:34:LEU:HD13	1:B:107:VAL:HG22	1.94	0.49
1:C:187:PHE:C	1:C:188:LEU:HD12	2.32	0.49
1:D:51:GLN:HB2	1:D:88:TYR:HA	1.94	0.49
1:B:174:LYS:HB2	1:B:186:TYR:CE1	2.47	0.49
1:C:73:GLU:CD	1:C:110:VAL:HG21	2.32	0.49
3:I:98:LYS:HB2	3:I:125:PHE:CZ	2.47	0.49
1:D:164:VAL:CG2	1:D:172:ILE:HG22	2.41	0.49
1:A:19:GLN:HG2	1:A:19:GLN:O	2.09	0.49
1:B:51:GLN:HG2	1:B:88:TYR:HA	1.94	0.49
1:D:1:TYR:CZ	1:D:123:GLU:HG3	2.47	0.49
3:K:108:LEU:N	3:K:108:LEU:CD1	2.75	0.49
1:B:67:LEU:HD22	2:R:81:SER:H	1.78	0.49
1:D:1:TYR:OH	1:D:123:GLU:HG3	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:92:ASN:HD22	3:K:92:ASN:N	2.10	0.49
1:D:81:MET:HE2	1:D:97:PHE:HD1	1.78	0.49
1:A:174:LYS:HB2	1:A:186:TYR:CE1	2.48	0.49
3:K:29:LYS:HD2	3:K:45:LEU:HD12	1.95	0.49
3:K:32:LEU:HD13	3:K:40:TYR:CE2	2.47	0.49
1:B:189:ILE:HG21	1:B:202:LEU:HD21	1.93	0.48
1:A:212(A):VAL:HG12	5:A:247:HOH:O	2.13	0.48
1:A:58(B):PHE:O	1:A:70:GLN:HB3	2.13	0.48
3:I:115:VAL:HG12	3:I:115(A):ASP:N	2.28	0.48
1:C:81:MET:HE1	1:C:97:PHE:CA	2.36	0.48
1:D:26:TRP:CD2	1:D:27:THR:HG22	2.49	0.48
1:B:5:MET:HB2	1:B:166:TYR:CZ	2.48	0.48
1:C:54:VAL:HG13	1:C:62:GLY:CA	2.43	0.48
1:A:26:TRP:HE1	1:A:71:ALA:HB2	1.78	0.48
3:L:103:PRO:HB2	5:L:151:HOH:O	2.12	0.48
1:C:171:TRP:CD1	1:C:202:LEU:HD11	2.49	0.48
1:A:149:TYR:N	1:A:188:LEU:O	2.45	0.48
1:A:81:MET:HE3	1:A:97:PHE:HA	1.94	0.48
1:C:144:TYR:CE2	1:C:187:PHE:HB2	2.49	0.48
4:B:213:NAG:O6	2:R:78:GLN:N	2.46	0.48
3:I:123:THR:O	3:I:125:PHE:CD2	2.66	0.48
1:C:16:VAL:HG21	1:C:184:ASN:O	2.13	0.48
1:C:21:SER:HB3	3:K:100:PHE:CD2	2.48	0.48
1:C:71:ALA:O	1:C:75:ILE:HG13	2.12	0.48
1:A:195:LYS:HE3	5:A:234:HOH:O	2.13	0.48
1:C:212(A):VAL:HG23	1:C:212(A):VAL:OXT	2.13	0.48
1:B:7:TRP:CD1	1:B:129:PRO:HG3	2.48	0.48
1:C:174:LYS:HB2	1:C:186:TYR:CE1	2.48	0.48
1:D:201:GLY:O	1:D:203:ALA:N	2.47	0.48
1:D:175:ASN:HB2	1:D:187:PHE:CE2	2.49	0.48
1:A:199:MET:O	1:A:200:CYS:HB2	2.14	0.48
3:L:40:TYR:HB3	3:L:45:LEU:CD1	2.42	0.48
3:L:59:ASN:HB3	3:L:61:TYR:CE1	2.48	0.48
1:D:147:GLY:O	1:D:188:LEU:HB2	2.13	0.48
3:J:11:LEU:HD22	3:J:53:GLN:HB2	1.95	0.48
1:D:86:TYR:CE1	1:D:96:LYS:HD2	2.48	0.47
3:I:94:TYR:HD2	3:I:94:TYR:N	2.12	0.47
1:A:70:GLN:NE2	2:P:81:SER:O	2.46	0.47
3:J:55:VAL:O	3:J:57:GLY:N	2.40	0.47
1:A:78:ASN:ND2	1:A:97:PHE:CE2	2.82	0.47
1:D:53:LEU:HD13	1:D:80:ILE:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ASN:ND2	1:D:203:ALA:HB3	2.28	0.47
1:C:164:VAL:HG11	1:C:186:TYR:HE1	1.79	0.47
1:B:81:MET:HE3	1:B:86:TYR:HD2	1.78	0.47
3:L:50:TYR:CE2	3:L:52:THR:HG23	2.49	0.47
1:C:81:MET:HE1	1:C:98:GLN:N	2.30	0.47
1:D:80:ILE:HG12	1:D:81:MET:N	2.30	0.47
1:D:125:VAL:HG21	1:D:171:TRP:HZ3	1.80	0.47
1:D:138:THR:O	1:D:140:ASP:N	2.48	0.47
1:D:49:ALA:CB	1:D:86:TYR:HB3	2.45	0.47
1:A:168(A):GLU:C	1:A:168(C):GLY:H	2.18	0.47
1:D:138:THR:O	1:D:141:PHE:N	2.47	0.47
1:B:13:VAL:CG1	1:B:174:LYS:HE3	2.45	0.47
1:A:61:HIS:O	1:A:64:GLN:HG2	2.14	0.47
3:I:67:GLY:O	3:I:68:ASP:C	2.52	0.47
1:B:177:TRP:CD1	3:J:56:ALA:HA	2.49	0.47
3:I:45:LEU:HA	3:I:66:ALA:HB2	1.95	0.47
1:B:58(B):PHE:CE1	1:B:74:TYR:HA	2.49	0.47
2:R:77:PRO:HB2	5:R:312:HOH:O	2.14	0.47
3:J:95:MET:HG3	3:J:115:VAL:HA	1.96	0.47
1:C:51:GLN:NE2	1:C:90:GLY:H	2.11	0.47
1:B:6:ASP:OD1	1:B:8:ARG:HB2	2.15	0.47
3:J:108:LEU:CD1	3:J:108:LEU:N	2.76	0.47
3:J:48:VAL:HG13	3:J:49:GLN:HG3	1.97	0.47
1:D:65:GLY:HA2	3:L:8:PRO:O	2.14	0.47
1:B:67:LEU:HD12	1:B:68:PRO:CD	2.45	0.47
1:A:21:SER:O	3:I:55:VAL:HG11	2.15	0.47
3:K:60:TYR:HE2	3:K:101:LYS:HD2	1.80	0.47
1:B:133:ALA:HA	1:B:159:HIS:O	2.14	0.47
3:K:24:ILE:HA	3:K:108:LEU:HD23	1.97	0.46
1:D:81:MET:HE2	1:D:97:PHE:CD1	2.51	0.46
1:B:26:TRP:CD2	1:B:66:GLY:HA3	2.50	0.46
1:D:138:THR:C	1:D:140:ASP:N	2.68	0.46
3:I:29:LYS:HG3	3:I:45:LEU:HD12	1.97	0.46
3:K:115:VAL:HG12	3:K:115(A):ASP:N	2.29	0.46
1:D:125:VAL:HA	1:D:128:ASN:O	2.15	0.46
1:B:115:MET:HE2	5:R:292:HOH:O	2.15	0.46
1:C:52:GLN:HE21	1:C:81:MET:N	2.12	0.46
1:B:26:TRP:NE1	1:B:60:ASN:OD1	2.48	0.46
1:A:132:PHE:O	1:A:160:ALA:HA	2.15	0.46
1:D:81:MET:CE	1:D:86:TYR:CD2	2.98	0.46
1:B:58(B):PHE:HD1	1:B:74:TYR:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLU:O	1:C:38:VAL:HG12	2.15	0.46
1:C:48:LEU:HG	1:C:80:ILE:CG2	2.44	0.46
1:C:202:LEU:C	1:C:202:LEU:HD23	2.35	0.46
1:D:55:ASP:HB2	1:D:95:CYS:HA	1.98	0.46
1:B:155:HIS:CD2	1:B:155:HIS:N	2.84	0.46
1:B:51:GLN:CG	1:B:89:LYS:H	2.29	0.46
3:L:96:HIS:CE1	3:L:116:LYS:HG2	2.51	0.46
1:D:157:VAL:HG21	2:T:80:CYS:SG	2.56	0.46
1:D:21:SER:O	3:L:55:VAL:HG11	2.16	0.46
3:L:20:GLU:O	3:L:24:ILE:HG13	2.16	0.46
3:I:63:LYS:NZ	3:I:120:ASP:O	2.40	0.46
1:D:53:LEU:CD1	1:D:80:ILE:HD12	2.45	0.46
1:B:154:CYS:SG	1:B:154:CYS:O	2.74	0.46
3:L:15:LYS:HD3	3:L:50:TYR:CD1	2.51	0.45
3:I:23:GLU:OE2	3:I:27:LYS:HE2	2.16	0.45
1:D:128:ASN:HD22	1:D:129:PRO:N	2.13	0.45
1:C:61:HIS:O	1:C:64:GLN:N	2.48	0.45
1:C:205:CYS:HB3	2:S:80:CYS:HB3	1.43	0.45
3:K:33:GLU:C	3:K:35:LYS:H	2.19	0.45
1:C:51:GLN:HG3	1:C:88:TYR:HA	1.96	0.45
1:A:48:LEU:CD1	1:A:48:LEU:N	2.79	0.45
1:D:2:PRO:O	1:D:166:TYR:HE1	1.98	0.45
3:L:94:TYR:CZ	3:L:118:LYS:HB2	2.52	0.45
1:C:18:ASN:HB3	5:C:279:HOH:O	2.17	0.45
1:A:16:VAL:HA	1:A:174:LYS:HE2	1.99	0.45
1:C:46:LEU:HD22	1:C:104:ILE:HD12	1.98	0.45
1:A:52:GLN:NE2	1:A:81:MET:H	2.14	0.45
1:D:48:LEU:HD11	1:D:105:ALA:HB2	1.98	0.45
3:I:96:HIS:HB2	3:I:114:GLN:HB2	1.98	0.45
2:S:81:SER:CA	3:K:7:ILE:HG22	2.46	0.45
1:C:66:GLY:O	3:K:8:PRO:HD2	2.16	0.45
1:D:171:TRP:N	1:D:189:ILE:O	2.49	0.45
1:C:26:TRP:CZ3	1:C:62:GLY:O	2.69	0.45
1:C:26:TRP:CE2	1:C:27:THR:HG22	2.52	0.45
1:B:48:LEU:N	1:B:48:LEU:HD13	2.32	0.45
1:A:184:ASN:N	1:A:184:ASN:OD1	2.50	0.45
3:J:96:HIS:HB2	3:J:114:GLN:HB2	1.97	0.45
1:A:22:CYS:SG	1:A:24:SER:HB2	2.56	0.45
1:A:113:ILE:HG23	1:A:120:ALA:HB3	1.99	0.45
1:A:151:SER:HB3	1:A:154:CYS:SG	2.57	0.45
3:L:65:ARG:HG2	3:L:94:TYR:CE2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:OG	4:B:213:NAG:H62	2.16	0.45
1:D:175:ASN:HD22	1:D:176:SER:N	2.14	0.45
1:A:132:PHE:HE1	1:A:202:LEU:HD12	1.81	0.45
1:D:110:VAL:HG22	1:D:110:VAL:O	2.17	0.45
1:A:136:VAL:HB	1:A:158:ASN:OD1	2.16	0.45
1:C:31:THR:O	1:C:35:GLU:HG3	2.17	0.45
1:B:148:ILE:HD13	1:B:170:TYR:HB3	1.99	0.45
1:B:170:TYR:HE1	1:B:172:ILE:HG12	1.82	0.45
1:D:198:ASN:ND2	1:D:203:ALA:H	2.13	0.45
1:A:58(B):PHE:CE1	1:A:74:TYR:HA	2.52	0.45
1:A:127:TYR:HE2	5:A:282:HOH:O	1.99	0.45
1:D:50:GLU:O	1:D:53:LEU:HB2	2.16	0.45
1:C:192:GLY:C	1:C:195:LYS:HD2	2.38	0.45
1:B:26:TRP:NE1	1:B:27:THR:HG22	2.32	0.44
1:D:154:CYS:O	1:D:154:CYS:SG	2.73	0.44
1:B:58(B):PHE:CD1	1:B:74:TYR:HB2	2.52	0.44
3:J:115:VAL:O	3:J:115(A):ASP:HB2	2.17	0.44
1:B:145:ARG:HA	1:B:182:GLY:HA2	2.00	0.44
1:B:22:CYS:HB2	1:B:90:GLY:O	2.17	0.44
1:D:5:MET:HB2	1:D:166:TYR:CE2	2.53	0.44
1:A:171:TRP:HB2	1:A:189:ILE:HG22	2.00	0.44
1:B:165:GLY:O	1:B:171:TRP:HE3	2.01	0.44
1:B:10:LYS:HA	1:B:10:LYS:HD2	1.42	0.44
3:I:40:TYR:HB3	3:I:45:LEU:HD21	1.99	0.44
3:K:92:ASN:N	3:K:92:ASN:ND2	2.66	0.44
3:J:21:ILE:HD13	3:J:24:ILE:HD12	1.98	0.44
1:D:191:ARG:HE	1:D:191:ARG:HB3	1.53	0.44
1:C:59:ASN:O	1:C:59:ASN:ND2	2.41	0.44
1:D:94:HIS:O	1:D:96:LYS:HG3	2.16	0.44
3:K:108:LEU:N	3:K:108:LEU:HD12	2.33	0.44
1:C:33:ALA:HB1	1:C:209:PRO:HD3	2.00	0.44
1:A:67:LEU:HG	1:A:68:PRO:HD2	2.00	0.44
1:B:13:VAL:HG12	1:B:14:SER:O	2.18	0.44
1:D:198:ASN:HD22	1:D:198:ASN:HA	1.71	0.44
1:D:67:LEU:HG	1:D:68:PRO:HD2	2.00	0.44
1:B:69:SER:HA	1:B:72:PHE:CD2	2.52	0.44
1:D:118:GLU:O	1:D:122:VAL:HG23	2.17	0.44
1:A:19:GLN:HE21	1:A:19:GLN:HB3	1.56	0.44
1:A:16:VAL:HG21	1:A:185:GLY:HA3	1.99	0.44
3:I:94:TYR:OH	3:I:118:LYS:HD2	2.18	0.44
1:D:118:GLU:OE1	1:D:198:ASN:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:TYR:CE2	1:C:187:PHE:CB	3.01	0.44
3:I:65:ARG:HG3	3:I:94:TYR:CE1	2.52	0.44
1:C:136:VAL:HB	1:C:158:ASN:OD1	2.17	0.44
3:L:115:VAL:HG12	3:L:115(A):ASP:N	2.33	0.44
1:C:67:LEU:HD11	1:C:205:CYS:SG	2.58	0.43
1:A:49:ALA:H	1:A:82:GLY:HA2	1.83	0.43
3:L:61:TYR:N	3:L:61:TYR:HD1	2.13	0.43
1:A:69:SER:CB	4:A:213:NAG:H62	2.49	0.43
1:C:67:LEU:HA	1:C:68:PRO:HD3	1.77	0.43
2:S:79:ASN:HB2	5:S:489:HOH:O	2.18	0.43
1:A:148:ILE:HD11	1:A:168(A):GLU:CB	2.46	0.43
1:B:61:HIS:N	1:B:65:GLY:O	2.49	0.43
1:D:134:PHE:HB2	1:D:200:CYS:O	2.18	0.43
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.85	0.43
1:B:5:MET:HG2	1:B:126:ALA:HA	1.99	0.43
1:B:58(A):ASN:HD22	1:B:58(A):ASN:HA	1.43	0.43
1:C:61:HIS:O	1:C:62:GLY:C	2.56	0.43
1:B:129:PRO:HB3	1:B:164:VAL:HG12	2.00	0.43
3:J:13:GLU:HG3	3:J:14:ALA:H	1.82	0.43
1:A:59:ASN:O	1:A:59:ASN:ND2	2.52	0.43
1:B:132:PHE:CZ	1:B:161:VAL:HG23	2.54	0.43
3:K:64:VAL:HG21	3:K:97:LEU:HD22	2.01	0.43
1:C:156:LYS:NZ	5:C:272:HOH:O	2.50	0.43
3:L:40:TYR:CB	3:L:45:LEU:HD11	2.47	0.43
1:D:121:MET:C	1:D:123:GLU:H	2.21	0.43
1:B:8:ARG:HD3	1:B:13:VAL:HG21	2.01	0.43
1:B:127:TYR:O	1:B:128:ASN:CB	2.67	0.43
1:B:162:LEU:O	1:B:164:VAL:HG13	2.18	0.43
1:B:134:PHE:CE2	1:B:187:PHE:HZ	2.37	0.43
1:B:187:PHE:HE1	1:B:189:ILE:HB	1.84	0.43
1:B:158:ASN:OD1	3:J:54:VAL:HG21	2.19	0.43
1:D:128:ASN:ND2	1:D:129:PRO:HD2	2.34	0.43
1:B:135:GLU:HB2	1:B:156:LYS:O	2.18	0.43
3:J:24:ILE:O	3:J:28:VAL:HB	2.18	0.43
1:B:78:ASN:O	1:B:78(A):LYS:HB2	2.19	0.43
3:J:49:GLN:NE2	3:J:63:LYS:HE3	2.33	0.43
3:J:13:GLU:HG3	3:J:14:ALA:N	2.34	0.43
1:A:140:ASP:O	1:A:142:LEU:N	2.51	0.43
1:B:202:LEU:HA	1:B:202:LEU:HD12	1.73	0.42
1:D:16:VAL:HG21	1:D:184:ASN:O	2.19	0.42
1:D:36:SER:O	1:D:37:ALA:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:28:VAL:HG22	3:L:110:LEU:HB2	2.00	0.42
3:L:13:GLU:O	3:L:15:LYS:HE3	2.18	0.42
3:K:96:HIS:CE1	3:K:116:LYS:CD	3.02	0.42
1:B:135:GLU:OE2	1:B:154:CYS:HA	2.19	0.42
1:B:78:ASN:ND2	1:B:79:GLY:O	2.51	0.42
1:C:188:LEU:N	1:C:188:LEU:HD12	2.34	0.42
1:B:117:ASP:O	1:B:121:MET:HG3	2.20	0.42
1:D:49:ALA:HB2	1:D:82:GLY:O	2.19	0.42
1:B:72:PHE:HB3	1:B:110:VAL:CG1	2.49	0.42
1:A:51:GLN:O	1:A:55:ASP:N	2.39	0.42
1:B:52:GLN:HE21	1:B:81:MET:HG3	1.84	0.42
3:L:53:GLN:HB3	3:L:59:ASN:HB2	2.02	0.42
1:A:21:SER:HA	3:I:55:VAL:HG21	1.99	0.42
4:D:215:BMA:C6	5:D:298:HOH:O	2.67	0.42
1:B:47:SER:O	1:B:82:GLY:HA2	2.19	0.42
3:I:21:ILE:HA	3:I:21:ILE:HD13	1.84	0.42
1:A:158:ASN:HB3	3:I:6:MET:HE1	2.02	0.42
1:D:49:ALA:HA	1:D:83:GLU:OE1	2.19	0.42
1:C:133:ALA:HB3	1:C:205:CYS:SG	2.60	0.42
3:J:98:LYS:HB2	3:J:125:PHE:CE2	2.54	0.42
1:D:98:GLN:HA	1:D:99:PRO:HD2	1.87	0.42
1:A:81:MET:HE1	1:A:98:GLN:N	2.34	0.42
3:I:48:VAL:CG2	3:I:65:ARG:HB2	2.45	0.42
1:D:146:LYS:HG3	1:D:183:MET:SD	2.59	0.42
3:J:68:ASP:C	3:J:93:LYS:H	2.23	0.42
1:D:81:MET:HG2	1:D:102(A):LYS:O	2.20	0.42
1:D:138:THR:O	1:D:139:ASN:C	2.58	0.42
3:J:11:LEU:HD13	3:J:61:TYR:CD1	2.54	0.42
3:I:11:LEU:CD2	3:I:53:GLN:HB2	2.50	0.42
3:K:46:GLU:O	3:K:48:VAL:HG23	2.20	0.42
3:K:95:MET:HG2	3:K:115:VAL:HA	2.02	0.42
1:C:148:ILE:CD1	1:C:168(A):GLU:HB3	2.50	0.42
1:A:161:VAL:HG11	1:A:187:PHE:CE2	2.54	0.42
1:A:69:SER:O	1:A:72:PHE:HB2	2.20	0.42
1:C:198:ASN:HA	1:C:202:LEU:HD22	2.02	0.42
3:L:102(A):LEU:O	3:L:104:GLY:O	2.38	0.42
1:B:187:PHE:CE1	1:B:189:ILE:HB	2.55	0.42
1:D:26:TRP:CE2	1:D:27:THR:HG22	2.54	0.42
1:A:63:CYS:SG	1:A:90:GLY:O	2.77	0.42
1:C:18:ASN:ND2	1:C:20:GLY:H	2.18	0.42
3:I:15:LYS:HD3	3:I:50:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLY:O	1:C:188:LEU:HB2	2.20	0.41
1:C:212(A):VAL:HG12	5:C:311:HOH:O	2.20	0.41
1:D:61:HIS:HE1	5:D:299:HOH:O	2.02	0.41
3:K:29:LYS:CD	3:K:45:LEU:HD12	2.50	0.41
1:D:121:MET:C	1:D:123:GLU:N	2.73	0.41
1:B:138:THR:O	1:B:139:ASN:C	2.58	0.41
1:D:19:GLN:NE2	1:D:177:TRP:CD1	2.88	0.41
1:B:2:PRO:O	1:B:166:TYR:HE1	2.03	0.41
1:D:7:TRP:O	1:D:12:PHE:HB2	2.20	0.41
3:L:125:PHE:N	3:L:125:PHE:CD1	2.88	0.41
1:B:161:VAL:HG12	1:B:175:ASN:HA	2.01	0.41
1:C:52:GLN:NE2	1:C:80:ILE:CA	2.81	0.41
1:D:81:MET:CE	1:D:97:PHE:HA	2.50	0.41
3:I:15:LYS:HB2	3:I:50:TYR:CE1	2.55	0.41
1:B:19:GLN:NE2	1:B:177:TRP:CD1	2.88	0.41
3:J:65:ARG:HG2	3:J:66:ALA:N	2.35	0.41
3:K:114:GLN:HA	5:K:360:HOH:O	2.19	0.41
1:B:8:ARG:HG3	5:B:301:HOH:O	2.20	0.41
1:B:52:GLN:NE2	1:B:81:MET:H	2.19	0.41
1:C:202:LEU:HD23	1:C:203:ALA:N	2.36	0.41
1:C:26:TRP:CG	1:C:27:THR:N	2.89	0.41
3:J:96:HIS:CG	3:J:116:LYS:HD3	2.56	0.41
3:K:95:MET:O	3:K:96:HIS:CD2	2.73	0.41
1:B:205:CYS:O	1:B:205:CYS:SG	2.78	0.41
1:D:5:MET:HA	5:D:283:HOH:O	2.21	0.41
1:C:118:GLU:O	1:C:121:MET:HB2	2.20	0.41
1:C:67:LEU:HD12	1:C:68:PRO:CD	2.50	0.41
1:C:138:THR:O	1:C:141:PHE:N	2.54	0.41
1:C:141:PHE:O	1:C:141:PHE:CG	2.73	0.41
1:C:158:ASN:OD1	1:C:158:ASN:C	2.58	0.41
3:I:39:THR:HG22	3:I:39:THR:O	2.19	0.41
3:I:119:ASP:O	3:I:120:ASP:C	2.59	0.41
2:R:79:ASN:O	2:R:80:CYS:HB2	2.20	0.41
3:L:28:VAL:HG21	3:L:99:VAL:HG13	2.03	0.41
3:K:33:GLU:O	3:K:37:ASN:N	2.53	0.41
1:B:62:GLY:C	1:B:64:GLN:H	2.24	0.41
1:B:51:GLN:HG2	1:B:89:LYS:H	1.85	0.41
3:L:33:GLU:OE1	3:L:40:TYR:N	2.51	0.41
3:J:53:GLN:OE1	3:J:61:TYR:HE1	2.04	0.41
3:L:23:GLU:O	3:L:27:LYS:HG3	2.20	0.41
1:C:136:VAL:HG21	1:C:159:HIS:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:CYS:HB3	2:R:80:CYS:HB2	1.90	0.41
1:A:130:VAL:HG22	1:A:208:TYR:HB3	2.03	0.41
3:J:102(A):LEU:O	3:J:104:GLY:N	2.54	0.41
1:B:121:MET:O	1:B:125:VAL:HG23	2.21	0.41
1:A:48:LEU:N	1:A:48:LEU:HD12	2.36	0.41
3:K:56:ALA:O	3:K:102(A):LEU:CG	2.69	0.41
3:K:36:THR:C	3:K:38:GLU:H	2.24	0.41
1:B:51:GLN:HE22	1:B:91:GLN:H	1.69	0.40
3:K:56:ALA:O	3:K:102(A):LEU:HD21	2.21	0.40
3:I:55:VAL:C	3:I:57:GLY:N	2.74	0.40
1:D:73:GLU:OE1	1:D:73:GLU:HA	2.21	0.40
3:I:31:GLN:HG2	3:I:34:GLU:OE2	2.21	0.40
1:C:183:MET:SD	1:C:188:LEU:HD13	2.62	0.40
4:C:213:NAG:O6	2:S:78:GLN:N	2.55	0.40
1:C:64:GLN:O	3:K:10:GLY:HA2	2.22	0.40
3:L:115:VAL:CG1	3:L:115(A):ASP:N	2.84	0.40
1:A:69:SER:HB2	4:A:213:NAG:C6	2.50	0.40
1:C:51:GLN:NE2	1:C:90:GLY:N	2.69	0.40
1:D:68:PRO:HG2	1:D:131:SER:HB3	2.03	0.40
1:A:76:ARG:NE	1:A:77:TYR:CE1	2.86	0.40
3:I:29:LYS:HG3	3:I:45:LEU:CD1	2.50	0.40
3:J:48:VAL:CG1	3:J:49:GLN:HG3	2.51	0.40
1:B:30:THR:HG23	1:B:72:PHE:CE1	2.56	0.40
3:K:94:TYR:CZ	3:K:118:LYS:HB2	2.56	0.40
1:D:26:TRP:CZ3	1:D:62:GLY:O	2.70	0.40
1:B:127:TYR:HD2	1:B:208:TYR:OH	2.03	0.40
1:C:27:THR:HA	1:C:53:LEU:HD23	2.02	0.40
1:A:148:ILE:CD1	1:A:168(A):GLU:HB3	2.50	0.40
3:L:59:ASN:HB3	3:L:61:TYR:HE1	1.85	0.40
3:K:102(A):LEU:O	3:K:103:PRO:C	2.59	0.40
1:C:159:HIS:NE2	1:C:175:ASN:ND2	2.58	0.40
3:J:66:ALA:O	3:J:93:LYS:HB3	2.21	0.40
3:K:117:ASN:O	3:K:120:ASP:HB2	2.21	0.40
1:C:58(A):ASN:HD22	1:C:58(A):ASN:HA	1.62	0.40

All (7) 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:68:ASP:OD2	5:C:292:HOH:O[2_747]	1.03	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:ASP:CG	5:C:292:HOH:O[2_747]	1.66	0.54
3:J:118:LYS:CD	3:K:105(A):ASN:OD1[2_747]	2.14	0.06
3:J:68:ASP:OD1	5:C:292:HOH:O[2_747]	2.15	0.05
5:D:301:HOH:O	5:L:131:HOH:O[1_655]	2.16	0.04
1:A:78(A):LYS:NZ	5:I:155:HOH:O[2_656]	2.17	0.03
1:A:78(A):LYS:CE	5:I:155:HOH:O[2_656]	2.19	0.01

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	218/220 (99%)	190 (87%)	22 (10%)	6 (3%)	6	21
1	B	218/220 (99%)	183 (84%)	25 (12%)	10 (5%)	3	9
1	C	218/220 (99%)	185 (85%)	31 (14%)	2 (1%)	21	55
1	D	218/220 (99%)	182 (84%)	30 (14%)	6 (3%)	6	21
2	P	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	R	6/8 (75%)	2 (33%)	3 (50%)	1 (17%)	0	0
2	S	6/8 (75%)	3 (50%)	3 (50%)	0	100	100
2	T	6/8 (75%)	2 (33%)	2 (33%)	2 (33%)	0	0
3	I	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	5	17
3	J	96/98 (98%)	81 (84%)	14 (15%)	1 (1%)	19	52
3	K	96/98 (98%)	78 (81%)	16 (17%)	2 (2%)	9	29
3	L	96/98 (98%)	83 (86%)	11 (12%)	2 (2%)	9	29
All	All	1280/1304 (98%)	1074 (84%)	170 (13%)	36 (3%)	6	21

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	11	ASN
1	B	37	ALA
2	R	80	CYS
3	K	92	ASN
1	D	202	LEU
1	A	58	GLN
2	P	80	CYS
3	I	68	ASP
3	I	104	GLY
1	B	38	VAL
1	B	63	CYS
3	K	55	VAL
1	D	49	ALA
1	D	139	ASN
1	D	176	SER
2	T	80	CYS
3	L	105	GLN
1	A	144	TYR
1	A	209	PRO
3	I	103	PRO
1	B	57	ALA
1	B	144	TYR
1	B	202	LEU
1	C	10	LYS
1	C	62	GLY
1	D	141	PHE
3	L	92	ASN
1	A	83	GLU
1	A	168(B)	ASN
1	B	99	PRO
1	D	168(B)	ASN
2	T	82	ALA
1	B	123	GLU
1	B	178	GLY
3	J	55	VAL

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	5
1	B	181/181 (100%)	146 (81%)	35 (19%)	2	5
1	C	181/181 (100%)	148 (82%)	33 (18%)	2	6
1	D	181/181 (100%)	151 (83%)	30 (17%)	3	8
2	P	7/7 (100%)	5 (71%)	2 (29%)	0	1
2	R	7/7 (100%)	6 (86%)	1 (14%)	4	12
2	S	7/7 (100%)	5 (71%)	2 (29%)	0	1
2	T	7/7 (100%)	4 (57%)	3 (43%)	0	0
3	I	85/85 (100%)	67 (79%)	18 (21%)	1	4
3	J	85/85 (100%)	65 (76%)	20 (24%)	1	2
3	K	85/85 (100%)	69 (81%)	16 (19%)	2	6
3	L	85/85 (100%)	67 (79%)	18 (21%)	1	4
All	All	1092/1092 (100%)	879 (80%)	213 (20%)	2	5

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	9	LYS
1	A	19	GLN
1	A	24	SER
1	A	26	TRP
1	A	29	SER
1	A	51	GLN
1	A	52	GLN
1	A	56	CYS
1	A	64	GLN
1	A	69	SER
1	A	77	TYR
1	A	80	ILE
1	A	81	MET
1	A	85	THR
1	A	86	TYR
1	A	99	PRO
1	A	102(A)	LYS
1	A	115	MET
1	A	118	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	126(A)	LEU
1	A	129	PRO
1	A	145	ARG
1	A	146	LYS
1	A	155(A)	LYS
1	A	157	VAL
1	A	161	VAL
1	A	168	GLU
1	A	168(D)	ILE
1	A	184	ASN
1	A	191	ARG
1	A	195	LYS
1	A	202	LEU
1	A	209	PRO
1	A	212	LEU
2	P	79	ASN
2	P	83	THR
3	I	6	MET
3	I	13	GLU
3	I	15	LYS
3	I	30	PRO
3	I	32	LEU
3	I	38	GLU
3	I	44	LYS
3	I	54	VAL
3	I	58	THR
3	I	64	VAL
3	I	65	ARG
3	I	93	LYS
3	I	94	TYR
3	I	95	MET
3	I	97	LEU
3	I	103	PRO
3	I	105(A)	ASN
3	I	108	LEU
1	B	5	MET
1	B	8	ARG
1	B	10	LYS
1	B	19	GLN
1	B	21	SER
1	B	26	TRP
1	B	27	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	36	SER
1	B	44	LYS
1	B	47	SER
1	B	48	LEU
1	B	52	GLN
1	B	53	LEU
1	B	58(A)	ASN
1	B	64	GLN
1	B	81	MET
1	B	85	THR
1	B	86	TYR
1	B	99	PRO
1	B	102(A)	LYS
1	B	128	ASN
1	B	129	PRO
1	B	136	VAL
1	B	139	ASN
1	B	140	ASP
1	B	155	HIS
1	B	155(A)	LYS
1	B	155(B)	THR
1	B	168	GLU
1	B	175	ASN
1	B	195	LYS
1	B	202	LEU
1	B	209	PRO
1	B	212	LEU
1	B	212(A)	VAL
2	R	83	THR
3	J	15	LYS
3	J	19	PRO
3	J	27	LYS
3	J	28	VAL
3	J	32	LEU
3	J	34	GLU
3	J	39	THR
3	J	44	LYS
3	J	48	VAL
3	J	52	THR
3	J	63	LYS
3	J	64	VAL
3	J	93	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	95	MET
3	J	100	PHE
3	J	101	LYS
3	J	103	PRO
3	J	105	GLN
3	J	118	LYS
3	J	123	THR
1	C	5	MET
1	C	18	ASN
1	C	21	SER
1	C	38	VAL
1	C	44	LYS
1	C	48	LEU
1	C	52	GLN
1	C	53	LEU
1	C	56	CYS
1	C	58(A)	ASN
1	C	59	ASN
1	C	78(A)	LYS
1	C	84	ASP
1	C	85	THR
1	C	86	TYR
1	C	87	PRO
1	C	89	LYS
1	C	91	GLN
1	C	94	HIS
1	C	96	LYS
1	C	128	ASN
1	C	139	ASN
1	C	145	ARG
1	C	152	THR
1	C	155	HIS
1	C	155(A)	LYS
1	C	155(B)	THR
1	C	157	VAL
1	C	164	VAL
1	C	173	VAL
1	C	175	ASN
1	C	195	LYS
1	C	202	LEU
2	S	79	ASN
2	S	80	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	6	MET
3	K	7	ILE
3	K	8	PRO
3	K	15	LYS
3	K	29	LYS
3	K	30	PRO
3	K	32	LEU
3	K	44	LYS
3	K	52	THR
3	K	55	VAL
3	K	63	LYS
3	K	92	ASN
3	K	97	LEU
3	K	103	PRO
3	K	111	THR
3	K	120	ASP
1	D	5	MET
1	D	26	TRP
1	D	27	THR
1	D	44	LYS
1	D	46	LEU
1	D	48	LEU
1	D	55	ASP
1	D	69	SER
1	D	76	ARG
1	D	86	TYR
1	D	96	LYS
1	D	102	ASP
1	D	108	LYS
1	D	110	VAL
1	D	115	MET
1	D	128	ASN
1	D	145	ARG
1	D	152	THR
1	D	154	CYS
1	D	155(A)	LYS
1	D	155(B)	THR
1	D	156	LYS
1	D	168	GLU
1	D	168(A)	GLU
1	D	168(D)	ILE
1	D	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	190	GLU
1	D	195	LYS
1	D	205	CYS
1	D	212(A)	VAL
2	T	76	GLU
2	T	80	CYS
2	T	83	THR
3	L	11	LEU
3	L	15	LYS
3	L	27	LYS
3	L	28	VAL
3	L	32	LEU
3	L	44	LYS
3	L	50	TYR
3	L	58	THR
3	L	61	TYR
3	L	65	ARG
3	L	97	LEU
3	L	99	VAL
3	L	103	PRO
3	L	116	LYS
3	L	118	LYS
3	L	119	ASP
3	L	120	ASP
3	L	121	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	52	GLN
1	A	58(A)	ASN
1	A	64	GLN
1	A	94	HIS
1	A	98	GLN
1	A	116	ASN
1	A	180	GLN
1	A	198	ASN
2	P	79	ASN
1	B	19	GLN
1	B	51	GLN
1	B	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	58(A)	ASN
1	B	60	ASN
1	B	64	GLN
1	B	70	GLN
1	B	98	GLN
1	B	116	ASN
1	B	155	HIS
1	B	175	ASN
1	B	198	ASN
2	R	79	ASN
1	C	18	ASN
1	C	19	GLN
1	C	51	GLN
1	C	52	GLN
1	C	58(A)	ASN
1	C	91	GLN
1	C	116	ASN
1	C	155	HIS
1	C	175	ASN
1	C	184	ASN
1	C	198	ASN
2	S	79	ASN
3	K	22	GLN
3	K	92	ASN
3	K	96	HIS
1	D	19	GLN
1	D	51	GLN
1	D	52	GLN
1	D	60	ASN
1	D	61	HIS
1	D	91	GLN
1	D	116	ASN
1	D	155	HIS
1	D	175	ASN
1	D	184	ASN
1	D	198	ASN
3	L	92	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	0.73	0	15,19,21	1.06	1 (6%)
4	NAG	A	214	4	14,14,15	0.72	0	15,19,21	0.83	0
4	BMA	A	215	4	11,11,12	1.01	1 (9%)	14,15,17	1.95	3 (21%)
4	NAG	B	213	1,4	14,14,15	0.98	0	15,19,21	1.45	2 (13%)
4	NAG	B	214	4	14,14,15	0.40	0	15,19,21	0.77	1 (6%)
4	BMA	B	215	4	11,11,12	1.01	1 (9%)	14,15,17	1.09	2 (14%)
4	NAG	C	213	1,4	14,14,15	0.85	0	15,19,21	0.66	0
4	NAG	C	214	4	14,14,15	0.59	0	15,19,21	0.97	1 (6%)
4	BMA	C	215	4	11,11,12	0.36	0	14,15,17	0.71	0
4	NAG	D	213	1,4	14,14,15	1.03	1 (7%)	15,19,21	1.01	0
4	NAG	D	214	4	14,14,15	0.75	0	15,19,21	0.84	1 (6%)
4	BMA	D	215	4	11,11,12	0.45	0	14,15,17	1.76	2 (14%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	B	215	BMA	C2-C3	2.32	1.55	1.52
4	D	213	NAG	C8-C7	2.43	1.55	1.50
4	A	215	BMA	C2-C3	2.59	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	213	NAG	C2-N2-C7	-3.46	118.59	123.04
4	C	214	NAG	C2-N2-C7	-3.08	119.08	123.04
4	B	214	NAG	C2-N2-C7	-2.25	120.15	123.04
4	B	215	BMA	C1-O5-C5	-2.17	109.50	112.25
4	D	214	NAG	C2-N2-C7	-2.06	120.39	123.04
4	B	215	BMA	C2-C3-C4	2.65	115.54	111.04
4	A	213	NAG	C4-C3-C2	2.77	115.53	111.23
4	B	213	NAG	C4-C3-C2	3.00	115.89	111.23
4	A	215	BMA	C3-C4-C5	3.37	116.07	110.20
4	D	215	BMA	C2-C3-C4	3.77	117.44	111.04
4	A	215	BMA	C2-C3-C4	4.03	117.89	111.04
4	D	215	BMA	C3-C4-C5	4.31	117.70	110.20
4	A	215	BMA	C1-C2-C3	4.70	115.10	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	213	NAG	3	0
4	B	213	NAG	2	0
4	B	215	BMA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	213	NAG	2	0
4	C	214	NAG	1	0
4	D	215	BMA	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/220 (98%)	-0.71	1 (0%) 91 88	10, 23, 38, 54	7 (3%)
1	B	216/220 (98%)	-0.57	0 100 100	8, 26, 42, 52	7 (3%)
1	C	216/220 (98%)	-0.75	0 100 100	5, 21, 38, 51	7 (3%)
1	D	216/220 (98%)	-0.63	1 (0%) 91 88	7, 25, 42, 54	8 (3%)
2	P	8/8 (100%)	0.40	1 (12%) 5 2	35, 40, 49, 51	3 (37%)
2	R	8/8 (100%)	1.09	2 (25%) 1 0	35, 42, 45, 47	3 (37%)
2	S	6/8 (75%)	0.09	1 (16%) 2 1	37, 40, 49, 52	2 (33%)
2	T	5/8 (62%)	0.64	0 100 100	45, 45, 50, 54	1 (20%)
3	I	95/98 (96%)	-0.49	1 (1%) 82 74	14, 28, 41, 51	6 (6%)
3	J	98/98 (100%)	-0.46	0 100 100	11, 29, 47, 54	12 (12%)
3	K	95/98 (96%)	-0.17	1 (1%) 82 74	17, 37, 53, 58	7 (7%)
3	L	95/98 (96%)	-0.25	1 (1%) 82 74	14, 33, 48, 57	8 (8%)
All	All	1274/1304 (97%)	-0.54	9 (0%) 89 84	5, 26, 46, 58	71 (5%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	83	THR	5.1
1	A	168(B)	ASN	2.9
3	L	105	GLN	2.8
2	P	83	THR	2.7
2	R	82	ALA	2.5
3	I	107	ASP	2.4
2	S	79	ASN	2.3
1	D	168(B)	ASN	2.2
3	K	39	THR	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	213	14/15	0.92	0.16	0.62	24,29,34,34	0
4	NAG	A	214	14/15	0.94	0.15	0.00	21,28,32,34	0
4	NAG	D	213	14/15	0.92	0.16	0.00	25,27,28,28	0
4	NAG	C	213	14/15	0.94	0.13	-0.23	16,18,21,21	0
4	NAG	B	213	14/15	0.91	0.15	-0.30	32,34,36,37	0
4	NAG	B	214	14/15	0.95	0.13	-1.32	31,33,34,37	0
4	NAG	C	214	14/15	0.97	0.11	-1.35	19,21,25,25	0
4	BMA	D	215	11/12	0.93	0.13	-	31,32,32,33	0
4	BMA	A	215	11/12	0.86	0.20	-	34,36,37,38	0
4	BMA	C	215	11/12	0.95	0.13	-	22,27,29,29	0
4	NAG	D	214	14/15	0.91	0.17	-	29,31,33,35	0
4	BMA	B	215	11/12	0.91	0.17	-	36,39,41,42	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.