



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:42 PM GMT

PDB ID : 4FQK
Title : Influenza B/Brisbane/60/2008 hemagglutinin Fab CR8059 complex
Authors : Dreyfus, C.; Laursen, N.S.; Wilson, I.A.
Deposited on : 2012-06-25
Resolution : 5.65 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

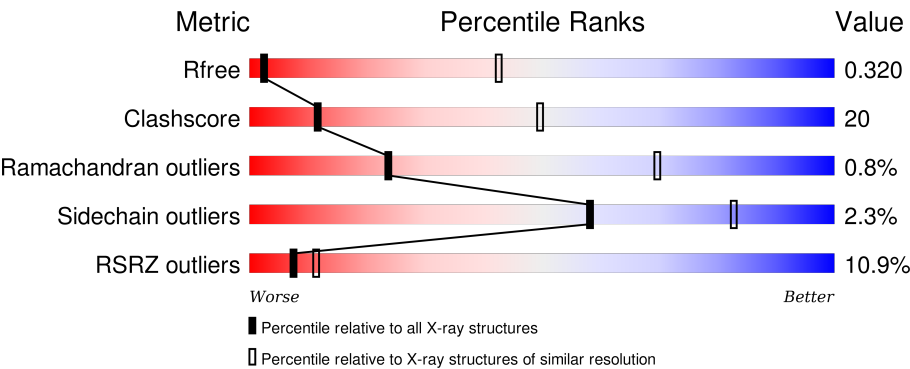
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.65 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	1006 (7.66-3.64)
Clashscore	102246	1036 (7.60-3.70)
Ramachandran outliers	100387	1011 (7.60-3.66)
Sidechain outliers	100360	1001 (7.60-3.64)
RSRZ outliers	91569	1005 (7.66-3.64)

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	347	<div><div>14%</div><div>56%</div><div>39%</div><div>• •</div></div>
1	C	347	<div><div>10%</div><div>57%</div><div>38%</div><div>• •</div></div>
2	B	179	<div><div>6%</div><div>56%</div><div>21%</div><div>• 22%</div></div>
2	D	179	<div><div>9%</div><div>56%</div><div>21%</div><div>• 22%</div></div>
3	E	234	<div><div>12%</div><div>71%</div><div>21%</div><div>• 6%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	234	<div><div></div><div>11%</div><div>71%</div><div>22%</div><div>6%</div></div>
4	F	216	<div><div></div><div>9%</div><div>79%</div><div>20%</div><div></div></div>
4	L	216	<div><div></div><div>7%</div><div>81%</div><div>17%</div><div></div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2560	1607	458	480	15			
1	C	337	Total	C	N	O	S	0	0	0
			2560	1607	458	480	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1054	652	182	215	5			
2	D	140	Total	C	N	O	S	0	0	0
			1062	658	183	216	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	LINKER	UNP C0LT38
B	525	GLY	-	LINKER	UNP C0LT38
B	526	ARG	-	LINKER	UNP C0LT38
D	524	SER	-	LINKER	UNP C0LT38
D	525	GLY	-	LINKER	UNP C0LT38
D	526	ARG	-	LINKER	UNP C0LT38

- Molecule 3 is a protein called Antibody CR8059 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	220	Total	C	N	O	S	0	0	0
			1673	1061	278	327	7			
3	H	221	Total	C	N	O	S	0	0	0
			1679	1064	279	328	8			

- Molecule 4 is a protein called Antibody CR8059 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	213	Total	C	N	O	S	0	0	0
			1606	1006	269	327	4			
4	L	214	Total	C	N	O	S	0	0	0
			1612	1009	270	328	5			

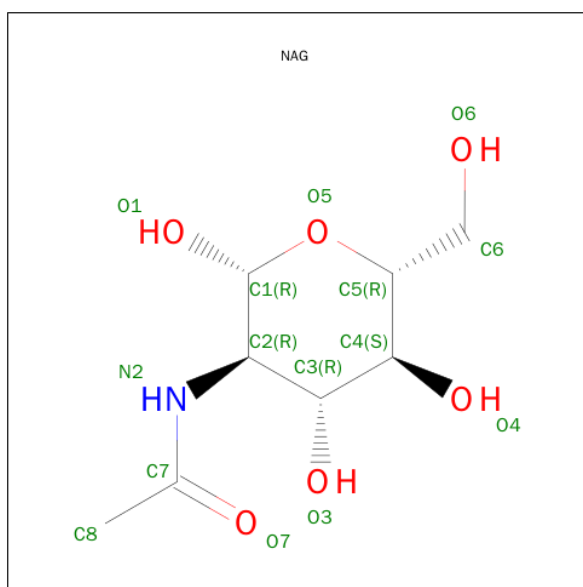
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

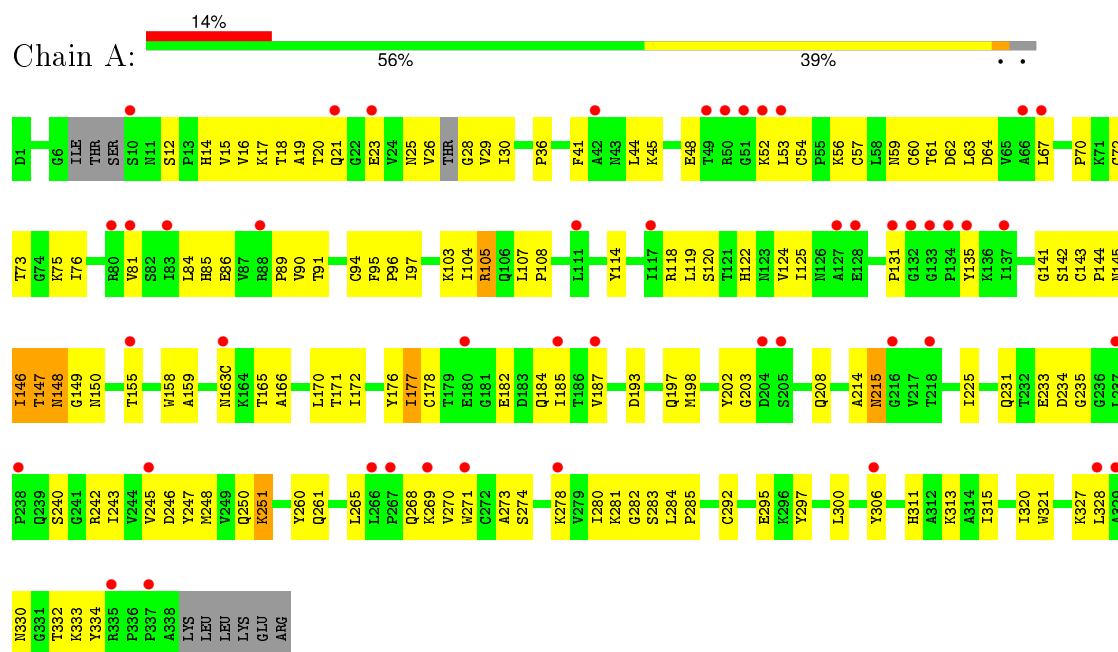


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0

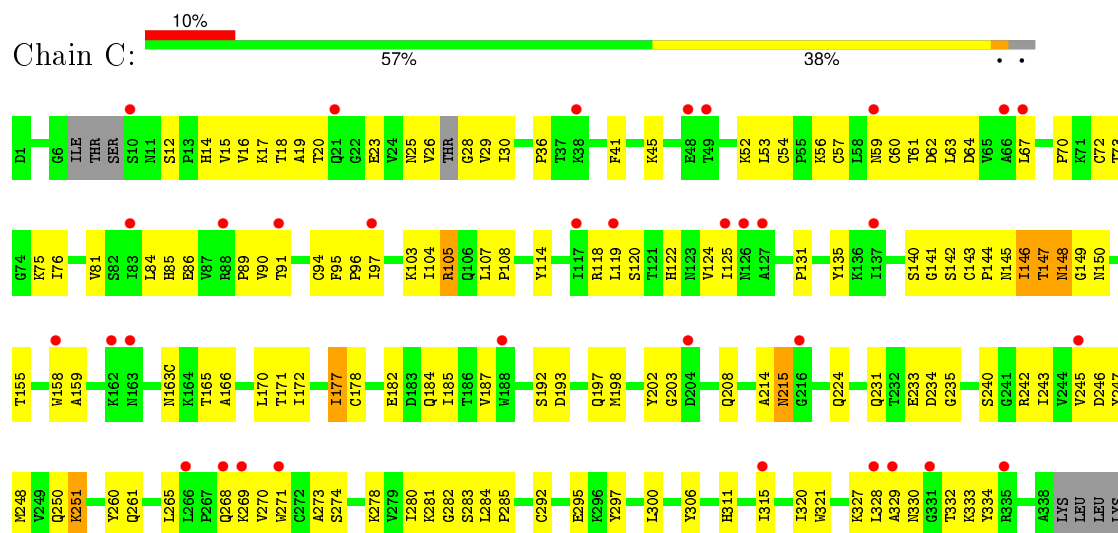
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Hemagglutinin HA1

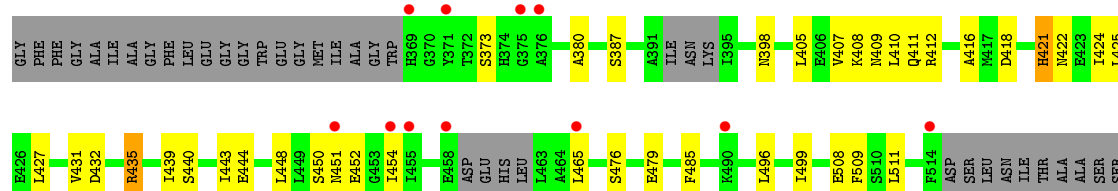


• Molecule 1: Hemagglutinin HA1



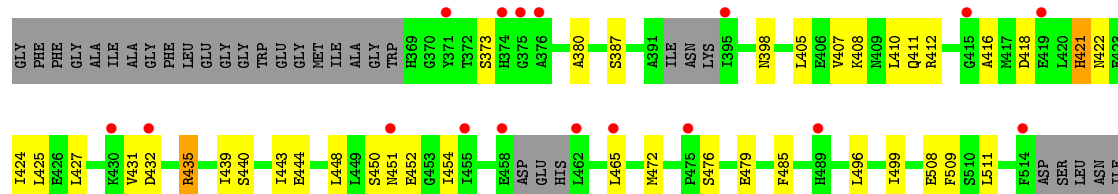
GLU
ARG

• Molecule 2: Hemagglutinin HA2



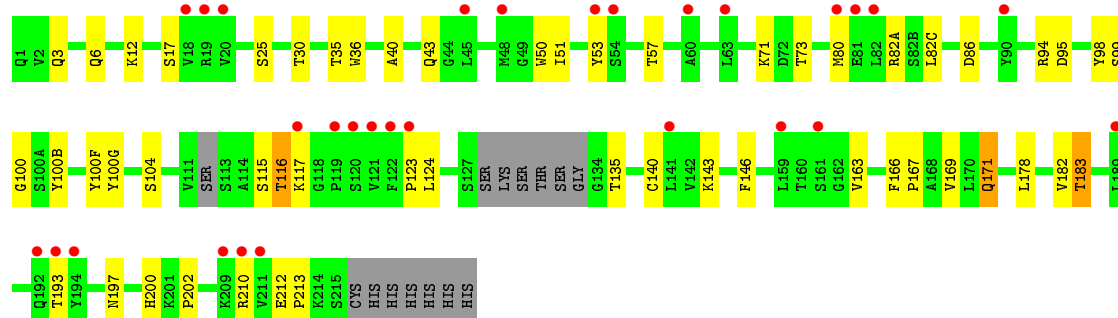
GLY
ARG

• Molecule 2: Hemagglutinin HA2



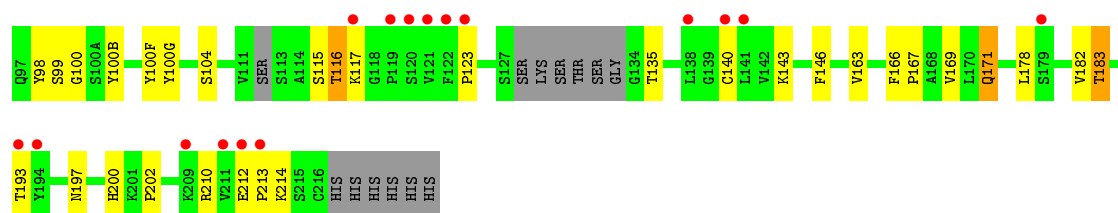
THR
ALA
ALA
SER
SER
GLY
ARG

• Molecule 3: Antibody CR8059 Heavy Chain

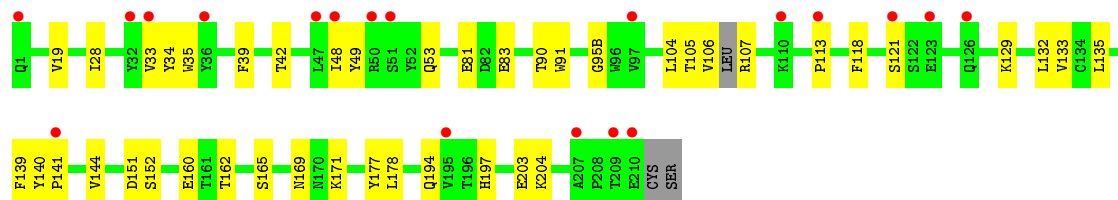
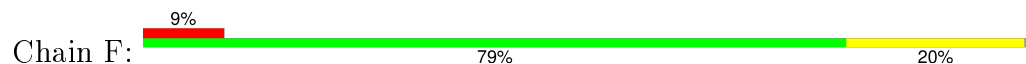


• Molecule 3: Antibody CR8059 Heavy Chain

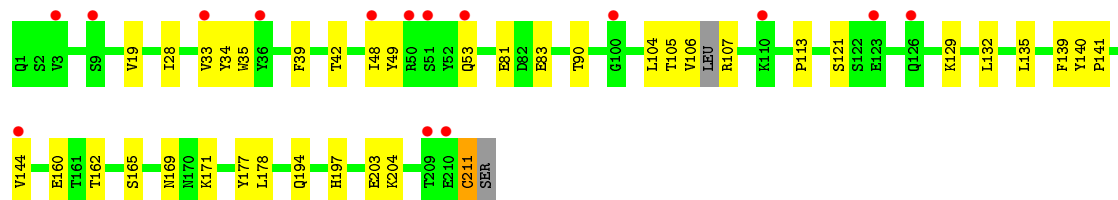
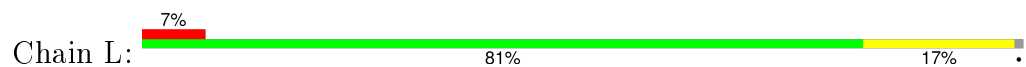




• Molecule 4: Antibody CR8059 Light Chain



• Molecule 4: Antibody CR8059 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	189.20Å 189.20Å 319.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 5.65 48.93 – 5.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.93–5.65) 99.9 (48.93–5.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 5.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.306 , 0.324 0.297 , 0.320	Depositor DCC
R_{free} test set	1268 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	243.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 139.0	EDS
Estimated twinning fraction	0.429 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 12751 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/2618	0.94	3/3553 (0.1%)
1	C	0.64	0/2618	0.94	2/3553 (0.1%)
2	B	0.45	0/1063	0.70	0/1429
2	D	0.45	0/1071	0.71	0/1440
3	E	0.44	0/1714	0.61	0/2335
3	H	0.44	0/1720	0.61	0/2343
4	F	0.43	0/1648	0.57	0/2250
4	L	0.43	0/1654	0.57	0/2258
All	All	0.52	0/14106	0.75	5/19161 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	84	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	C	67	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	A	67	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	A	44	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2559	201	0
1	C	2560	0	2559	195	0
2	B	1054	0	1043	65	0
2	D	1062	0	1054	59	0
3	E	1673	0	1633	50	0
3	H	1679	0	1638	49	0
4	F	1606	0	1541	34	0
4	L	1612	0	1546	29	0
5	A	84	0	75	1	0
5	C	84	0	75	5	0
6	A	39	0	34	3	0
6	C	39	0	34	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
All	All	14080	0	13817	567	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (567) 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:C:214:ALA:HB2	1:C:248:MET:CE	1.62	1.29
1:A:214:ALA:HB2	1:A:248:MET:CE	1.62	1.27
1:A:20:THR:CG2	2:B:452:GLU:HG3	1.78	1.13
1:A:320:ILE:CD1	2:B:405:LEU:HD22	1.78	1.12
1:C:320:ILE:CD1	2:D:405:LEU:HD22	1.80	1.11
1:C:131:PRO:HG2	1:C:172:ILE:HD11	1.33	1.11
1:A:280:ILE:HD11	1:A:315:ILE:HG23	1.25	1.10
1:C:280:ILE:HD11	1:C:315:ILE:HG23	1.25	1.10
1:C:214:ALA:HB2	1:C:248:MET:HE3	1.32	1.10
1:A:20:THR:CG2	2:B:452:GLU:CG	2.31	1.08
1:A:214:ALA:HB2	1:A:248:MET:HE3	1.32	1.06
1:A:124:VAL:HG12	1:A:177:ILE:HG13	1.38	1.06
1:A:56:LYS:NZ	1:A:75:LYS:HE3	1.72	1.05
1:C:124:VAL:HG12	1:C:177:ILE:HG13	1.38	1.04
1:A:280:ILE:CD1	1:A:315:ILE:HG12	1.87	1.04
1:C:56:LYS:NZ	1:C:75:LYS:HE3	1.72	1.04
1:C:280:ILE:CD1	1:C:315:ILE:HG12	1.87	1.03
1:A:131:PRO:HG2	1:A:172:ILE:HD11	1.33	1.03
1:C:96:PRO:O	1:C:243:ILE:HG22	1.59	1.02
1:C:283:SER:HB2	3:E:99:SER:O	1.57	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:O	1:A:243:ILE:HG22	1.59	1.01
1:A:20:THR:HG22	2:B:452:GLU:CG	1.91	1.01
4:F:105:THR:HG21	4:F:141:PRO:HB3	1.43	1.01
1:A:119:LEU:HD21	1:A:269:LYS:HB3	1.43	1.01
1:C:131:PRO:HG2	1:C:172:ILE:CD1	1.91	1.00
2:D:416:ALA:HB1	2:D:425:LEU:HD21	1.42	1.00
1:A:328:LEU:HD12	2:B:451:ASN:OD1	1.62	1.00
1:C:328:LEU:HD12	2:D:451:ASN:OD1	1.62	0.99
1:A:131:PRO:HG2	1:A:172:ILE:CD1	1.91	0.99
2:B:416:ALA:HB1	2:B:425:LEU:HD21	1.42	0.99
1:C:119:LEU:HD21	1:C:269:LYS:HB3	1.43	0.98
1:A:283:SER:HB2	3:H:99:SER:O	1.63	0.97
1:A:20:THR:HG21	2:B:452:GLU:CG	1.93	0.97
1:A:215:ASN:OD1	1:A:251:LYS:HG2	1.65	0.97
1:C:215:ASN:OD1	1:C:251:LYS:HG2	1.65	0.96
1:C:283:SER:HB3	3:E:100:GLY:HA3	1.48	0.96
1:C:214:ALA:HB2	1:C:248:MET:HE2	1.47	0.96
1:A:280:ILE:HD12	1:A:315:ILE:HG12	1.48	0.94
1:A:281:LYS:HD2	2:B:412:ARG:CZ	1.98	0.94
1:C:280:ILE:HD12	1:C:315:ILE:HG12	1.48	0.94
4:L:105:THR:HG21	4:L:141:PRO:HB3	1.50	0.94
1:A:214:ALA:HB2	1:A:248:MET:HE2	1.48	0.94
2:D:421:HIS:O	2:D:425:LEU:HG	1.68	0.93
2:B:421:HIS:O	2:B:425:LEU:HG	1.68	0.93
1:A:240:SER:OG	6:A:407:NAG:H82	1.69	0.93
1:A:280:ILE:HD11	1:A:315:ILE:CG2	1.99	0.92
1:A:285:PRO:HD2	3:H:100(F):TYR:CE2	2.04	0.92
1:C:280:ILE:HD11	1:C:315:ILE:CG2	1.99	0.92
1:C:240:SER:OG	5:C:408:NAG:H82	1.69	0.92
1:A:171:THR:O	1:A:172:ILE:HD13	1.71	0.91
1:A:119:LEU:HD23	1:A:120:SER:N	1.86	0.91
1:C:171:THR:O	1:C:172:ILE:HD13	1.71	0.90
1:A:20:THR:HG21	2:B:452:GLU:HG3	1.50	0.90
1:C:285:PRO:HD2	3:E:100(F):TYR:CE2	2.07	0.89
1:C:278:LYS:HD2	2:D:411:GLN:NE2	1.87	0.89
1:C:131:PRO:CG	1:C:172:ILE:HD11	2.01	0.89
1:A:131:PRO:CG	1:A:172:ILE:HD11	2.01	0.89
1:C:119:LEU:HD23	1:C:120:SER:N	1.87	0.89
3:E:167:PRO:HG2	4:F:165:SER:OG	1.70	0.89
1:A:20:THR:CG2	2:B:452:GLU:HG2	2.03	0.89
1:C:281:LYS:HD2	2:D:412:ARG:NH2	1.87	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ILE:HD11	2:D:405:LEU:HD22	1.54	0.88
3:H:167:PRO:HG2	4:L:165:SER:OG	1.73	0.88
1:A:320:ILE:HD11	2:B:405:LEU:HD22	1.54	0.86
1:C:215:ASN:ND2	1:C:215:ASN:O	2.09	0.86
1:C:155:THR:CG2	1:C:187:VAL:HB	2.05	0.86
1:A:155:THR:CG2	1:A:187:VAL:HB	2.05	0.86
1:A:18:THR:HG22	2:B:451:ASN:HB2	1.58	0.85
1:A:215:ASN:ND2	1:A:215:ASN:O	2.09	0.85
1:C:281:LYS:HD2	2:D:412:ARG:CZ	2.07	0.84
1:A:56:LYS:NZ	1:A:75:LYS:CE	2.40	0.84
1:C:56:LYS:NZ	1:C:75:LYS:CE	2.40	0.84
1:A:283:SER:HB3	3:H:100:GLY:HA3	1.58	0.84
1:C:26:VAL:HG12	1:C:28:GLY:O	1.78	0.83
1:A:214:ALA:CB	1:A:248:MET:HE3	2.08	0.83
1:C:214:ALA:CB	1:C:248:MET:HE3	2.09	0.83
1:C:56:LYS:HZ3	1:C:75:LYS:HE3	1.42	0.82
1:A:281:LYS:HD2	2:B:412:ARG:NH2	1.92	0.82
1:A:320:ILE:CD1	2:B:405:LEU:CD2	2.58	0.82
2:B:416:ALA:HB1	2:B:425:LEU:CD2	2.09	0.82
1:C:18:THR:HG22	2:D:451:ASN:HB2	1.61	0.81
2:D:416:ALA:HB1	2:D:425:LEU:CD2	2.09	0.81
1:A:18:THR:HG22	2:B:451:ASN:CB	2.11	0.80
1:C:52:LYS:HE3	3:E:53:TYR:CE1	2.17	0.79
1:A:20:THR:HG22	2:B:452:GLU:HG3	1.50	0.79
1:C:18:THR:HG22	2:D:451:ASN:CB	2.13	0.78
1:A:26:VAL:HG12	1:A:28:GLY:O	1.84	0.77
1:A:320:ILE:HD11	2:B:405:LEU:CD2	2.15	0.77
1:A:284:LEU:HB3	1:A:285:PRO:HA	1.67	0.76
1:A:52:LYS:HE3	3:H:53:TYR:CE1	2.21	0.76
1:A:59:ASN:OD1	3:H:30:THR:HG21	1.85	0.75
1:C:320:ILE:CD1	2:D:405:LEU:CD2	2.64	0.75
1:C:52:LYS:CE	3:E:53:TYR:CE1	2.70	0.75
1:A:278:LYS:HD2	2:B:411:GLN:NE2	2.01	0.74
1:C:284:LEU:HB3	1:C:285:PRO:HA	1.67	0.74
1:A:215:ASN:HD22	1:A:215:ASN:C	1.91	0.74
1:A:56:LYS:HZ3	1:A:75:LYS:HE3	1.48	0.74
1:C:20:THR:HB	2:D:452:GLU:HG3	1.69	0.74
1:C:59:ASN:OD1	3:E:30:THR:HG21	1.88	0.74
1:C:215:ASN:C	1:C:215:ASN:HD22	1.91	0.73
1:C:283:SER:CB	3:E:99:SER:O	2.35	0.73
1:A:119:LEU:HD21	1:A:269:LYS:CB	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PRO:HB2	1:C:297:TYR:CD1	2.24	0.73
1:A:52:LYS:CE	3:H:53:TYR:CE1	2.72	0.73
1:C:283:SER:CB	3:E:100:GLY:HA3	2.18	0.73
1:A:56:LYS:HZ3	1:A:75:LYS:CE	2.01	0.73
1:A:36:PRO:HB2	1:A:297:TYR:CD1	2.24	0.73
1:C:193:ASP:OD1	1:C:198:MET:SD	2.46	0.73
1:A:193:ASP:OD1	1:A:198:MET:SD	2.46	0.72
1:A:158:TRP:HA	1:A:265:LEU:HD23	1.70	0.72
1:A:280:ILE:HG23	1:A:295:GLU:HG3	1.71	0.72
4:F:106:VAL:HG22	4:F:106:VAL:O	1.89	0.72
1:C:119:LEU:HD23	1:C:120:SER:H	1.54	0.72
1:C:119:LEU:HD21	1:C:269:LYS:CB	2.18	0.72
1:A:292:CYS:HB3	1:A:300:LEU:HB3	1.72	0.72
1:C:280:ILE:HD11	1:C:315:ILE:HG12	1.73	0.71
1:C:158:TRP:HA	1:C:265:LEU:HD23	1.70	0.71
1:C:292:CYS:HB3	1:C:300:LEU:HB3	1.72	0.71
4:L:106:VAL:O	4:L:106:VAL:HG22	1.89	0.71
1:A:56:LYS:HZ1	1:A:75:LYS:HE3	1.54	0.71
2:B:479:GLU:OE1	2:B:485:PHE:CE2	2.44	0.71
1:C:320:ILE:HD11	2:D:405:LEU:CD2	2.20	0.70
1:A:16:VAL:CG2	1:A:29:VAL:CG1	2.69	0.70
1:C:280:ILE:HG23	1:C:295:GLU:HG3	1.72	0.70
1:A:19:ALA:H	2:B:448:LEU:HB3	1.57	0.70
1:A:119:LEU:HD23	1:A:120:SER:H	1.54	0.70
1:C:172:ILE:HG13	1:C:260:TYR:HE2	1.56	0.70
2:B:479:GLU:OE1	2:B:485:PHE:CZ	2.45	0.70
2:D:479:GLU:OE1	2:D:485:PHE:CE2	2.44	0.70
1:A:85:HIS:HB2	3:H:99:SER:HB3	1.74	0.70
2:D:479:GLU:OE1	2:D:485:PHE:CZ	2.45	0.69
1:C:56:LYS:HZ3	1:C:75:LYS:CE	2.02	0.69
1:A:243:ILE:HD11	1:A:265:LEU:HD11	1.73	0.69
1:A:280:ILE:HD11	1:A:315:ILE:HG12	1.73	0.69
1:A:16:VAL:HG13	1:A:327:LYS:O	1.93	0.69
1:A:172:ILE:HG13	1:A:260:TYR:HE2	1.56	0.69
1:A:85:HIS:HB2	3:H:99:SER:CB	2.23	0.69
1:C:14:HIS:CD2	1:C:28:GLY:HA2	2.28	0.68
1:A:283:SER:CB	3:H:99:SER:O	2.40	0.68
1:C:243:ILE:HD11	1:C:265:LEU:HD11	1.73	0.68
1:C:85:HIS:HB2	3:E:99:SER:CB	2.24	0.68
1:A:284:LEU:HD13	3:H:98:TYR:OH	1.93	0.68
1:A:16:VAL:CG2	1:A:29:VAL:HG12	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:HZ3	1:A:75:LYS:NZ	1.92	0.67
1:A:26:VAL:HA	1:A:332:THR:O	1.93	0.67
1:C:36:PRO:HB2	1:C:297:TYR:HD1	1.58	0.67
1:A:19:ALA:N	2:B:448:LEU:HB3	2.09	0.67
1:C:53:LEU:CD1	1:C:62:ASP:HB3	2.25	0.67
1:C:284:LEU:HD13	3:E:98:TYR:OH	1.95	0.67
1:A:52:LYS:HE2	3:H:53:TYR:HE1	1.60	0.67
1:C:56:LYS:HZ1	1:C:75:LYS:HE3	1.60	0.67
1:C:85:HIS:HB2	3:E:99:SER:HB3	1.77	0.66
1:A:16:VAL:HG23	1:A:29:VAL:CG1	2.25	0.66
1:C:56:LYS:NZ	1:C:75:LYS:NZ	2.44	0.66
1:C:52:LYS:HE2	3:E:53:TYR:HE1	1.59	0.66
1:A:53:LEU:CD1	1:A:62:ASP:HB3	2.25	0.66
4:F:83:GLU:HG2	4:F:106:VAL:HG13	1.77	0.66
1:A:56:LYS:NZ	1:A:75:LYS:NZ	2.44	0.66
1:A:85:HIS:HD2	1:A:86:GLU:HG3	1.61	0.66
1:A:36:PRO:HB2	1:A:297:TYR:HD1	1.58	0.66
3:H:166:PHE:CZ	4:L:135:LEU:HB3	2.29	0.66
2:D:373:SER:HB2	2:D:380:ALA:HB3	1.77	0.66
3:E:3:GLN:HB2	3:E:25:SER:HB2	1.78	0.66
2:B:373:SER:HB2	2:B:380:ALA:HB3	1.78	0.65
3:H:3:GLN:HB2	3:H:25:SER:HB2	1.78	0.65
1:C:89:PRO:HG2	1:C:105:ARG:O	1.96	0.65
1:A:14:HIS:CD2	1:A:28:GLY:HA2	2.31	0.65
4:F:33:VAL:HA	4:F:90:THR:HG22	1.78	0.65
1:A:214:ALA:O	1:A:215:ASN:ND2	2.30	0.65
1:C:85:HIS:HD2	1:C:86:GLU:HG3	1.61	0.65
1:C:16:VAL:HG13	1:C:327:LYS:O	1.97	0.65
4:L:33:VAL:HA	4:L:90:THR:HG22	1.78	0.65
1:A:306:TYR:CE2	2:B:443:ILE:HD13	2.32	0.65
4:L:83:GLU:HG2	4:L:106:VAL:HG13	1.77	0.65
1:A:89:PRO:HG2	1:A:105:ARG:O	1.96	0.65
1:C:214:ALA:O	1:C:215:ASN:ND2	2.30	0.64
1:A:20:THR:HG23	1:A:21:GLN:HG2	1.78	0.64
2:D:508:GLU:HG3	2:D:509:PHE:H	1.63	0.64
3:E:169:VAL:HA	4:F:162:THR:HG22	1.79	0.64
1:C:172:ILE:CG1	1:C:260:TYR:HE2	2.11	0.64
2:D:427:LEU:O	2:D:431:VAL:HG23	1.97	0.64
2:B:427:LEU:O	2:B:431:VAL:HG23	1.97	0.64
3:H:212:GLU:CG	3:H:213:PRO:HD2	2.28	0.64
3:E:212:GLU:CG	3:E:213:PRO:HD2	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:THR:O	1:A:148:ASN:CG	2.37	0.63
1:C:147:THR:O	1:C:148:ASN:CG	2.37	0.63
1:C:26:VAL:CG1	1:C:28:GLY:O	2.46	0.63
2:B:508:GLU:HG3	2:B:509:PHE:H	1.63	0.63
1:C:214:ALA:CB	1:C:248:MET:CE	2.57	0.63
1:C:26:VAL:HA	1:C:332:THR:O	1.98	0.63
1:A:16:VAL:HG23	1:A:29:VAL:HG11	1.80	0.63
1:C:94:CYS:HA	1:C:142:SER:O	1.99	0.63
1:A:172:ILE:CG1	1:A:260:TYR:HE2	2.10	0.62
1:C:171:THR:O	1:C:172:ILE:CD1	2.46	0.62
1:A:214:ALA:CB	1:A:248:MET:CE	2.57	0.62
1:A:94:CYS:HA	1:A:142:SER:O	1.99	0.62
4:F:106:VAL:CG2	4:F:106:VAL:O	2.48	0.61
1:A:171:THR:O	1:A:172:ILE:CD1	2.46	0.61
1:A:16:VAL:CG2	1:A:29:VAL:HG11	2.30	0.61
1:C:85:HIS:HB2	3:E:99:SER:OG	2.01	0.61
2:D:435:ARG:HD3	2:D:439:ILE:CG1	2.31	0.61
1:C:311:HIS:HB2	1:C:321:TRP:CD1	2.36	0.61
1:C:320:ILE:HD13	2:D:405:LEU:HD22	1.78	0.61
1:A:311:HIS:HB2	1:A:321:TRP:CD1	2.36	0.61
1:A:283:SER:CB	3:H:100:GLY:HA3	2.28	0.60
2:D:398:ASN:HD21	2:D:450:SER:HB3	1.66	0.60
4:L:106:VAL:O	4:L:106:VAL:CG2	2.48	0.60
3:H:169:VAL:HA	4:L:162:THR:HG22	1.82	0.60
2:B:398:ASN:HD21	2:B:450:SER:HB3	1.66	0.60
3:E:163:VAL:HG22	3:E:182:VAL:HG22	1.83	0.60
2:B:435:ARG:HD3	2:B:439:ILE:CG1	2.31	0.60
1:A:41:PHE:CZ	1:A:282:GLY:HA2	2.37	0.60
1:C:280:ILE:CD1	1:C:315:ILE:CG1	2.73	0.60
1:A:119:LEU:CD2	1:A:269:LYS:HB3	2.27	0.59
4:L:83:GLU:CG	4:L:106:VAL:HG13	2.32	0.59
1:C:70:PRO:HB2	1:C:144:PRO:O	2.01	0.59
1:A:280:ILE:CD1	1:A:315:ILE:CG1	2.73	0.59
1:A:26:VAL:CG1	1:A:28:GLY:O	2.48	0.59
1:A:16:VAL:HG21	1:A:29:VAL:HG12	1.82	0.59
2:D:418:ASP:O	2:D:422:ASN:ND2	2.35	0.59
2:B:418:ASP:O	2:B:422:ASN:ND2	2.36	0.59
3:H:163:VAL:HG22	3:H:182:VAL:HG22	1.83	0.59
1:C:41:PHE:CZ	1:C:282:GLY:HA2	2.37	0.59
1:A:70:PRO:HB2	1:A:144:PRO:O	2.01	0.59
4:F:83:GLU:CG	4:F:106:VAL:HG13	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:HIS:HB3	2:B:424:ILE:HD12	1.84	0.59
2:D:421:HIS:HB3	2:D:424:ILE:HD12	1.84	0.59
1:A:283:SER:O	3:H:100(F):TYR:OH	2.20	0.58
3:H:212:GLU:HG3	3:H:213:PRO:HD2	1.85	0.58
1:C:25:ASN:O	1:C:333:LYS:HA	2.02	0.58
1:C:281:LYS:CD	2:D:412:ARG:NH2	2.65	0.58
2:B:421:HIS:O	2:B:425:LEU:CG	2.48	0.58
3:E:193:THR:HG22	3:E:210:ARG:HH22	1.69	0.58
1:C:16:VAL:CG2	1:C:29:VAL:CG1	2.81	0.58
1:C:119:LEU:CD2	1:C:269:LYS:HB3	2.26	0.58
1:A:155:THR:HG23	1:A:187:VAL:HB	1.84	0.58
1:A:281:LYS:CD	2:B:412:ARG:NH2	2.65	0.58
1:C:292:CYS:SG	1:C:300:LEU:HD23	2.44	0.58
1:A:131:PRO:CD	1:A:172:ILE:HD11	2.34	0.57
1:C:131:PRO:CD	1:C:172:ILE:HD11	2.34	0.57
1:C:328:LEU:HD11	2:D:454:ILE:HD12	1.87	0.57
1:A:85:HIS:HB2	3:H:99:SER:OG	2.05	0.57
3:E:212:GLU:HG3	3:E:213:PRO:HD2	1.85	0.57
3:H:193:THR:HG22	3:H:210:ARG:HH22	1.69	0.57
1:A:320:ILE:HD12	2:B:405:LEU:HD22	1.81	0.56
1:A:18:THR:HG22	2:B:451:ASN:HB3	1.86	0.56
1:C:155:THR:HG23	1:C:187:VAL:HB	1.84	0.56
1:A:104:ILE:HD13	1:A:245:VAL:HG12	1.87	0.56
1:C:131:PRO:CG	1:C:172:ILE:CD1	2.71	0.56
1:A:292:CYS:SG	1:A:300:LEU:HD23	2.44	0.56
1:C:19:ALA:N	2:D:448:LEU:HB3	2.20	0.56
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.06	0.56
1:C:280:ILE:HD12	1:C:315:ILE:CG1	2.30	0.56
1:C:197:GLN:HA	1:C:197:GLN:OE1	2.06	0.56
1:C:16:VAL:HG23	1:C:29:VAL:CG1	2.35	0.56
1:C:104:ILE:HD13	1:C:245:VAL:HG12	1.87	0.56
1:C:59:ASN:OD1	3:E:73:THR:CG2	2.53	0.56
3:H:36:TRP:CE2	3:H:80:MET:HB2	2.41	0.56
3:E:166:PHE:CZ	4:F:135:LEU:HB3	2.41	0.56
1:A:25:ASN:O	1:A:333:LYS:HA	2.05	0.56
1:C:16:VAL:CG2	1:C:29:VAL:HG12	2.36	0.55
2:D:508:GLU:HG3	2:D:509:PHE:CD1	2.42	0.55
3:E:36:TRP:CE2	3:E:80:MET:HB2	2.41	0.55
2:D:421:HIS:O	2:D:425:LEU:CG	2.48	0.55
1:C:19:ALA:H	2:D:448:LEU:HB3	1.71	0.55
2:D:476:SER:HB3	2:D:511:LEU:HD13	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:83:GLU:HG2	4:L:106:VAL:CG1	2.37	0.55
2:B:435:ARG:HD3	2:B:439:ILE:HG13	1.89	0.55
3:E:200:HIS:NE2	3:E:202:PRO:HG2	2.22	0.55
1:C:26:VAL:O	1:C:28:GLY:N	2.41	0.54
3:H:200:HIS:NE2	3:H:202:PRO:HG2	2.22	0.54
1:C:280:ILE:HD11	1:C:315:ILE:CG1	2.37	0.54
2:B:476:SER:HB3	2:B:511:LEU:HD13	1.89	0.54
1:C:56:LYS:HZ3	1:C:75:LYS:NZ	2.05	0.54
1:C:278:LYS:HD2	2:D:411:GLN:HE21	1.67	0.54
1:C:16:VAL:HG23	1:C:29:VAL:HG11	1.89	0.54
2:D:435:ARG:HD3	2:D:439:ILE:HG13	1.89	0.54
1:A:59:ASN:OD1	3:H:73:THR:CG2	2.56	0.54
2:D:410:LEU:HG	2:D:432:ASP:OD2	2.08	0.54
4:F:83:GLU:HG2	4:F:106:VAL:CG1	2.37	0.54
3:H:35:THR:HG22	3:H:50:TRP:HB2	1.88	0.54
2:B:508:GLU:HG3	2:B:509:PHE:CD1	2.42	0.54
1:A:20:THR:HG21	2:B:452:GLU:HG2	1.76	0.53
1:C:283:SER:O	3:E:100(F):TYR:OH	2.26	0.53
3:E:35:THR:HG22	3:E:50:TRP:HB2	1.89	0.53
1:A:284:LEU:CB	1:A:285:PRO:HA	2.36	0.53
2:D:422:ASN:HA	2:D:425:LEU:HD12	1.90	0.53
2:B:410:LEU:HG	2:B:432:ASP:OD2	2.08	0.53
1:C:124:VAL:HG12	1:C:177:ILE:CG1	2.26	0.53
2:D:508:GLU:HG3	2:D:509:PHE:N	2.24	0.53
1:C:85:HIS:CD2	1:C:86:GLU:HG3	2.42	0.53
1:A:280:ILE:HD12	1:A:315:ILE:CG1	2.30	0.53
1:A:18:THR:CG2	2:B:451:ASN:HB3	2.39	0.53
1:A:240:SER:OG	6:A:407:NAG:C8	2.51	0.53
1:C:306:TYR:CE2	2:D:443:ILE:HD13	2.44	0.53
1:C:18:THR:HG22	2:D:451:ASN:HB3	1.89	0.53
2:B:422:ASN:HA	2:B:425:LEU:HD12	1.90	0.52
1:C:16:VAL:CG1	1:C:327:LYS:O	2.58	0.52
2:B:408:LYS:O	2:B:435:ARG:NH2	2.42	0.52
3:H:123:PRO:O	4:L:121:SER:HB3	2.10	0.52
1:A:280:ILE:CG2	1:A:295:GLU:HG3	2.39	0.52
1:A:56:LYS:HZ3	1:A:75:LYS:HZ2	1.58	0.52
2:B:508:GLU:CG	2:B:509:PHE:H	2.22	0.52
1:C:53:LEU:HD11	1:C:62:ASP:HB3	1.91	0.52
1:A:16:VAL:CG1	1:A:327:LYS:O	2.57	0.52
1:A:208:GLN:HB3	1:A:261:GLN:HB2	1.92	0.52
1:A:20:THR:HG22	2:B:452:GLU:HG2	1.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:GLU:CG	2:D:509:PHE:H	2.22	0.52
1:A:85:HIS:CD2	1:A:86:GLU:HG3	2.42	0.52
1:C:56:LYS:HZ2	1:C:75:LYS:NZ	2.07	0.52
1:A:53:LEU:HD11	1:A:62:ASP:HB3	1.91	0.52
1:C:208:GLN:HB3	1:C:261:GLN:HB2	1.92	0.52
3:H:115:SER:O	3:H:115:SER:OG	2.23	0.52
1:A:103:LYS:NZ	1:A:246:ASP:OD1	2.38	0.52
1:A:52:LYS:HE2	3:H:53:TYR:CE1	2.38	0.51
4:L:28:ILE:HG12	4:L:90:THR:HG21	1.92	0.51
2:B:439:ILE:O	2:B:443:ILE:HG13	2.10	0.51
1:C:103:LYS:NZ	1:C:246:ASP:OD1	2.38	0.51
1:A:280:ILE:HD11	1:A:315:ILE:CG1	2.37	0.51
2:B:508:GLU:HG3	2:B:509:PHE:N	2.24	0.51
3:E:115:SER:OG	3:E:115:SER:O	2.23	0.51
1:C:16:VAL:HG22	1:C:327:LYS:HB2	1.92	0.51
1:A:320:ILE:HD13	2:B:405:LEU:HD22	1.81	0.51
1:A:94:CYS:O	1:A:235:GLY:N	2.43	0.51
2:D:408:LYS:O	2:D:435:ARG:NH2	2.42	0.51
1:A:26:VAL:O	1:A:28:GLY:N	2.44	0.51
1:C:131:PRO:O	1:C:170:LEU:HD13	2.11	0.51
1:C:97:ILE:HA	1:C:243:ILE:HG23	1.93	0.51
2:D:439:ILE:O	2:D:443:ILE:HG13	2.10	0.51
2:D:416:ALA:O	2:D:421:HIS:ND1	2.43	0.51
3:H:167:PRO:CG	4:L:165:SER:OG	2.55	0.51
4:F:28:ILE:HG12	4:F:90:THR:HG21	1.92	0.51
2:B:416:ALA:O	2:B:421:HIS:ND1	2.43	0.50
1:C:59:ASN:OD1	3:E:73:THR:HG23	2.11	0.50
1:A:105:ARG:NH2	1:A:233:GLU:OE1	2.45	0.50
1:A:59:ASN:OD1	3:H:73:THR:HG23	2.12	0.50
1:A:131:PRO:O	1:A:170:LEU:HD13	2.11	0.50
1:C:145:ASN:O	1:C:146:ILE:C	2.50	0.50
1:C:94:CYS:O	1:C:235:GLY:N	2.43	0.50
1:C:105:ARG:NH2	1:C:233:GLU:OE1	2.44	0.50
1:C:16:VAL:CG2	1:C:29:VAL:HG11	2.41	0.50
1:A:149:GLY:HA3	5:A:401:NAG:O6	2.11	0.50
1:C:18:THR:CG2	2:D:451:ASN:HB3	2.41	0.50
1:A:145:ASN:O	1:A:146:ILE:C	2.50	0.50
1:C:240:SER:OG	5:C:408:NAG:C8	2.51	0.50
4:F:144:VAL:HG12	4:F:197:HIS:HB2	1.94	0.50
1:C:149:GLY:HA3	6:C:401:NAG:O6	2.11	0.50
3:H:212:GLU:HG2	3:H:213:PRO:HD2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:95:ASP:OD2	3:E:100(B):TYR:OH	2.30	0.50
1:A:124:VAL:HG12	1:A:177:ILE:CG1	2.26	0.49
3:E:167:PRO:CG	4:F:165:SER:OG	2.53	0.49
3:H:171:GLN:HG3	4:L:160:GLU:HG3	1.93	0.49
3:H:6:GLN:OE1	3:H:104:SER:OG	2.29	0.49
3:E:171:GLN:HG3	4:F:160:GLU:HG3	1.93	0.49
1:A:131:PRO:HD2	1:A:172:ILE:HD11	1.94	0.49
3:H:169:VAL:HG11	4:L:177:TYR:CD1	2.47	0.49
1:C:131:PRO:HD2	1:C:172:ILE:HD11	1.94	0.49
4:F:105:THR:CG2	4:F:141:PRO:HB3	2.28	0.49
1:A:172:ILE:HG13	1:A:260:TYR:CE2	2.44	0.49
1:A:97:ILE:HA	1:A:243:ILE:HG23	1.93	0.49
3:E:12:LYS:HE2	3:E:17:SER:O	2.12	0.49
4:L:144:VAL:HG12	4:L:197:HIS:HB2	1.94	0.49
1:C:16:VAL:HG22	1:C:327:LYS:CB	2.42	0.49
3:E:6:GLN:OE1	3:E:104:SER:OG	2.29	0.49
1:C:97:ILE:HA	1:C:243:ILE:CG2	2.43	0.49
1:C:280:ILE:CG2	1:C:295:GLU:HG3	2.39	0.48
3:H:12:LYS:HE2	3:H:17:SER:O	2.12	0.48
1:C:36:PRO:HB2	1:C:297:TYR:CE1	2.48	0.48
3:E:212:GLU:HG2	3:E:213:PRO:HD2	1.94	0.48
3:H:214:LYS:HG3	4:L:211:CYS:SG	2.52	0.48
4:F:107:ARG:N	4:F:140:TYR:HH	2.11	0.48
1:C:172:ILE:HG13	1:C:260:TYR:CE2	2.44	0.48
1:A:131:PRO:CG	1:A:172:ILE:CD1	2.72	0.48
4:L:107:ARG:N	4:L:140:TYR:HH	2.11	0.48
1:A:163(C):ASN:O	1:A:165:THR:HG22	2.14	0.48
1:A:36:PRO:HB2	1:A:297:TYR:CE1	2.48	0.48
3:H:100(G):TYR:HB3	4:L:34:TYR:CZ	2.49	0.47
1:C:26:VAL:C	1:C:28:GLY:N	2.67	0.47
1:C:52:LYS:HD3	1:C:62:ASP:OD1	2.14	0.47
1:A:16:VAL:HG22	1:A:327:LYS:CB	2.44	0.47
1:C:163(C):ASN:O	1:C:165:THR:HG22	2.14	0.47
1:C:16:VAL:HG21	1:C:29:VAL:HG12	1.95	0.47
1:C:182:GLU:HG2	1:C:274:SER:HB3	1.96	0.47
1:C:63:LEU:HA	1:C:108:PRO:HG3	1.96	0.47
1:C:30:ILE:HG13	1:C:330:ASN:HB2	1.97	0.47
1:A:63:LEU:HA	1:A:108:PRO:HG3	1.95	0.47
1:A:122:HIS:O	1:A:269:LYS:HD3	2.15	0.47
1:A:52:LYS:HD3	1:A:62:ASP:OD1	2.14	0.47
1:C:193:ASP:OD1	1:C:198:MET:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:ARG:HD3	2:B:439:ILE:HG12	1.96	0.47
2:D:435:ARG:HD3	2:D:439:ILE:HG12	1.96	0.47
1:A:81:VAL:CG1	1:A:315:ILE:HD11	2.45	0.47
1:A:193:ASP:OD1	1:A:198:MET:HB2	2.14	0.47
1:A:197:GLN:CD	6:A:407:NAG:O7	2.54	0.47
1:A:97:ILE:HA	1:A:243:ILE:CG2	2.44	0.47
1:C:122:HIS:O	1:C:269:LYS:HD3	2.15	0.47
1:C:178:CYS:SG	1:C:184:GLN:HG3	2.55	0.47
3:E:100(G):TYR:HB3	4:F:34:TYR:CZ	2.50	0.47
1:A:313:LYS:HB3	2:B:411:GLN:HA	1.98	0.46
1:C:81:VAL:CG1	1:C:315:ILE:HD11	2.45	0.46
1:C:197:GLN:CD	5:C:408:NAG:O7	2.54	0.46
3:H:95:ASP:OD2	3:H:100(B):TYR:OH	2.30	0.46
1:C:114:TYR:CG	1:C:273:ALA:HB1	2.51	0.46
1:C:197:GLN:HE21	5:C:408:NAG:H81	1.81	0.46
1:A:292:CYS:HB3	1:A:300:LEU:HD23	1.98	0.46
1:C:103:LYS:HG3	1:C:247:TYR:CE1	2.50	0.46
1:A:12:SER:HB2	1:A:334:TYR:HB2	1.96	0.46
1:A:26:VAL:C	1:A:28:GLY:N	2.69	0.46
1:A:103:LYS:HG3	1:A:247:TYR:CE1	2.50	0.46
1:A:182:GLU:HG2	1:A:274:SER:HB3	1.96	0.46
4:L:204:LYS:HD3	4:L:204:LYS:HA	1.76	0.46
1:A:30:ILE:HG13	1:A:330:ASN:HB2	1.97	0.46
1:C:135:TYR:CD1	1:C:159:ALA:HB1	2.50	0.46
1:A:250:GLN:O	1:A:251:LYS:O	2.33	0.46
3:E:169:VAL:HG11	4:F:177:TYR:CD1	2.50	0.46
1:C:184:GLN:NE2	1:C:270:VAL:HG11	2.31	0.46
1:A:184:GLN:NE2	1:A:270:VAL:HG11	2.31	0.46
1:C:231:GLN:HG2	1:C:242:ARG:NH2	2.31	0.46
1:A:114:TYR:CG	1:A:273:ALA:HB1	2.51	0.46
1:A:231:GLN:HG2	1:A:242:ARG:NH2	2.31	0.46
1:C:250:GLN:O	1:C:251:LYS:O	2.33	0.46
1:A:178:CYS:SG	1:A:184:GLN:HG3	2.55	0.46
1:C:215:ASN:C	1:C:215:ASN:ND2	2.63	0.45
1:A:16:VAL:HG22	1:A:327:LYS:HB2	1.98	0.45
2:B:407:VAL:HG12	2:B:435:ARG:HH21	1.82	0.45
3:E:116:THR:HA	3:E:146:PHE:O	2.17	0.45
1:A:135:TYR:CD1	1:A:159:ALA:HB1	2.50	0.45
1:C:61:THR:O	1:C:64:ASP:HB2	2.16	0.45
2:D:407:VAL:HG12	2:D:435:ARG:HH21	1.82	0.45
1:C:292:CYS:HB3	1:C:300:LEU:HD23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PRO:CD	1:C:172:ILE:CD1	2.95	0.45
1:A:59:ASN:OD1	3:H:30:THR:CG2	2.62	0.45
1:A:313:LYS:HD3	2:B:412:ARG:N	2.32	0.45
1:A:61:THR:O	1:A:64:ASP:HB2	2.16	0.45
1:A:131:PRO:CD	1:A:172:ILE:CD1	2.95	0.45
1:C:131:PRO:HD2	1:C:172:ILE:CD1	2.47	0.45
1:C:26:VAL:HG21	1:C:329:ALA:HB1	1.99	0.45
1:C:165:THR:HA	1:C:203:GLY:HA3	1.99	0.44
1:C:231:GLN:HB3	1:C:234:ASP:OD2	2.18	0.44
1:C:72:CYS:O	1:C:73:THR:HG23	2.17	0.44
3:E:51:ILE:HB	3:E:57:THR:HG22	1.99	0.44
1:A:147:THR:O	1:A:148:ASN:OD1	2.36	0.44
1:A:165:THR:HA	1:A:203:GLY:HA3	1.98	0.44
1:C:20:THR:HB	2:D:452:GLU:CG	2.45	0.44
4:F:49:TYR:CE1	4:F:53:GLN:HB3	2.52	0.44
1:A:72:CYS:O	1:A:73:THR:HG23	2.17	0.44
4:L:39:PHE:O	4:L:42:THR:OG1	2.33	0.44
3:H:17:SER:HB3	3:H:82(A):ARG:HA	2.00	0.44
1:C:53:LEU:HG	1:C:62:ASP:CG	2.38	0.44
1:C:165:THR:OG1	1:C:166:ALA:N	2.51	0.44
4:F:194:GLN:HB3	4:F:203:GLU:HG3	2.00	0.44
3:H:51:ILE:HB	3:H:57:THR:HG22	1.99	0.44
1:A:131:PRO:HD2	1:A:172:ILE:CD1	2.47	0.44
1:C:185:ILE:HB	1:C:271:TRP:HB2	2.00	0.44
3:H:117:LYS:HE2	3:H:117:LYS:HB3	1.86	0.44
1:A:53:LEU:HG	1:A:62:ASP:CG	2.38	0.43
2:B:444:GLU:O	2:B:448:LEU:HG	2.17	0.43
3:E:123:PRO:O	4:F:121:SER:HB3	2.18	0.43
4:L:169:ASN:OD1	4:L:171:LYS:HB2	2.18	0.43
4:L:49:TYR:CE1	4:L:53:GLN:HB3	2.52	0.43
1:A:185:ILE:HB	1:A:271:TRP:HB2	2.00	0.43
1:C:95:PHE:CD1	1:C:96:PRO:HD2	2.53	0.43
4:L:105:THR:CG2	4:L:141:PRO:HB3	2.36	0.43
1:C:17:LYS:O	2:D:448:LEU:HD23	2.18	0.43
1:A:165:THR:OG1	1:A:166:ALA:N	2.51	0.43
1:C:320:ILE:HD13	2:D:405:LEU:CD2	2.44	0.43
1:C:320:ILE:HG21	2:D:443:ILE:HD11	2.01	0.43
1:A:95:PHE:CD1	1:A:96:PRO:HD2	2.53	0.43
3:E:117:LYS:HE2	3:E:117:LYS:HB3	1.86	0.43
1:C:125:ILE:O	1:C:268:GLN:NE2	2.47	0.43
2:D:444:GLU:O	2:D:448:LEU:HG	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:GLU:CG	2:D:509:PHE:N	2.81	0.43
4:F:169:ASN:OD1	4:F:171:LYS:HB2	2.18	0.43
3:H:135:THR:OG1	3:H:183:THR:HG23	2.19	0.43
3:H:116:THR:HA	3:H:146:PHE:O	2.17	0.43
2:D:496:LEU:HD12	2:D:499:ILE:HD12	2.01	0.43
4:L:35:TRP:HB2	4:L:48:ILE:HB	2.00	0.43
1:C:81:VAL:HG13	1:C:315:ILE:CD1	2.49	0.43
1:A:328:LEU:HD11	2:B:454:ILE:HD12	2.00	0.43
3:E:17:SER:HB3	3:E:82(A):ARG:HA	2.00	0.43
1:A:48:GLU:HG2	1:A:48:GLU:H	1.69	0.43
2:B:496:LEU:HD12	2:B:499:ILE:HD12	2.01	0.43
1:A:231:GLN:HB3	1:A:234:ASP:OD2	2.18	0.43
3:E:135:THR:OG1	3:E:183:THR:HG23	2.19	0.43
4:F:204:LYS:HA	4:F:204:LYS:HD3	1.77	0.43
1:C:56:LYS:HZ3	1:C:75:LYS:HZ2	1.66	0.43
1:C:147:THR:O	1:C:148:ASN:OD1	2.36	0.43
1:C:292:CYS:CB	1:C:300:LEU:HD23	2.49	0.42
2:B:508:GLU:CG	2:B:509:PHE:N	2.82	0.42
2:D:387:SER:HB2	2:D:465:LEU:HD11	2.01	0.42
1:A:90:VAL:HG12	1:A:91:THR:O	2.19	0.42
1:C:329:ALA:N	2:D:451:ASN:OD1	2.43	0.42
1:A:155:THR:HG21	1:A:187:VAL:HB	1.97	0.42
1:C:12:SER:HB2	1:C:334:TYR:HB2	2.01	0.42
2:B:387:SER:HB2	2:B:465:LEU:HD11	2.01	0.42
1:A:150:ASN:N	1:A:150:ASN:OD1	2.50	0.42
1:A:17:LYS:O	2:B:448:LEU:HD23	2.18	0.42
4:L:113:PRO:HB3	4:L:139:PHE:HB3	2.01	0.42
4:L:194:GLN:HB3	4:L:203:GLU:HG3	2.00	0.42
3:H:212:GLU:CG	3:H:213:PRO:CD	2.97	0.42
1:C:107:LEU:HB3	1:C:108:PRO:HD3	2.01	0.42
1:C:150:ASN:N	1:C:150:ASN:OD1	2.50	0.42
1:C:57:CYS:O	1:C:60:CYS:HB2	2.20	0.42
4:F:39:PHE:O	4:F:42:THR:OG1	2.33	0.42
1:A:320:ILE:HD13	2:B:405:LEU:CD2	2.42	0.42
1:C:284:LEU:CB	1:C:285:PRO:HA	2.36	0.42
1:C:141:GLY:C	1:C:143:CYS:H	2.23	0.42
4:L:132:LEU:HD12	4:L:178:LEU:HD23	2.02	0.42
1:A:292:CYS:CB	1:A:300:LEU:HD23	2.49	0.42
4:F:35:TRP:HB2	4:F:48:ILE:HB	2.00	0.42
2:D:435:ARG:CD	2:D:439:ILE:HG13	2.50	0.42
1:A:81:VAL:HG13	1:A:315:ILE:CD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:HG12	1:C:91:THR:O	2.19	0.42
1:C:192:SER:OG	1:C:224:GLN:O	2.28	0.42
1:C:81:VAL:HG11	1:C:315:ILE:HD11	2.02	0.42
1:C:59:ASN:OD1	3:E:30:THR:CG2	2.65	0.42
1:A:145:ASN:O	1:A:147:THR:N	2.52	0.42
1:C:15:VAL:HG22	1:C:23:GLU:HG2	2.02	0.42
3:H:82(C):LEU:HA	3:H:86:ASP:OD2	2.20	0.42
2:D:440:SER:O	2:D:444:GLU:HG3	2.20	0.41
3:E:169:VAL:CA	4:F:162:THR:HG22	2.47	0.41
1:C:281:LYS:HB2	1:C:295:GLU:HG2	2.02	0.41
1:C:158:TRP:C	1:C:158:TRP:CD1	2.92	0.41
4:F:132:LEU:HD12	4:F:178:LEU:HD23	2.02	0.41
1:A:176:TYR:OH	1:A:182:GLU:O	2.35	0.41
1:A:20:THR:CG2	1:A:21:GLN:HG2	2.47	0.41
1:A:81:VAL:HG11	1:A:315:ILE:HD11	2.02	0.41
2:B:440:SER:O	2:B:444:GLU:HG3	2.20	0.41
1:C:145:ASN:O	1:C:147:THR:N	2.53	0.41
1:A:107:LEU:HB3	1:A:108:PRO:HD3	2.01	0.41
1:C:278:LYS:HD2	2:D:411:GLN:CD	2.39	0.41
3:E:82(C):LEU:HA	3:E:86:ASP:OD2	2.19	0.41
4:F:113:PRO:HB3	4:F:139:PHE:HB3	2.02	0.41
1:A:141:GLY:C	1:A:143:CYS:H	2.23	0.41
1:C:214:ALA:CB	1:C:248:MET:HE2	2.33	0.41
1:A:243:ILE:HD11	1:A:265:LEU:CD1	2.47	0.41
1:A:285:PRO:HD3	3:H:96:VAL:O	2.21	0.41
3:E:169:VAL:HG11	4:F:177:TYR:CE1	2.56	0.41
1:A:57:CYS:O	1:A:60:CYS:HB2	2.20	0.41
2:D:472:MET:HG2	2:D:472:MET:H	1.70	0.41
1:A:53:LEU:O	1:A:76:ILE:HG23	2.21	0.41
3:E:212:GLU:CG	3:E:213:PRO:CD	2.97	0.41
1:A:225:ILE:HA	1:A:225:ILE:HD13	1.71	0.41
1:A:172:ILE:CG1	1:A:260:TYR:CE2	2.97	0.41
1:C:53:LEU:O	1:C:76:ILE:HG23	2.21	0.41
1:C:41:PHE:CE1	1:C:282:GLY:HA2	2.56	0.41
4:F:118:PHE:HB2	4:F:133:VAL:HB	2.03	0.41
1:A:158:TRP:C	1:A:158:TRP:CD1	2.92	0.41
1:C:197:GLN:NE2	5:C:408:NAG:H81	2.35	0.41
2:B:435:ARG:CD	2:B:439:ILE:HG13	2.50	0.41
2:B:409:ASN:O	2:B:410:LEU:HB2	2.21	0.41
1:A:125:ILE:O	1:A:268:GLN:NE2	2.47	0.41
4:F:91:TRP:CZ3	4:F:95(B):GLY:HA2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG22	1:A:23:GLU:HG2	2.02	0.41
1:C:52:LYS:HE2	3:E:53:TYR:CE1	2.39	0.41
1:C:16:VAL:HG12	1:C:17:LYS:N	2.36	0.41
3:E:124:LEU:HB3	4:F:118:PHE:CD1	2.56	0.41
3:H:40:ALA:HB3	3:H:43:GLN:HG3	2.03	0.40
3:E:40:ALA:HB3	3:E:43:GLN:HG3	2.03	0.40
4:L:19:VAL:HG21	4:L:104:LEU:CD1	2.52	0.40
4:F:19:VAL:HG21	4:F:104:LEU:CD1	2.52	0.40
2:D:418:ASP:HA	2:D:425:LEU:HD11	2.03	0.40
2:B:418:ASP:HA	2:B:425:LEU:HD11	2.03	0.40
1:A:16:VAL:HG12	1:A:17:LYS:N	2.36	0.40
1:C:140:SER:C	1:C:141:GLY:O	2.60	0.40
1:A:281:LYS:HB2	1:A:295:GLU:HG2	2.02	0.40
4:F:151:ASP:HB2	4:F:152:SER:H	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	11	53
1	C	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	11	53
2	B	133/179 (74%)	128 (96%)	5 (4%)	0	100	100
2	D	134/179 (75%)	129 (96%)	5 (4%)	0	100	100
3	E	214/234 (92%)	202 (94%)	11 (5%)	1 (0%)	34	77
3	H	215/234 (92%)	203 (94%)	11 (5%)	1 (0%)	34	77
4	F	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
4	L	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
All	All	1777/1952 (91%)	1673 (94%)	90 (5%)	14 (1%)	24	70

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS
1	A	148	ASN
1	C	148	ASN
3	E	116	THR
3	H	116	THR
1	A	45	LYS
1	A	146	ILE
1	A	147	THR
1	C	45	LYS
1	C	146	ILE
1	C	147	THR

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	284/294 (97%)	279 (98%)	5 (2%)	66	87
1	C	284/294 (97%)	279 (98%)	5 (2%)	66	87
2	B	116/143 (81%)	114 (98%)	2 (2%)	68	87
2	D	117/143 (82%)	115 (98%)	2 (2%)	68	87
3	E	185/198 (93%)	177 (96%)	8 (4%)	35	70
3	H	186/198 (94%)	178 (96%)	8 (4%)	35	70
4	F	180/183 (98%)	178 (99%)	2 (1%)	80	91
4	L	181/183 (99%)	178 (98%)	3 (2%)	68	87
All	All	1533/1636 (94%)	1498 (98%)	35 (2%)	58	83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	105	ARG
1	A	118	ARG
1	A	202	TYR
1	A	215	ASN
2	B	421	HIS
2	B	435	ARG
1	C	54	CYS
1	C	105	ARG
1	C	118	ARG
1	C	202	TYR
1	C	215	ASN
2	D	421	HIS
2	D	435	ARG
3	E	71	LYS
3	E	94	ARG
3	E	140	CYS
3	E	143	LYS
3	E	171	GLN
3	E	178	LEU
3	E	183	THR
3	E	197	ASN
4	F	81	GLU
4	F	129	LYS
3	H	71	LYS
3	H	94	ARG
3	H	140	CYS
3	H	143	LYS
3	H	171	GLN
3	H	178	LEU
3	H	183	THR
3	H	197	ASN
4	L	81	GLU
4	L	129	LYS
4	L	211	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	85	HIS
1	A	126	ASN
1	A	129	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	398	ASN
2	B	409	ASN
1	C	14	HIS
1	C	85	HIS
1	C	126	ASN
1	C	129	ASN
2	D	398	ASN
2	D	409	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

18 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	$\# Z > 2$
5	NAG	A	401	1,5	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
5	NAG	A	402	5	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
5	NAG	A	403	1,5	14,14,15	0.38	0	15,19,21	1.85	2 (13%)
5	NAG	A	404	5	14,14,15	0.43	0	15,19,21	1.24	2 (13%)
5	NAG	A	405	1,5	14,14,15	0.51	0	15,19,21	1.07	1 (6%)
5	NAG	A	406	5	14,14,15	0.46	0	15,19,21	0.86	1 (6%)
6	NAG	A	407	1,6	14,14,15	0.49	0	15,19,21	1.54	4 (26%)
6	NAG	A	408	6	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
6	BMA	A	409	6	11,11,12	0.63	0	14,15,17	1.45	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	401	1,6	14,14,15	0.51	0	15,19,21	1.05	1 (6%)
6	NAG	C	402	6	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
6	BMA	C	403	6	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
5	NAG	C	404	1,5	14,14,15	0.38	0	15,19,21	1.84	2 (13%)
5	NAG	C	405	5	14,14,15	0.42	0	15,19,21	1.24	2 (13%)
5	NAG	C	406	1,5	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
5	NAG	C	407	5	14,14,15	0.46	0	15,19,21	0.85	1 (6%)
5	NAG	C	408	1,5	14,14,15	0.50	0	15,19,21	1.52	3 (20%)
5	NAG	C	409	5	14,14,15	0.48	0	15,19,21	1.17	2 (13%)

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
5	NAG	A	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	402	5	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	404	5	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	406	5	-	0/6/23/26	0/1/1/1
6	NAG	A	407	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	408	6	-	0/6/23/26	0/1/1/1
6	BMA	A	409	6	-	0/2/19/22	0/1/1/1
6	NAG	C	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	402	6	-	0/6/23/26	0/1/1/1
6	BMA	C	403	6	-	0/2/19/22	0/1/1/1
5	NAG	C	404	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	405	5	-	0/6/23/26	0/1/1/1
5	NAG	C	406	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	407	5	-	0/6/23/26	0/1/1/1
5	NAG	C	408	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	409	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	405	NAG	C2-N2-C7	-2.89	119.32	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	NAG	C2-N2-C7	-2.84	119.39	123.04
6	A	407	NAG	O7-C7-C8	-2.82	116.88	122.06
5	C	408	NAG	O7-C7-C8	-2.81	116.91	122.06
6	A	408	NAG	O5-C5-C6	-2.66	101.59	107.35
6	A	407	NAG	C4-C3-C2	-2.65	107.12	111.23
5	C	409	NAG	O5-C5-C6	-2.63	101.66	107.35
5	C	408	NAG	C4-C3-C2	-2.62	107.15	111.23
5	A	406	NAG	C2-N2-C7	-2.58	119.72	123.04
5	C	407	NAG	C2-N2-C7	-2.52	119.80	123.04
5	A	402	NAG	C2-N2-C7	-2.47	119.86	123.04
6	A	409	BMA	O4-C4-C5	-2.44	102.77	109.24
6	C	402	NAG	C2-N2-C7	-2.44	119.91	123.04
6	A	409	BMA	C6-C5-C4	-2.30	107.34	113.02
6	A	408	NAG	C4-C3-C2	-2.24	107.75	111.23
5	C	409	NAG	C4-C3-C2	-2.23	107.76	111.23
5	A	404	NAG	C4-C3-C2	-2.08	108.00	111.23
5	C	405	NAG	C4-C3-C2	-2.03	108.08	111.23
6	C	403	BMA	O5-C1-C2	-2.02	107.58	110.86
6	A	407	NAG	C3-C4-C5	2.02	113.71	110.20
5	C	404	NAG	C3-C4-C5	2.32	114.24	110.20
5	A	403	NAG	C3-C4-C5	2.35	114.29	110.20
5	C	408	NAG	C3-C2-N2	2.44	116.40	110.56
6	A	407	NAG	C3-C2-N2	2.44	116.41	110.56
6	A	409	BMA	O2-C2-C3	2.94	116.02	110.12
5	A	401	NAG	C1-O5-C5	3.31	116.44	112.25
6	C	401	NAG	C1-O5-C5	3.32	116.46	112.25
5	C	406	NAG	C1-O5-C5	3.34	116.48	112.25
5	A	405	NAG	C1-O5-C5	3.37	116.52	112.25
5	C	404	NAG	C1-O5-C5	6.28	120.21	112.25
5	A	403	NAG	C1-O5-C5	6.30	120.24	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	NAG	1	0
6	A	407	NAG	3	0
6	C	401	NAG	1	0
5	C	408	NAG	5	0

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	410	1	14,14,15	0.47	0	15,19,21	1.02	1 (6%)
7	NAG	C	410	1	14,14,15	0.48	0	15,19,21	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	410	1	-	0/6/23/26	0/1/1/1
7	NAG	C	410	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	410	NAG	C1-O5-C5	2.58	115.52	112.25
7	A	410	NAG	C1-O5-C5	2.59	115.53	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	337/347 (97%)	0.63	47 (13%) 4 8	100, 100, 100, 100	0
1	C	337/347 (97%)	0.59	34 (10%) 9 13	100, 100, 100, 100	0
2	B	139/179 (77%)	0.73	11 (7%) 15 18	100, 100, 100, 100	0
2	D	140/179 (78%)	0.88	17 (12%) 6 10	100, 100, 100, 100	0
3	E	220/234 (94%)	0.74	29 (13%) 4 9	100, 100, 100, 100	0
3	H	221/234 (94%)	0.64	26 (11%) 6 10	100, 100, 100, 100	0
4	F	213/216 (98%)	0.45	19 (8%) 12 15	100, 100, 100, 100	0
4	L	214/216 (99%)	0.36	15 (7%) 19 21	100, 100, 100, 100	0
All	All	1821/1952 (93%)	0.61	198 (10%) 7 11	100, 100, 100, 100	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	194	TYR	7.3
1	C	329	ALA	6.7
4	L	123	GLU	5.6
1	A	329	ALA	5.3
4	F	210	GLU	5.0
1	A	23	GLU	4.9
2	D	376	ALA	4.7
4	F	1	GLN	4.7
1	A	132	GLY	4.6
3	E	193	THR	4.6
3	E	121	VAL	4.5
1	C	127	ALA	4.4
1	C	83	ILE	4.3
2	D	465	LEU	4.2
3	H	121	VAL	4.1
3	E	123	PRO	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	47	LEU	4.0
4	F	32	TYR	4.0
3	E	20	VAL	4.0
1	C	21	GLN	3.9
1	A	216	GLY	3.8
3	E	211	VAL	3.8
1	C	245	VAL	3.8
2	B	376	ALA	3.8
3	E	209	LYS	3.7
2	D	458	GLU	3.7
1	A	133	GLY	3.6
1	A	127	ALA	3.5
1	A	271	TRP	3.5
2	D	375	GLY	3.5
2	B	371	TYR	3.5
3	H	179	SER	3.4
4	L	48	ILE	3.4
1	A	218	THR	3.4
2	B	454	ILE	3.4
2	B	465	LEU	3.4
1	C	49	THR	3.4
3	E	119	PRO	3.3
3	H	193	THR	3.3
3	E	82	LEU	3.3
3	E	122	PHE	3.3
3	H	211	VAL	3.2
1	C	269	LYS	3.2
2	D	455	ILE	3.2
1	A	50	ARG	3.1
1	A	245	VAL	3.1
2	D	451	ASN	3.1
1	A	21	GLN	3.1
2	B	458	GLU	3.1
2	D	432	ASP	3.1
3	E	80	MET	3.1
3	E	117	LYS	3.0
1	A	67	LEU	3.0
1	A	80	ARG	3.0
4	L	100	GLY	3.0
1	C	271	TRP	3.0
4	L	210	GLU	3.0
3	H	194	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	123	GLU	3.0
4	F	48	ILE	3.0
1	C	315	ILE	3.0
2	B	455	ILE	3.0
4	L	50	ARG	2.9
1	C	67	LEU	2.9
1	A	51	GLY	2.9
3	H	209	LYS	2.9
3	H	212	GLU	2.9
3	E	45	LEU	2.9
1	C	158	TRP	2.9
3	H	19	ARG	2.9
3	H	20	VAL	2.9
3	E	63	LEU	2.8
3	E	120	SER	2.8
1	A	163(C)	ASN	2.8
1	C	266	LEU	2.8
4	L	126	GLN	2.8
1	A	328	LEU	2.8
2	B	369	HIS	2.7
2	D	514	PHE	2.7
4	L	51	SER	2.7
1	C	216	GLY	2.7
3	E	54	SER	2.7
3	E	53	TYR	2.7
4	F	51	SER	2.7
2	D	415	GLY	2.7
3	H	67	VAL	2.6
1	C	38	LYS	2.6
2	D	371	TYR	2.6
1	A	131	PRO	2.6
4	F	33	VAL	2.6
1	A	83	ILE	2.6
1	A	269	LYS	2.6
3	H	123	PRO	2.6
1	A	49	THR	2.6
1	A	10	SER	2.6
2	D	419	GLU	2.6
4	F	209	THR	2.6
3	E	18	VAL	2.6
3	E	210	ARG	2.6
4	L	33	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	54	SER	2.5
3	E	159	LEU	2.5
1	A	335	ARG	2.5
3	H	63	LEU	2.5
4	F	50	ARG	2.5
1	A	88	ARG	2.5
1	C	328	LEU	2.5
1	A	81	VAL	2.5
1	A	134	PRO	2.5
4	F	97	VAL	2.5
3	H	213	PRO	2.5
1	C	88	ARG	2.5
1	A	306	TYR	2.5
1	C	331	GLY	2.5
3	E	48	MET	2.4
1	A	137	ILE	2.4
2	B	375	GLY	2.4
3	H	45	LEU	2.4
4	F	113	PRO	2.4
1	C	97	ILE	2.4
4	F	36	TYR	2.4
3	E	90	TYR	2.4
2	D	475	PRO	2.4
3	H	120	SER	2.4
1	C	66	ALA	2.4
1	A	135	TYR	2.4
4	F	195	VAL	2.4
1	C	48	GLU	2.4
2	B	490	LYS	2.4
3	H	38	ARG	2.3
3	E	60	ALA	2.3
1	C	59	ASN	2.3
1	C	204	ASP	2.3
3	E	19	ARG	2.3
4	L	3	VAL	2.3
1	C	126	ASN	2.3
1	A	278	LYS	2.3
3	E	81	GLU	2.3
1	A	266	LEU	2.3
4	F	126	GLN	2.3
1	A	42	ALA	2.3
1	C	163	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	335	ARG	2.3
2	D	489	HIS	2.3
1	C	137	ILE	2.3
1	A	180	GLU	2.3
1	A	52	LYS	2.2
1	C	188	TRP	2.2
4	L	144	VAL	2.2
2	D	462	LEU	2.2
3	E	189	LEU	2.2
1	A	117	ILE	2.2
1	A	204	ASP	2.2
2	B	514	PHE	2.2
4	L	9	SER	2.2
4	F	207	ALA	2.2
4	L	36	TYR	2.2
1	C	117	ILE	2.2
3	H	122	PHE	2.2
4	L	53	GLN	2.2
1	A	53	LEU	2.1
3	E	141	LEU	2.1
4	F	110	LYS	2.1
1	A	337	PRO	2.1
3	H	119	PRO	2.1
3	H	141	LEU	2.1
1	A	66	ALA	2.1
1	C	91	THR	2.1
3	H	138	LEU	2.1
3	H	90	TYR	2.1
4	F	141	PRO	2.1
2	B	451	ASN	2.1
1	A	205	SER	2.1
4	F	121	SER	2.1
1	A	238	PRO	2.1
1	C	268	GLN	2.1
2	D	395	ILE	2.1
3	H	46	GLU	2.1
4	L	209	THR	2.1
3	H	117	LYS	2.1
1	A	187	VAL	2.1
1	C	119	LEU	2.1
3	H	140	CYS	2.1
2	D	430	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	GLU	2.0
1	A	111	LEU	2.0
1	A	237	LEU	2.0
3	E	161	SER	2.0
3	H	60	ALA	2.0
3	E	192	GLN	2.0
1	A	185	ILE	2.0
1	C	125	ILE	2.0
1	C	162	LYS	2.0
1	A	155	THR	2.0
1	C	10	SER	2.0
2	D	374	HIS	2.0
1	A	267	PRO	2.0
4	L	110	LYS	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(Å ²)	Q<0.9
5	NAG	A	402	14/15	0.60	0.57	-	100,100,100,100	0
5	NAG	C	406	14/15	0.85	0.50	-	100,100,100,100	0
6	NAG	C	401	14/15	0.89	0.29	-	100,100,100,100	0
5	NAG	A	406	14/15	0.67	0.45	-	100,100,100,100	0
6	NAG	A	407	14/15	0.77	0.47	-	100,100,100,100	0
5	NAG	C	409	14/15	0.76	0.31	-	100,100,100,100	0
5	NAG	C	407	14/15	0.76	0.41	-	100,100,100,100	0
6	BMA	A	409	11/12	0.75	0.35	-	100,100,100,100	0
5	NAG	A	404	14/15	0.81	0.37	-	100,100,100,100	0
5	NAG	A	403	14/15	0.91	0.36	-	100,100,100,100	0
5	NAG	C	404	14/15	0.96	0.19	-	100,100,100,100	0
6	NAG	A	408	14/15	0.80	0.25	-	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	C	405	14/15	0.89	0.32	-	100,100,100,100	0
5	NAG	C	408	14/15	0.85	0.35	-	100,100,100,100	0
5	NAG	A	401	14/15	0.91	0.27	-	100,100,100,100	0
6	BMA	C	403	11/12	0.67	0.38	-	100,100,100,100	0
5	NAG	A	405	14/15	0.82	0.45	-	100,100,100,100	0
6	NAG	C	402	14/15	0.81	0.38	-	100,100,100,100	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	NAG	C	410	14/15	0.62	0.50	-	100,100,100,100	0
7	NAG	A	410	14/15	0.73	0.47	-	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.