Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:09 AM GMT

PDB ID	:	2PMV
Title	:	Crystal Structure of Human Intrinsic Factor- Cobalamin Complex at 2.6 A Resolution
Authors	:	Mathews, F.S.; Gordon, M.M.; Chen, Z.; Rajashankar, K.R.; Ealick, S.E.; Alpers, D.H.; Sukumar, N.
Deposited on	:	2007-04-23
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

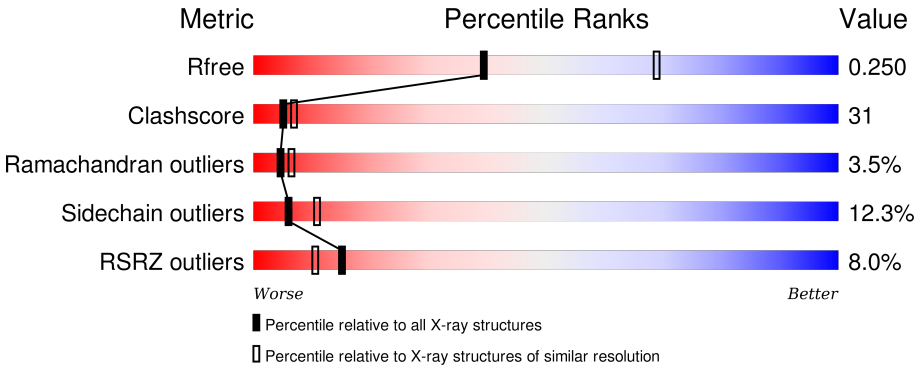
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	399	10%, 52%, 31%, 11%, • 5%
1	B	399	2%, 41%, 21%, 5% •, 33%
1	C	399	13%, 49%, 34%, 10%, • 5%
1	D	399	2%, 41%, 21%, 5% •, 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10457 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 Gastric intrinsic factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	3	0	0
			2871	1820	475	557	19			
1	B	267	Total	C	N	O	S	0	0	0
			2009	1268	332	392	17			
1	C	378	Total	C	N	O	S	5	0	0
			2871	1820	475	557	19			
1	D	267	Total	C	N	O	S	0	0	0
			2009	1268	332	392	17			

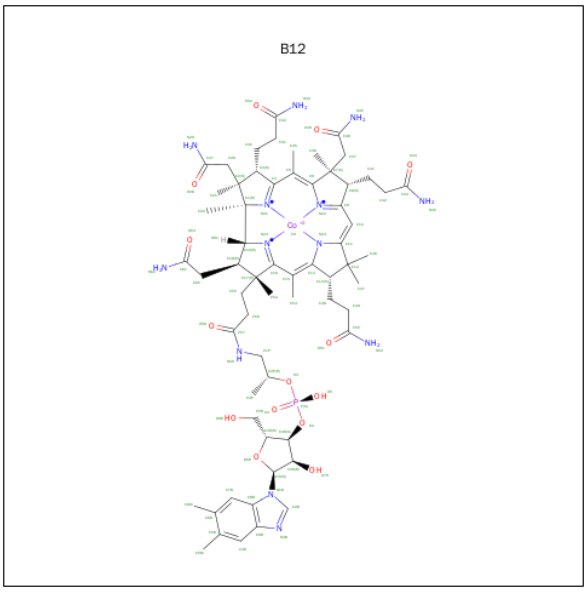
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIS	GLN	CONFLICT	UNP P27352
B	73	HIS	GLN	CONFLICT	UNP P27352
C	73	HIS	GLN	CONFLICT	UNP P27352
D	73	HIS	GLN	CONFLICT	UNP P27352

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

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

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is water.

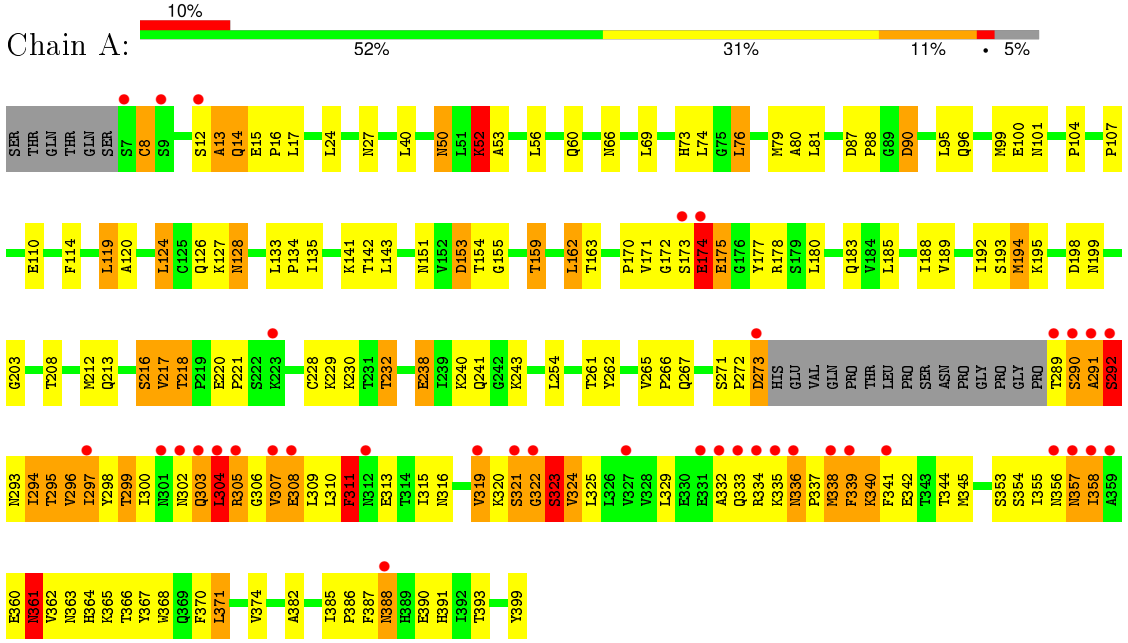
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	100	Total	O	0	0
			100	100		
4	C	129	Total	O	0	0
			129	129		
4	D	95	Total	O	0	0
			95	95		

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.

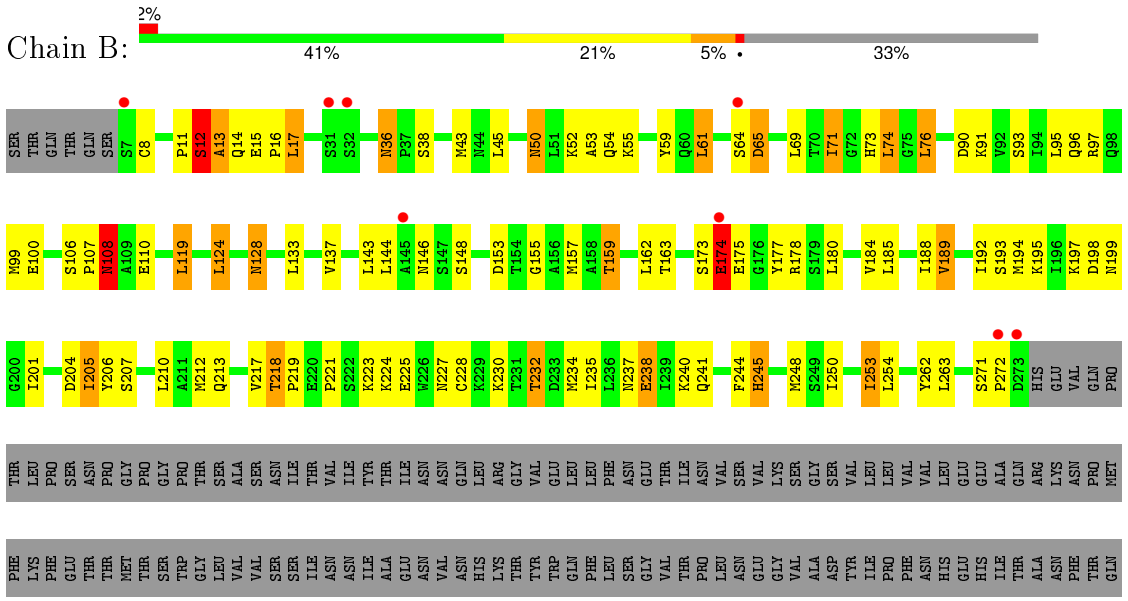
- Molecule 1: Gastric intrinsic factor

Chain A:



- Molecule 1: Gastric intrinsic factor

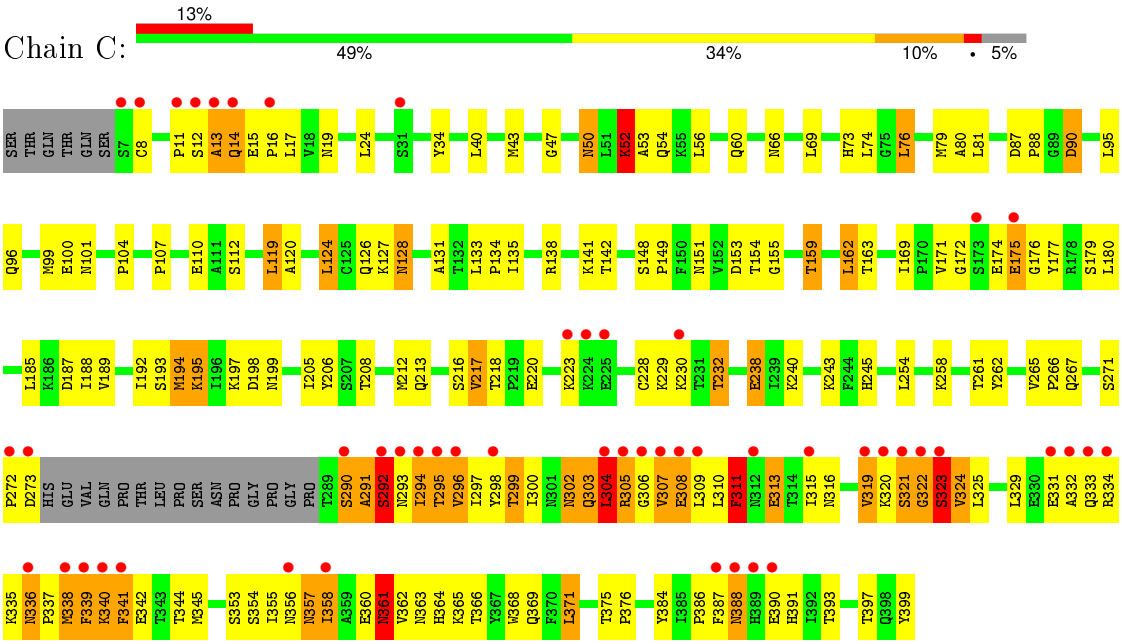
Chain B:



TYR

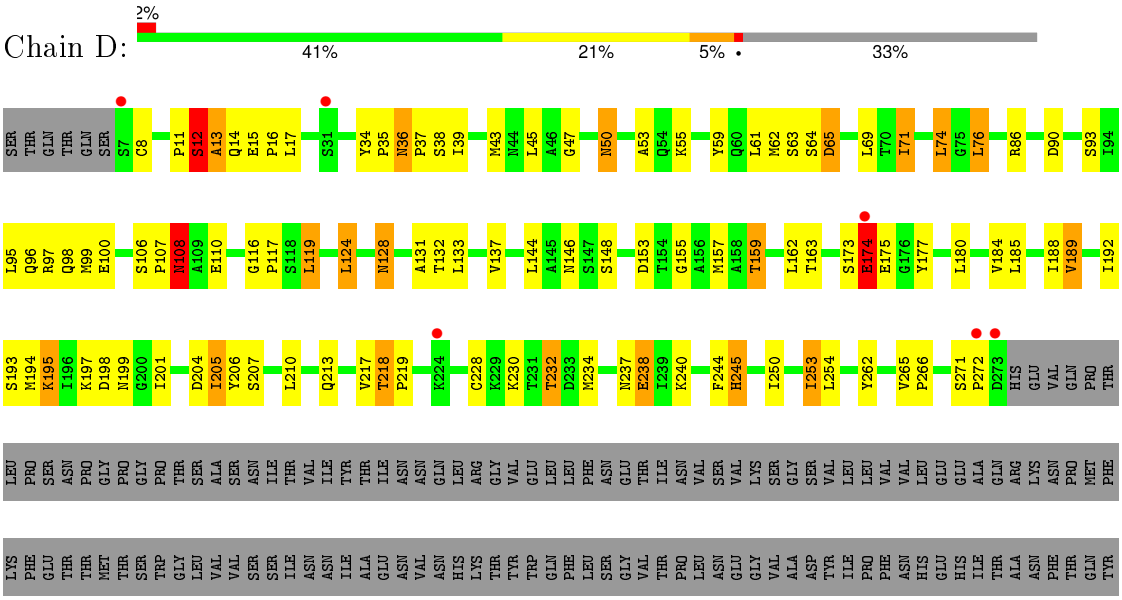
- Molecule 1: Gastric intrinsic factor

Chain C:



- Molecule 1: Gastric intrinsic factor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.10Å 67.30Å 147.70Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	37.53 – 2.60 37.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.4 (37.53-2.60) 88.6 (37.53-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.249 0.213 , 0.250	Depositor DCC
R_{free} test set	1564 reflections (3.17%)	DCC
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 55706 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10457	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: B12, 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	0.63	2/2925 (0.1%)	0.97	13/3978 (0.3%)
1	B	0.56	0/2044	0.76	1/2775 (0.0%)
1	C	0.64	5/2925 (0.2%)	0.94	12/3978 (0.3%)
1	D	0.55	0/2044	0.76	2/2775 (0.1%)
All	All	0.60	7/9938 (0.1%)	0.88	28/13506 (0.2%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	GLU	CB-CG	-8.85	1.35	1.52
1	C	52	LYS	CB-CG	-8.64	1.29	1.52
1	A	308	GLU	CD-OE1	-6.67	1.18	1.25
1	C	308	GLU	CD-OE1	-6.52	1.18	1.25
1	C	52	LYS	CG-CD	-6.31	1.30	1.52
1	C	52	LYS	CA-CB	-5.60	1.41	1.53
1	C	175	GLU	CD-OE2	5.06	1.31	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	GLU	N-CA-CB	-13.05	87.12	110.60
1	C	52	LYS	CD-CE-NZ	-12.87	82.11	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	LYS	CD-CE-NZ	-12.63	82.66	111.70
1	A	321	SER	N-CA-C	-11.86	78.97	111.00
1	C	304	LEU	N-CA-C	11.50	142.05	111.00
1	A	304	LEU	N-CA-C	11.24	141.36	111.00
1	C	321	SER	N-CA-C	-10.63	82.29	111.00
1	A	175	GLU	CA-CB-CG	10.16	135.76	113.40
1	A	290	SER	N-CA-C	10.15	138.40	111.00
1	C	290	SER	N-CA-C	10.06	138.17	111.00
1	C	304	LEU	CA-CB-CG	-9.97	92.38	115.30
1	C	322	GLY	N-CA-C	-9.45	89.47	113.10
1	A	304	LEU	CA-CB-CG	-9.21	94.12	115.30
1	A	174	GLU	O-C-N	-8.04	109.84	122.70
1	C	52	LYS	CB-CA-C	-7.32	95.76	110.40
1	C	52	LYS	CB-CG-CD	-6.88	93.70	111.60
1	A	304	LEU	CB-CG-CD1	-6.26	100.36	111.00
1	A	322	GLY	N-CA-C	-5.97	98.16	113.10
1	A	175	GLU	CB-CG-CD	-5.79	98.56	114.20
1	C	175	GLU	CA-C-N	5.56	127.32	116.20
1	C	47	GLY	N-CA-C	-5.52	99.31	113.10
1	A	203	GLY	N-CA-C	-5.22	100.05	113.10
1	C	175	GLU	CA-CB-CG	5.19	124.82	113.40
1	B	174	GLU	CA-CB-CG	-5.18	102.00	113.40
1	C	195	LYS	N-CA-C	-5.07	97.33	111.00
1	D	195	LYS	N-CA-C	-5.05	97.37	111.00
1	A	308	GLU	OE1-CD-OE2	-5.03	117.27	123.30
1	D	47	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLU	Mainchain

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	2871	0	2861	214	1
1	B	2009	0	2043	99	0
1	C	2871	0	2861	223	1
1	D	2009	0	2043	84	0
2	A	28	0	25	1	0
2	C	28	0	25	2	0
3	A	91	0	87	10	0
3	C	91	0	87	2	0
4	A	135	0	0	8	0
4	B	100	0	0	15	0
4	C	129	0	0	12	0
4	D	95	0	0	8	0
All	All	10457	0	10032	617	1

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 31.

All (617) 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:175:GLU:OE1	1:A:177:TYR:CE1	1.89	1.24
1:C:305:ARG:O	1:C:307:VAL:N	1.80	1.14
1:A:333:GLN:HE21	1:A:340:LYS:HB2	1.09	1.13
1:C:304:LEU:CD1	1:C:305:ARG:HG3	1.77	1.13
1:C:302:ASN:HD22	1:C:303:GLN:N	1.46	1.12
1:C:292:SER:HB2	1:C:319:VAL:HA	1.30	1.10
1:A:305:ARG:O	1:A:307:VAL:N	1.85	1.07
1:A:304:LEU:HD13	1:A:305:ARG:H	1.05	1.06
1:C:333:GLN:HE21	1:C:340:LYS:HB2	1.12	1.06
1:A:292:SER:HB2	1:A:319:VAL:HA	1.33	1.05
1:C:304:LEU:HD13	1:C:305:ARG:N	1.75	0.99
1:C:133:LEU:HD22	1:C:177:TYR:CD2	1.98	0.97
1:C:304:LEU:HD13	1:C:305:ARG:HG3	1.43	0.96
1:A:304:LEU:CD1	1:A:305:ARG:H	1.78	0.96
1:C:292:SER:CB	1:C:319:VAL:HA	1.95	0.95
1:C:302:ASN:HD22	1:C:303:GLN:H	1.10	0.95
1:A:292:SER:CB	1:A:319:VAL:HA	1.95	0.95
1:A:107:PRO:HD3	1:C:107:PRO:HB3	1.48	0.95
1:A:289:THR:O	1:A:289:THR:HG22	1.66	0.95
1:A:299:THR:HG23	1:A:313:GLU:HG3	1.46	0.95
1:A:304:LEU:HD13	1:A:305:ARG:N	1.81	0.94
1:C:299:THR:HG23	1:C:313:GLU:HG3	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:HD13	1:C:305:ARG:H	1.29	0.94
1:C:310:LEU:HD21	1:C:356:ASN:HD22	1.33	0.93
1:A:310:LEU:HD21	1:A:356:ASN:HD22	1.32	0.92
1:D:250:ILE:HA	1:D:253:ILE:HD11	1.50	0.91
1:C:304:LEU:CD1	1:C:305:ARG:H	1.82	0.91
1:C:304:LEU:H	1:C:309:LEU:CD2	1.83	0.91
1:C:133:LEU:HD22	1:C:177:TYR:HD2	1.32	0.90
1:D:199:ASN:HD21	1:D:201:ILE:HD12	1.38	0.89
1:B:12:SER:HA	1:B:15:GLU:HG3	1.55	0.89
1:C:304:LEU:H	1:C:309:LEU:HD21	1.36	0.88
1:C:14:GLN:HE21	1:C:14:GLN:HA	1.37	0.88
1:D:12:SER:HA	1:D:15:GLU:HG3	1.55	0.87
1:A:310:LEU:HD21	1:A:356:ASN:ND2	1.89	0.87
1:A:370:PHE:H	3:A:1001:B12:H402	1.21	0.86
1:A:333:GLN:NE2	1:A:340:LYS:HB2	1.91	0.86
1:C:175:GLU:OE1	1:C:177:TYR:CE1	2.28	0.86
1:C:310:LEU:HD21	1:C:356:ASN:ND2	1.90	0.86
1:B:199:ASN:HD21	1:B:201:ILE:HD12	1.38	0.86
1:A:107:PRO:CD	1:C:107:PRO:HB3	2.06	0.86
1:B:250:ILE:HA	1:B:253:ILE:HD11	1.55	0.86
1:A:304:LEU:CD1	1:A:305:ARG:HG3	2.07	0.85
1:A:133:LEU:HD13	1:A:177:TYR:HE2	1.41	0.84
1:A:304:LEU:H	1:A:309:LEU:HD21	1.42	0.84
1:A:175:GLU:OE1	1:A:177:TYR:HE1	1.59	0.84
1:A:14:GLN:HE21	1:A:14:GLN:HA	1.42	0.83
1:C:185:LEU:O	1:C:189:VAL:HG23	1.78	0.83
1:A:185:LEU:O	1:A:189:VAL:HG23	1.79	0.82
1:A:133:LEU:HD22	1:A:177:TYR:CD2	2.15	0.82
1:C:333:GLN:NE2	1:C:340:LYS:HB2	1.94	0.82
1:A:133:LEU:HD13	1:A:177:TYR:CE2	2.15	0.82
1:D:155:GLY:O	1:D:159:THR:HG23	1.79	0.82
1:B:155:GLY:O	1:B:159:THR:HG23	1.81	0.81
1:A:304:LEU:H	1:A:309:LEU:CD2	1.93	0.81
3:A:1001:B12:H8	3:A:1001:B12:H401	1.46	0.81
1:C:290:SER:OG	1:C:291:ALA:N	2.14	0.80
1:C:340:LYS:NZ	1:C:357:ASN:HD22	1.79	0.80
1:C:304:LEU:CD1	1:C:305:ARG:CG	2.58	0.80
1:A:299:THR:HG23	1:A:313:GLU:CG	2.11	0.80
1:A:322:GLY:O	1:A:323:SER:C	2.19	0.80
1:C:302:ASN:ND2	1:C:303:GLN:N	2.29	0.79
1:A:183:GLN:HG2	1:C:179:SER:OG	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:NZ	1:A:357:ASN:HD22	1.81	0.78
1:C:17:LEU:HD21	1:C:240:LYS:HG2	1.66	0.77
1:A:304:LEU:HD13	1:A:305:ARG:HG3	1.66	0.77
1:A:290:SER:OG	1:A:291:ALA:N	2.17	0.77
1:A:304:LEU:HD13	1:A:305:ARG:CG	2.15	0.77
1:C:299:THR:HG23	1:C:313:GLU:CG	2.13	0.77
1:A:305:ARG:C	1:A:307:VAL:H	1.89	0.76
1:A:151:ASN:ND2	1:A:154:THR:H	1.82	0.76
1:C:336:ASN:C	1:C:338:MET:H	1.89	0.76
1:A:178:ARG:NH1	4:A:1018:HOH:O	2.18	0.76
1:C:303:GLN:O	1:C:304:LEU:HD23	1.86	0.75
1:A:271:SER:N	1:A:272:PRO:HD3	2.01	0.75
1:C:151:ASN:ND2	1:C:154:THR:H	1.85	0.75
1:A:335:LYS:C	1:A:337:PRO:HD3	2.06	0.75
1:C:335:LYS:C	1:C:337:PRO:HD3	2.06	0.75
1:B:193:SER:O	1:B:194:MET:HG2	1.85	0.75
1:B:163:THR:HG21	1:B:217:VAL:HG13	1.67	0.74
1:D:163:THR:HG21	1:D:217:VAL:HG13	1.67	0.74
1:C:360:GLU:O	1:C:366:THR:HG23	1.87	0.74
1:C:336:ASN:O	1:C:338:MET:N	2.21	0.73
1:C:322:GLY:O	1:C:323:SER:C	2.26	0.73
1:A:355:ILE:O	1:A:358:ILE:HG23	1.88	0.73
1:A:50:ASN:HD22	1:A:50:ASN:C	1.90	0.73
1:A:289:THR:O	1:A:289:THR:CG2	2.37	0.73
1:B:50:ASN:C	1:B:50:ASN:HD22	1.91	0.73
1:A:336:ASN:C	1:A:338:MET:H	1.91	0.73
1:C:294:ILE:HD13	1:C:388:ASN:HA	1.71	0.72
1:C:176:GLY:HA2	4:C:1199:HOH:O	1.89	0.72
1:C:304:LEU:HD13	1:C:305:ARG:CG	2.20	0.72
1:A:304:LEU:CD1	1:A:305:ARG:CG	2.67	0.71
1:C:361:ASN:HD21	1:C:363:ASN:HB2	1.55	0.71
1:A:360:GLU:O	1:A:366:THR:HG23	1.90	0.71
1:C:50:ASN:HD21	1:C:52:LYS:HB2	1.55	0.71
1:C:305:ARG:C	1:C:307:VAL:H	1.91	0.71
1:A:340:LYS:HZ1	1:A:357:ASN:HD22	1.37	0.71
1:C:271:SER:N	1:C:272:PRO:HD3	2.06	0.70
1:A:300:ILE:HD13	1:A:339:PHE:HD2	1.56	0.70
1:A:319:VAL:HG22	1:A:323:SER:OG	1.92	0.70
1:C:50:ASN:HD22	1:C:50:ASN:C	1.94	0.70
1:C:332:ALA:HB1	1:C:339:PHE:CZ	2.26	0.70
1:D:36:ASN:HD22	1:D:36:ASN:C	1.96	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:O	1:A:338:MET:N	2.23	0.69
1:D:173:SER:O	1:D:175:GLU:N	2.21	0.69
1:C:175:GLU:OE1	1:C:177:TYR:HE1	1.74	0.69
1:A:332:ALA:HB1	1:A:339:PHE:CZ	2.28	0.69
1:A:304:LEU:HD13	1:A:305:ARG:CB	2.23	0.68
3:A:1001:B12:H362	3:A:1001:B12:H351	1.75	0.68
1:A:304:LEU:HD11	1:A:305:ARG:HG3	1.76	0.68
1:C:175:GLU:CD	1:C:177:TYR:HE1	1.96	0.68
1:D:193:SER:O	1:D:194:MET:HG2	1.94	0.68
1:A:133:LEU:HD22	1:A:177:TYR:HD2	1.56	0.68
1:D:155:GLY:O	1:D:159:THR:CG2	2.42	0.68
1:B:36:ASN:C	1:B:36:ASN:HD22	1.97	0.67
1:A:294:ILE:HD13	1:A:388:ASN:HA	1.76	0.67
1:C:245:HIS:HB3	4:C:1186:HOH:O	1.94	0.67
1:A:213:GLN:HE21	1:A:261:THR:HB	1.60	0.67
1:B:144:LEU:HD13	1:B:184:VAL:HG22	1.76	0.67
1:C:340:LYS:HZ1	1:C:357:ASN:HD22	1.40	0.67
1:A:50:ASN:ND2	1:A:53:ALA:H	1.92	0.67
3:C:1002:B12:H351	3:C:1002:B12:H362	1.77	0.67
1:C:303:GLN:O	1:C:304:LEU:CG	2.43	0.66
1:D:17:LEU:HD21	1:D:240:LYS:HG3	1.76	0.66
1:A:107:PRO:HD3	1:C:107:PRO:CB	2.22	0.66
1:C:193:SER:O	1:C:194:MET:HG2	1.96	0.65
1:B:146:ASN:HD21	1:B:148:SER:HB3	1.61	0.65
1:C:355:ILE:O	1:C:358:ILE:HG23	1.96	0.65
1:B:244:PHE:CE2	1:B:253:ILE:HG12	2.32	0.65
1:A:213:GLN:NE2	1:A:262:TYR:H	1.95	0.65
1:A:361:ASN:HD21	1:A:363:ASN:HB2	1.62	0.65
1:B:93:SER:O	1:B:97:ARG:HG3	1.97	0.65
1:C:128:ASN:HD22	1:C:128:ASN:C	2.00	0.64
1:C:155:GLY:O	1:C:159:THR:CG2	2.45	0.64
1:A:193:SER:O	1:A:194:MET:HG2	1.98	0.64
1:B:173:SER:O	1:B:175:GLU:N	2.28	0.64
1:A:303:GLN:O	1:A:304:LEU:HD23	1.98	0.63
1:C:299:THR:HB	1:C:393:THR:HG23	1.80	0.63
1:D:250:ILE:HA	1:D:253:ILE:CD1	2.28	0.63
1:A:299:THR:HG23	1:A:313:GLU:CD	2.19	0.63
1:D:76:LEU:HD13	1:D:119:LEU:HG	1.80	0.63
1:C:213:GLN:HE22	1:C:262:TYR:H	1.45	0.63
1:A:17:LEU:HD21	1:A:240:LYS:HG2	1.80	0.63
1:C:300:ILE:HD13	1:C:339:PHE:HD2	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:HG23	1:C:313:GLU:CD	2.19	0.63
1:D:144:LEU:HB3	4:D:422:HOH:O	1.98	0.63
1:A:216:SER:HB3	4:A:1109:HOH:O	1.99	0.63
1:C:155:GLY:O	1:C:159:THR:HG22	1.98	0.63
1:D:50:ASN:HD22	1:D:50:ASN:C	2.02	0.63
1:D:144:LEU:HD13	1:D:184:VAL:HG22	1.81	0.63
1:C:303:GLN:O	1:C:304:LEU:CD2	2.47	0.62
1:A:319:VAL:HG22	1:A:323:SER:CB	2.29	0.62
1:C:17:LEU:HD21	1:C:240:LYS:CG	2.29	0.62
1:C:228:CYS:O	1:C:232:THR:HG22	1.99	0.62
1:B:245:HIS:HB2	4:B:484:HOH:O	1.99	0.62
1:C:319:VAL:HG22	1:C:323:SER:OG	1.98	0.62
1:C:295:THR:HA	1:C:316:ASN:O	2.00	0.62
1:A:69:LEU:HD22	1:A:73:HIS:HB3	1.80	0.62
1:C:294:ILE:CD1	1:C:388:ASN:HA	2.30	0.62
1:A:213:GLN:HE22	1:A:262:TYR:H	1.46	0.62
1:B:228:CYS:O	1:B:232:THR:HG22	2.00	0.62
1:C:76:LEU:HD13	1:C:119:LEU:HG	1.81	0.62
1:C:310:LEU:O	1:C:311:PHE:HB2	2.00	0.61
1:C:308:GLU:O	1:C:308:GLU:HG3	2.00	0.61
1:C:365:LYS:HG3	1:C:399:TYR:CE1	2.35	0.61
1:C:213:GLN:NE2	1:C:262:TYR:H	1.99	0.61
1:A:310:LEU:O	1:A:311:PHE:HB2	2.00	0.61
1:A:365:LYS:HG3	1:A:399:TYR:CE1	2.35	0.61
1:A:163:THR:HG21	1:A:217:VAL:HG13	1.81	0.61
1:C:304:LEU:HD11	1:C:305:ARG:HG3	1.76	0.61
1:C:358:ILE:O	1:C:358:ILE:HG12	2.00	0.61
1:C:151:ASN:HD22	1:C:154:THR:H	1.47	0.60
1:C:213:GLN:HE21	1:C:261:THR:HB	1.65	0.60
1:A:304:LEU:HD11	1:A:305:ARG:HD2	1.82	0.60
1:B:163:THR:HG21	1:B:217:VAL:CG1	2.31	0.60
1:C:361:ASN:ND2	1:C:363:ASN:H	1.99	0.60
1:B:205:ILE:HG13	1:B:206:TYR:CE2	2.36	0.60
1:D:163:THR:HG21	1:D:217:VAL:CG1	2.31	0.60
1:C:172:GLY:N	1:C:174:GLU:OE1	2.34	0.60
1:C:336:ASN:N	1:C:337:PRO:HD3	2.16	0.60
1:A:17:LEU:HD21	1:A:240:LYS:CG	2.31	0.60
1:A:128:ASN:C	1:A:128:ASN:HD22	2.04	0.60
1:A:238:GLU:HG3	1:A:243:LYS:HG3	1.81	0.60
1:D:228:CYS:O	1:D:232:THR:HG22	2.02	0.59
1:D:106:SER:OG	1:D:107:PRO:HD2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:HE3	4:C:1142:HOH:O	2.02	0.59
1:A:303:GLN:O	1:A:304:LEU:CG	2.50	0.59
1:C:199:ASN:O	1:C:230:LYS:HE3	2.03	0.59
1:D:110:GLU:OE1	1:D:110:GLU:N	2.34	0.59
1:B:174:GLU:HB3	4:B:474:HOH:O	2.02	0.59
1:A:341:PHE:HB2	1:A:354:SER:O	2.03	0.59
1:A:50:ASN:C	1:A:50:ASN:ND2	2.57	0.58
1:D:119:LEU:HD13	1:D:157:MET:SD	2.43	0.58
1:D:8:CYS:HB2	1:D:232:THR:HG21	1.84	0.58
1:D:93:SER:O	1:D:97:ARG:HG3	2.03	0.58
1:A:175:GLU:OE1	1:A:177:TYR:CD1	2.53	0.58
1:B:8:CYS:HB2	1:B:232:THR:HG21	1.85	0.58
1:C:303:GLN:O	1:C:304:LEU:HG	2.04	0.58
1:A:370:PHE:N	3:A:1001:B12:H402	1.97	0.58
1:B:250:ILE:HA	1:B:253:ILE:CD1	2.28	0.58
1:B:159:THR:HG22	1:B:188:ILE:HG21	1.84	0.58
1:C:197:LYS:HE3	4:C:1121:HOH:O	2.03	0.58
1:D:137:VAL:HG21	1:D:177:TYR:CE1	2.39	0.58
1:C:305:ARG:HH12	1:C:364:HIS:CG	2.22	0.58
1:C:340:LYS:NZ	1:C:357:ASN:ND2	2.51	0.58
1:C:299:THR:OG1	1:C:391:HIS:NE2	2.35	0.58
1:D:205:ILE:HG13	1:D:206:TYR:CE2	2.37	0.58
1:D:146:ASN:HD21	1:D:148:SER:HB3	1.69	0.58
1:A:340:LYS:NZ	1:A:357:ASN:ND2	2.52	0.58
1:A:208:THR:O	1:A:212:MET:HG3	2.03	0.58
1:B:76:LEU:HD13	1:B:119:LEU:HG	1.85	0.57
1:C:138:ARG:HD2	4:C:1107:HOH:O	2.03	0.57
1:A:299:THR:CG2	1:A:313:GLU:CD	2.73	0.57
1:A:295:THR:HA	1:A:316:ASN:O	2.04	0.57
1:A:294:ILE:CD1	1:A:388:ASN:HA	2.34	0.57
1:C:336:ASN:C	1:C:338:MET:N	2.57	0.57
1:A:358:ILE:O	1:A:358:ILE:HG12	2.03	0.57
1:A:361:ASN:ND2	1:A:363:ASN:H	2.02	0.57
1:C:305:ARG:HH12	1:C:364:HIS:HB3	1.68	0.57
1:A:76:LEU:HD13	1:A:119:LEU:HG	1.86	0.57
1:A:336:ASN:N	1:A:337:PRO:HD3	2.19	0.57
1:B:64:SER:O	1:B:65:ASP:C	2.43	0.57
1:A:300:ILE:HD13	1:A:339:PHE:CD2	2.39	0.56
1:B:184:VAL:O	1:B:188:ILE:HG13	2.05	0.56
1:C:95:LEU:HD23	1:C:124:LEU:HD13	1.87	0.56
1:A:171:VAL:HG11	1:B:54:GLN:HG2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:CD1	1:C:305:ARG:N	2.50	0.56
1:A:170:PRO:HB2	1:A:173:SER:HB3	1.88	0.56
1:C:50:ASN:ND2	1:C:50:ASN:C	2.58	0.56
1:B:224:LYS:HE2	4:B:475:HOH:O	2.06	0.56
1:D:244:PHE:CE2	1:D:253:ILE:HG12	2.40	0.56
1:C:238:GLU:HG3	1:C:243:LYS:HG3	1.86	0.56
1:D:128:ASN:ND2	1:D:131:ALA:H	2.03	0.56
1:A:155:GLY:O	1:A:159:THR:CG2	2.54	0.56
1:C:341:PHE:HB2	1:C:354:SER:O	2.06	0.56
1:B:17:LEU:HD21	1:B:240:LYS:HG3	1.87	0.55
1:D:184:VAL:O	1:D:188:ILE:HG13	2.06	0.55
1:C:50:ASN:ND2	1:C:53:ALA:H	2.04	0.55
1:D:128:ASN:C	1:D:128:ASN:HD22	2.08	0.55
1:C:110:GLU:OE1	1:C:110:GLU:N	2.39	0.55
1:C:69:LEU:HD22	1:C:73:HIS:HB3	1.87	0.55
1:A:189:VAL:HG22	1:A:218:THR:HG21	1.89	0.55
1:D:106:SER:OG	1:D:107:PRO:CD	2.54	0.55
1:B:14:GLN:O	1:B:17:LEU:HB2	2.06	0.55
1:A:228:CYS:O	1:A:232:THR:HG22	2.06	0.55
1:A:303:GLN:O	1:A:304:LEU:HG	2.06	0.55
1:B:137:VAL:HG21	1:B:177:TYR:CE1	2.42	0.55
1:A:265:VAL:HB	1:A:266:PRO:HD3	1.88	0.55
1:B:91:LYS:HE2	4:B:426:HOH:O	2.06	0.55
1:C:163:THR:HG21	1:C:217:VAL:HG13	1.88	0.55
1:C:302:ASN:ND2	1:C:303:GLN:H	1.92	0.55
1:A:172:GLY:N	1:A:174:GLU:OE1	2.39	0.55
1:C:19:ASN:HA	4:C:1106:HOH:O	2.05	0.55
1:C:319:VAL:HG22	1:C:323:SER:CB	2.37	0.54
1:C:342:GLU:HB2	1:C:354:SER:HB3	1.90	0.54
1:A:199:ASN:O	1:A:230:LYS:HE3	2.08	0.54
1:A:386:PRO:HA	4:A:1103:HOH:O	2.07	0.54
1:B:155:GLY:O	1:B:159:THR:CG2	2.54	0.54
1:A:336:ASN:C	1:A:338:MET:N	2.59	0.54
1:C:371:LEU:HD23	1:C:371:LEU:N	2.22	0.54
1:A:175:GLU:HB2	1:C:223:LYS:NZ	2.22	0.54
1:C:305:ARG:NH1	1:C:364:HIS:HB3	2.22	0.54
1:A:307:VAL:O	1:A:308:GLU:HB3	2.08	0.54
1:B:238:GLU:HA	1:B:238:GLU:OE1	2.06	0.54
1:B:71:ILE:CD1	1:B:99:MET:SD	2.96	0.54
1:D:95:LEU:HD23	1:D:124:LEU:HD13	1.89	0.54
1:A:310:LEU:CD2	1:A:356:ASN:HD22	2.14	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:O	1:A:366:THR:CG2	2.55	0.53
1:C:300:ILE:HD13	1:C:339:PHE:CD2	2.43	0.53
1:C:310:LEU:CD2	1:C:356:ASN:HD22	2.14	0.53
1:A:303:GLN:O	1:A:304:LEU:CD2	2.57	0.53
1:C:310:LEU:CD2	1:C:356:ASN:ND2	2.70	0.53
1:C:174:GLU:HG3	4:D:441:HOH:O	2.09	0.53
1:A:79:MET:HG2	1:A:126:GLN:HE22	1.73	0.53
1:D:272:PRO:HD2	4:D:463:HOH:O	2.06	0.53
1:D:64:SER:O	1:D:65:ASP:C	2.46	0.53
1:C:220:GLU:HB2	4:C:1213:HOH:O	2.08	0.53
1:C:304:LEU:H	1:C:309:LEU:HD22	1.68	0.53
1:B:241:GLN:HG3	4:B:413:HOH:O	2.07	0.53
1:C:302:ASN:O	1:C:303:GLN:HG3	2.09	0.53
1:C:133:LEU:HD22	1:C:177:TYR:CE2	2.41	0.53
1:C:265:VAL:HB	1:C:266:PRO:HD3	1.90	0.53
1:A:133:LEU:CD2	1:A:177:TYR:HD2	2.22	0.53
1:C:40:LEU:HD23	1:C:80:ALA:HB1	1.91	0.53
1:B:71:ILE:HD11	1:B:99:MET:SD	2.49	0.52
1:C:315:ILE:O	1:C:335:LYS:NZ	2.42	0.52
1:C:171:VAL:O	1:D:86:ARG:NH2	2.35	0.52
1:B:106:SER:OG	1:B:107:PRO:HD2	2.09	0.52
1:A:299:THR:HB	1:A:393:THR:HG23	1.90	0.52
1:A:151:ASN:HD22	1:A:154:THR:H	1.54	0.52
1:C:258:LYS:NZ	4:C:1106:HOH:O	2.40	0.52
1:B:218:THR:HG22	1:B:219:PRO:HD2	1.91	0.52
1:A:319:VAL:HG22	1:A:323:SER:HB2	1.91	0.52
1:B:245:HIS:CB	4:B:484:HOH:O	2.57	0.52
1:C:34:TYR:HA	4:C:1111:HOH:O	2.10	0.52
1:A:95:LEU:HD23	1:A:124:LEU:HD13	1.91	0.52
1:C:205:ILE:HD12	1:C:206:TYR:CZ	2.45	0.52
1:C:304:LEU:N	1:C:309:LEU:CD2	2.64	0.52
1:C:340:LYS:HZ3	1:C:357:ASN:HD22	1.55	0.52
1:C:332:ALA:HB1	1:C:339:PHE:HZ	1.70	0.52
1:A:371:LEU:N	1:A:371:LEU:HD23	2.25	0.52
1:C:208:THR:O	1:C:212:MET:HG3	2.10	0.52
1:A:304:LEU:N	1:A:309:LEU:CD2	2.69	0.51
1:B:199:ASN:O	1:B:234:MET:HG2	2.10	0.51
1:B:50:ASN:C	1:B:50:ASN:ND2	2.62	0.51
1:A:66:ASN:ND2	1:A:90:ASP:OD2	2.42	0.51
1:A:304:LEU:CD1	1:A:305:ARG:HD2	2.39	0.51
1:C:299:THR:CG2	1:C:313:GLU:CD	2.77	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:HB2	1:A:267:GLN:NE2	2.26	0.51
1:A:304:LEU:HD11	1:A:305:ARG:CG	2.39	0.51
1:C:361:ASN:C	1:C:361:ASN:HD22	2.14	0.51
1:C:133:LEU:HD13	1:C:177:TYR:CE2	2.46	0.51
1:A:299:THR:OG1	1:A:391:HIS:NE2	2.41	0.51
1:A:334:ARG:C	1:A:336:ASN:N	2.63	0.51
1:B:106:SER:OG	1:B:107:PRO:CD	2.59	0.51
1:A:340:LYS:HZ1	1:A:357:ASN:ND2	2.08	0.51
1:A:355:ILE:HB	1:A:368:TRP:CZ2	2.46	0.51
1:A:311:PHE:CZ	4:A:1094:HOH:O	2.55	0.51
1:C:337:PRO:C	1:C:339:PHE:H	2.14	0.50
1:A:339:PHE:CG	1:A:339:PHE:O	2.64	0.50
1:B:36:ASN:ND2	1:B:38:SER:H	2.09	0.50
1:D:14:GLN:O	1:D:17:LEU:HB2	2.10	0.50
1:A:96:GLN:O	1:A:100:GLU:HG3	2.10	0.50
1:A:183:GLN:CG	1:C:179:SER:OG	2.56	0.50
1:A:151:ASN:HD22	1:A:154:THR:CB	2.24	0.50
1:C:334:ARG:C	1:C:336:ASN:N	2.65	0.50
1:C:14:GLN:NE2	1:C:14:GLN:HA	2.18	0.50
1:C:50:ASN:ND2	1:C:52:LYS:H	2.09	0.50
1:D:237:ASN:HA	1:D:240:LYS:HE3	1.94	0.50
1:C:8:CYS:HB2	1:C:232:THR:HG21	1.94	0.50
1:A:297:ILE:HD12	1:A:391:HIS:HB2	1.94	0.50
1:A:334:ARG:C	1:A:336:ASN:H	2.15	0.50
1:C:298:TYR:CZ	1:C:329:LEU:HD22	2.47	0.50
1:A:304:LEU:HD13	1:A:305:ARG:CA	2.42	0.50
1:D:157:MET:CE	1:D:210:LEU:HD13	2.42	0.50
1:A:390:GLU:CB	4:A:1103:HOH:O	2.59	0.50
1:C:344:THR:HG22	1:C:353:SER:HB3	1.93	0.50
1:C:296:VAL:HG12	1:C:390:GLU:O	2.12	0.50
1:C:290:SER:OG	1:C:331:GLU:OE2	2.23	0.50
1:A:110:GLU:N	1:A:110:GLU:OE1	2.44	0.50
1:C:339:PHE:O	1:C:339:PHE:CG	2.65	0.49
1:C:304:LEU:HD12	1:C:305:ARG:HD2	1.94	0.49
1:C:199:ASN:C	1:C:230:LYS:HE3	2.32	0.49
1:A:337:PRO:C	1:A:339:PHE:H	2.15	0.49
1:A:296:VAL:HG12	1:A:390:GLU:O	2.13	0.49
1:A:298:TYR:CZ	1:A:329:LEU:HD22	2.47	0.49
1:C:302:ASN:C	1:C:302:ASN:HD22	2.04	0.49
1:C:189:VAL:HG22	1:C:218:THR:HG21	1.94	0.49
1:C:355:ILE:HB	1:C:368:TRP:CZ2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1074:HOH:O	1:C:141:LYS:HE2	2.12	0.49
1:A:305:ARG:HH12	1:A:364:HIS:CG	2.30	0.49
1:A:310:LEU:CD2	1:A:356:ASN:ND2	2.71	0.49
1:C:399:TYR:CD2	3:C:1002:B12:H461	2.47	0.49
1:A:304:LEU:H	1:A:309:LEU:HD22	1.75	0.49
1:A:315:ILE:O	1:A:335:LYS:NZ	2.45	0.49
1:C:66:ASN:ND2	1:C:90:ASP:OD2	2.45	0.49
1:C:325:LEU:O	1:C:325:LEU:HD13	2.12	0.49
1:B:95:LEU:HD23	1:B:124:LEU:HD13	1.94	0.49
1:D:90:ASP:HB2	4:D:420:HOH:O	2.12	0.49
1:B:12:SER:HA	1:B:15:GLU:CG	2.35	0.49
1:D:96:GLN:O	1:D:100:GLU:HG3	2.13	0.49
1:A:344:THR:HG22	1:A:353:SER:HB3	1.93	0.49
1:A:340:LYS:HZ3	1:A:357:ASN:HD22	1.61	0.48
1:A:305:ARG:HH12	1:A:364:HIS:HB3	1.77	0.48
1:B:50:ASN:ND2	1:B:53:ALA:H	2.11	0.48
1:A:189:VAL:CG2	1:A:218:THR:HG21	2.43	0.48
1:C:335:LYS:HB2	1:C:337:PRO:HD3	1.95	0.48
1:A:332:ALA:HB1	1:A:339:PHE:HZ	1.74	0.48
1:D:238:GLU:HA	1:D:238:GLU:OE1	2.13	0.48
1:B:119:LEU:HD13	1:B:157:MET:SD	2.54	0.48
1:C:304:LEU:HD13	1:C:305:ARG:CA	2.41	0.48
1:A:213:GLN:NE2	1:A:261:THR:HB	2.28	0.48
1:A:342:GLU:HB2	1:A:354:SER:HB3	1.95	0.48
1:A:175:GLU:HG3	1:C:223:LYS:CG	2.44	0.48
1:A:322:GLY:O	1:A:324:VAL:N	2.47	0.48
1:D:250:ILE:O	1:D:253:ILE:HD12	2.13	0.48
1:D:12:SER:HA	1:D:15:GLU:CG	2.37	0.48
1:A:361:ASN:C	1:A:361:ASN:HD22	2.16	0.48
1:C:155:GLY:O	1:C:159:THR:HG23	2.14	0.48
1:A:159:THR:HG22	1:A:188:ILE:HG21	1.95	0.48
1:D:159:THR:HG22	1:D:188:ILE:HG21	1.95	0.48
1:C:294:ILE:HD13	1:C:388:ASN:CA	2.44	0.48
1:A:133:LEU:HD22	1:A:177:TYR:CE2	2.49	0.47
1:A:302:ASN:HD22	1:A:309:LEU:HA	1.79	0.47
1:D:36:ASN:ND2	1:D:38:SER:H	2.11	0.47
1:B:205:ILE:HG13	1:B:206:TYR:CD2	2.49	0.47
1:B:157:MET:HE2	1:B:210:LEU:HD13	1.96	0.47
1:C:198:ASP:O	1:C:230:LYS:HE2	2.14	0.47
1:A:40:LEU:HD23	1:A:80:ALA:HB1	1.95	0.47
1:D:55:LYS:HE3	1:D:59:TYR:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLY:O	1:A:159:THR:HG22	2.14	0.47
1:D:218:THR:HG22	1:D:219:PRO:HD2	1.96	0.47
1:B:52:LYS:HG2	4:B:430:HOH:O	2.14	0.47
1:C:56:LEU:O	1:C:60:GLN:HG3	2.15	0.47
1:C:185:LEU:HD22	1:C:218:THR:HG22	1.96	0.47
1:A:271:SER:H	1:A:272:PRO:HD3	1.79	0.47
1:B:213:GLN:NE2	1:B:262:TYR:H	2.11	0.47
1:A:302:ASN:O	1:A:303:GLN:HG3	2.14	0.47
1:A:322:GLY:H	1:A:385:ILE:HG23	1.80	0.47
3:A:1001:B12:H8	3:A:1001:B12:N40	2.18	0.47
1:A:50:ASN:ND2	1:A:52:LYS:H	2.13	0.47
1:D:205:ILE:HG21	1:D:238:GLU:HG2	1.96	0.47
1:A:199:ASN:C	1:A:230:LYS:HE3	2.35	0.47
1:B:237:ASN:HA	1:B:240:LYS:HE3	1.97	0.47
1:C:322:GLY:O	1:C:324:VAL:N	2.47	0.47
1:A:155:GLY:O	1:A:159:THR:HG23	2.14	0.47
1:A:194:MET:HG3	1:A:194:MET:O	2.15	0.47
1:C:172:GLY:O	1:C:174:GLU:HG2	2.15	0.47
1:C:361:ASN:ND2	1:C:363:ASN:HB2	2.27	0.46
1:B:157:MET:CE	1:B:210:LEU:HD13	2.45	0.46
1:C:308:GLU:CG	1:C:308:GLU:O	2.61	0.46
1:D:194:MET:HG3	1:D:194:MET:O	2.14	0.46
1:A:304:LEU:CD1	1:A:305:ARG:CD	2.94	0.46
1:C:128:ASN:ND2	1:C:131:ALA:H	2.13	0.46
1:A:220:GLU:OE1	1:A:221:PRO:HD2	2.15	0.46
1:A:175:GLU:HG3	1:C:223:LYS:HG3	1.98	0.46
1:C:305:ARG:HH12	1:C:364:HIS:CB	2.26	0.46
1:B:36:ASN:HD21	1:B:38:SER:HB2	1.81	0.46
1:D:192:ILE:O	1:D:195:LYS:HB2	2.16	0.46
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.16	0.46
1:A:335:LYS:HB2	1:A:337:PRO:HD3	1.97	0.46
1:D:36:ASN:ND2	1:D:36:ASN:C	2.66	0.46
1:C:79:MET:HG2	1:C:126:GLN:HE22	1.81	0.46
1:A:297:ILE:HG13	1:A:297:ILE:H	1.48	0.46
1:D:144:LEU:HA	1:D:144:LEU:HD12	1.80	0.46
1:C:151:ASN:HD22	1:C:154:THR:CB	2.28	0.46
1:C:192:ILE:O	1:C:195:LYS:HB2	2.15	0.46
1:B:198:ASP:O	1:B:230:LYS:HE3	2.15	0.46
2:C:901:NAG:H83	4:C:1216:HOH:O	2.15	0.46
1:D:71:ILE:CD1	1:D:99:MET:SD	3.04	0.46
1:A:304:LEU:HD11	1:A:305:ARG:CD	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLN:NE2	1:C:261:THR:HB	2.29	0.46
2:C:901:NAG:H61	2:C:902:NAG:HN2	1.81	0.46
1:B:192:ILE:O	1:B:195:LYS:HB2	2.16	0.46
1:B:144:LEU:HA	1:B:144:LEU:HD12	1.82	0.45
1:B:205:ILE:H	1:B:205:ILE:HG12	1.57	0.45
1:C:266:PRO:HB2	1:C:267:GLN:NE2	2.31	0.45
1:C:334:ARG:C	1:C:336:ASN:H	2.19	0.45
1:B:205:ILE:HG21	1:B:238:GLU:HG2	1.98	0.45
1:B:110:GLU:N	1:B:110:GLU:OE1	2.44	0.45
1:D:15:GLU:N	1:D:16:PRO:CD	2.79	0.45
1:D:98:GLN:HG2	4:D:411:HOH:O	2.17	0.45
1:A:162:LEU:HA	1:A:162:LEU:HD12	1.81	0.45
1:D:62:MET:O	1:D:63:SER:CB	2.63	0.45
1:D:153:ASP:OD1	1:D:207:SER:HB2	2.16	0.45
1:D:71:ILE:HD11	1:D:99:MET:SD	2.57	0.45
1:A:192:ILE:O	1:A:195:LYS:HB2	2.16	0.45
1:C:313:GLU:OE1	1:C:313:GLU:N	2.49	0.45
1:A:56:LEU:O	1:A:60:GLN:HG3	2.16	0.45
1:A:141:LYS:NZ	1:C:187:ASP:OD1	2.30	0.45
1:C:159:THR:HG22	1:C:188:ILE:HG21	1.99	0.45
1:C:95:LEU:HD11	1:C:120:ALA:HB1	1.98	0.45
1:C:11:PRO:O	1:C:13:ALA:N	2.49	0.45
1:B:204:ASP:OD1	1:B:204:ASP:C	2.55	0.45
1:B:193:SER:O	1:B:194:MET:CG	2.61	0.45
1:B:213:GLN:HE22	1:B:262:TYR:H	1.65	0.45
1:C:104:PRO:HG3	1:C:142:THR:CG2	2.47	0.45
1:A:87:ASP:HA	1:A:88:PRO:HD3	1.79	0.45
1:B:90:ASP:HB2	4:B:466:HOH:O	2.16	0.45
1:A:133:LEU:HB2	1:A:134:PRO:HD3	1.99	0.44
1:D:11:PRO:O	1:D:13:ALA:N	2.50	0.44
1:D:205:ILE:CG2	1:D:238:GLU:HG2	2.47	0.44
1:D:174:GLU:H	1:D:174:GLU:HG2	1.40	0.44
1:B:128:ASN:HD22	1:B:128:ASN:C	2.19	0.44
1:D:39:ILE:O	1:D:43:MET:HG2	2.17	0.44
1:C:336:ASN:N	1:C:337:PRO:CD	2.80	0.44
1:D:106:SER:C	1:D:108:ASN:H	2.21	0.44
1:A:344:THR:CG2	1:A:353:SER:HB3	2.47	0.44
2:A:901:NAG:H61	2:A:902:NAG:HN2	1.82	0.44
1:D:213:GLN:NE2	1:D:262:TYR:H	2.15	0.44
1:C:307:VAL:O	1:C:308:GLU:HB3	2.17	0.44
1:A:305:ARG:NH1	1:A:364:HIS:HB3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:TYR:CE2	3:A:1001:B12:H463	2.52	0.44
1:B:271:SER:N	1:B:272:PRO:HD3	2.32	0.44
1:C:303:GLN:HA	1:C:309:LEU:HD22	1.99	0.44
1:A:305:ARG:C	1:A:307:VAL:N	2.56	0.44
1:C:360:GLU:O	1:C:366:THR:CG2	2.61	0.44
1:C:15:GLU:N	1:C:16:PRO:CD	2.81	0.44
1:A:325:LEU:HD13	1:A:325:LEU:O	2.17	0.44
1:C:172:GLY:C	1:C:174:GLU:HG2	2.38	0.44
1:C:344:THR:CG2	1:C:353:SER:HB3	2.48	0.44
1:C:96:GLN:O	1:C:100:GLU:HG3	2.17	0.44
1:B:55:LYS:HE3	1:B:59:TYR:CZ	2.52	0.44
1:D:204:ASP:OD1	1:D:204:ASP:C	2.56	0.44
1:C:303:GLN:OE1	4:C:1220:HOH:O	2.21	0.44
1:C:333:GLN:HG3	1:C:340:LYS:HB2	2.00	0.44
3:A:1001:B12:H533	3:A:1001:B12:H482	1.99	0.44
1:C:240:LYS:CE	4:C:1142:HOH:O	2.61	0.44
1:C:229:LYS:HA	1:C:232:THR:CG2	2.48	0.44
1:C:148:SER:HB3	1:C:149:PRO:HD2	1.99	0.44
1:C:133:LEU:HB2	1:C:134:PRO:HD3	2.00	0.43
1:A:8:CYS:HB2	1:A:232:THR:HG21	1.99	0.43
1:D:69:LEU:HD12	1:D:74:LEU:HD13	2.00	0.43
1:B:11:PRO:O	1:B:13:ALA:N	2.51	0.43
1:B:69:LEU:HD22	1:B:73:HIS:HB3	2.00	0.43
1:D:205:ILE:HG13	1:D:206:TYR:CD2	2.54	0.43
1:C:335:LYS:CB	1:C:337:PRO:HD3	2.49	0.43
1:C:323:SER:O	1:C:324:VAL:O	2.36	0.43
1:D:36:ASN:HD22	1:D:37:PRO:N	2.15	0.43
1:D:271:SER:N	1:D:272:PRO:HD3	2.32	0.43
1:C:340:LYS:HZ3	1:C:357:ASN:ND2	2.13	0.43
1:D:34:TYR:HA	1:D:35:PRO:HD3	1.88	0.43
1:C:271:SER:H	1:C:272:PRO:HD3	1.81	0.43
1:C:292:SER:O	1:C:293:ASN:OD1	2.36	0.43
1:B:248:MET:HE1	4:B:412:HOH:O	2.18	0.43
1:C:189:VAL:CG2	1:C:218:THR:HG21	2.49	0.43
1:A:229:LYS:HA	1:A:232:THR:CG2	2.48	0.43
1:A:290:SER:O	1:A:291:ALA:O	2.36	0.43
1:B:217:VAL:HG11	1:B:263:LEU:HD11	2.00	0.43
1:C:362:VAL:HG23	1:C:399:TYR:OH	2.19	0.43
1:D:50:ASN:ND2	1:D:53:ALA:H	2.17	0.43
1:A:104:PRO:HG3	1:A:142:THR:CG2	2.49	0.43
1:D:205:ILE:HG12	4:D:477:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:LEU:CD2	1:C:371:LEU:N	2.81	0.43
1:C:43:MET:HE2	1:C:54:GLN:HB2	2.00	0.43
1:D:198:ASP:O	1:D:230:LYS:HE3	2.18	0.43
1:C:87:ASP:HA	1:C:88:PRO:HD3	1.80	0.43
1:B:210:LEU:HB2	4:B:470:HOH:O	2.19	0.42
1:B:106:SER:C	1:B:108:ASN:H	2.21	0.42
1:A:114:PHE:CZ	1:A:142:THR:HG22	2.54	0.42
1:C:319:VAL:HG22	1:C:323:SER:HB2	2.00	0.42
1:C:290:SER:CB	1:C:331:GLU:OE2	2.67	0.42
1:D:124:LEU:HB3	1:D:132:THR:OG1	2.20	0.42
1:C:133:LEU:HB3	1:C:177:TYR:HE2	1.85	0.42
1:B:228:CYS:O	1:B:232:THR:CG2	2.65	0.42
1:A:172:GLY:C	1:A:174:GLU:HG2	2.40	0.42
1:A:304:LEU:CG	1:A:305:ARG:N	2.82	0.42
1:A:128:ASN:C	1:A:128:ASN:ND2	2.72	0.42
1:A:95:LEU:HD23	1:A:124:LEU:CD1	2.49	0.42
1:B:143:LEU:HA	1:B:143:LEU:HD12	1.88	0.42
1:B:225:GLU:HG2	4:B:454:HOH:O	2.18	0.42
1:D:50:ASN:ND2	1:D:50:ASN:C	2.71	0.42
1:B:43:MET:HE2	1:B:54:GLN:HB2	2.01	0.42
1:B:185:LEU:O	1:B:189:VAL:HG22	2.19	0.42
1:C:162:LEU:HA	1:C:162:LEU:HD12	1.85	0.42
1:C:290:SER:O	1:C:291:ALA:O	2.37	0.42
1:A:27:ASN:HB3	4:A:1136:HOH:O	2.18	0.42
1:A:399:TYR:CD2	3:A:1001:B12:H461	2.55	0.42
1:B:36:ASN:ND2	1:B:36:ASN:C	2.68	0.42
1:B:108:ASN:HA	1:B:108:ASN:HD22	1.69	0.42
1:B:221:PRO:HB2	4:B:454:HOH:O	2.20	0.42
1:B:153:ASP:OD1	1:B:207:SER:HB2	2.20	0.42
1:A:99:MET:HB3	1:A:135:ILE:HD13	2.02	0.42
1:B:212:MET:HB3	4:B:442:HOH:O	2.18	0.42
1:D:11:PRO:HG2	1:D:14:GLN:HG2	2.02	0.42
1:B:224:LYS:HB3	4:B:489:HOH:O	2.19	0.42
1:A:298:TYR:CE2	1:A:329:LEU:HD22	2.54	0.42
1:A:195:LYS:HA	1:A:195:LYS:HD3	1.92	0.42
1:D:185:LEU:O	1:D:189:VAL:HG22	2.19	0.42
1:A:313:GLU:N	1:A:313:GLU:OE1	2.53	0.42
1:D:157:MET:HE2	1:D:210:LEU:HD13	2.02	0.42
1:A:114:PHE:CD1	1:A:143:LEU:HD13	2.54	0.42
1:D:116:GLY:N	1:D:117:PRO:CD	2.82	0.42
1:C:333:GLN:HG3	1:C:340:LYS:CB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:CG2	1:B:238:GLU:HG2	2.49	0.41
1:A:266:PRO:HB2	1:A:267:GLN:HE22	1.85	0.41
1:D:228:CYS:O	1:D:232:THR:CG2	2.68	0.41
1:B:43:MET:CE	1:B:54:GLN:HB2	2.50	0.41
1:D:199:ASN:O	1:D:234:MET:HG2	2.20	0.41
1:A:151:ASN:HD21	1:A:153:ASP:HB2	1.85	0.41
1:C:361:ASN:C	1:C:361:ASN:ND2	2.72	0.41
1:C:50:ASN:HD22	1:C:52:LYS:H	1.68	0.41
1:B:212:MET:HE2	4:B:442:HOH:O	2.20	0.41
1:A:175:GLU:HB2	1:C:223:LYS:HZ2	1.84	0.41
1:C:305:ARG:C	1:C:307:VAL:N	2.55	0.41
1:A:292:SER:O	1:A:293:ASN:OD1	2.37	0.41
1:A:362:VAL:HG23	1:A:399:TYR:OH	2.20	0.41
1:A:52:LYS:HE3	1:A:52:LYS:HB2	1.44	0.41
1:B:119:LEU:HD13	1:B:157:MET:HG2	2.03	0.41
1:A:325:LEU:O	1:A:325:LEU:HD22	2.19	0.41
1:A:127:LYS:HA	1:A:127:LYS:HD3	1.79	0.41
1:C:375:THR:HA	1:C:376:PRO:HD3	1.89	0.41
1:A:336:ASN:N	1:A:337:PRO:CD	2.84	0.41
1:B:36:ASN:HD22	1:B:38:SER:H	1.69	0.41
1:A:361:ASN:C	1:A:361:ASN:ND2	2.73	0.41
1:A:95:LEU:HD11	1:A:120:ALA:HB1	2.02	0.41
1:C:127:LYS:HD3	1:C:127:LYS:HA	1.83	0.41
1:A:12:SER:O	1:A:13:ALA:HB2	2.20	0.41
1:A:367:TYR:CD1	1:A:399:TYR:HD2	2.39	0.41
1:A:391:HIS:HB3	4:A:1127:HOH:O	2.20	0.41
1:C:128:ASN:ND2	1:C:128:ASN:C	2.70	0.41
1:C:325:LEU:N	1:C:384:TYR:O	2.50	0.41
1:C:303:GLN:C	1:C:304:LEU:HD23	2.39	0.41
1:C:304:LEU:HB3	1:C:305:ARG:H	1.36	0.41
3:A:1001:B12:C6	3:A:1001:B12:H4B	2.50	0.41
1:B:227:ASN:ND2	1:B:230:LYS:HB2	2.35	0.41
1:C:369:GLN:HE21	1:C:397:THR:HG21	1.86	0.41
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.88	0.41
1:A:324:VAL:HG11	1:A:382:ALA:O	2.21	0.41
1:C:337:PRO:O	1:C:339:PHE:N	2.54	0.41
1:B:173:SER:O	1:B:175:GLU:HG2	2.21	0.41
1:D:213:GLN:HE22	1:D:262:TYR:H	1.69	0.41
1:B:223:LYS:HD3	1:B:223:LYS:O	2.21	0.41
1:B:96:GLN:O	1:B:100:GLU:HG3	2.20	0.41
1:A:303:GLN:HB2	1:A:303:GLN:HE21	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:O	1:A:230:LYS:HE2	2.21	0.41
1:C:325:LEU:HD23	1:C:386:PRO:CG	2.51	0.41
1:B:69:LEU:HD12	1:B:74:LEU:HD13	2.03	0.41
1:C:304:LEU:N	1:C:309:LEU:HD22	2.33	0.40
1:C:169:ILE:HB	4:D:407:HOH:O	2.20	0.40
1:A:81:LEU:HA	1:A:81:LEU:HD23	1.83	0.40
1:B:15:GLU:N	1:B:16:PRO:CD	2.83	0.40
1:D:110:GLU:O	1:D:110:GLU:HG2	2.21	0.40
1:A:371:LEU:HD12	1:A:374:VAL:O	2.21	0.40
1:B:223:LYS:HD3	1:B:223:LYS:C	2.42	0.40
1:A:273:ASP:CG	1:B:178:ARG:HH21	2.25	0.40
1:D:245:HIS:HB2	4:D:465:HOH:O	2.22	0.40
1:D:265:VAL:HB	1:D:266:PRO:HD3	2.03	0.40
1:A:15:GLU:N	1:A:16:PRO:CD	2.85	0.40
3:A:1001:B12:H552	3:A:1001:B12:H531	2.03	0.40
1:C:112:SER:HA	1:C:154:THR:OG1	2.21	0.40
1:B:194:MET:HG3	1:B:194:MET:O	2.21	0.40
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.83	0.40
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.96	0.40
1:A:193:SER:O	1:A:194:MET:CG	2.68	0.40
1:C:99:MET:HB3	1:C:135:ILE:HD13	2.04	0.40

All (1) 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)
1:A:241:GLN:O	1:C:52:LYS:NZ[1_655]	1.87	0.33

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	374/399 (94%)	333 (89%)	24 (6%)	17 (4%)	3 4
1	B	265/399 (66%)	240 (91%)	20 (8%)	5 (2%)	10 19
1	C	374/399 (94%)	334 (89%)	22 (6%)	18 (5%)	3 3
1	D	265/399 (66%)	243 (92%)	17 (6%)	5 (2%)	10 19
All	All	1278/1596 (80%)	1150 (90%)	83 (6%)	45 (4%)	4 6

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ALA
1	A	291	ALA
1	A	306	GLY
1	A	311	PHE
1	A	320	LYS
1	A	321	SER
1	A	324	VAL
1	A	388	ASN
1	B	12	SER
1	B	13	ALA
1	B	108	ASN
1	B	174	GLU
1	C	13	ALA
1	C	291	ALA
1	C	305	ARG
1	C	306	GLY
1	C	311	PHE
1	C	320	LYS
1	C	321	SER
1	C	324	VAL
1	C	388	ASN
1	D	13	ALA
1	D	108	ASN
1	D	174	GLU
1	A	307	VAL
1	A	323	SER
1	A	361	ASN
1	B	65	ASP
1	C	307	VAL
1	C	323	SER
1	D	12	SER
1	D	65	ASP
1	A	292	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	305	ARG
1	A	338	MET
1	C	292	SER
1	C	338	MET
1	C	361	ASN
1	A	90	ASP
1	A	336	ASN
1	C	12	SER
1	C	90	ASP
1	C	336	ASN
1	A	319	VAL
1	C	319	VAL

5.3.2 Protein sidechains (i)

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	322/349 (92%)	281 (87%)	41 (13%)	5 10
1	B	229/349 (66%)	203 (89%)	26 (11%)	7 12
1	C	322/349 (92%)	280 (87%)	42 (13%)	5 9
1	D	229/349 (66%)	203 (89%)	26 (11%)	7 12
All	All	1102/1396 (79%)	967 (88%)	135 (12%)	6 11

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	14	GLN
1	A	24	LEU
1	A	50	ASN
1	A	52	LYS
1	A	74	LEU
1	A	76	LEU
1	A	101	ASN
1	A	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	LEU
1	A	128	ASN
1	A	153	ASP
1	A	159	THR
1	A	162	LEU
1	A	180	LEU
1	A	194	MET
1	A	216	SER
1	A	217	VAL
1	A	218	THR
1	A	232	THR
1	A	238	GLU
1	A	254	LEU
1	A	273	ASP
1	A	292	SER
1	A	294	ILE
1	A	295	THR
1	A	296	VAL
1	A	297	ILE
1	A	299	THR
1	A	303	GLN
1	A	304	LEU
1	A	311	PHE
1	A	323	SER
1	A	339	PHE
1	A	340	LYS
1	A	345	MET
1	A	357	ASN
1	A	358	ILE
1	A	361	ASN
1	A	371	LEU
1	A	387	PHE
1	B	12	SER
1	B	17	LEU
1	B	36	ASN
1	B	45	LEU
1	B	50	ASN
1	B	61	LEU
1	B	71	ILE
1	B	74	LEU
1	B	76	LEU
1	B	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	119	LEU
1	B	124	LEU
1	B	128	ASN
1	B	133	LEU
1	B	159	THR
1	B	162	LEU
1	B	180	LEU
1	B	189	VAL
1	B	197	LYS
1	B	205	ILE
1	B	218	THR
1	B	232	THR
1	B	238	GLU
1	B	245	HIS
1	B	253	ILE
1	B	254	LEU
1	C	14	GLN
1	C	24	LEU
1	C	50	ASN
1	C	52	LYS
1	C	74	LEU
1	C	76	LEU
1	C	101	ASN
1	C	119	LEU
1	C	124	LEU
1	C	128	ASN
1	C	153	ASP
1	C	159	THR
1	C	162	LEU
1	C	180	LEU
1	C	194	MET
1	C	216	SER
1	C	217	VAL
1	C	232	THR
1	C	238	GLU
1	C	254	LEU
1	C	273	ASP
1	C	292	SER
1	C	294	ILE
1	C	295	THR
1	C	296	VAL
1	C	297	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	299	THR
1	C	302	ASN
1	C	303	GLN
1	C	304	LEU
1	C	311	PHE
1	C	313	GLU
1	C	323	SER
1	C	339	PHE
1	C	340	LYS
1	C	341	PHE
1	C	345	MET
1	C	357	ASN
1	C	358	ILE
1	C	361	ASN
1	C	371	LEU
1	C	387	PHE
1	D	12	SER
1	D	36	ASN
1	D	45	LEU
1	D	50	ASN
1	D	61	LEU
1	D	71	ILE
1	D	74	LEU
1	D	76	LEU
1	D	108	ASN
1	D	119	LEU
1	D	124	LEU
1	D	128	ASN
1	D	133	LEU
1	D	159	THR
1	D	162	LEU
1	D	174	GLU
1	D	180	LEU
1	D	189	VAL
1	D	197	LYS
1	D	205	ILE
1	D	218	THR
1	D	232	THR
1	D	238	GLU
1	D	245	HIS
1	D	253	ILE
1	D	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	50	ASN
1	A	54	GLN
1	A	67	ASN
1	A	98	GLN
1	A	126	GLN
1	A	128	ASN
1	A	146	ASN
1	A	151	ASN
1	A	213	GLN
1	A	245	HIS
1	A	267	GLN
1	A	293	ASN
1	A	302	ASN
1	A	303	GLN
1	A	333	GLN
1	A	356	ASN
1	A	357	ASN
1	A	361	ASN
1	A	363	ASN
1	B	27	ASN
1	B	36	ASN
1	B	50	ASN
1	B	54	GLN
1	B	67	ASN
1	B	108	ASN
1	B	126	GLN
1	B	128	ASN
1	B	146	ASN
1	B	151	ASN
1	B	213	GLN
1	B	246	ASN
1	B	267	GLN
1	C	14	GLN
1	C	50	ASN
1	C	54	GLN
1	C	66	ASN
1	C	67	ASN
1	C	98	GLN
1	C	126	GLN
1	C	128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	146	ASN
1	C	151	ASN
1	C	213	GLN
1	C	267	GLN
1	C	302	ASN
1	C	303	GLN
1	C	333	GLN
1	C	356	ASN
1	C	357	ASN
1	C	361	ASN
1	C	363	ASN
1	D	27	ASN
1	D	36	ASN
1	D	50	ASN
1	D	54	GLN
1	D	67	ASN
1	D	108	ASN
1	D	126	GLN
1	D	128	ASN
1	D	146	ASN
1	D	151	ASN
1	D	213	GLN
1	D	246	ASN
1	D	267	GLN

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

4 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	$\#\|Z\| > 2$
2	NAG	A	901	1,2	14,14,15	1.31	2 (14%)	15,19,21	1.96	4 (26%)
2	NAG	A	902	2	14,14,15	1.32	2 (14%)	15,19,21	1.39	2 (13%)
2	NAG	C	901	1,2	14,14,15	1.68	3 (21%)	15,19,21	2.09	4 (26%)
2	NAG	C	902	2	14,14,15	1.15	1 (7%)	15,19,21	1.27	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
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	902	2	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	O5-C5	2.03	1.47	1.43
2	C	901	NAG	C2-N2	2.22	1.50	1.46
2	A	901	NAG	C4-C5	2.31	1.58	1.53
2	C	902	NAG	C4-C5	2.45	1.58	1.53
2	C	901	NAG	C4-C5	2.81	1.59	1.53
2	A	902	NAG	C4-C5	2.83	1.59	1.53
2	A	901	NAG	C1-C2	3.00	1.56	1.52
2	C	901	NAG	C1-C2	3.95	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	901	NAG	O7-C7-C8	-3.63	115.40	122.06
2	A	901	NAG	O7-C7-C8	-3.33	115.96	122.06
2	A	902	NAG	C1-O5-C5	-2.95	108.51	112.25
2	C	901	NAG	C4-C3-C2	-2.88	106.75	111.23
2	A	901	NAG	C4-C3-C2	-2.79	106.89	111.23
2	C	902	NAG	C1-O5-C5	-2.58	108.97	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	NAG	C2-N2-C7	2.59	126.37	123.04
2	C	902	NAG	C2-N2-C7	2.59	126.37	123.04
2	A	901	NAG	C8-C7-N2	3.63	123.05	116.11
2	C	901	NAG	C8-C7-N2	3.72	123.23	116.11
2	A	901	NAG	C2-N2-C7	4.75	129.14	123.04
2	C	901	NAG	C2-N2-C7	5.19	129.71	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0
2	A	902	NAG	1	0
2	C	901	NAG	2	0
2	C	902	NAG	1	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	$\#\|Z\| > 2$
3	B12	A	1001	-	74,101,101	1.70	16 (21%)	111,166,166	1.36	15 (13%)
3	B12	C	1002	-	74,101,101	1.62	10 (13%)	111,166,166	1.34	13 (11%)

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
3	B12	A	1001	-	-	0/51/223/223	0/3/11/11
3	B12	C	1002	-	-	0/51/223/223	0/3/11/11

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	B12	C8B-N1B	-3.36	1.34	1.38
3	C	1002	B12	C2R-C3R	-3.36	1.45	1.53
3	A	1001	B12	C2R-C3R	-3.31	1.45	1.53
3	A	1001	B12	P-O4	-2.08	1.43	1.48
3	A	1001	B12	P-O3	-2.04	1.54	1.59
3	A	1001	B12	C54-C17	2.05	1.58	1.54
3	A	1001	B12	O44-C43	2.20	1.30	1.24
3	C	1002	B12	C8B-C9B	2.25	1.44	1.40
3	A	1001	B12	C8B-C9B	2.44	1.45	1.40
3	C	1002	B12	C54-C17	2.47	1.59	1.54
3	A	1001	B12	C36-C7	2.55	1.59	1.54
3	C	1002	B12	C48-C13	2.61	1.58	1.54
3	A	1001	B12	O58-C57	2.70	1.28	1.23
3	A	1001	B12	C7B-C6B	2.81	1.45	1.37
3	C	1002	B12	C36-C7	2.93	1.59	1.54
3	A	1001	B12	O6R-C4R	2.94	1.51	1.45
3	C	1002	B12	O58-C57	3.00	1.29	1.23
3	C	1002	B12	C7B-C6B	3.06	1.46	1.37
3	A	1001	B12	C48-C13	3.28	1.59	1.54
3	C	1002	B12	C6B-C5B	3.30	1.49	1.41
3	A	1001	B12	C1-C2	3.35	1.67	1.58
3	A	1001	B12	C6B-C5B	3.57	1.50	1.41
3	A	1001	B12	C41-C8	4.74	1.61	1.54
3	C	1002	B12	C30-C3	5.60	1.63	1.54
3	A	1001	B12	C30-C3	5.60	1.63	1.54
3	C	1002	B12	C41-C8	6.15	1.64	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	B12	C37-C7-C8	-3.21	99.32	108.27
3	C	1002	B12	C41-C8-C7	-2.83	106.09	114.16
3	C	1002	B12	C37-C7-C8	-2.71	100.71	108.27
3	C	1002	B12	O58-C57-C56	-2.70	117.33	121.98
3	C	1002	B12	C48-C13-C12	-2.65	109.28	116.53
3	A	1001	B12	C41-C8-C7	-2.61	106.72	114.16
3	A	1001	B12	C3-C4-C5	-2.58	123.17	131.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	B12	C48-C13-C12	-2.58	109.47	116.53
3	A	1001	B12	O58-C57-C56	-2.51	117.66	121.98
3	C	1002	B12	C3-C4-C5	-2.50	123.44	131.88
3	A	1001	B12	C2R-C1R-N1B	-2.49	110.50	114.29
3	C	1002	B12	P-O3-C2P	-2.34	117.85	120.92
3	A	1001	B12	C47-C12-C46	-2.33	103.81	109.56
3	A	1001	B12	C25-C2-C3	-2.29	111.70	115.56
3	C	1002	B12	C47-C12-C46	-2.04	104.53	109.56
3	C	1002	B12	C47-C12-C13	2.07	121.55	112.81
3	A	1001	B12	C2R-C3R-C4R	2.25	107.52	103.29
3	C	1002	B12	C8-C7-C6	2.27	104.83	101.09
3	A	1001	B12	C8-C7-C6	2.31	104.89	101.09
3	A	1001	B12	C42-C41-C8	2.42	122.01	114.80
3	A	1001	B12	C49-C48-C13	2.43	122.06	114.80
3	C	1002	B12	C35-C5-C6	2.48	122.69	118.25
3	C	1002	B12	C18-C60-C61	2.52	120.16	113.92
3	A	1001	B12	C47-C12-C13	2.61	123.83	112.81
3	A	1001	B12	C35-C5-C6	2.66	123.01	118.25
3	C	1002	B12	C42-C41-C8	2.92	123.51	114.80
3	A	1001	B12	C60-C18-C17	5.32	125.99	115.68
3	C	1002	B12	C60-C18-C17	5.79	126.91	115.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	B12	10	0
3	C	1002	B12	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	378/399 (94%)	0.27	38 (10%) 9 5	29, 49, 97, 99	1 (0%)
1	B	267/399 (66%)	0.08	8 (2%) 54 47	31, 48, 85, 99	0
1	C	378/399 (94%)	0.47	51 (13%) 4 2	30, 52, 99, 99	2 (0%)
1	D	267/399 (66%)	-0.06	6 (2%) 65 59	30, 46, 81, 99	0
All	All	1290/1596 (80%)	0.22	103 (7%) 15 10	29, 49, 97, 99	3 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	LEU	7.0
1	C	272	PRO	6.6
1	A	305	ARG	6.3
1	B	174	GLU	6.2
1	C	338	MET	6.2
1	A	307	VAL	6.1
1	D	273	ASP	6.1
1	D	272	PRO	5.6
1	C	12	SER	5.5
1	C	307	VAL	5.4
1	C	334	ARG	5.3
1	A	174	GLU	5.3
1	B	273	ASP	5.1
1	C	305	ARG	4.9
1	A	292	SER	4.8
1	C	341	PHE	4.7
1	C	389	HIS	4.6
1	D	174	GLU	4.6
1	A	273	ASP	4.6
1	C	273	ASP	4.5
1	C	306	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	336	ASN	4.5
1	A	338	MET	4.4
1	C	224	LYS	4.3
1	C	332	ALA	4.1
1	C	388	ASN	4.1
1	C	323	SER	4.0
1	A	308	GLU	3.9
1	A	7	SER	3.8
1	C	31	SER	3.8
1	A	312	ASN	3.8
1	C	298	TYR	3.8
1	B	32	SER	3.7
1	C	308	GLU	3.7
1	B	272	PRO	3.7
1	C	336	ASN	3.6
1	C	340	LYS	3.6
1	D	224	LYS	3.6
1	A	297	ILE	3.5
1	C	304	LEU	3.4
1	C	295	THR	3.4
1	C	223	LYS	3.4
1	A	289	THR	3.3
1	C	333	GLN	3.2
1	C	358	ILE	3.2
1	A	334	ARG	3.2
1	A	290	SER	3.2
1	C	296	VAL	3.1
1	C	331	GLU	3.0
1	A	357	ASN	3.0
1	C	321	SER	3.0
1	C	387	PHE	2.9
1	C	356	ASN	2.9
1	C	309	LEU	2.9
1	C	11	PRO	2.9
1	C	173	SER	2.8
1	A	321	SER	2.8
1	C	8	CYS	2.8
1	C	225	GLU	2.8
1	A	223	LYS	2.7
1	C	175	GLU	2.7
1	B	7	SER	2.7
1	C	293	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	339	PHE	2.6
1	C	14	GLN	2.5
1	A	335	LYS	2.5
1	C	7	SER	2.5
1	A	359	ALA	2.4
1	B	31	SER	2.4
1	B	64	SER	2.4
1	C	13	ALA	2.4
1	A	173	SER	2.4
1	A	339	PHE	2.4
1	A	322	GLY	2.4
1	C	294	ILE	2.4
1	C	312	ASN	2.4
1	A	332	ALA	2.3
1	A	356	ASN	2.3
1	A	388	ASN	2.3
1	A	358	ILE	2.3
1	C	390	GLU	2.3
1	A	333	GLN	2.3
1	A	302	ASN	2.3
1	A	9	SER	2.2
1	D	7	SER	2.2
1	C	319	VAL	2.2
1	A	341	PHE	2.2
1	A	291	ALA	2.2
1	C	230	LYS	2.2
1	C	320	LYS	2.2
1	B	145	ALA	2.2
1	A	319	VAL	2.2
1	A	12	SER	2.1
1	C	290	SER	2.1
1	D	31	SER	2.1
1	C	315	ILE	2.1
1	C	322	GLY	2.1
1	A	303	GLN	2.0
1	A	327	VAL	2.0
1	C	16	PRO	2.0
1	A	331	GLU	2.0
1	A	301	ASN	2.0
1	C	292	SER	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
2	NAG	A	901	14/15	0.88	0.20	-0.73	94,97,99,99	0
2	NAG	C	901	14/15	0.87	0.18	-0.81	86,87,91,94	0
2	NAG	C	902	14/15	0.85	0.32	-	95,98,99,99	0
2	NAG	A	902	14/15	0.78	0.43	-	97,99,99,99	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, 95^{th} 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
3	B12	A	1001	91/91	0.96	0.21	0.73	30,41,53,68	0
3	B12	C	1002	91/91	0.95	0.20	0.36	37,47,60,66	0

6.5 Other polymers (i)

There are no such residues in this entry.