Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 03:59 PM EDT

PDB ID	:	2RFW
Title	:	Crystal Structure of Cellobiohydrolase from Melanocarpus albomyces
Authors	:	Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on	:	2007-10-02
Resolution	:	1.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

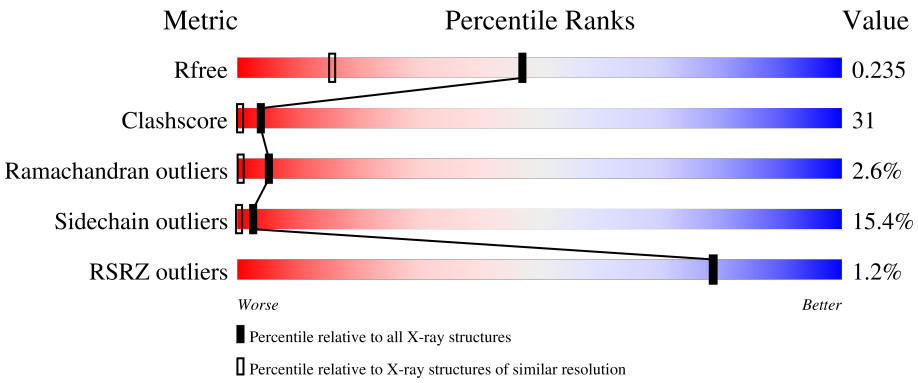
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	430	2%, 34%, 50%, 14%, •
1	B	430	3%, 30%, 53%, 16%, •
1	C	430	61%, 33%, 5%
1	D	430	65%, 30%, •, •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14021 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 Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	3333	2075	558	669	31	0	0	0
1	B	430	3333	2075	558	669	31	0	0	0
1	C	430	3333	2075	558	669	31	0	0	0
1	D	430	3333	2075	558	669	31	0	0	0

- Molecule 2 is water.

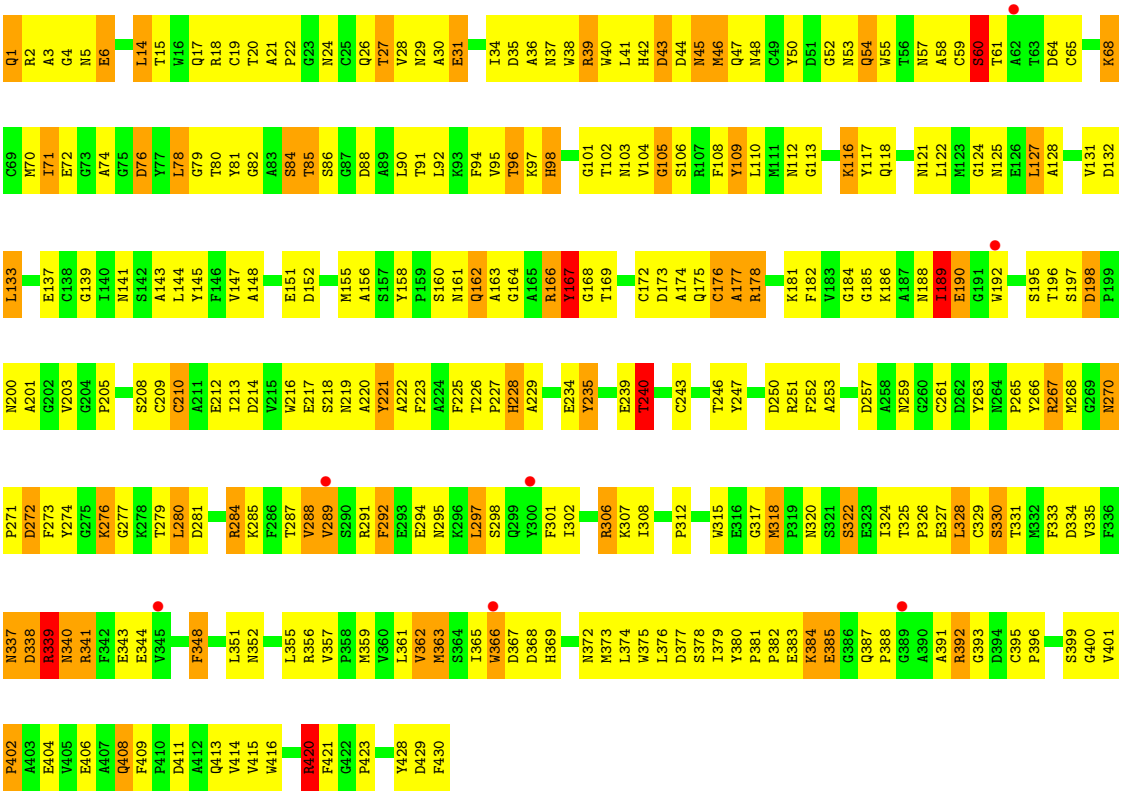
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	139	139	139	0	0
2	B	147	147	147	0	0
2	C	187	187	187	0	0
2	D	216	216	216	0	0

3 Residue-property plots (i)

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

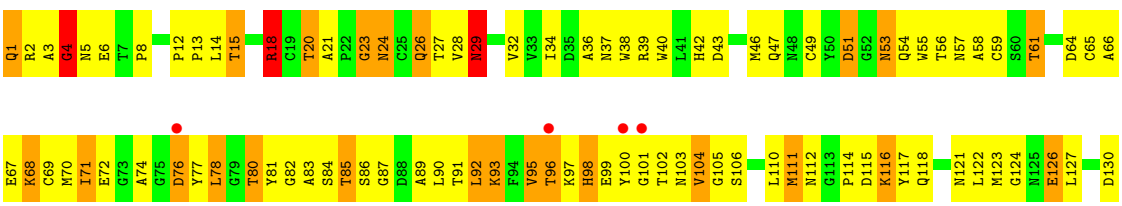
• Molecule 1: Cellulose 1,4-beta-cellobiosidase

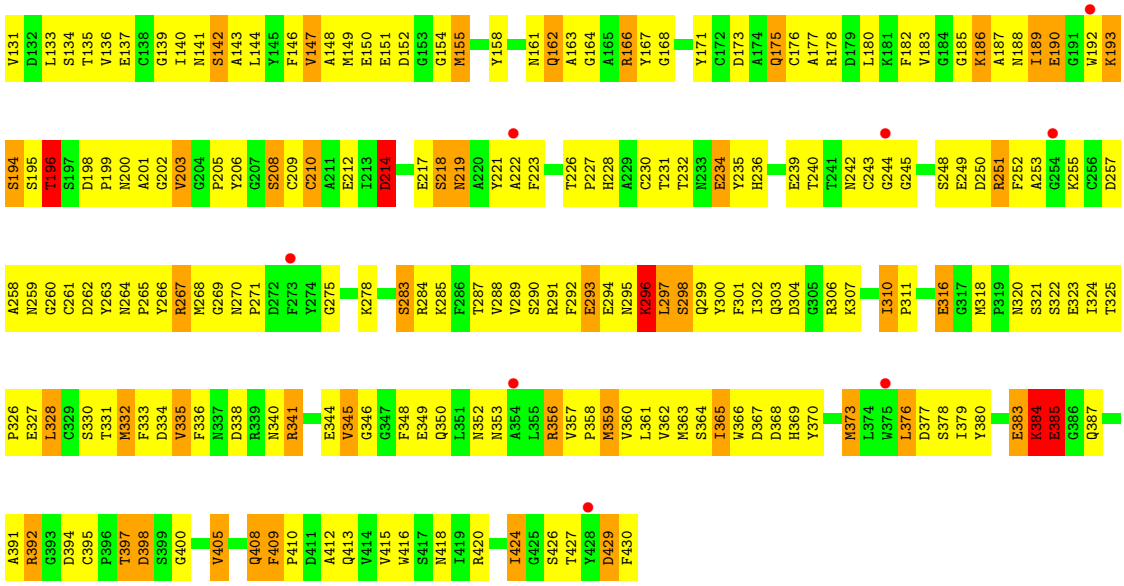
Chain A: 2% 34% 50% 14%



• Molecule 1: Cellulose 1,4-beta-cellobiosidase

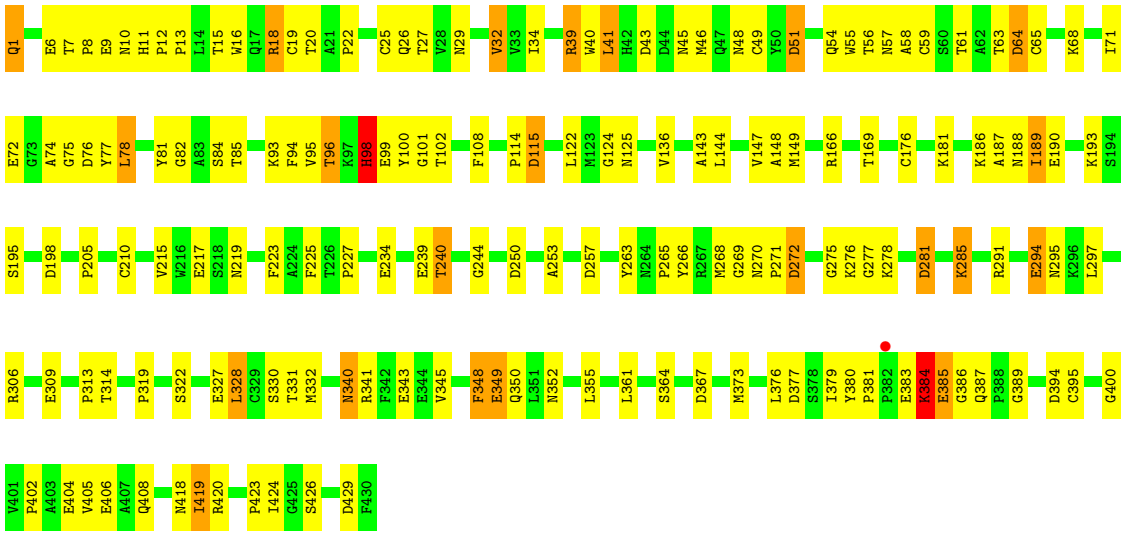
Chain B: 3% 30% 53% 16%





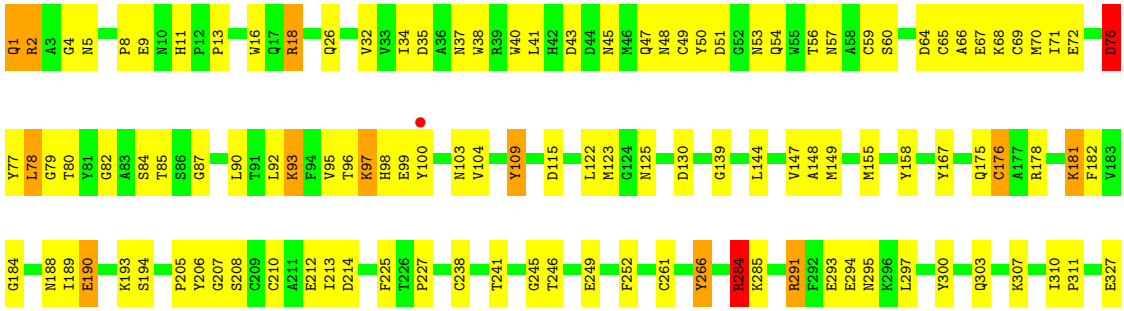
- Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain C:



- Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain D:



L328
C329
S330
T331
M332
F333
D334
V335
F336
N340
R341
F342
E343
F348
L351
N352
L355
L361
V362
W366
D367
D377
S378
I379
Y380
P381
P382
E383
K384
E385
C395
D398
S399
G400
E406
N418
P423
I424
F430

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.94Å 94.52Å 189.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 24.67 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-1.60) 99.4 (24.67-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 1.60Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.199 , 0.243 0.200 , 0.235	Depositor DCC
R_{free} test set	11783 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	9.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.437 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.37	0/3416	1.16	16/4648 (0.3%)
1	B	0.36	0/3416	1.13	7/4648 (0.2%)
1	C	0.42	0/3416	1.21	4/4648 (0.1%)
1	D	0.43	0/3416	1.24	13/4648 (0.3%)
All	All	0.40	0/13664	1.18	40/18592 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	148	ALA	C-N-CA	9.83	146.27	121.70
1	A	267	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	397	THR	C-N-CA	8.63	143.28	121.70
1	A	382	PRO	C-N-CA	8.37	142.61	121.70
1	D	341	ARG	CD-NE-CZ	8.33	135.27	123.60
1	D	284	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	D	109	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	C	98	HIS	CA-CB-CG	6.96	125.44	113.60
1	A	221	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	167	TYR	CB-CG-CD2	6.41	124.85	121.00
1	C	384	LYS	C-N-CA	6.33	137.53	121.70
1	A	176	CYS	C-N-CA	6.29	137.43	121.70
1	B	18	ARG	CD-NE-CZ	6.29	132.41	123.60
1	C	18	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	A	306	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	4	GLY	O-C-N	-5.79	113.43	122.70
1	D	284	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	109	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	B	98	HIS	C-N-CA	5.66	135.84	121.70
1	A	339	ARG	CD-NE-CZ	5.64	131.50	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	HIS	CA-CB-CG	5.52	122.99	113.60
1	D	266	TYR	CA-CB-CG	5.50	123.86	113.40
1	A	98	HIS	CA-CB-CG	5.46	122.89	113.60
1	A	284	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	303	GLN	O-C-N	5.45	131.41	122.70
1	A	167	TYR	CA-CB-CG	5.42	123.69	113.40
1	C	253	ALA	CB-CA-C	-5.37	102.04	110.10
1	A	420	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	57	ASN	C-N-CA	5.33	135.01	121.70
1	D	225	PHE	CB-CG-CD1	-5.28	117.11	120.80
1	A	306	ARG	CD-NE-CZ	5.25	130.95	123.60
1	A	55	TRP	C-N-CA	5.22	134.75	121.70
1	D	366	TRP	CA-CB-CG	5.16	123.51	113.70
1	B	49	CYS	C-N-CA	5.13	134.52	121.70
1	D	225	PHE	CB-CG-CD2	5.10	124.37	120.80
1	D	300	TYR	CB-CG-CD1	5.09	124.06	121.00
1	D	291	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	D	109	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	235	TYR	CB-CG-CD2	5.02	124.01	121.00
1	D	76	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3333	0	3027	256	0
1	B	3333	0	3026	303	0
1	C	3333	0	3028	139	0
1	D	3333	0	3030	110	0
2	A	139	0	0	14	0
2	B	147	0	0	18	0
2	C	187	0	0	13	0
2	D	216	0	0	9	0
All	All	14021	0	12111	780	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 31.

All (780) 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:21:ALA:HB3	1:A:24:ASN:HD22	1.25	1.00
1:A:141:ASN:HD21	1:A:217:GLU:HG2	1.33	0.90
1:B:2:ARG:HB2	1:B:70:MET:HG2	1.54	0.89
1:C:22:PRO:HD3	1:C:426:SER:HA	1.56	0.86
1:B:287:THR:HB	1:B:302:ILE:HB	1.58	0.86
1:A:95:VAL:HG22	1:A:104:VAL:HG22	1.56	0.85
1:B:115:ASP:HA	1:B:166:ARG:HG3	1.59	0.84
1:A:132:ASP:HB2	1:A:285:LYS:HD3	1.60	0.84
1:D:59:CYS:HG	1:D:65:CYS:HG	0.97	0.83
1:B:99:GLU:HG3	1:C:40:TRP:HB2	1.61	0.82
1:C:379:ILE:HG21	1:C:385:GLU:HG3	1.61	0.82
1:A:295:ASN:H	1:A:352:ASN:HD21	1.27	0.82
1:A:128:ALA:HB2	1:A:289:VAL:HG13	1.61	0.81
1:B:163:ALA:HB1	1:B:167:TYR:HB2	1.61	0.80
1:A:90:LEU:HD23	1:A:363:MET:HE3	1.63	0.80
1:C:295:ASN:H	1:C:352:ASN:HD21	1.27	0.79
1:A:381:PRO:HB2	1:A:383:GLU:HG3	1.65	0.79
1:B:218:SER:HB3	1:B:223:PHE:HA	1.65	0.79
1:A:34:ILE:HG22	1:A:39:ARG:HH21	1.46	0.78
1:A:3:ALA:HB1	1:A:167:TYR:OH	1.83	0.78
1:B:144:LEU:HD12	1:B:363:MET:HG2	1.66	0.77
1:D:227:PRO:HD2	1:D:261:CYS:O	1.84	0.77
1:C:195:SER:HB3	1:C:198:ASP:O	1.86	0.76
1:D:125:ASN:HD22	1:D:423:PRO:HA	1.50	0.76
1:A:227:PRO:HD2	1:A:261:CYS:O	1.84	0.76
1:B:252:PHE:HA	2:B:434:HOH:O	1.84	0.75
1:B:173:ASP:HB2	1:B:212:GLU:OE1	1.86	0.75
1:B:267:ARG:HG3	1:B:392:ARG:HG2	1.67	0.74
1:B:408:GLN:O	1:B:410:PRO:HD3	1.87	0.74
1:B:265:PRO:HA	1:B:268:MET:HB2	1.70	0.73
1:D:64:ASP:O	1:D:68:LYS:HB2	1.88	0.73
1:B:55:TRP:HB3	1:B:189:ILE:HD12	1.69	0.73
1:C:419:ILE:HD12	1:C:419:ILE:H	1.54	0.73
1:A:105:GLY:HA2	1:A:365:ILE:HG23	1.72	0.72
1:A:198:ASP:OD2	1:A:201:ALA:HB3	1.89	0.72
1:B:364:SER:HB2	2:B:566:HOH:O	1.88	0.72
1:D:327:GLU:O	1:D:331:THR:HG23	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:O	1:A:125:ASN:HB2	1.89	0.72
1:A:218:SER:HA	1:A:376:LEU:HD21	1.72	0.72
1:A:374:LEU:HD22	1:A:379:ILE:O	1.90	0.72
1:A:145:TYR:HB2	1:A:213:ILE:O	1.90	0.72
1:A:189:ILE:HG23	1:A:190:GLU:H	1.55	0.72
1:A:331:THR:O	1:A:335:VAL:HG23	1.89	0.72
1:B:8:PRO:HG2	1:C:78:LEU:HD11	1.72	0.72
1:C:297:LEU:HD11	1:C:355:LEU:HD11	1.71	0.71
1:B:267:ARG:HA	1:B:391:ALA:O	1.91	0.71
1:A:361:LEU:HD12	1:A:362:VAL:H	1.55	0.71
1:B:420:ARG:HB3	1:B:427:THR:HG22	1.70	0.71
1:A:116:LYS:HB2	1:A:151:GLU:HG2	1.71	0.71
1:B:214:ASP:HB2	1:B:226:THR:O	1.91	0.70
1:A:340:ASN:O	1:A:344:GLU:HG3	1.92	0.70
1:C:169:THR:HG22	2:C:565:HOH:O	1.91	0.70
1:B:150:GLU:HG3	2:B:466:HOH:O	1.91	0.70
1:A:4:GLY:HA2	1:A:70:MET:SD	2.33	0.69
1:B:2:ARG:HA	1:B:162:GLN:HB2	1.75	0.69
1:A:178:ARG:HG3	1:A:247:TYR:HB2	1.74	0.69
1:C:328:LEU:O	1:C:332:MET:HG3	1.93	0.69
1:A:132:ASP:HB3	1:A:415:VAL:HB	1.73	0.69
1:B:96:THR:O	1:B:102:THR:HA	1.91	0.69
1:B:111:MET:HB3	1:B:116:LYS:O	1.92	0.69
1:B:287:THR:HG23	2:B:521:HOH:O	1.92	0.69
1:D:26:GLN:HB2	2:D:516:HOH:O	1.93	0.69
1:B:76:ASP:HB3	1:C:76:ASP:OD2	1.93	0.69
1:C:11:HIS:HB3	1:C:32:VAL:O	1.93	0.69
1:B:408:GLN:HG3	1:B:409:PHE:H	1.57	0.68
1:C:82:GLY:HA3	1:C:96:THR:HG21	1.73	0.68
1:B:53:ASN:HB3	1:B:201:ALA:O	1.94	0.68
1:B:144:LEU:HD21	1:B:361:LEU:HD11	1.75	0.68
1:A:291:ARG:O	1:A:297:LEU:HA	1.93	0.68
1:B:91:THR:OG1	1:B:415:VAL:HG22	1.94	0.68
1:D:85:THR:HG23	2:D:619:HOH:O	1.92	0.68
1:C:144:LEU:HD21	1:C:361:LEU:HD11	1.74	0.68
1:A:257:ASP:HA	1:A:341:ARG:HG2	1.74	0.68
1:B:47:GLN:OE1	1:B:58:ALA:HB2	1.93	0.68
1:D:18:ARG:HH11	1:D:18:ARG:HB2	1.59	0.68
1:A:34:ILE:HG22	1:A:39:ARG:NH2	2.08	0.67
1:B:147:VAL:HG21	1:B:171:TYR:HE1	1.60	0.67
1:D:340:ASN:ND2	1:D:343:GLU:H	1.91	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:HB3	1:A:50:TYR:O	1.93	0.67
1:B:175:GLN:HG3	1:B:258:ALA:HB1	1.76	0.67
1:A:287:THR:HB	1:A:302:ILE:HB	1.77	0.67
1:C:384:LYS:HG2	1:C:387:GLN:HE22	1.60	0.67
1:A:173:ASP:HB2	1:A:212:GLU:OE1	1.95	0.67
1:D:4:GLY:HA3	1:D:72:GLU:OE2	1.94	0.66
1:B:124:GLY:O	1:B:424:ILE:HD12	1.95	0.66
1:A:21:ALA:HB3	1:A:24:ASN:ND2	2.05	0.66
1:B:331:THR:O	1:B:334:ASP:HB2	1.95	0.66
1:B:76:ASP:HB3	1:C:76:ASP:HA	1.78	0.66
1:B:328:LEU:HD22	1:B:332:MET:HG3	1.76	0.66
1:C:74:ALA:HB1	1:C:81:TYR:HE2	1.60	0.66
1:C:115:ASP:HB2	2:C:585:HOH:O	1.96	0.66
1:D:95:VAL:HG22	1:D:104:VAL:HG22	1.78	0.65
1:A:341:ARG:HA	1:A:344:GLU:HG3	1.79	0.65
1:B:245:GLY:HA2	1:B:258:ALA:HB2	1.79	0.65
1:D:123:MET:HB3	2:D:535:HOH:O	1.95	0.65
1:B:426:SER:HB3	2:B:478:HOH:O	1.95	0.65
1:A:141:ASN:ND2	1:A:217:GLU:HG2	2.09	0.65
1:A:92:LEU:HD22	1:A:106:SER:OG	1.97	0.64
1:B:90:LEU:HD23	1:B:363:MET:SD	2.37	0.64
1:A:188:ASN:OD1	1:A:205:PRO:HD2	1.96	0.64
1:B:190:GLU:O	1:B:205:PRO:HD3	1.98	0.64
1:C:93:LYS:NZ	1:C:96:THR:HB	2.13	0.64
1:C:64:ASP:O	1:C:68:LYS:HG3	1.97	0.64
1:B:368:ASP:OD1	1:B:370:TYR:HB2	1.98	0.63
1:B:39:ARG:HD3	1:B:72:GLU:O	1.99	0.63
1:B:288:VAL:HG12	2:B:431:HOH:O	1.97	0.63
1:D:98:HIS:HE1	1:D:103:ASN:HB2	1.62	0.63
1:A:110:LEU:HB3	2:A:511:HOH:O	1.97	0.63
1:C:239:GLU:HG3	1:C:240:THR:HG23	1.80	0.63
1:B:195:SER:HA	2:B:573:HOH:O	1.98	0.63
1:A:52:GLY:O	1:A:200:ASN:HA	1.99	0.63
1:B:97:LYS:HA	1:B:102:THR:HA	1.79	0.63
1:B:147:VAL:HG22	1:B:362:VAL:HG21	1.80	0.63
1:D:41:LEU:HD12	1:D:181:LYS:NZ	2.14	0.63
1:A:423:PRO:HB3	2:A:524:HOH:O	1.99	0.62
1:A:195:SER:HA	2:A:520:HOH:O	1.98	0.62
1:A:333:PHE:O	1:A:337:ASN:HA	1.99	0.62
1:C:384:LYS:HE2	2:C:477:HOH:O	2.00	0.62
1:B:29:ASN:H	1:B:29:ASN:ND2	1.95	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:HD21	1:A:221:TYR:HB2	1.64	0.62
1:C:41:LEU:HG	1:C:71:ILE:HG12	1.81	0.62
1:D:189:ILE:HG23	1:D:190:GLU:HG3	1.81	0.62
1:C:309:GLU:HG2	2:C:467:HOH:O	1.99	0.62
1:A:80:THR:HG23	1:A:98:HIS:CE1	2.35	0.62
1:B:143:ALA:HB3	1:B:364:SER:OG	1.99	0.62
1:B:209:CYS:HB2	1:B:236:HIS:CE1	2.35	0.62
1:C:383:GLU:O	1:C:384:LYS:HB2	2.00	0.62
1:D:331:THR:HA	1:D:334:ASP:OD1	2.00	0.62
1:A:361:LEU:HD12	1:A:362:VAL:N	2.15	0.62
1:A:208:SER:HB2	1:A:235:TYR:CE1	2.35	0.61
1:A:41:LEU:HG	1:A:71:ILE:HG22	1.82	0.61
1:A:178:ARG:HG3	1:A:247:TYR:HD2	1.64	0.61
1:D:80:THR:HG23	1:D:98:HIS:CD2	2.35	0.61
1:A:250:ASP:OD2	1:A:253:ALA:HB2	2.01	0.61
1:D:178:ARG:HG2	1:D:206:TYR:O	2.00	0.61
1:A:1:PCA:OE	1:A:161:ASN:HB2	2.00	0.61
1:B:99:GLU:HA	1:C:40:TRP:CE3	2.36	0.61
1:B:349:GLU:O	1:B:352:ASN:HB2	2.01	0.61
1:B:212:GLU:O	1:B:228:HIS:HB2	2.01	0.60
1:A:274:TYR:CD1	1:A:280:LEU:HD12	2.36	0.60
1:B:121:ASN:HB2	2:B:548:HOH:O	2.01	0.60
1:B:405:VAL:HA	1:B:408:GLN:HG2	1.83	0.60
1:C:48:ASN:O	1:C:56:THR:HG21	2.00	0.60
1:B:122:LEU:HD22	1:B:359:MET:HG3	1.81	0.60
1:B:18:ARG:HD3	2:B:550:HOH:O	2.01	0.60
1:A:317:GLY:O	1:A:331:THR:HB	2.01	0.60
1:D:385:GLU:O	1:D:385:GLU:HG2	2.02	0.60
1:A:324:ILE:HG22	1:A:348:PHE:CE1	2.36	0.60
1:A:178:ARG:NH1	1:A:243:CYS:HB2	2.17	0.59
1:B:117:TYR:OH	1:B:168:GLY:HA2	2.03	0.59
1:C:82:GLY:CA	1:C:96:THR:HG21	2.32	0.59
1:A:288:VAL:HG13	1:A:301:PHE:CD2	2.37	0.59
1:B:55:TRP:CH2	1:B:187:ALA:HB1	2.37	0.59
1:C:12:PRO:HB3	1:C:85:THR:HG22	1.84	0.59
1:B:180:LEU:HD12	1:B:208:SER:OG	2.02	0.59
1:D:13:PRO:O	1:D:85:THR:HG21	2.02	0.59
1:B:183:VAL:HG11	1:B:206:TYR:HB3	1.84	0.59
1:C:124:GLY:O	1:C:424:ILE:HG12	2.02	0.59
1:B:264:ASN:O	1:B:268:MET:HG2	2.01	0.59
1:A:384:LYS:CB	1:A:387:GLN:HE21	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASN:H	1:B:352:ASN:HD21	1.51	0.59
1:D:41:LEU:HD11	1:D:182:PHE:HE2	1.68	0.58
1:A:315:TRP:HB2	1:A:318:MET:HG3	1.84	0.58
1:B:78:LEU:HD13	1:C:10:ASN:ND2	2.18	0.58
1:B:97:LYS:HE3	1:C:6:GLU:HA	1.83	0.58
1:C:125:ASN:HD22	1:C:423:PRO:HA	1.68	0.58
1:B:136:VAL:HG11	1:B:142:SER:OG	2.03	0.58
1:C:27:THR:HG22	1:C:29:ASN:HD21	1.67	0.58
1:A:174:ALA:H	1:A:212:GLU:HB2	1.67	0.58
1:A:239:GLU:HA	1:A:239:GLU:OE1	2.03	0.58
1:B:8:PRO:HG2	1:C:78:LEU:CD1	2.34	0.58
1:A:5:ASN:H	1:A:70:MET:HE1	1.67	0.58
1:A:127:LEU:HG	1:A:128:ALA:N	2.17	0.58
1:B:80:THR:HB	1:B:81:TYR:CD2	2.38	0.58
1:C:266:TYR:CD2	1:C:271:PRO:HA	2.38	0.58
1:B:97:LYS:HD2	1:C:6:GLU:OE1	2.03	0.58
1:D:125:ASN:HD22	1:D:423:PRO:CA	2.16	0.58
1:A:356:ARG:HB3	1:B:24:ASN:HD21	1.69	0.58
1:B:55:TRP:CB	1:B:189:ILE:HD12	2.34	0.58
1:D:54:GLN:HG3	1:D:194:SER:OG	2.04	0.58
1:B:6:GLU:HB2	1:B:72:GLU:OE2	2.04	0.57
1:B:230:CYS:HB2	1:B:232:THR:O	2.04	0.57
1:B:78:LEU:HG	1:B:84:SER:HB3	1.84	0.57
1:B:126:GLU:OE1	1:B:291:ARG:HG2	2.04	0.57
1:C:78:LEU:HG	1:C:84:SER:HB3	1.86	0.57
1:B:51:ASP:HB2	1:B:56:THR:CG2	2.34	0.57
1:B:205:PRO:O	1:B:206:TYR:HD2	1.87	0.57
1:B:141:ASN:HD21	1:B:217:GLU:HB3	1.69	0.57
1:B:377:ASP:HB2	1:B:395:CYS:SG	2.45	0.57
1:C:59:CYS:HA	1:C:68:LYS:NZ	2.20	0.57
1:C:385:GLU:HG2	1:C:386:GLY:N	2.18	0.57
1:B:146:PHE:HB3	1:B:359:MET:HB3	1.85	0.57
1:B:245:GLY:HA2	1:B:258:ALA:CB	2.34	0.57
1:C:13:PRO:O	1:C:85:THR:HG21	2.04	0.57
1:D:148:ALA:HB3	1:D:210:CYS:HB2	1.87	0.57
1:B:373:MET:SD	1:B:376:LEU:HD23	2.45	0.57
1:D:50:TYR:OH	1:D:53:ASN:HA	2.04	0.57
1:A:209:CYS:O	1:A:235:TYR:HA	2.05	0.57
1:A:324:ILE:HG22	1:A:348:PHE:CZ	2.40	0.57
1:B:226:THR:HG1	1:B:262:ASP:HA	1.69	0.57
1:B:209:CYS:O	1:B:210:CYS:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:CYS:SG	1:A:235:TYR:HD1	2.28	0.56
1:C:19:CYS:HA	1:C:25:CYS:HA	1.87	0.56
1:D:18:ARG:HH11	1:D:18:ARG:CB	2.18	0.56
1:D:85:THR:HA	2:D:578:HOH:O	2.05	0.56
1:B:295:ASN:HA	1:B:348:PHE:CE2	2.41	0.56
1:C:63:THR:OG1	1:C:186:LYS:HE2	2.05	0.56
1:D:188:ASN:OD1	1:D:205:PRO:HD2	2.04	0.56
1:A:127:LEU:HD23	2:A:534:HOH:O	2.05	0.56
1:A:267:ARG:HA	1:A:391:ALA:O	2.04	0.56
1:A:368:ASP:HB2	1:A:373:MET:CE	2.35	0.56
1:B:68:LYS:HZ2	1:B:68:LYS:HB3	1.70	0.56
1:A:144:LEU:HG	1:A:363:MET:HG3	1.87	0.56
1:A:178:ARG:HG3	1:A:247:TYR:CD2	2.40	0.56
1:B:333:PHE:HE2	1:B:338:ASP:HB2	1.70	0.56
1:A:90:LEU:HD12	1:A:91:THR:N	2.21	0.56
1:A:158:TYR:HB3	1:A:184:GLY:O	2.06	0.56
1:C:380:TYR:CD1	1:C:381:PRO:HA	2.40	0.56
1:D:16:TRP:HH2	2:D:579:HOH:O	1.88	0.56
1:B:244:GLY:HA2	1:B:248:SER:HB2	1.87	0.56
1:A:155:MET:HG2	1:A:161:ASN:O	2.06	0.56
1:A:38:TRP:CZ2	1:A:106:SER:HA	2.41	0.56
1:A:252:PHE:CD1	1:A:339:ARG:HD3	2.40	0.56
1:B:219:ASN:OD1	1:B:376:LEU:HD21	2.06	0.55
1:A:270:ASN:HB3	2:A:488:HOH:O	2.06	0.55
1:B:218:SER:HB3	1:B:223:PHE:CA	2.35	0.55
1:C:27:THR:HG22	1:C:29:ASN:ND2	2.21	0.55
1:C:74:ALA:HB1	1:C:81:TYR:CE2	2.41	0.55
1:A:21:ALA:HB1	1:A:22:PRO:HD2	1.87	0.55
1:B:333:PHE:CE2	1:B:338:ASP:HB2	2.42	0.55
1:D:241:THR:HG22	1:D:249:GLU:OE1	2.06	0.55
1:A:266:TYR:HB2	2:A:541:HOH:O	2.05	0.55
1:B:144:LEU:HA	1:B:362:VAL:O	2.06	0.55
1:B:266:TYR:CD2	1:B:271:PRO:HA	2.41	0.55
1:D:295:ASN:H	1:D:352:ASN:HD21	1.53	0.55
1:A:132:ASP:HB3	1:A:415:VAL:CB	2.36	0.55
1:B:198:ASP:OD1	1:B:199:PRO:HD2	2.06	0.55
1:B:188:ASN:O	1:B:192:TRP:HE3	1.90	0.55
1:C:400:GLY:HA2	1:C:405:VAL:HG11	1.88	0.55
1:D:307:LYS:HE3	1:D:430:PHE:HB3	1.89	0.55
1:C:404:GLU:O	1:C:408:GLN:HG2	2.06	0.55
1:A:144:LEU:CD2	1:A:361:LEU:HD11	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TYR:CE1	1:B:268:MET:HG3	2.42	0.55
1:C:7:THR:HG22	1:C:8:PRO:O	2.06	0.55
1:B:55:TRP:CD2	1:B:189:ILE:HB	2.42	0.55
1:B:231:THR:OG1	1:B:255:LYS:HB3	2.07	0.54
1:B:379:ILE:HG21	1:B:385:GLU:HB2	1.89	0.54
1:B:97:LYS:HA	1:B:102:THR:OG1	2.07	0.54
1:D:34:ILE:HB	1:D:77:TYR:HE2	1.71	0.54
1:D:379:ILE:HG21	1:D:385:GLU:HB2	1.89	0.54
1:A:139:GLY:CA	1:A:400:GLY:HA2	2.37	0.54
1:A:139:GLY:HA3	1:A:400:GLY:HA2	1.90	0.54
1:A:147:VAL:HG12	1:A:212:GLU:HG3	1.88	0.54
1:A:315:TRP:HB2	1:A:318:MET:SD	2.47	0.54
1:D:40:TRP:CE3	1:D:72:GLU:HG3	2.42	0.54
1:B:12:PRO:HD3	1:B:77:TYR:CE1	2.43	0.54
1:B:64:ASP:O	1:B:67:GLU:HB2	2.07	0.54
1:D:96:THR:OG1	1:D:103:ASN:HB3	2.08	0.54
1:B:149:MET:HB2	1:B:360:VAL:HG21	1.90	0.54
1:C:93:LYS:HE3	1:C:96:THR:CG2	2.37	0.54
1:D:35:ASP:HB3	1:D:38:TRP:CE3	2.43	0.54
1:B:152:ASP:OD2	1:B:155:MET:HB2	2.08	0.54
1:B:147:VAL:CG1	1:B:212:GLU:HG3	2.38	0.54
1:B:316:GLU:HA	1:B:316:GLU:OE1	2.06	0.54
1:D:50:TYR:CD1	1:D:181:LYS:HD2	2.42	0.54
1:A:6:GLU:OE2	1:A:42:HIS:HE1	1.91	0.54
1:A:6:GLU:O	1:D:97:LYS:HG3	2.08	0.54
1:A:380:TYR:HB3	1:A:392:ARG:NE	2.23	0.54
1:B:81:TYR:O	1:B:96:THR:HG21	2.08	0.54
1:B:209:CYS:HB2	1:B:236:HIS:NE2	2.23	0.54
1:D:379:ILE:HD13	1:D:385:GLU:HG3	1.90	0.54
1:A:137:GLU:HG3	1:A:409:PHE:CE1	2.43	0.53
1:B:287:THR:O	1:B:301:PHE:HA	2.07	0.53
1:D:293:GLU:HG3	1:D:424:ILE:HD11	1.90	0.53
1:C:384:LYS:HG2	1:C:387:GLN:NE2	2.22	0.53
1:A:68:LYS:NZ	1:A:68:LYS:HB3	2.16	0.53
1:A:292:PHE:HB3	1:A:355:LEU:HD22	1.90	0.53
1:B:23:GLY:O	1:B:24:ASN:HB2	2.09	0.53
1:B:267:ARG:HD3	1:B:336:PHE:CE2	2.43	0.53
1:A:64:ASP:O	1:A:68:LYS:HG2	2.08	0.53
1:A:263:TYR:CZ	1:A:322:SER:HA	2.43	0.53
1:B:36:ALA:O	1:B:39:ARG:HB2	2.09	0.53
1:A:112:ASN:HB2	1:A:118:GLN:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:CYS:HA	1:A:208:SER:OG	2.09	0.53
1:D:48:ASN:O	1:D:56:THR:HG21	2.08	0.53
1:A:401:VAL:HG23	2:A:548:HOH:O	2.09	0.53
1:C:327:GLU:O	1:C:331:THR:HG23	2.09	0.53
1:D:80:THR:HG23	1:D:98:HIS:NE2	2.24	0.53
1:A:15:THR:HB	1:A:27:THR:CG2	2.38	0.53
1:A:178:ARG:HH22	1:A:240:THR:HA	1.74	0.53
1:A:372:ASN:O	1:A:400:GLY:HA3	2.09	0.53
1:B:147:VAL:HG21	1:B:171:TYR:CE1	2.40	0.53
1:A:92:LEU:O	1:A:413:GLN:HB2	2.09	0.53
1:A:295:ASN:H	1:A:352:ASN:ND2	2.03	0.53
1:A:363:MET:HG2	1:A:416:TRP:CD1	2.44	0.53
1:A:271:PRO:HD2	1:A:272:ASP:OD1	2.09	0.52
1:C:9:GLU:OE2	1:C:9:GLU:HA	2.08	0.52
1:D:249:GLU:HG3	2:D:580:HOH:O	2.09	0.52
1:A:137:GLU:HG3	1:A:409:PHE:CD1	2.44	0.52
1:A:210:CYS:HB3	1:A:235:TYR:HA	1.92	0.52
1:B:134:SER:HB3	1:B:283:SER:HA	1.92	0.52
1:C:148:ALA:HB3	1:C:210:CYS:HB2	1.92	0.52
1:D:82:GLY:O	1:D:93:LYS:HD3	2.08	0.52
1:A:315:TRP:HB2	1:A:318:MET:CG	2.40	0.52
1:C:59:CYS:HA	1:C:68:LYS:HZ3	1.73	0.52
1:A:76:ASP:OD2	1:D:76:ASP:HB3	2.09	0.52
1:B:96:THR:HG23	1:B:103:ASN:HB3	1.91	0.52
1:B:302:ILE:O	1:B:302:ILE:HG22	2.09	0.52
1:C:269:GLY:HA3	1:C:314:THR:OG1	2.09	0.52
1:D:71:ILE:HD12	1:D:167:TYR:HB3	1.91	0.52
1:A:341:ARG:O	1:A:344:GLU:HB2	2.10	0.52
1:B:51:ASP:HB2	1:B:56:THR:HG22	1.92	0.52
1:B:341:ARG:HA	1:B:344:GLU:OE2	2.10	0.52
1:A:176:CYS:HA	1:A:208:SER:O	2.10	0.52
1:B:3:ALA:O	1:B:4:GLY:O	2.28	0.52
1:A:109:TYR:CD1	1:A:362:VAL:HG13	2.44	0.51
1:A:128:ALA:HB1	1:A:428:TYR:HE1	1.75	0.51
1:A:172:CYS:O	1:A:173:ASP:HB3	2.10	0.51
1:B:98:HIS:CD2	1:B:100:TYR:H	2.27	0.51
1:A:60:SER:O	1:A:189:ILE:HD13	2.09	0.51
1:A:266:TYR:CD2	1:A:393:GLY:HA2	2.46	0.51
1:B:367:ASP:HB2	2:B:531:HOH:O	2.09	0.51
1:C:114:PRO:O	1:C:166:ARG:HG2	2.10	0.51
1:D:41:LEU:HD12	1:D:181:LYS:HZ1	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:TRP:CZ2	1:C:181:LYS:HB3	2.45	0.51
1:D:311:PRO:HG3	2:D:551:HOH:O	2.10	0.51
1:B:350:GLN:O	1:B:353:ASN:HB2	2.10	0.51
1:C:328:LEU:HD22	1:C:332:MET:HG3	1.93	0.51
1:A:45:ASN:O	1:A:46:MET:HB2	2.10	0.51
1:B:163:ALA:O	1:B:166:ARG:HD3	2.11	0.51
1:A:365:ILE:O	1:A:366:TRP:HB3	2.11	0.51
1:A:5:ASN:H	1:A:70:MET:CE	2.24	0.51
1:B:163:ALA:HB1	1:B:167:TYR:CB	2.38	0.51
1:B:290:SER:OG	1:B:299:GLN:HG3	2.11	0.51
1:B:327:GLU:O	1:B:330:SER:OG	2.29	0.51
1:C:41:LEU:HD12	2:C:466:HOH:O	2.11	0.51
1:A:92:LEU:HD21	1:A:108:PHE:CD1	2.46	0.51
1:A:268:MET:HA	1:A:315:TRP:HE1	1.76	0.51
1:A:356:ARG:HB3	1:B:24:ASN:ND2	2.26	0.51
1:C:275:GLY:O	1:C:281:ASP:HA	2.10	0.51
1:A:78:LEU:HD21	1:D:8:PRO:HD2	1.93	0.50
1:B:155:MET:CE	1:B:164:GLY:HA3	2.41	0.50
1:A:15:THR:OG1	1:A:88:ASP:HB3	2.11	0.50
1:A:341:ARG:HD2	1:A:344:GLU:OE1	2.11	0.50
1:C:217:GLU:O	1:C:223:PHE:HA	2.12	0.50
1:A:3:ALA:HB1	1:A:167:TYR:CZ	2.45	0.50
1:B:95:VAL:HG23	1:B:410:PRO:HA	1.94	0.50
1:C:268:MET:O	1:C:313:PRO:HA	2.11	0.50
1:A:102:THR:O	1:A:102:THR:HG22	2.12	0.50
1:B:53:ASN:OD1	1:B:199:PRO:O	2.30	0.50
1:B:65:CYS:SG	1:B:189:ILE:HG21	2.50	0.50
1:B:365:ILE:HG23	1:B:365:ILE:O	2.11	0.50
1:A:125:ASN:HD21	1:B:18:ARG:HH12	1.58	0.50
1:A:178:ARG:O	1:A:203:VAL:HA	2.12	0.50
1:B:61:THR:O	1:B:64:ASP:OD2	2.30	0.50
1:C:383:GLU:HA	1:C:383:GLU:OE2	2.12	0.50
1:D:41:LEU:HD22	1:D:69:CYS:HB3	1.94	0.50
1:A:128:ALA:CB	1:A:289:VAL:HG13	2.37	0.50
1:B:346:GLY:HA3	1:B:350:GLN:HB2	1.94	0.50
1:A:35:ASP:OD1	1:A:109:TYR:OH	2.30	0.50
1:A:377:ASP:O	1:A:393:GLY:HA3	2.12	0.50
1:A:379:ILE:O	1:A:379:ILE:HG22	2.12	0.50
1:A:384:LYS:O	1:A:385:GLU:O	2.30	0.50
1:B:76:ASP:OD1	1:C:75:GLY:O	2.30	0.50
1:B:295:ASN:O	1:B:296:LYS:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:HD21	1:D:92:LEU:HD21	1.93	0.50
1:D:241:THR:HG22	1:D:249:GLU:OE2	2.12	0.50
1:C:143:ALA:HB3	1:C:364:SER:OG	2.12	0.49
1:D:333:PHE:O	1:D:336:PHE:O	2.30	0.49
1:A:29:ASN:HB3	2:A:553:HOH:O	2.12	0.49
1:A:132:ASP:CB	1:A:285:LYS:HD3	2.35	0.49
1:A:141:ASN:HD21	1:A:217:GLU:CG	2.16	0.49
1:A:295:ASN:OD1	1:A:352:ASN:OD1	2.29	0.49
1:B:95:VAL:HG12	1:B:102:THR:HG23	1.95	0.49
1:B:244:GLY:HA2	1:B:250:ASP:O	2.12	0.49
1:C:306:ARG:HH12	1:D:418:ASN:ND2	2.10	0.49
1:A:19:CYS:HA	1:A:24:ASN:O	2.13	0.49
1:A:47:GLN:HG2	1:A:58:ALA:HB2	1.93	0.49
1:A:144:LEU:HD21	1:A:361:LEU:HD11	1.94	0.49
1:C:40:TRP:HB3	1:C:72:GLU:HB2	1.92	0.49
1:A:53:ASN:HB3	1:A:201:ALA:N	2.28	0.49
1:A:121:ASN:O	1:A:125:ASN:OD1	2.30	0.49
1:B:299:GLN:O	1:B:310:ILE:HD11	2.11	0.49
1:B:32:VAL:HG12	1:B:110:LEU:HA	1.95	0.49
1:B:96:THR:OG1	1:B:103:ASN:HB3	2.13	0.49
1:B:303:GLN:O	1:B:304:ASP:HB2	2.12	0.49
1:B:361:LEU:HD12	1:B:362:VAL:N	2.27	0.49
1:B:76:ASP:H	1:C:76:ASP:CG	2.15	0.49
1:B:198:ASP:HB3	1:B:201:ALA:HB3	1.94	0.49
1:B:323:GLU:HA	2:B:448:HOH:O	2.12	0.49
1:A:39:ARG:HD3	1:A:72:GLU:O	2.11	0.49
1:C:6:GLU:HB2	1:C:72:GLU:OE2	2.12	0.49
1:A:315:TRP:CH2	1:A:388:PRO:HA	2.47	0.49
1:B:263:TYR:OH	1:B:311:PRO:O	2.30	0.49
1:C:63:THR:HG21	2:C:593:HOH:O	2.12	0.49
1:A:356:ARG:HA	2:A:557:HOH:O	2.13	0.49
1:B:226:THR:HG23	1:B:262:ASP:N	2.28	0.49
1:C:15:THR:O	1:C:419:ILE:HD13	2.13	0.49
1:C:144:LEU:CD2	1:C:361:LEU:HD11	2.43	0.49
1:C:349:GLU:OE2	1:C:349:GLU:O	2.31	0.49
1:A:43:ASP:OD1	1:A:45:ASN:OD1	2.30	0.48
1:A:198:ASP:HB3	1:A:369:HIS:CD2	2.48	0.48
1:A:295:ASN:ND2	1:A:326:PRO:HG2	2.28	0.48
1:B:226:THR:OG1	1:B:262:ASP:HA	2.13	0.48
1:C:295:ASN:H	1:C:352:ASN:ND2	2.05	0.48
1:A:163:ALA:O	1:A:166:ARG:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LYS:HG2	1:A:387:GLN:NE2	2.27	0.48
1:A:402:PRO:O	1:A:406:GLU:HG3	2.13	0.48
1:B:291:ARG:HB3	1:B:424:ILE:HG12	1.94	0.48
1:C:55:TRP:HB3	1:C:189:ILE:HD12	1.94	0.48
1:A:143:ALA:HA	1:A:216:TRP:O	2.13	0.48
1:B:37:ASN:OD1	1:B:180:LEU:HA	2.13	0.48
1:B:122:LEU:HG	1:B:292:PHE:CE1	2.47	0.48
1:B:182:PHE:HD2	2:B:442:HOH:O	1.95	0.48
1:C:188:ASN:OD1	1:C:205:PRO:HD2	2.12	0.48
1:D:50:TYR:CE1	1:D:181:LYS:HD2	2.47	0.48
1:A:95:VAL:HG22	1:A:104:VAL:CG2	2.37	0.48
1:D:175:GLN:O	1:D:245:GLY:HA3	2.13	0.48
1:A:325:THR:OG1	1:A:327:GLU:OE1	2.30	0.48
1:A:375:TRP:HA	1:A:392:ARG:HD3	1.95	0.48
1:B:74:ALA:HB3	1:B:77:TYR:CE1	2.49	0.48
1:A:307:LYS:HE3	1:A:430:PHE:HB3	1.96	0.48
1:B:122:LEU:HG	1:B:292:PHE:CD1	2.48	0.48
1:D:125:ASN:HA	1:D:423:PRO:HA	1.96	0.48
1:A:113:GLY:HA3	2:A:451:HOH:O	2.14	0.48
1:B:15:THR:OG1	1:B:87:GLY:O	2.30	0.48
1:B:127:LEU:HD22	1:B:146:PHE:CE1	2.49	0.48
1:B:361:LEU:HD12	1:B:362:VAL:H	1.78	0.48
1:A:90:LEU:HD12	1:A:91:THR:H	1.78	0.48
1:A:214:ASP:HB2	1:A:226:THR:HB	1.96	0.48
1:B:40:TRP:CE3	1:B:72:GLU:HG3	2.49	0.48
1:B:136:VAL:HG13	1:B:140:ILE:CG2	2.44	0.48
1:B:275:GLY:C	1:B:278:LYS:HG3	2.33	0.48
1:C:227:PRO:HG3	1:C:297:LEU:HD22	1.95	0.48
1:A:84:SER:HB2	1:A:91:THR:HB	1.95	0.48
1:A:131:VAL:O	1:A:285:LYS:HG3	2.14	0.48
1:A:177:ALA:HB3	1:A:208:SER:OG	2.14	0.48
1:B:210:CYS:HB3	1:B:235:TYR:HA	1.95	0.48
1:D:252:PHE:HD2	1:D:341:ARG:HD3	1.79	0.48
1:A:366:TRP:HB3	2:A:457:HOH:O	2.14	0.48
1:B:227:PRO:HG3	1:B:297:LEU:HD23	1.96	0.48
1:B:239:GLU:HG3	1:B:240:THR:HG23	1.95	0.48
1:B:384:LYS:HG2	1:B:387:GLN:NE2	2.28	0.48
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.14	0.47
1:B:185:GLY:C	1:B:186:LYS:HE3	2.34	0.47
1:B:296:LYS:HE3	1:B:298:SER:OG	2.14	0.47
1:D:158:TYR:CD2	1:D:184:GLY:HA2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:HB2	1:A:26:GLN:O	2.13	0.47
1:A:218:SER:CA	1:A:376:LEU:HD21	2.44	0.47
1:B:2:ARG:HD2	1:B:70:MET:CG	2.44	0.47
1:B:257:ASP:CG	1:B:260:GLY:H	2.18	0.47
1:C:93:LYS:HZ2	1:C:96:THR:HB	1.78	0.47
1:C:319:PRO:CG	1:C:328:LEU:HD23	2.44	0.47
1:D:59:CYS:HG	1:D:65:CYS:CB	2.24	0.47
1:A:20:THR:HB	1:B:112:ASN:OD1	2.14	0.47
1:A:297:LEU:CD1	1:A:355:LEU:HD11	2.45	0.47
1:D:348:PHE:CE2	1:D:351:LEU:HD23	2.49	0.47
1:B:269:GLY:O	1:B:271:PRO:HD3	2.15	0.47
1:B:380:TYR:HB3	1:B:392:ARG:NE	2.30	0.47
1:C:12:PRO:HB2	1:C:32:VAL:HG23	1.97	0.47
1:C:94:PHE:CD2	1:C:95:VAL:HG23	2.50	0.47
1:C:291:ARG:HB3	1:C:424:ILE:HD12	1.97	0.47
1:A:17:GLN:HA	1:A:28:VAL:HG23	1.97	0.47
1:A:155:MET:HG3	1:A:164:GLY:HA3	1.97	0.47
1:A:326:PRO:O	1:A:330:SER:OG	2.31	0.47
1:A:356:ARG:HG2	1:B:24:ASN:HD21	1.80	0.47
1:B:166:ARG:HH11	1:B:166:ARG:HB2	1.80	0.47
1:B:405:VAL:HA	1:B:408:GLN:CG	2.44	0.47
1:C:115:ASP:HA	1:C:166:ARG:HG2	1.96	0.47
1:B:65:CYS:O	1:B:69:CYS:HB2	2.15	0.47
1:B:64:ASP:HA	1:B:67:GLU:OE1	2.15	0.47
1:B:126:GLU:HB2	1:B:290:SER:O	2.14	0.47
1:A:37:ASN:OD1	1:A:181:LYS:HD2	2.15	0.47
1:A:372:ASN:HB3	1:A:400:GLY:HA3	1.95	0.47
1:B:13:PRO:O	1:B:85:THR:HG21	2.15	0.47
1:D:54:GLN:HG3	1:D:194:SER:HG	1.80	0.47
1:A:43:ASP:HB2	2:A:489:HOH:O	2.15	0.46
1:A:125:ASN:HB3	1:A:421:PHE:CZ	2.50	0.46
1:B:112:ASN:O	1:B:116:LYS:HE2	2.16	0.46
1:B:360:VAL:O	1:B:362:VAL:HG23	2.15	0.46
1:B:4:GLY:N	1:B:71:ILE:O	2.48	0.46
1:A:84:SER:CB	1:A:91:THR:HB	2.46	0.46
1:B:112:ASN:HB2	1:B:118:GLN:HA	1.95	0.46
1:B:177:ALA:HB3	1:B:180:LEU:HD12	1.97	0.46
1:B:297:LEU:HD22	1:B:348:PHE:HZ	1.80	0.46
1:D:241:THR:HG22	1:D:249:GLU:CD	2.36	0.46
1:D:377:ASP:O	1:D:395:CYS:HB2	2.15	0.46
1:B:105:GLY:O	1:B:106:SER:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:HG23	1:C:64:ASP:OD2	2.16	0.46
1:C:61:THR:OG1	1:C:64:ASP:OD2	2.30	0.46
1:C:367:ASP:OD2	1:C:406:GLU:OE2	2.32	0.46
1:D:367:ASP:OD2	1:D:406:GLU:OE2	2.34	0.46
1:A:378:SER:O	1:A:392:ARG:HB2	2.16	0.46
1:B:89:ALA:HA	1:B:416:TRP:O	2.15	0.46
1:C:18:ARG:HH11	1:C:18:ARG:HD2	1.54	0.46
1:D:147:VAL:HG23	1:D:149:MET:HG3	1.98	0.46
1:A:128:ALA:HB3	1:A:420:ARG:HG3	1.96	0.46
1:A:294:GLU:O	1:A:295:ASN:HB2	2.16	0.46
1:A:315:TRP:O	1:A:318:MET:HG3	2.16	0.46
1:B:384:LYS:O	1:B:385:GLU:O	2.33	0.46
1:D:380:TYR:CG	1:D:381:PRO:HA	2.50	0.46
1:A:92:LEU:HD21	1:A:108:PHE:CE1	2.51	0.46
1:B:2:ARG:HD2	1:B:70:MET:HG3	1.98	0.46
1:B:4:GLY:N	1:B:70:MET:HE2	2.31	0.46
1:B:20:THR:O	1:B:21:ALA:HB2	2.15	0.46
1:C:285:LYS:NZ	2:C:509:HOH:O	2.48	0.46
1:D:41:LEU:HD12	1:D:181:LYS:HZ2	1.80	0.46
1:D:291:ARG:HB3	1:D:424:ILE:HD13	1.97	0.46
1:A:74:ALA:HB1	1:A:81:TYR:CE2	2.51	0.45
1:A:223:PHE:CE2	1:A:265:PRO:HG2	2.50	0.45
1:B:37:ASN:OD1	1:B:180:LEU:HD23	2.16	0.45
1:C:405:VAL:HA	1:C:408:GLN:HG2	1.98	0.45
1:D:53:ASN:CG	1:D:194:SER:HB3	2.36	0.45
1:A:214:ASP:OD2	1:A:228:HIS:NE2	2.49	0.45
1:A:287:THR:HG21	1:A:428:TYR:CE1	2.51	0.45
1:B:218:SER:HB3	1:B:223:PHE:CB	2.46	0.45
1:B:291:ARG:NH2	1:B:430:PHE:OXT	2.49	0.45
1:B:357:VAL:HG13	1:B:358:PRO:HD2	1.98	0.45
1:A:20:THR:OG1	1:B:116:LYS:NZ	2.49	0.45
1:A:41:LEU:HA	1:A:70:MET:O	2.17	0.45
1:B:78:LEU:O	1:B:82:GLY:N	2.50	0.45
1:B:324:ILE:O	1:B:324:ILE:HG22	2.15	0.45
1:A:124:GLY:O	1:A:125:ASN:ND2	2.50	0.45
1:A:219:ASN:CG	1:A:221:TYR:H	2.20	0.45
1:B:66:ALA:HB2	1:B:182:PHE:HE1	1.81	0.45
1:B:80:THR:HB	1:B:81:TYR:CE2	2.52	0.45
1:B:116:LYS:HB3	1:B:151:GLU:HG2	1.98	0.45
1:B:121:ASN:N	2:B:548:HOH:O	2.50	0.45
1:B:328:LEU:HD22	1:B:332:MET:CG	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASN:ND2	2:C:600:HOH:O	2.50	0.45
1:C:429:ASP:C	1:D:284:ARG:HH22	2.19	0.45
1:D:329:CYS:O	1:D:333:PHE:HD1	2.00	0.45
1:A:76:ASP:CG	1:D:76:ASP:H	2.20	0.45
1:A:133:LEU:O	1:A:220:ALA:HB2	2.17	0.45
1:A:408:GLN:O	1:A:408:GLN:HG3	2.17	0.45
1:B:23:GLY:HA2	2:B:553:HOH:O	2.16	0.45
1:B:251:ARG:O	1:B:251:ARG:HG2	2.14	0.45
1:C:340:ASN:ND2	1:C:343:GLU:H	2.14	0.45
1:A:64:ASP:OD2	1:A:65:CYS:N	2.50	0.45
1:A:197:SER:OG	1:A:198:ASP:N	2.50	0.45
1:B:131:VAL:O	1:B:131:VAL:HG13	2.15	0.45
1:B:141:ASN:N	1:B:366:TRP:O	2.50	0.45
1:A:217:GLU:O	1:A:218:SER:HB3	2.15	0.45
1:B:53:ASN:HD22	1:B:194:SER:HB3	1.80	0.45
1:D:307:LYS:HB2	1:D:430:PHE:CD2	2.52	0.45
1:A:2:ARG:HA	1:A:162:GLN:HG3	1.98	0.45
1:A:287:THR:HG21	1:A:428:TYR:CZ	2.52	0.45
1:A:357:VAL:O	1:A:359:MET:HG3	2.16	0.45
1:B:137:GLU:OE2	1:B:221:TYR:HE1	2.00	0.45
1:D:76:ASP:OD2	1:D:78:LEU:N	2.50	0.45
1:D:181:LYS:HE3	1:D:181:LYS:HB2	1.29	0.45
1:A:98:HIS:ND1	1:A:101:GLY:O	2.50	0.45
1:B:55:TRP:CD1	1:B:189:ILE:HA	2.52	0.45
1:B:98:HIS:N	1:B:101:GLY:O	2.50	0.45
1:B:139:GLY:HA3	1:B:400:GLY:HA2	1.98	0.45
1:B:154:GLY:O	1:B:158:TYR:HB2	2.16	0.45
1:B:275:GLY:O	1:B:278:LYS:HG3	2.17	0.45
1:D:93:LYS:HD2	2:D:589:HOH:O	2.16	0.45
1:D:98:HIS:O	1:D:100:TYR:N	2.50	0.45
1:B:64:ASP:O	1:B:67:GLU:N	2.50	0.45
1:B:397:THR:OG1	1:B:398:ASP:N	2.50	0.45
1:D:2:ARG:NH1	1:D:67:GLU:O	2.50	0.45
1:D:11:HIS:HB3	1:D:32:VAL:O	2.17	0.45
1:D:43:ASP:OD2	1:D:45:ASN:N	2.49	0.45
1:D:380:TYR:CE1	1:D:382:PRO:HD3	2.52	0.45
1:B:53:ASN:ND2	1:B:195:SER:O	2.50	0.44
1:B:152:ASP:CG	1:B:155:MET:HB2	2.37	0.44
1:B:408:GLN:HG3	1:B:409:PHE:N	2.29	0.44
1:A:44:ASP:OD1	1:A:45:ASN:ND2	2.50	0.44
1:A:117:TYR:OH	1:A:168:GLY:HA2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:TYR:O	1:A:222:ALA:HB2	2.18	0.44
1:B:192:TRP:CZ2	1:B:202:GLY:HA3	2.52	0.44
1:C:65:CYS:HB2	1:C:187:ALA:HB2	1.98	0.44
1:C:345:VAL:O	1:C:350:GLN:HG2	2.18	0.44
1:A:92:LEU:O	1:A:413:GLN:HA	2.18	0.44
1:A:189:ILE:O	1:A:192:TRP:N	2.50	0.44
1:A:272:ASP:OD1	1:A:272:ASP:N	2.50	0.44
1:A:384:LYS:O	1:A:385:GLU:HB3	2.16	0.44
1:A:402:PRO:HB2	2:A:478:HOH:O	2.17	0.44
1:B:2:ARG:NH2	1:B:67:GLU:O	2.49	0.44
1:B:122:LEU:HD22	1:B:359:MET:CG	2.47	0.44
1:D:1:PCA:HA	1:D:66:ALA:O	2.18	0.44
1:A:3:ALA:HB1	1:A:167:TYR:HH	1.79	0.44
1:B:12:PRO:HA	1:B:13:PRO:HD3	1.89	0.44
1:B:135:THR:O	1:B:412:ALA:HA	2.18	0.44
1:B:155:MET:HE2	1:B:164:GLY:HA3	1.99	0.44
1:C:41:LEU:HD11	1:C:71:ILE:HD11	1.99	0.44
1:C:244:GLY:HA2	1:C:250:ASP:O	2.18	0.44
1:A:312:PRO:HG2	1:A:320:ASN:HD21	1.82	0.44
1:B:198:ASP:HB3	1:B:201:ALA:CB	2.47	0.44
1:B:222:ALA:HB3	1:B:376:LEU:O	2.17	0.44
1:B:318:MET:CE	1:B:335:VAL:HG21	2.47	0.44
1:B:341:ARG:O	1:B:344:GLU:N	2.50	0.44
1:C:257:ASP:HA	1:C:341:ARG:HG3	1.98	0.44
1:A:414:VAL:HG11	1:A:416:TRP:NE1	2.32	0.44
1:B:266:TYR:OH	1:B:394:ASP:OD1	2.29	0.44
1:B:267:ARG:HD3	1:B:336:PHE:HE2	1.83	0.44
1:C:98:HIS:HB2	1:C:101:GLY:CA	2.47	0.44
1:C:380:TYR:CG	1:C:381:PRO:HA	2.52	0.44
1:A:5:ASN:N	1:A:72:GLU:OE2	2.50	0.44
1:A:384:LYS:HD2	1:A:384:LYS:HA	1.76	0.44
1:B:42:HIS:ND1	1:B:43:ASP:O	2.50	0.44
1:B:61:THR:N	1:B:64:ASP:OD2	2.50	0.44
1:C:16:TRP:HB2	1:C:419:ILE:HB	1.99	0.44
1:C:306:ARG:NH1	1:D:130:ASP:OD2	2.50	0.44
1:D:207:GLY:HA3	1:D:238:CYS:SG	2.57	0.44
1:A:348:PHE:O	1:A:352:ASN:N	2.50	0.44
1:B:76:ASP:CG	1:C:76:ASP:HA	2.38	0.44
1:B:341:ARG:NE	2:B:434:HOH:O	2.50	0.44
1:C:48:ASN:ND2	1:C:51:ASP:OD1	2.50	0.44
1:C:373:MET:HG3	1:C:376:LEU:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ARG:O	1:A:344:GLU:N	2.50	0.44
1:C:306:ARG:HH12	1:D:418:ASN:HD22	1.66	0.44
1:D:297:LEU:HD11	1:D:355:LEU:HD11	2.00	0.44
1:B:195:SER:CB	1:B:201:ALA:HB3	2.48	0.43
1:C:41:LEU:CD2	1:C:71:ILE:HG12	2.48	0.43
1:D:144:LEU:HD21	1:D:361:LEU:HD11	2.00	0.43
1:A:273:PHE:CD1	1:A:279:THR:HB	2.53	0.43
1:B:383:GLU:H	1:B:383:GLU:HG2	1.24	0.43
1:C:349:GLU:OE2	1:C:352:ASN:HB2	2.18	0.43
1:A:141:ASN:HB2	1:A:373:MET:SD	2.58	0.43
1:A:188:ASN:HB3	1:A:192:TRP:CZ3	2.53	0.43
1:C:295:ASN:HA	1:C:348:PHE:CE2	2.53	0.43
1:A:53:ASN:O	1:A:54:GLN:HG2	2.19	0.43
1:B:352:ASN:O	1:B:356:ARG:HG3	2.19	0.43
1:C:41:LEU:CG	1:C:71:ILE:HG12	2.46	0.43
1:C:49:CYS:HA	1:C:58:ALA:HB3	1.99	0.43
1:C:57:ASN:ND2	2:C:606:HOH:O	2.50	0.43
1:A:30:ALA:O	1:A:31:GLU:HB3	2.18	0.43
1:B:38:TRP:CE2	1:B:106:SER:HA	2.54	0.43
1:B:103:ASN:OD1	1:B:104:VAL:N	2.52	0.43
1:C:64:ASP:OD1	1:C:68:LYS:NZ	2.50	0.43
1:D:109:TYR:CD1	1:D:362:VAL:HG22	2.53	0.43
1:D:213:ILE:N	1:D:213:ILE:HD12	2.34	0.43
1:B:14:LEU:HD12	1:B:14:LEU:HA	1.75	0.43
1:B:96:THR:CG2	1:B:103:ASN:HB3	2.49	0.43
1:B:182:PHE:HB2	2:B:563:HOH:O	2.19	0.43
1:B:310:ILE:O	1:B:322:SER:HB3	2.19	0.43
1:C:9:GLU:CD	1:C:39:ARG:HH12	2.22	0.43
1:C:34:ILE:HB	1:C:108:PHE:CE2	2.53	0.43
1:C:147:VAL:HG23	1:C:149:MET:HG3	2.00	0.43
1:A:164:GLY:O	1:A:169:THR:HG23	2.18	0.43
1:A:404:GLU:O	1:A:408:GLN:HB3	2.19	0.43
1:B:155:MET:CE	1:B:166:ARG:HD2	2.49	0.43
1:A:395:CYS:HA	1:A:396:PRO:HD3	1.85	0.43
1:B:97:LYS:HB3	1:B:102:THR:OG1	2.17	0.43
1:B:144:LEU:CD2	1:B:361:LEU:HD11	2.45	0.43
1:B:296:LYS:HE3	2:B:504:HOH:O	2.19	0.43
1:D:79:GLY:O	1:D:98:HIS:HB3	2.19	0.43
1:B:53:ASN:OD1	1:B:53:ASN:N	2.51	0.43
1:C:389:GLY:HA3	2:C:507:HOH:O	2.19	0.43
1:C:418:ASN:HD21	1:C:420:ARG:HH21	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LEU:HG	1:D:84:SER:HB3	1.99	0.43
1:B:264:ASN:OD1	1:B:266:TYR:N	2.49	0.43
1:C:61:THR:HG1	1:C:64:ASP:H	1.66	0.43
1:A:161:ASN:OD1	1:A:164:GLY:N	2.49	0.42
1:A:329:CYS:SG	1:A:348:PHE:HE1	2.42	0.42
1:A:363:MET:HG2	1:A:416:TRP:CG	2.54	0.42
1:B:76:ASP:CB	1:C:76:ASP:HA	2.46	0.42
1:A:36:ALA:HA	1:A:39:ARG:HG3	2.00	0.42
1:A:297:LEU:HD11	1:A:355:LEU:HD11	2.01	0.42
1:B:231:THR:HG22	1:B:345:VAL:O	2.19	0.42
1:B:295:ASN:ND2	1:B:326:PRO:HG2	2.34	0.42
1:A:178:ARG:CG	1:A:247:TYR:HB2	2.46	0.42
1:B:4:GLY:HA3	1:B:71:ILE:O	2.20	0.42
1:B:152:ASP:O	1:B:155:MET:HG3	2.19	0.42
1:C:39:ARG:HD3	1:C:72:GLU:O	2.19	0.42
1:D:2:ARG:O	1:D:70:MET:HA	2.19	0.42
1:D:43:ASP:OD1	1:D:47:GLN:N	2.50	0.42
1:D:59:CYS:CB	1:D:65:CYS:HG	2.27	0.42
1:D:348:PHE:CZ	1:D:351:LEU:HD23	2.54	0.42
1:A:139:GLY:HA2	1:A:400:GLY:HA2	2.01	0.42
1:A:160:SER:OG	1:A:185:GLY:O	2.29	0.42
1:A:234:GLU:CD	1:A:234:GLU:H	2.22	0.42
1:B:257:ASP:OD1	1:B:259:ASN:HB3	2.19	0.42
1:B:293:GLU:OE1	1:B:424:ILE:HD13	2.20	0.42
1:C:277:GLY:HA2	1:C:281:ASP:OD2	2.19	0.42
1:D:334:ASP:HB2	1:D:335:VAL:H	1.64	0.42
1:A:280:LEU:HD22	1:A:280:LEU:HA	1.87	0.42
1:B:36:ALA:O	1:B:39:ARG:N	2.50	0.42
1:B:198:ASP:HB2	1:B:369:HIS:CE1	2.54	0.42
1:C:136:VAL:HG12	1:C:219:ASN:CB	2.50	0.42
1:A:219:ASN:ND2	1:A:221:TYR:HD1	2.18	0.42
1:A:257:ASP:OD1	1:A:341:ARG:HB3	2.19	0.42
1:B:149:MET:HB2	1:B:360:VAL:CG2	2.49	0.42
1:B:234:GLU:H	1:B:234:GLU:HG2	1.22	0.42
1:C:272:ASP:OD1	1:C:278:LYS:NZ	2.49	0.42
1:D:9:GLU:OE1	1:D:77:TYR:OH	2.33	0.42
1:A:221:TYR:CE1	1:A:276:LYS:HE3	2.55	0.42
1:A:229:ALA:HB2	1:A:351:LEU:HA	2.02	0.42
1:B:6:GLU:N	1:B:72:GLU:OE2	2.49	0.42
1:B:122:LEU:HD22	1:B:359:MET:SD	2.60	0.42
1:D:176:CYS:HA	1:D:208:SER:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:HB3	1:A:415:VAL:CG2	2.50	0.42
1:B:76:ASP:OD2	1:B:76:ASP:O	2.37	0.42
1:B:412:ALA:O	1:B:413:GLN:HB3	2.20	0.42
1:B:77:TYR:O	1:B:81:TYR:HB2	2.19	0.42
1:B:178:ARG:O	1:B:203:VAL:HA	2.20	0.42
1:B:195:SER:HB2	1:B:201:ALA:HB3	2.01	0.42
1:B:270:ASN:ND2	1:B:311:PRO:HB2	2.34	0.42
1:B:300:TYR:CG	1:B:307:LYS:HE3	2.54	0.42
1:C:405:VAL:HA	1:C:408:GLN:CG	2.49	0.42
1:D:49:CYS:C	1:D:56:THR:HG23	2.40	0.42
1:A:36:ALA:O	1:A:39:ARG:HG3	2.20	0.41
1:B:196:THR:N	2:B:570:HOH:O	2.52	0.41
1:C:6:GLU:HB2	1:C:72:GLU:CD	2.40	0.41
1:C:40:TRP:CE3	1:C:72:GLU:HG3	2.55	0.41
1:C:96:THR:HG23	2:C:550:HOH:O	2.19	0.41
1:B:1:PCA:N	1:B:161:ASN:HA	2.35	0.41
1:B:26:GLN:H	1:B:26:GLN:HG3	1.64	0.41
1:B:147:VAL:HG13	1:B:212:GLU:HG3	2.02	0.41
1:B:289:VAL:HG21	1:B:300:TYR:CE1	2.55	0.41
1:C:187:ALA:HB3	1:C:189:ILE:HG22	2.01	0.41
1:A:277:GLY:HA2	1:A:281:ASP:CG	2.39	0.41
1:B:83:ALA:HA	1:B:91:THR:O	2.20	0.41
1:B:193:LYS:HD2	1:B:193:LYS:HA	1.69	0.41
1:B:295:ASN:O	1:B:325:THR:HG22	2.20	0.41
1:C:402:PRO:HA	1:C:405:VAL:HG22	2.01	0.41
1:D:310:ILE:HA	1:D:311:PRO:HD3	1.96	0.41
1:A:82:GLY:CA	1:A:96:THR:HG21	2.51	0.41
1:A:96:THR:O	1:A:102:THR:HA	2.19	0.41
1:A:266:TYR:HB3	1:A:392:ARG:O	2.21	0.41
1:B:53:ASN:HB2	1:B:194:SER:OG	2.20	0.41
1:C:65:CYS:HB2	1:C:187:ALA:CB	2.51	0.41
1:C:215:VAL:HA	1:C:225:PHE:CE2	2.56	0.41
1:A:14:LEU:HD12	1:A:85:THR:OG1	2.21	0.41
1:A:374:LEU:HD23	1:A:378:SER:HB3	2.01	0.41
1:B:55:TRP:NE1	1:B:189:ILE:HA	2.36	0.41
1:B:83:ALA:HB2	1:B:92:LEU:HD23	2.02	0.41
1:B:139:GLY:HA2	1:B:373:MET:CB	2.50	0.41
1:C:1:PCA:HB2	1:C:71:ILE:HG13	2.01	0.41
1:A:182:PHE:HA	1:A:186:LYS:O	2.21	0.41
1:A:208:SER:HB2	1:A:235:TYR:HE1	1.81	0.41
1:A:263:TYR:CE1	1:A:322:SER:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASN:HA	1:A:348:PHE:CD2	2.56	0.41
1:B:126:GLU:HA	1:B:290:SER:O	2.20	0.41
1:B:144:LEU:HG	1:B:362:VAL:O	2.20	0.41
1:B:195:SER:HB3	1:B:198:ASP:O	2.20	0.41
1:B:261:CYS:HA	1:B:332:MET:HE1	2.02	0.41
1:B:266:TYR:CE2	1:B:271:PRO:HB3	2.55	0.41
1:D:212:GLU:OE2	1:D:214:ASP:OD1	2.38	0.41
1:A:152:ASP:OD2	1:A:156:ALA:N	2.53	0.41
1:A:414:VAL:HG11	1:A:416:TRP:CE2	2.56	0.41
1:B:114:PRO:O	1:B:166:ARG:HB3	2.20	0.41
1:B:263:TYR:HA	1:B:268:MET:HE2	2.02	0.41
1:B:379:ILE:HD12	1:B:379:ILE:N	2.36	0.41
1:C:294:GLU:O	1:C:294:GLU:HG2	2.21	0.41
1:C:377:ASP:O	1:C:395:CYS:HB2	2.20	0.41
1:A:127:LEU:HB2	1:A:421:PHE:HD1	1.86	0.41
1:A:147:VAL:CG1	1:A:212:GLU:HG3	2.50	0.41
1:A:252:PHE:HE2	1:A:259:ASN:ND2	2.18	0.41
1:A:266:TYR:N	2:A:541:HOH:O	2.53	0.41
1:D:361:LEU:HD12	1:D:362:VAL:N	2.35	0.41
1:B:71:ILE:HD13	1:B:71:ILE:HG21	1.86	0.41
1:C:263:TYR:CE1	1:C:322:SER:HA	2.56	0.41
1:A:223:PHE:CZ	1:A:301:PHE:HZ	2.39	0.40
1:A:341:ARG:O	1:A:341:ARG:HG3	2.20	0.40
1:B:175:GLN:HG3	1:B:258:ALA:CB	2.46	0.40
1:B:243:CYS:O	1:B:253:ALA:HB3	2.20	0.40
1:C:98:HIS:ND1	1:C:102:THR:N	2.69	0.40
1:D:381:PRO:HA	1:D:382:PRO:HD3	1.87	0.40
1:A:367:ASP:OD1	1:A:367:ASP:N	2.50	0.40
1:C:268:MET:HB2	2:C:600:HOH:O	2.20	0.40
1:D:125:ASN:ND2	2:D:598:HOH:O	2.49	0.40
1:B:53:ASN:ND2	1:B:194:SER:HB3	2.37	0.40
1:B:93:LYS:HA	1:B:413:GLN:HB3	2.03	0.40
1:B:111:MET:HA	1:B:118:GLN:H	1.87	0.40
1:B:284:ARG:HB3	1:B:303:GLN:NE2	2.36	0.40
1:B:291:ARG:HB3	1:B:424:ILE:CG1	2.51	0.40
1:C:265:PRO:HA	2:C:600:HOH:O	2.20	0.40
1:D:139:GLY:HA3	1:D:400:GLY:HA2	2.03	0.40
1:D:383:GLU:OE2	1:D:383:GLU:HA	2.21	0.40
1:B:143:ALA:CB	1:B:366:TRP:HE1	2.33	0.40
1:B:175:GLN:OE1	1:B:258:ALA:HA	2.22	0.40
1:D:41:LEU:HD22	1:D:69:CYS:CB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HG3	1:A:247:TYR:CB	2.48	0.40
1:A:356:ARG:CB	1:B:24:ASN:HD21	2.33	0.40
1:B:127:LEU:HD22	1:B:146:PHE:CZ	2.56	0.40
1:B:349:GLU:O	1:B:352:ASN:N	2.54	0.40
1:D:307:LYS:HE3	1:D:430:PHE:O	2.20	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	428/430 (100%)	356 (83%)	52 (12%)	20 (5%)	2 0
1	B	428/430 (100%)	356 (83%)	57 (13%)	15 (4%)	3 0
1	C	428/430 (100%)	409 (96%)	15 (4%)	4 (1%)	17 4
1	D	428/430 (100%)	398 (93%)	24 (6%)	6 (1%)	11 2
All	All	1712/1720 (100%)	1519 (89%)	148 (9%)	45 (3%)	5 0

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ALA
1	A	190	GLU
1	A	240	THR
1	A	337	ASN
1	A	399	SER
1	B	4	GLY
1	B	24	ASN
1	B	29	ASN
1	B	46	MET
1	B	429	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	384	LYS
1	D	99	GLU
1	D	385	GLU
1	A	60	SER
1	A	189	ILE
1	A	210	CYS
1	A	339	ARG
1	A	385	GLU
1	B	23	GLY
1	B	196	THR
1	B	210	CYS
1	B	296	LYS
1	B	385	GLU
1	C	240	THR
1	D	334	ASP
1	D	382	PRO
1	A	94	PHE
1	A	402	PRO
1	B	214	ASP
1	B	418	ASN
1	C	98	HIS
1	C	176	CYS
1	A	31	GLU
1	A	43	ASP
1	A	328	LEU
1	A	429	ASP
1	B	249	GLU
1	D	176	CYS
1	A	148	ALA
1	B	176	CYS
1	B	384	LYS
1	D	87	GLY
1	A	79	GLY
1	A	338	ASP
1	A	105	GLY

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	354/354 (100%)	286 (81%)	68 (19%)	1 0
1	B	354/354 (100%)	266 (75%)	88 (25%)	0 0
1	C	354/354 (100%)	319 (90%)	35 (10%)	8 1
1	D	354/354 (100%)	327 (92%)	27 (8%)	13 2
All	All	1416/1416 (100%)	1198 (85%)	218 (15%)	2 0

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	14	LEU
1	A	18	ARG
1	A	27	THR
1	A	39	ARG
1	A	40	TRP
1	A	45	ASN
1	A	46	MET
1	A	54	GLN
1	A	57	ASN
1	A	59	CYS
1	A	60	SER
1	A	61	THR
1	A	68	LYS
1	A	71	ILE
1	A	76	ASP
1	A	78	LEU
1	A	84	SER
1	A	85	THR
1	A	86	SER
1	A	96	THR
1	A	97	LYS
1	A	103	ASN
1	A	116	LYS
1	A	127	LEU
1	A	133	LEU
1	A	162	GLN
1	A	166	ARG
1	A	167	TYR
1	A	175	GLN
1	A	178	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	189	ILE
1	A	196	THR
1	A	198	ASP
1	A	225	PHE
1	A	240	THR
1	A	246	THR
1	A	251	ARG
1	A	270	ASN
1	A	272	ASP
1	A	276	LYS
1	A	280	LEU
1	A	284	ARG
1	A	288	VAL
1	A	289	VAL
1	A	292	PHE
1	A	297	LEU
1	A	298	SER
1	A	306	ARG
1	A	308	ILE
1	A	318	MET
1	A	322	SER
1	A	328	LEU
1	A	330	SER
1	A	334	ASP
1	A	338	ASP
1	A	340	ASN
1	A	341	ARG
1	A	343	GLU
1	A	348	PHE
1	A	362	VAL
1	A	363	MET
1	A	366	TRP
1	A	384	LYS
1	A	392	ARG
1	A	408	GLN
1	A	411	ASP
1	A	420	ARG
1	B	5	ASN
1	B	15	THR
1	B	18	ARG
1	B	20	THR
1	B	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	27	THR
1	B	28	VAL
1	B	29	ASN
1	B	34	ILE
1	B	51	ASP
1	B	53	ASN
1	B	54	GLN
1	B	59	CYS
1	B	61	THR
1	B	68	LYS
1	B	71	ILE
1	B	76	ASP
1	B	78	LEU
1	B	80	THR
1	B	85	THR
1	B	86	SER
1	B	92	LEU
1	B	93	LYS
1	B	95	VAL
1	B	96	THR
1	B	104	VAL
1	B	111	MET
1	B	116	LYS
1	B	123	MET
1	B	126	GLU
1	B	130	ASP
1	B	133	LEU
1	B	142	SER
1	B	147	VAL
1	B	155	MET
1	B	162	GLN
1	B	166	ARG
1	B	175	GLN
1	B	186	LYS
1	B	189	ILE
1	B	190	GLU
1	B	193	LYS
1	B	194	SER
1	B	196	THR
1	B	200	ASN
1	B	203	VAL
1	B	208	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	214	ASP
1	B	218	SER
1	B	219	ASN
1	B	234	GLU
1	B	242	ASN
1	B	251	ARG
1	B	267	ARG
1	B	283	SER
1	B	285	LYS
1	B	293	GLU
1	B	294	GLU
1	B	296	LYS
1	B	297	LEU
1	B	298	SER
1	B	306	ARG
1	B	310	ILE
1	B	316	GLU
1	B	320	ASN
1	B	321	SER
1	B	328	LEU
1	B	332	MET
1	B	335	VAL
1	B	340	ASN
1	B	341	ARG
1	B	345	VAL
1	B	356	ARG
1	B	359	MET
1	B	365	ILE
1	B	373	MET
1	B	376	LEU
1	B	378	SER
1	B	383	GLU
1	B	384	LYS
1	B	385	GLU
1	B	392	ARG
1	B	398	ASP
1	B	405	VAL
1	B	408	GLN
1	B	409	PHE
1	B	424	ILE
1	B	429	ASP
1	C	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	26	GLN
1	C	32	VAL
1	C	39	ARG
1	C	41	LEU
1	C	43	ASP
1	C	45	ASN
1	C	46	MET
1	C	51	ASP
1	C	54	GLN
1	C	64	ASP
1	C	77	TYR
1	C	78	LEU
1	C	96	THR
1	C	99	GLU
1	C	100	TYR
1	C	115	ASP
1	C	122	LEU
1	C	189	ILE
1	C	190	GLU
1	C	193	LYS
1	C	234	GLU
1	C	272	ASP
1	C	276	LYS
1	C	281	ASP
1	C	285	LYS
1	C	294	GLU
1	C	328	LEU
1	C	330	SER
1	C	340	ASN
1	C	348	PHE
1	C	349	GLU
1	C	385	GLU
1	C	394	ASP
1	C	419	ILE
1	D	2	ARG
1	D	5	ASN
1	D	18	ARG
1	D	37	ASN
1	D	51	ASP
1	D	57	ASN
1	D	60	SER
1	D	76	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	78	LEU
1	D	93	LYS
1	D	97	LYS
1	D	115	ASP
1	D	122	LEU
1	D	155	MET
1	D	181	LYS
1	D	190	GLU
1	D	193	LYS
1	D	246	THR
1	D	266	TYR
1	D	284	ARG
1	D	285	LYS
1	D	294	GLU
1	D	332	MET
1	D	340	ASN
1	D	385	GLU
1	D	398	ASP
1	D	424	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	GLN
1	A	24	ASN
1	A	29	ASN
1	A	42	HIS
1	A	125	ASN
1	A	175	GLN
1	A	270	ASN
1	A	320	ASN
1	A	340	ASN
1	A	352	ASN
1	A	369	HIS
1	A	387	GLN
1	A	408	GLN
1	B	5	ASN
1	B	24	ASN
1	B	26	GLN
1	B	29	ASN
1	B	200	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	270	ASN
1	B	320	ASN
1	B	340	ASN
1	B	352	ASN
1	B	369	HIS
1	B	372	ASN
1	C	29	ASN
1	C	125	ASN
1	C	162	GLN
1	C	320	ASN
1	C	340	ASN
1	C	352	ASN
1	C	353	ASN
1	C	369	HIS
1	C	387	GLN
1	D	5	ASN
1	D	57	ASN
1	D	125	ASN
1	D	320	ASN
1	D	340	ASN
1	D	352	ASN
1	D	353	ASN
1	D	369	HIS
1	D	408	GLN
1	D	413	GLN
1	D	418	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	B	1	1	7,8,9	2.22	1 (14%)	9,10,12	1.74	4 (44%)
1	PCA	C	1	1	7,8,9	2.06	1 (14%)	9,10,12	1.53	2 (22%)
1	PCA	A	1	1	7,8,9	2.11	1 (14%)	9,10,12	1.59	2 (22%)
1	PCA	D	1	1	7,8,9	1.98	1 (14%)	9,10,12	1.34	1 (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
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	CD-N	5.48	1.48	1.34
1	A	1	PCA	CD-N	5.14	1.47	1.34
1	C	1	PCA	CD-N	4.97	1.46	1.34
1	D	1	PCA	CD-N	4.89	1.46	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	PCA	CB-CA-C	-3.03	108.50	112.66
1	B	1	PCA	CB-CG-CD	2.95	108.97	104.41
1	B	1	PCA	OE-CD-CG	-2.66	121.97	126.72
1	C	1	PCA	OE-CD-CG	-2.64	122.01	126.72
1	A	1	PCA	CB-CA-C	-2.54	109.17	112.66
1	A	1	PCA	CB-CG-CD	2.36	108.07	104.41
1	C	1	PCA	CB-CG-CD	2.29	107.96	104.41
1	B	1	PCA	CB-CA-C	-2.04	109.86	112.66
1	B	1	PCA	CG-CD-N	-2.02	103.44	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	PCA	1	0
1	C	1	PCA	1	0
1	A	1	PCA	1	0
1	D	1	PCA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	429/430 (99%)	0.25	7 (1%)	72	71	14, 27, 42, 58	0
1	B	429/430 (99%)	0.29	12 (2%)	53	50	13, 28, 44, 70	0
1	C	429/430 (99%)	-0.46	1 (0%)	95	94	5, 13, 28, 62	0
1	D	429/430 (99%)	-0.50	1 (0%)	95	94	4, 12, 26, 62	0
All	All	1716/1720 (99%)	-0.10	21 (1%)	79	78	4, 21, 40, 70	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	382	PRO	5.8
1	B	101	GLY	4.9
1	D	100	TYR	3.8
1	B	100	TYR	3.7
1	B	192	TRP	3.4
1	A	192	TRP	3.2
1	B	375	TRP	3.1
1	A	300	TYR	3.0
1	B	428	TYR	2.9
1	A	289	VAL	2.7
1	B	76	ASP	2.5
1	B	222	ALA	2.5
1	B	254	GLY	2.5
1	A	389	GLY	2.4
1	A	345	VAL	2.3
1	B	273	PHE	2.3
1	B	244	GLY	2.3
1	A	366	TRP	2.2
1	B	96	THR	2.2
1	A	62	ALA	2.1
1	B	354	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	PCA	A	1	8/9	0.93	0.14	12,23,30,58	0
1	PCA	B	1	8/9	0.93	0.08	16,28,39,63	0
1	PCA	C	1	8/9	0.96	0.07	13,17,21,21	0
1	PCA	D	1	8/9	0.97	0.08	6,11,19,20	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.