



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:38 pm BST

PDB ID : 4PRG
Title : 0072 PARTIAL AGONIST PPAR GAMMA COCRYSTAL
Authors : Milburn, M.V.
Deposited on : 1999-05-07
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

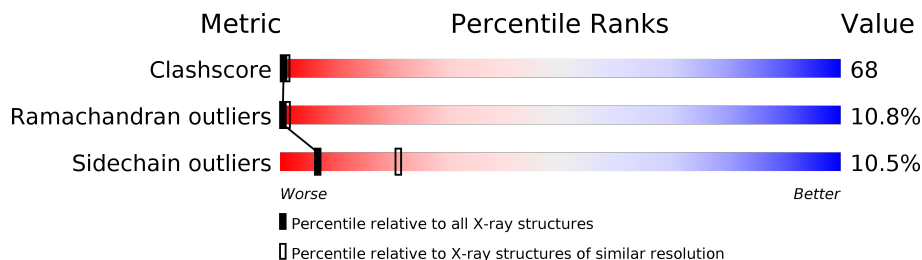
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	270	 20% 63% 15% .
1	B	270	 20% 65% 14% .
1	C	270	 17% 68% 14% .
1	D	270	 22% 65% 12% .

2 Entry composition [i](#)

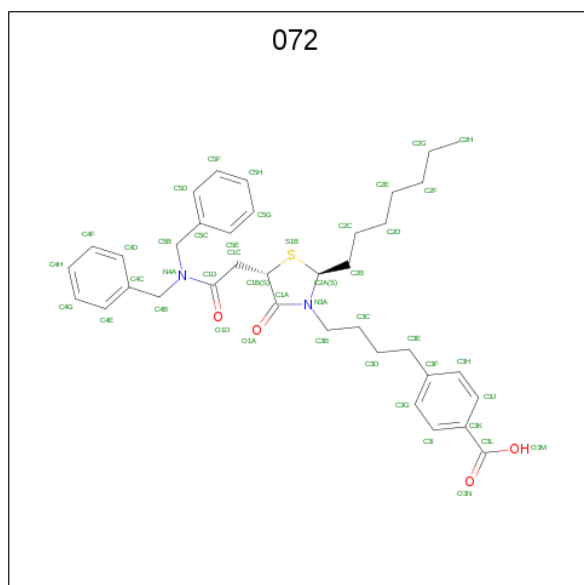
There are 2 unique types of molecules in this entry. The entry contains 8840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	Total 2166	C 1397	N 354	O 405	S 10	0	0	0
1	B	270	Total 2166	C 1397	N 354	O 405	S 10	0	0	0
1	C	270	Total 2166	C 1397	N 354	O 405	S 10	0	0	0
1	D	270	Total 2166	C 1397	N 354	O 405	S 10	0	0	0

- Molecule 2 is (+/-)-(2S,5S)-3-(4-(4-CARBOXYPHENYL)BUTYL)-2-HEPTYL-4-OXO-5-T HIAZOLIDINE (three-letter code: 072) (formula: C₃₇H₄₆N₂O₄S).

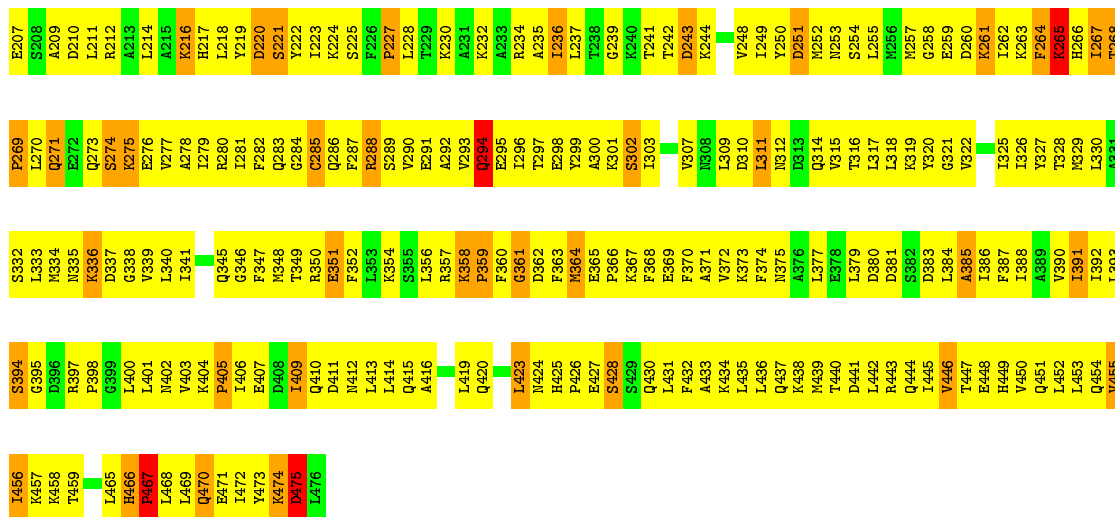
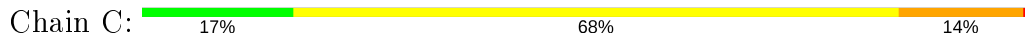


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 44	C 37	N 2	O 4	S 1	0	0

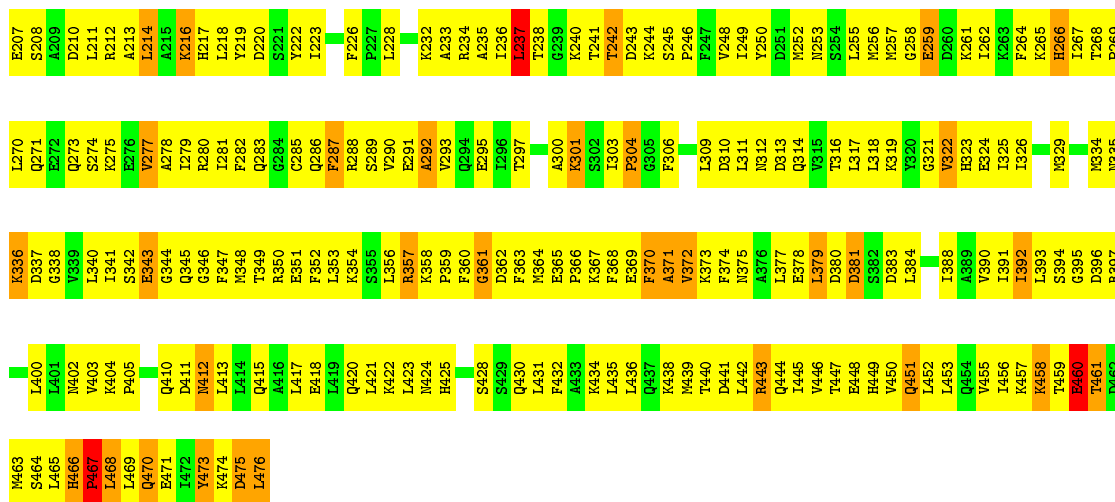
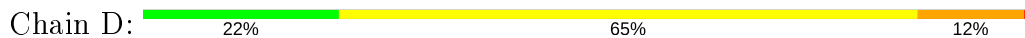
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			44	37	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			44	37	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			44	37	2	4	1		



● Molecule 1: PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.72Å 61.54Å 118.81Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 19.88 – 2.59	Depositor EDS
% Data completeness (in resolution range)	78.6 (10.00-2.90) 71.1 (19.88-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.59Å)	Xtrriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.240 , 0.283 0.275 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtrriage
Anisotropy	0.527	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 92.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9712e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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:
072

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	0.46	0/2203	0.71	1/2967 (0.0%)
1	B	0.45	0/2203	0.72	0/2967
1	C	0.46	0/2203	0.72	0/2967
1	D	0.49	0/2203	0.73	0/2967
All	All	0.46	0/8812	0.72	1/11868 (0.0%)

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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	270	LEU	CA-CB-CG	5.65	128.31	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	473	TYR	Sidechain

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	2166	0	2232	312	0
1	B	2166	0	2232	305	0
1	C	2166	0	2232	325	0
1	D	2166	0	2232	301	1
2	A	44	0	45	6	0
2	B	44	0	45	4	0
2	C	44	0	45	4	0
2	D	44	0	45	1	0
All	All	8840	0	9108	1220	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 68.

All (1220) 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:400:LEU:HD12	1:A:403:VAL:HG22	1.27	1.10
1:D:290:VAL:HG21	1:D:473:TYR:HD1	1.17	1.08
1:D:452:LEU:O	1:D:456:ILE:HG12	1.54	1.07
1:C:320:TYR:HB2	1:C:397:ARG:HH11	1.22	1.02
1:D:259:GLU:HA	1:D:262:ILE:HG22	1.35	1.02
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.36	1.02
1:B:311:LEU:HD12	1:B:311:LEU:H	1.24	1.01
1:C:212:ARG:HH11	1:C:423:LEU:HD13	1.26	0.99
1:B:419:LEU:HA	1:B:422:LYS:HD2	1.41	0.99
1:A:212:ARG:O	1:A:216:LYS:HD3	1.60	0.99
1:A:288:ARG:NH1	1:A:289:SER:HA	1.77	0.99
1:C:276:GLU:O	1:C:280:ARG:HB2	1.64	0.98
1:C:358:LYS:H	1:C:358:LYS:HE2	1.29	0.97
1:D:259:GLU:HB3	1:D:269:PRO:HD3	1.49	0.94
1:D:233:ALA:O	1:D:237:LEU:HB2	1.68	0.94
1:C:370:PHE:HD1	1:C:373:LYS:HZ1	1.00	0.93
1:C:271:GLN:O	1:C:276:GLU:HA	1.69	0.93
1:B:462:ASP:HB3	1:D:423:LEU:HB3	1.51	0.93
1:B:279:ILE:HD12	1:B:279:ILE:H	1.34	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:GLU:HA	1:C:294:GLN:HG2	1.49	0.92
1:C:357:ARG:HG2	1:C:359:PRO:HD2	1.48	0.92
1:C:212:ARG:NH1	1:C:423:LEU:HD13	1.84	0.92
1:D:290:VAL:HG21	1:D:473:TYR:CD1	2.04	0.91
1:D:358:LYS:HD2	1:D:358:LYS:H	1.35	0.91
1:D:460:GLU:HG2	1:D:463:MET:SD	2.11	0.91
1:A:288:ARG:C	1:A:288:ARG:HD2	1.91	0.91
1:C:286:GLN:HA	1:C:289:SER:OG	1.71	0.90
1:D:270:LEU:HB3	1:D:274:SER:HB3	1.51	0.90
1:D:402:ASN:O	1:D:405:PRO:HD2	1.73	0.89
1:C:370:PHE:HA	1:C:373:LYS:HE3	1.54	0.89
1:A:454:GLN:HG2	1:A:475:ASP:OD2	1.73	0.89
1:A:448:GLU:O	1:A:451:GLN:HG2	1.73	0.88
1:C:212:ARG:O	1:C:216:LYS:HD3	1.73	0.88
1:D:447:THR:O	1:D:450:VAL:HG22	1.73	0.88
1:D:288:ARG:NH2	1:D:342:SER:HA	1.89	0.87
1:C:442:LEU:O	1:C:446:VAL:HG23	1.72	0.87
1:A:271:GLN:O	1:A:276:GLU:HA	1.75	0.87
1:B:466:HIS:CB	1:B:470:GLN:HB2	2.05	0.87
1:C:440:THR:HG23	1:C:441:ASP:H	1.39	0.87
1:D:476:LEU:H	1:D:476:LEU:HD23	1.39	0.87
1:C:268:THR:H	1:C:269:PRO:HD2	1.38	0.86
1:A:270:LEU:HD22	1:A:271:GLN:H	1.41	0.85
1:A:469:LEU:HD12	1:A:472:ILE:HD11	1.58	0.85
1:B:212:ARG:HA	1:B:212:ARG:NH1	1.91	0.84
1:B:234:ARG:HH12	1:B:237:LEU:HD13	1.42	0.84
1:B:312:ASN:N	1:B:312:ASN:HD22	1.73	0.84
1:C:437:GLN:O	1:C:440:THR:HG22	1.77	0.84
1:B:321:GLY:O	1:B:325:ILE:HG12	1.77	0.83
1:C:294:GLN:HE21	1:C:294:GLN:HA	1.41	0.83
1:A:256:MET:HA	1:A:259:GLU:HG3	1.60	0.83
1:C:212:ARG:HH21	1:C:216:LYS:HE3	1.44	0.83
1:D:259:GLU:OE2	1:D:264:PHE:HB3	1.79	0.82
1:D:252:MET:O	1:D:255:LEU:HB3	1.78	0.82
1:C:290:VAL:O	1:C:293:VAL:HB	1.80	0.82
1:D:343:GLU:HB3	1:D:345:GLN:HG2	1.61	0.81
1:B:381:ASP:HA	1:B:384:LEU:HD13	1.63	0.80
1:D:288:ARG:HH21	1:D:342:SER:HA	1.45	0.80
1:D:208:SER:HA	1:D:211:LEU:HD12	1.62	0.80
1:D:311:LEU:H	1:D:311:LEU:HD12	1.44	0.79
1:C:287:PHE:O	1:C:290:VAL:HG12	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:O	1:B:341:ILE:HD12	1.82	0.79
1:D:264:PHE:CZ	1:D:266:HIS:HB3	2.18	0.79
1:B:439:MET:HA	1:B:442:LEU:HD12	1.64	0.79
1:C:419:LEU:HG	1:C:423:LEU:HD11	1.64	0.79
1:A:425:HIS:HB3	1:A:428:SER:HB2	1.63	0.79
1:C:449:HIS:NE2	1:C:453:LEU:HD12	1.98	0.79
1:C:232:LYS:O	1:C:236:ILE:HD12	1.83	0.78
1:D:357:ARG:HG2	1:D:358:LYS:N	1.97	0.78
1:A:359:PRO:HG2	1:A:360:PHE:HD1	1.48	0.78
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.65	0.78
1:B:380:ASP:O	1:B:384:LEU:HD12	1.83	0.78
1:B:476:LEU:H	1:B:476:LEU:HD22	1.49	0.78
1:C:341:ILE:HD13	1:C:348:MET:HB2	1.66	0.77
1:A:350:ARG:NH2	1:A:368:PHE:HB2	2.00	0.77
1:A:465:LEU:HD21	1:A:473:TYR:HD2	1.50	0.77
1:B:411:ASP:O	1:B:415:GLN:HG3	1.85	0.77
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.67	0.77
1:A:220:ASP:O	1:A:223:ILE:HB	1.85	0.77
1:C:207:GLU:HG2	1:C:209:ALA:H	1.50	0.77
1:B:288:ARG:HH12	1:B:343:GLU:H	1.30	0.77
1:A:290:VAL:O	1:A:294:GLN:HG2	1.84	0.76
1:A:460:GLU:O	1:A:463:MET:HB3	1.84	0.76
1:B:258:GLY:HA2	1:B:261:LYS:HD2	1.65	0.76
1:D:289:SER:O	1:D:292:ALA:HB3	1.85	0.76
1:B:212:ARG:HH11	1:B:212:ARG:HA	1.49	0.76
1:C:320:TYR:OH	1:C:398:PRO:HB2	1.86	0.76
1:D:430:GLN:O	1:D:434:LYS:HG3	1.86	0.76
1:A:430:GLN:HG2	1:B:414:LEU:HD12	1.67	0.76
1:A:212:ARG:HE	1:A:216:LYS:HE3	1.51	0.76
1:B:355:SER:O	1:B:356:LEU:HD23	1.86	0.76
1:A:252:MET:HB3	1:A:256:MET:CE	2.15	0.76
1:A:439:MET:HA	1:A:442:LEU:HD13	1.68	0.75
1:D:358:LYS:N	1:D:358:LYS:HD2	1.99	0.75
1:B:312:ASN:H	1:B:312:ASN:HD22	1.32	0.75
1:D:259:GLU:HA	1:D:262:ILE:CG2	2.12	0.75
1:A:230:LYS:O	1:A:234:ARG:HG2	1.86	0.75
1:B:264:PHE:CZ	1:B:266:HIS:HB3	2.22	0.75
1:C:265:LYS:HA	1:C:265:LYS:NZ	2.02	0.75
1:D:357:ARG:HG2	1:D:358:LYS:H	1.51	0.74
1:A:265:LYS:HB3	1:A:265:LYS:NZ	2.03	0.74
1:C:455:VAL:HG12	1:C:459:THR:HG21	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG22	1:A:281:ILE:HG13	1.68	0.74
1:B:343:GLU:HG2	1:B:345:GLN:HE21	1.52	0.74
1:D:465:LEU:O	1:D:466:HIS:HD2	1.71	0.74
1:C:320:TYR:HB2	1:C:397:ARG:NH1	1.99	0.74
1:D:264:PHE:HE2	1:D:267:ILE:H	1.36	0.74
1:B:343:GLU:HB3	1:B:345:GLN:HG2	1.70	0.73
1:C:288:ARG:NH1	1:C:326:ILE:HD13	2.04	0.73
1:A:465:LEU:HD21	1:A:473:TYR:CD2	2.23	0.73
1:A:309:LEU:HD21	1:A:409:ILE:CD1	2.19	0.73
1:A:441:ASP:O	1:A:445:ILE:HG13	1.88	0.73
1:D:364:MET:HA	1:D:367:LYS:HG2	1.68	0.73
1:B:466:HIS:HB3	1:B:470:GLN:HB2	1.71	0.73
1:D:440:THR:O	1:D:444:GLN:HG2	1.89	0.73
1:A:379:LEU:HD21	1:A:435:LEU:HD22	1.69	0.73
1:A:466:HIS:CE1	1:A:468:LEU:HG	2.24	0.73
1:B:421:LEU:HD12	1:B:432:PHE:HA	1.71	0.73
1:A:320:TYR:CB	1:A:397:ARG:HH11	2.02	0.72
1:A:212:ARG:HB3	1:A:216:LYS:NZ	2.04	0.72
1:D:411:ASP:O	1:D:415:GLN:HG3	1.89	0.72
1:A:427:GLU:CD	1:A:427:GLU:H	1.92	0.72
1:A:449:HIS:O	1:A:452:LEU:HB2	1.90	0.72
1:C:318:LEU:O	1:C:322:VAL:HB	1.90	0.72
1:A:257:MET:O	1:A:261:LYS:HG2	1.90	0.72
1:B:441:ASP:O	1:B:445:ILE:HG12	1.89	0.72
1:C:425:HIS:HB3	1:C:428:SER:OG	1.89	0.72
1:A:292:ALA:O	1:A:296:ILE:HG13	1.90	0.71
1:B:343:GLU:CG	1:B:345:GLN:HE21	2.03	0.71
1:A:456:ILE:O	1:A:460:GLU:HB2	1.91	0.71
1:C:358:LYS:H	1:C:358:LYS:CE	2.03	0.71
1:D:269:PRO:HA	1:D:280:ARG:NH2	2.05	0.71
1:D:466:HIS:H	1:D:467:PRO:HD2	1.55	0.71
1:A:247:PHE:CE2	1:A:261:LYS:HG3	2.26	0.71
1:B:341:ILE:HG12	1:B:348:MET:HE3	1.72	0.71
1:C:405:PRO:O	1:C:409:ILE:HG13	1.89	0.71
1:B:260:ASP:OD1	1:B:269:PRO:HG3	1.91	0.71
1:D:234:ARG:CZ	1:D:237:LEU:HD13	2.20	0.71
1:D:311:LEU:N	1:D:311:LEU:HD12	2.04	0.71
1:A:400:LEU:CD1	1:A:403:VAL:HG22	2.12	0.71
1:C:393:LEU:CD1	1:C:409:ILE:HB	2.22	0.70
1:A:324:GLU:HG2	1:A:446:VAL:HG21	1.74	0.70
1:D:365:GLU:O	1:D:369:GLU:HG3	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:SER:O	1:C:275:LYS:HB2	1.90	0.70
1:A:350:ARG:HH21	1:A:368:PHE:HB2	1.56	0.70
1:A:437:GLN:O	1:A:440:THR:HG22	1.90	0.70
1:B:430:GLN:HE21	1:B:433:ALA:CB	2.03	0.70
1:C:251:ASP:OD1	1:C:253:ASN:HB3	1.91	0.70
1:A:403:VAL:C	1:A:405:PRO:HD2	2.12	0.70
1:B:460:GLU:HG2	1:B:463:MET:SD	2.32	0.70
1:C:291:GLU:HA	1:C:294:GLN:CG	2.21	0.70
1:C:440:THR:HG23	1:C:441:ASP:N	2.07	0.70
1:D:292:ALA:HA	1:D:295:GLU:OE1	1.92	0.70
1:D:476:LEU:H	1:D:476:LEU:CD2	2.05	0.70
1:A:348:MET:SD	1:A:353:LEU:HD21	2.31	0.69
1:D:358:LYS:CD	1:D:358:LYS:H	2.05	0.69
1:B:341:ILE:HD13	1:B:348:MET:HB2	1.73	0.69
1:B:369:GLU:O	1:B:372:VAL:HB	1.91	0.69
1:C:403:VAL:HG12	1:C:407:GLU:HG3	1.75	0.69
1:C:293:VAL:HG11	1:C:468:LEU:HD13	1.74	0.69
1:D:371:ALA:HB1	1:D:375:ASN:HD21	1.56	0.69
1:B:461:THR:HB	1:D:423:LEU:HD21	1.73	0.69
1:B:460:GLU:OE2	1:B:463:MET:HB2	1.93	0.69
1:C:419:LEU:HG	1:C:423:LEU:CD1	2.22	0.69
1:C:455:VAL:O	1:C:459:THR:HG23	1.91	0.69
1:B:417:LEU:O	1:B:420:GLN:HB3	1.92	0.69
1:A:214:LEU:HD23	1:A:416:ALA:HB2	1.75	0.69
1:D:232:LYS:HD2	1:D:235:ALA:HB3	1.74	0.69
1:B:475:ASP:OD1	1:B:476:LEU:HD22	1.93	0.69
1:A:330:LEU:O	1:A:333:LEU:HB2	1.93	0.69
1:A:288:ARG:O	1:A:291:GLU:HB2	1.93	0.69
1:B:463:MET:C	1:B:465:LEU:H	1.96	0.69
1:B:462:ASP:H	1:D:423:LEU:HD22	1.57	0.69
1:D:468:LEU:H	1:D:468:LEU:HD12	1.57	0.69
1:C:268:THR:N	1:C:269:PRO:HD2	2.07	0.69
1:D:271:GLN:HA	1:D:271:GLN:HE21	1.58	0.68
1:D:364:MET:HA	1:D:367:LYS:CG	2.22	0.68
1:B:286:GLN:O	1:B:290:VAL:HG23	1.92	0.68
1:B:317:LEU:HD22	1:B:393:LEU:HA	1.74	0.68
1:B:357:ARG:HB3	1:B:360:PHE:HD2	1.58	0.68
1:B:466:HIS:HB2	1:B:470:GLN:HB2	1.75	0.68
1:C:474:LYS:HB2	1:C:474:LYS:NZ	2.06	0.68
1:A:252:MET:HB3	1:A:256:MET:HE3	1.74	0.68
1:D:445:ILE:HA	1:D:448:GLU:HG3	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HB3	1:A:344:GLY:HA2	1.76	0.68
1:A:286:GLN:HA	1:A:289:SER:OG	1.94	0.68
1:B:466:HIS:N	1:B:467:PRO:CD	2.57	0.68
1:D:410:GLN:HA	1:D:413:LEU:HD12	1.75	0.68
1:A:309:LEU:HD21	1:A:409:ILE:HD11	1.74	0.68
1:D:301:LYS:HD2	1:D:301:LYS:N	2.09	0.68
1:A:310:ASP:OD2	1:A:312:ASN:HB2	1.94	0.67
1:B:466:HIS:N	1:B:467:PRO:HD2	2.09	0.67
1:A:270:LEU:HD13	1:A:271:GLN:N	2.09	0.67
1:A:438:LYS:O	1:A:442:LEU:HD12	1.95	0.67
1:C:370:PHE:HD1	1:C:373:LYS:NZ	1.86	0.67
1:D:417:LEU:O	1:D:420:GLN:HB3	1.94	0.67
1:C:366:PRO:HA	1:C:369:GLU:CD	2.15	0.67
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.58	0.67
1:D:455:VAL:O	1:D:458:LYS:HG2	1.95	0.67
1:A:334:MET:HB3	1:A:339:VAL:HB	1.76	0.67
1:B:424:ASN:ND2	1:B:425:HIS:NE2	2.43	0.67
1:C:433:ALA:O	1:C:437:GLN:HG2	1.95	0.67
1:D:311:LEU:CD1	1:D:311:LEU:H	2.07	0.67
1:B:247:PHE:CE2	1:B:258:GLY:HA3	2.30	0.67
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.77	0.67
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.29	0.67
1:B:230:LYS:HA	1:B:332:SER:HB3	1.76	0.67
1:B:430:GLN:HE21	1:B:433:ALA:HB3	1.59	0.67
1:C:330:LEU:HD12	1:C:333:LEU:HD12	1.77	0.67
1:B:457:LYS:HG3	1:B:458:LYS:N	2.09	0.66
1:D:270:LEU:HD13	1:D:274:SER:OG	1.94	0.66
1:D:271:GLN:HA	1:D:271:GLN:NE2	2.10	0.66
1:D:256:MET:SD	1:D:269:PRO:HB2	2.35	0.66
1:C:400:LEU:HD22	1:C:406:ILE:CD1	2.25	0.66
1:C:465:LEU:HB3	1:C:470:GLN:NE2	2.11	0.66
1:A:212:ARG:NE	1:A:216:LYS:HE3	2.10	0.66
1:C:339:VAL:HG22	1:C:340:LEU:O	1.95	0.66
1:C:358:LYS:N	1:C:358:LYS:HE2	2.08	0.66
1:A:288:ARG:CD	1:A:288:ARG:C	2.63	0.65
1:A:411:ASP:O	1:A:415:GLN:HG3	1.96	0.65
1:A:374:PHE:HA	1:A:438:LYS:HZ3	1.61	0.65
1:C:419:LEU:O	1:C:423:LEU:HD12	1.95	0.65
1:A:219:TYR:CE1	1:A:382:SER:HA	2.30	0.65
1:A:370:PHE:HA	1:A:373:LYS:HE3	1.78	0.65
1:A:427:GLU:O	1:A:429:SER:N	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:HIS:H	1:D:467:PRO:CD	2.08	0.65
1:A:225:SER:O	1:A:295:GLU:HB3	1.96	0.65
1:D:212:ARG:NH1	1:D:212:ARG:HA	2.12	0.65
1:C:359:PRO:HG2	1:C:360:PHE:H	1.61	0.65
1:D:214:LEU:O	1:D:218:LEU:HG	1.97	0.65
1:D:232:LYS:C	1:D:234:ARG:H	1.98	0.65
1:D:357:ARG:HB3	1:D:360:PHE:HD2	1.62	0.65
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.78	0.64
1:A:453:LEU:HD13	1:A:473:TYR:CE1	2.32	0.64
1:C:230:LYS:O	1:C:234:ARG:HG2	1.97	0.64
1:A:366:PRO:HG2	1:A:367:LYS:HE3	1.79	0.64
1:B:348:MET:HG2	1:B:353:LEU:HD21	1.80	0.64
1:D:301:LYS:HD2	1:D:301:LYS:H	1.62	0.64
1:C:309:LEU:HD21	1:C:409:ILE:HD11	1.78	0.64
1:A:329:MET:O	1:A:331:ALA:N	2.30	0.64
1:C:214:LEU:HD21	1:C:413:LEU:HD23	1.78	0.64
1:C:268:THR:H	1:C:269:PRO:CD	2.09	0.64
1:C:307:VAL:HA	1:C:314:GLN:OE1	1.97	0.64
1:C:404:LYS:N	1:C:405:PRO:HD2	2.13	0.64
1:D:208:SER:O	1:D:212:ARG:HG2	1.97	0.64
1:D:439:MET:O	1:D:443:ARG:HB2	1.96	0.64
1:A:320:TYR:HB3	1:A:397:ARG:HH11	1.61	0.64
1:A:336:LYS:HZ2	1:A:350:ARG:HH12	1.46	0.64
1:C:288:ARG:C	1:C:288:ARG:HD2	2.18	0.64
1:A:369:GLU:O	1:A:373:LYS:HG2	1.98	0.64
1:D:453:LEU:HD23	1:D:475:ASP:OD2	1.97	0.63
1:A:295:GLU:O	1:A:298:GLU:HB3	1.98	0.63
1:A:297:THR:OG1	1:A:318:LEU:HD13	1.98	0.63
1:A:319:LYS:HA	1:A:472:ILE:HG22	1.79	0.63
1:B:253:ASN:HB3	1:B:257:MET:SD	2.39	0.63
1:A:230:LYS:HG3	1:A:332:SER:HB3	1.78	0.63
1:A:469:LEU:HA	1:A:472:ILE:HG12	1.80	0.63
1:B:312:ASN:ND2	1:B:312:ASN:N	2.46	0.63
1:A:364:MET:SD	2:A:1:072:H4F	2.39	0.63
1:A:373:LYS:HG3	1:A:438:LYS:HE3	1.81	0.63
1:C:357:ARG:CG	1:C:359:PRO:HD2	2.25	0.63
1:B:357:ARG:HG2	1:B:359:PRO:CD	2.29	0.63
1:B:402:ASN:OD1	1:B:405:PRO:HD3	1.99	0.63
1:B:223:ILE:HG22	1:B:224:LYS:HD3	1.80	0.62
1:D:412:ASN:HA	1:D:415:GLN:NE2	2.14	0.62
1:C:250:TYR:O	1:C:251:ASP:HB3	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:CG	1:A:359:PRO:HD2	2.24	0.62
1:B:264:PHE:CG	1:B:265:LYS:N	2.68	0.62
1:B:353:LEU:O	1:B:356:LEU:HG	2.00	0.62
1:B:357:ARG:HB3	1:B:360:PHE:CD2	2.34	0.62
1:D:232:LYS:C	1:D:234:ARG:N	2.52	0.62
1:A:428:SER:HB3	1:A:431:LEU:HB2	1.81	0.62
1:B:475:ASP:CG	1:B:476:LEU:HD22	2.19	0.62
1:C:364:MET:HB3	1:C:368:PHE:HE1	1.64	0.62
1:D:259:GLU:C	1:D:261:LYS:H	2.02	0.62
1:A:288:ARG:O	1:A:288:ARG:HD2	1.99	0.62
1:D:325:ILE:O	1:D:329:MET:HE2	2.00	0.62
1:D:466:HIS:N	1:D:467:PRO:HD2	2.14	0.62
1:C:454:GLN:O	1:C:457:LYS:N	2.28	0.62
1:B:282:PHE:C	1:B:284:GLY:H	2.01	0.62
1:C:440:THR:HB	1:D:440:THR:HG22	1.82	0.62
1:B:421:LEU:HD11	1:B:435:LEU:HD23	1.81	0.62
1:C:466:HIS:CG	1:C:467:PRO:HD2	2.35	0.62
1:A:276:GLU:OE2	1:A:279:ILE:HG12	1.99	0.61
1:B:348:MET:HG2	1:B:353:LEU:CG	2.29	0.61
1:C:294:GLN:HE21	1:C:294:GLN:CA	2.05	0.61
1:D:232:LYS:HD2	1:D:235:ALA:CB	2.29	0.61
1:A:336:LYS:NZ	1:A:350:ARG:HH12	1.98	0.61
1:A:324:GLU:OE2	1:A:443:ARG:HD3	2.00	0.61
1:B:381:ASP:HA	1:B:384:LEU:CD1	2.30	0.61
1:C:311:LEU:HD23	1:C:312:ASN:N	2.15	0.61
1:A:363:PHE:HE1	2:A:1:072:H4H	1.65	0.61
1:B:462:ASP:CA	1:D:423:LEU:HD13	2.30	0.61
1:A:277:VAL:HG13	1:A:278:ALA:N	2.13	0.61
1:A:288:ARG:CZ	1:A:289:SER:HA	2.30	0.61
1:C:393:LEU:HD11	1:C:409:ILE:HB	1.81	0.61
1:A:267:ILE:HD13	1:A:274:SER:O	2.01	0.61
1:C:453:LEU:HD13	1:C:473:TYR:CE1	2.35	0.61
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.15	0.61
1:A:251:ASP:OD1	1:A:253:ASN:N	2.34	0.61
1:B:458:LYS:HE3	1:B:458:LYS:O	1.99	0.61
1:C:265:LYS:HA	1:C:265:LYS:HZ3	1.64	0.61
1:C:277:VAL:HG13	1:C:278:ALA:N	2.15	0.61
1:D:356:LEU:O	1:D:361:GLY:HA3	2.00	0.61
1:A:364:MET:HA	1:A:367:LYS:HG2	1.83	0.61
1:D:318:LEU:O	1:D:322:VAL:HG23	2.01	0.61
1:A:276:GLU:OE2	1:A:278:ALA:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:O	1:B:329:MET:HG3	2.01	0.61
1:A:320:TYR:HB2	1:A:397:ARG:HH11	1.66	0.60
1:A:433:ALA:O	1:A:437:GLN:HG2	2.01	0.60
1:C:296:ILE:O	1:C:300:ALA:N	2.19	0.60
1:C:349:THR:HG22	1:C:350:ARG:H	1.65	0.60
1:C:249:ILE:HG21	1:C:255:LEU:HD13	1.82	0.60
1:D:325:ILE:O	1:D:329:MET:HG3	2.00	0.60
1:D:417:LEU:HD21	1:D:435:LEU:CD2	2.31	0.60
1:A:288:ARG:HH11	1:A:289:SER:HA	1.65	0.60
1:A:218:LEU:HD11	1:A:413:LEU:HD22	1.82	0.60
1:A:458:LYS:HE3	1:C:210:ASP:OD1	2.00	0.60
1:B:234:ARG:HH22	1:B:237:LEU:CD1	2.14	0.60
1:C:212:ARG:HD3	1:C:423:LEU:CD1	2.32	0.60
1:D:249:ILE:O	1:D:349:THR:HG23	2.01	0.60
1:D:341:ILE:HD13	1:D:348:MET:H	1.67	0.60
1:B:404:LYS:N	1:B:405:PRO:HD2	2.17	0.60
1:C:249:ILE:HD12	1:C:255:LEU:HA	1.82	0.60
1:D:358:LYS:HB2	1:D:359:PRO:HD3	1.84	0.60
1:D:325:ILE:HG23	1:D:388:ILE:HG23	1.82	0.60
1:D:450:VAL:CG2	1:D:451:GLN:N	2.64	0.60
1:C:248:VAL:HG22	1:C:347:PHE:HB3	1.83	0.60
1:A:404:LYS:N	1:A:405:PRO:HD2	2.17	0.60
1:B:271:GLN:HE21	1:B:271:GLN:HA	1.67	0.60
1:D:340:LEU:C	1:D:341:ILE:HD12	2.21	0.60
1:A:265:LYS:HZ3	1:A:265:LYS:HB3	1.66	0.60
1:A:474:LYS:HZ2	1:A:474:LYS:HB2	1.67	0.60
1:D:232:LYS:O	1:D:236:ILE:HG12	2.02	0.60
1:A:274:SER:O	1:A:275:LYS:HB3	2.02	0.59
1:C:349:THR:HG22	1:C:350:ARG:N	2.17	0.59
1:B:384:LEU:O	1:B:388:ILE:HG13	2.01	0.59
1:B:472:ILE:C	1:B:473:TYR:HD1	2.05	0.59
1:D:314:GLN:O	1:D:318:LEU:HD13	2.01	0.59
1:A:360:PHE:HD1	1:A:360:PHE:H	1.50	0.59
1:A:433:ALA:O	1:A:437:GLN:CG	2.50	0.59
1:A:374:PHE:HA	1:A:438:LYS:NZ	2.16	0.59
1:D:356:LEU:HB2	1:D:361:GLY:HA2	1.84	0.59
1:B:343:GLU:O	1:B:345:GLN:NE2	2.35	0.59
1:B:214:LEU:HD23	1:B:416:ALA:HB2	1.83	0.59
1:A:234:ARG:NH1	1:A:332:SER:HA	2.17	0.59
1:C:288:ARG:O	1:C:292:ALA:N	2.36	0.59
1:B:327:TYR:CE1	1:B:367:LYS:HD2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:GLN:O	1:D:424:ASN:N	2.35	0.59
1:B:288:ARG:HH12	1:B:343:GLU:N	2.00	0.58
1:B:451:GLN:C	1:B:451:GLN:NE2	2.56	0.58
1:D:421:LEU:HD23	1:D:421:LEU:N	2.17	0.58
1:B:268:THR:HB	1:B:269:PRO:HD2	1.85	0.58
1:C:250:TYR:CE1	1:C:254:SER:HB3	2.38	0.58
1:A:218:LEU:HD11	1:A:413:LEU:CD2	2.33	0.58
1:A:451:GLN:O	1:A:455:VAL:HG23	2.03	0.58
1:B:348:MET:HG2	1:B:353:LEU:CD2	2.33	0.58
1:D:417:LEU:HD21	1:D:435:LEU:HD21	1.85	0.58
1:D:411:ASP:C	1:D:415:GLN:HE21	2.07	0.58
1:A:214:LEU:HD21	1:A:413:LEU:HD23	1.85	0.58
1:C:336:LYS:HE2	1:C:372:VAL:HG11	1.85	0.58
1:A:271:GLN:HB3	1:A:280:ARG:NH2	2.18	0.58
1:B:288:ARG:NH1	1:B:343:GLU:H	2.02	0.58
1:B:466:HIS:O	1:B:470:GLN:N	2.30	0.58
1:D:380:ASP:O	1:D:384:LEU:HD12	2.02	0.58
1:A:288:ARG:HD2	1:A:289:SER:N	2.18	0.58
1:C:403:VAL:C	1:C:405:PRO:HD2	2.25	0.58
1:D:379:LEU:HD12	1:D:425:HIS:HE2	1.68	0.58
1:C:259:GLU:HG2	1:C:264:PHE:CD2	2.39	0.57
1:D:338:GLY:HA3	1:D:347:PHE:CZ	2.38	0.57
1:D:279:ILE:O	1:D:283:GLN:HG3	2.04	0.57
1:B:461:THR:HG22	1:D:212:ARG:HD3	1.86	0.57
1:C:397:ARG:H	1:C:400:LEU:HD12	1.69	0.57
1:B:322:VAL:HG13	1:B:323:HIS:N	2.19	0.57
1:B:348:MET:HG2	1:B:353:LEU:HG	1.85	0.57
1:D:370:PHE:HA	1:D:373:LYS:CE	2.34	0.57
1:A:365:GLU:N	1:A:366:PRO:HD2	2.19	0.57
1:B:306:PHE:O	1:B:308:ASN:N	2.37	0.57
1:B:343:GLU:HG2	1:B:345:GLN:NE2	2.20	0.57
1:B:445:ILE:HA	1:B:448:GLU:OE1	2.05	0.57
1:C:360:PHE:O	1:C:362:ASP:N	2.38	0.57
1:D:288:ARG:HH22	1:D:343:GLU:H	1.53	0.57
1:C:320:TYR:CB	1:C:397:ARG:HH11	2.07	0.57
1:C:430:GLN:HG3	1:C:433:ALA:HB3	1.87	0.57
1:D:259:GLU:CA	1:D:262:ILE:HG22	2.24	0.57
1:A:220:ASP:HB2	1:A:224:LYS:HE3	1.86	0.56
1:A:207:GLU:HB3	1:A:210:ASP:HB2	1.86	0.56
1:A:465:LEU:HD23	1:A:470:GLN:HA	1.88	0.56
1:C:252:MET:SD	1:C:255:LEU:HD23	2.45	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:GLN:O	1:C:448:GLU:HG3	2.06	0.56
1:D:286:GLN:O	1:D:290:VAL:HG23	2.05	0.56
1:A:282:PHE:C	1:A:284:GLY:H	2.08	0.56
1:C:368:PHE:O	1:C:372:VAL:HG23	2.05	0.56
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.85	0.56
1:C:288:ARG:HH12	1:C:326:ILE:HD13	1.70	0.56
1:D:222:TYR:O	1:D:226:PHE:HD2	1.88	0.56
1:D:432:PHE:O	1:D:435:LEU:HB3	2.06	0.56
1:C:371:ALA:O	1:C:375:ASN:ND2	2.39	0.56
1:C:379:LEU:HD11	1:C:435:LEU:HD22	1.86	0.56
1:C:440:THR:CG2	1:C:441:ASP:H	2.14	0.56
1:D:255:LEU:HD22	1:D:352:PHE:HZ	1.70	0.56
1:D:340:LEU:HB3	1:D:344:GLY:HA2	1.87	0.56
1:D:450:VAL:HG23	1:D:451:GLN:N	2.21	0.56
1:D:470:GLN:HE22	1:D:471:GLU:CD	2.09	0.56
1:D:418:GLU:O	1:D:422:LYS:HG3	2.06	0.56
1:C:220:ASP:O	1:C:224:LYS:N	2.36	0.56
1:C:230:LYS:HG3	1:C:332:SER:HB2	1.87	0.56
1:C:264:PHE:C	1:C:266:HIS:H	2.09	0.56
1:C:271:GLN:HE22	1:C:277:VAL:N	2.04	0.56
1:C:366:PRO:HA	1:C:369:GLU:OE2	2.06	0.56
1:C:270:LEU:HD22	1:C:271:GLN:H	1.71	0.56
1:A:305:GLY:O	1:A:308:ASN:HB2	2.05	0.56
1:A:458:LYS:HB2	1:A:458:LYS:NZ	2.20	0.56
1:B:402:ASN:OD1	1:B:405:PRO:CD	2.54	0.56
1:B:468:LEU:O	1:B:472:ILE:HG13	2.06	0.56
1:A:430:GLN:O	1:A:434:LYS:HG2	2.07	0.55
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.87	0.55
1:B:325:ILE:HD12	1:B:388:ILE:CG2	2.36	0.55
1:B:433:ALA:O	1:B:437:GLN:HG2	2.07	0.55
1:C:291:GLU:CA	1:C:294:GLN:HG2	2.32	0.55
1:C:387:PHE:O	1:C:391:ILE:HG13	2.06	0.55
1:D:340:LEU:O	1:D:341:ILE:HD12	2.07	0.55
1:D:371:ALA:O	1:D:372:VAL:C	2.45	0.55
1:D:397:ARG:O	1:D:400:LEU:HD12	2.05	0.55
1:A:277:VAL:HG23	1:A:280:ARG:HH21	1.71	0.55
1:A:334:MET:HB3	1:A:339:VAL:CB	2.35	0.55
1:A:400:LEU:HD11	1:A:406:ILE:HD12	1.87	0.55
1:D:278:ALA:HB1	1:D:360:PHE:CD2	2.42	0.55
1:D:384:LEU:O	1:D:388:ILE:HG13	2.07	0.55
1:C:410:GLN:HG2	1:C:414:LEU:HG	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:TYR:CE2	1:A:398:PRO:HD2	2.42	0.55
1:D:325:ILE:N	1:D:325:ILE:HD13	2.22	0.55
1:A:300:ALA:HA	1:A:303:ILE:CD1	2.37	0.55
1:D:457:LYS:HD2	1:D:461:THR:HG21	1.87	0.55
1:A:410:GLN:O	1:A:414:LEU:HG	2.07	0.55
1:B:232:LYS:O	1:B:236:ILE:HG13	2.07	0.55
1:B:252:MET:O	1:B:255:LEU:HB3	2.06	0.55
1:D:338:GLY:O	1:D:368:PHE:HE1	1.89	0.55
1:D:357:ARG:CG	1:D:358:LYS:H	2.16	0.55
1:A:412:ASN:HA	1:A:415:GLN:OE1	2.06	0.55
1:C:225:SER:O	1:C:295:GLU:HG2	2.07	0.55
1:C:230:LYS:HG3	1:C:332:SER:CB	2.36	0.55
1:B:357:ARG:HG2	1:B:359:PRO:HD2	1.88	0.55
1:C:454:GLN:O	1:C:455:VAL:C	2.45	0.55
1:C:249:ILE:HG23	1:C:255:LEU:HA	1.88	0.55
1:D:222:TYR:HE2	1:D:388:ILE:HD11	1.72	0.55
1:A:457:LYS:HD2	1:A:460:GLU:O	2.07	0.55
1:B:311:LEU:N	1:B:311:LEU:HD12	2.08	0.55
1:B:357:ARG:HG2	1:B:359:PRO:HD3	1.88	0.54
1:D:240:LYS:HG2	1:D:242:THR:H	1.71	0.54
1:D:344:GLY:C	1:D:346:GLY:H	2.11	0.54
1:D:383:ASP:OD2	1:D:425:HIS:NE2	2.39	0.54
1:B:336:LYS:O	1:B:350:ARG:HD2	2.07	0.54
1:C:242:THR:O	1:C:243:ASP:C	2.45	0.54
1:D:241:THR:O	1:D:242:THR:C	2.44	0.54
1:D:237:LEU:HD11	1:D:334:MET:O	2.06	0.54
1:A:470:GLN:NE2	1:A:470:GLN:HA	2.22	0.54
1:B:326:ILE:HG23	2:B:2:072:H5E	1.88	0.54
1:D:222:TYR:HD1	1:D:223:ILE:HD13	1.72	0.54
1:A:289:SER:O	1:A:290:VAL:C	2.46	0.54
1:A:350:ARG:HG3	1:A:368:PHE:CZ	2.43	0.54
1:A:421:LEU:CD1	1:A:432:PHE:HA	2.38	0.54
1:B:282:PHE:C	1:B:284:GLY:N	2.61	0.54
1:B:474:LYS:O	1:B:475:ASP:HB3	2.07	0.54
1:C:290:VAL:HG13	1:C:291:GLU:N	2.23	0.54
1:C:393:LEU:HD11	1:C:409:ILE:HD12	1.90	0.54
1:D:213:ALA:O	1:D:214:LEU:C	2.45	0.54
1:A:383:ASP:OD1	1:A:383:ASP:N	2.41	0.54
1:B:292:ALA:HA	1:B:295:GLU:HG3	1.88	0.54
1:A:370:PHE:HA	1:A:373:LYS:CE	2.37	0.54
1:B:348:MET:SD	1:B:353:LEU:HD21	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:GLN:CA	1:D:271:GLN:HE21	2.21	0.54
1:D:277:VAL:O	1:D:278:ALA:C	2.44	0.54
1:B:241:THR:O	1:B:243:ASP:N	2.41	0.54
1:B:330:LEU:HD23	1:B:330:LEU:O	2.08	0.54
1:C:212:ARG:HD3	1:C:423:LEU:HD11	1.90	0.54
1:D:322:VAL:O	1:D:326:ILE:HG13	2.08	0.54
1:D:457:LYS:C	1:D:459:THR:H	2.10	0.54
1:D:364:MET:O	1:D:367:LYS:N	2.41	0.53
1:C:264:PHE:O	1:C:266:HIS:N	2.40	0.53
1:D:358:LYS:HB2	1:D:359:PRO:CD	2.37	0.53
1:B:418:GLU:O	1:B:422:LYS:HG3	2.08	0.53
1:B:444:GLN:O	1:B:448:GLU:HG3	2.07	0.53
1:B:453:LEU:O	1:B:456:ILE:N	2.42	0.53
1:A:400:LEU:HD12	1:A:403:VAL:CG2	2.18	0.53
1:B:325:ILE:CD1	1:B:388:ILE:HG23	2.37	0.53
1:C:281:ILE:O	1:C:284:GLY:N	2.41	0.53
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.88	0.53
1:A:474:LYS:HE3	1:A:474:LYS:HA	1.90	0.53
1:B:271:GLN:HE22	1:B:276:GLU:HA	1.73	0.53
1:B:436:LEU:O	1:B:438:LYS:N	2.33	0.53
1:C:293:VAL:O	1:C:297:THR:OG1	2.21	0.53
1:A:401:LEU:C	1:A:402:ASN:HD22	2.12	0.53
1:B:234:ARG:NH1	1:B:237:LEU:HD13	2.17	0.53
1:B:404:LYS:HB3	1:B:405:PRO:CD	2.38	0.53
1:C:251:ASP:OD1	1:C:253:ASN:N	2.41	0.53
1:D:268:THR:O	1:D:270:LEU:N	2.42	0.53
1:B:341:ILE:CD1	1:B:348:MET:HB2	2.39	0.53
1:D:451:GLN:O	1:D:455:VAL:HB	2.09	0.53
1:A:373:LYS:HZ3	1:A:438:LYS:HE3	1.73	0.53
1:A:457:LYS:HE2	1:A:463:MET:O	2.08	0.53
1:C:290:VAL:HG23	1:C:468:LEU:HD12	1.90	0.53
1:B:234:ARG:HH22	1:B:237:LEU:HD12	1.74	0.53
1:B:371:ALA:O	1:B:375:ASN:HB2	2.08	0.53
1:A:293:VAL:HG22	1:A:322:VAL:CG2	2.39	0.53
1:B:234:ARG:HH21	1:B:332:SER:C	2.13	0.53
1:C:370:PHE:HA	1:C:373:LYS:HG2	1.91	0.53
1:C:381:ASP:HA	1:C:384:LEU:HD12	1.91	0.53
1:C:384:LEU:O	1:C:388:ILE:HG12	2.08	0.53
1:C:448:GLU:HA	1:C:451:GLN:HG2	1.91	0.53
1:D:217:HIS:O	1:D:220:ASP:HB2	2.09	0.53
1:D:343:GLU:C	1:D:345:GLN:H	2.13	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASN:OD1	1:A:347:PHE:HZ	1.91	0.52
1:A:288:ARG:HG3	2:A:1:072:C1D	2.39	0.52
1:A:342:SER:O	1:A:343:GLU:HB2	2.08	0.52
1:B:424:ASN:OD1	1:B:424:ASN:O	2.26	0.52
1:C:440:THR:CB	1:D:440:THR:HG22	2.38	0.52
1:D:351:GLU:O	1:D:354:LYS:N	2.40	0.52
1:A:216:LYS:HD3	1:A:216:LYS:H	1.74	0.52
1:A:291:GLU:O	1:A:295:GLU:HG3	2.09	0.52
1:A:358:LYS:HE3	1:A:358:LYS:HA	1.91	0.52
1:B:393:LEU:O	1:B:410:GLN:HG3	2.10	0.52
1:C:239:GLY:C	1:C:241:THR:H	2.12	0.52
1:B:270:LEU:HB2	1:B:274:SER:OG	2.10	0.52
1:B:279:ILE:HG22	1:B:283:GLN:OE1	2.09	0.52
1:B:457:LYS:CG	1:B:458:LYS:N	2.73	0.52
1:C:288:ARG:CZ	1:C:289:SER:OG	2.57	0.52
1:C:403:VAL:O	1:C:404:LYS:C	2.47	0.52
1:A:212:ARG:HB3	1:A:216:LYS:HZ1	1.75	0.52
1:B:271:GLN:HG3	1:B:271:GLN:O	2.08	0.52
1:B:410:GLN:O	1:B:413:LEU:HB2	2.10	0.52
1:C:288:ARG:C	1:C:288:ARG:CD	2.78	0.52
1:C:357:ARG:HG2	1:C:358:LYS:N	2.24	0.52
1:C:410:GLN:O	1:C:413:LEU:N	2.43	0.52
1:C:474:LYS:HZ2	1:C:474:LYS:HB2	1.72	0.52
1:A:270:LEU:CD2	1:A:271:GLN:H	2.15	0.52
1:C:363:PHE:O	1:C:367:LYS:HE3	2.09	0.52
1:D:259:GLU:C	1:D:261:LYS:N	2.62	0.52
1:D:451:GLN:HE22	1:D:455:VAL:HG21	1.74	0.52
1:C:251:ASP:OD1	1:C:253:ASN:CB	2.57	0.52
1:C:258:GLY:HA3	1:C:264:PHE:CZ	2.44	0.52
1:C:334:MET:HB3	1:C:339:VAL:HB	1.91	0.52
1:C:251:ASP:HA	1:C:352:PHE:CD1	2.45	0.52
1:C:397:ARG:HB2	1:C:400:LEU:HG	1.92	0.52
1:C:393:LEU:HD12	1:C:409:ILE:HB	1.92	0.52
1:D:232:LYS:O	1:D:234:ARG:N	2.42	0.52
1:D:258:GLY:O	1:D:262:ILE:N	2.43	0.52
1:D:412:ASN:HD22	1:D:412:ASN:C	2.12	0.52
1:B:463:MET:O	1:B:465:LEU:N	2.40	0.52
1:C:288:ARG:HD2	1:C:289:SER:N	2.24	0.52
1:D:365:GLU:N	1:D:366:PRO:HD2	2.25	0.52
1:A:276:GLU:O	1:A:279:ILE:HB	2.10	0.52
1:B:463:MET:C	1:B:465:LEU:N	2.63	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:THR:N	1:C:269:PRO:CD	2.71	0.52
1:C:450:VAL:HG11	1:C:475:ASP:HA	1.91	0.52
1:D:222:TYR:CE1	1:D:381:ASP:HB3	2.45	0.52
1:D:392:ILE:HG22	1:D:393:LEU:HD22	1.91	0.52
1:B:209:ALA:O	1:B:212:ARG:HB2	2.09	0.52
1:C:212:ARG:NH1	1:C:420:GLN:HA	2.24	0.52
1:D:268:THR:HB	1:D:269:PRO:HD2	1.92	0.52
1:B:237:LEU:O	1:B:239:GLY:N	2.43	0.51
1:B:436:LEU:C	1:B:438:LYS:H	2.12	0.51
1:D:349:THR:O	1:D:353:LEU:HD12	2.09	0.51
1:C:220:ASP:HA	1:C:223:ILE:HB	1.93	0.51
1:C:394:SER:CB	1:C:397:ARG:HE	2.23	0.51
1:D:273:GLN:HA	1:D:273:GLN:OE1	2.10	0.51
1:D:394:SER:HB3	1:D:397:ARG:NE	2.25	0.51
1:B:462:ASP:HA	1:D:423:LEU:HD13	1.90	0.51
1:A:276:GLU:OE2	1:A:279:ILE:N	2.43	0.51
1:B:317:LEU:CD2	1:B:393:LEU:HA	2.39	0.51
1:B:384:LEU:H	1:B:384:LEU:HD12	1.75	0.51
1:D:379:LEU:HD12	1:D:383:ASP:OD2	2.11	0.51
1:D:434:LYS:O	1:D:438:LYS:HD3	2.10	0.51
1:A:249:ILE:HB	1:A:348:MET:HA	1.93	0.51
1:A:290:VAL:CG1	1:A:291:GLU:N	2.74	0.51
1:A:331:ALA:O	1:A:333:LEU:N	2.44	0.51
1:C:350:ARG:HB3	1:C:351:GLU:OE1	2.11	0.51
1:C:364:MET:O	1:C:367:LYS:HB2	2.10	0.51
1:D:270:LEU:HB3	1:D:274:SER:CB	2.34	0.51
1:A:313:ASP:OD1	1:A:401:LEU:HB2	2.10	0.51
1:B:421:LEU:HD12	1:B:432:PHE:CA	2.39	0.51
1:D:216:LYS:O	1:D:220:ASP:CG	2.49	0.51
1:D:370:PHE:O	1:D:371:ALA:C	2.49	0.51
1:A:230:LYS:HG3	1:A:332:SER:CB	2.41	0.51
1:B:333:LEU:O	1:B:339:VAL:HA	2.11	0.51
1:D:435:LEU:O	1:D:438:LYS:HB2	2.11	0.51
1:D:459:THR:HG22	1:D:460:GLU:N	2.26	0.51
1:A:467:PRO:HA	1:A:470:GLN:HB3	1.91	0.51
1:C:370:PHE:O	1:C:373:LYS:HG2	2.11	0.51
1:A:325:ILE:O	1:A:329:MET:HG3	2.11	0.51
1:B:208:SER:O	1:B:211:LEU:N	2.44	0.51
1:C:368:PHE:O	1:C:369:GLU:C	2.49	0.51
1:C:363:PHE:HZ	1:C:449:HIS:HD2	1.59	0.51
1:C:466:HIS:CD2	1:C:467:PRO:HD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:LYS:O	1:D:459:THR:N	2.43	0.51
1:C:266:HIS:HB2	2:C:3:072:H3I	1.93	0.51
1:C:370:PHE:HA	1:C:373:LYS:CE	2.33	0.51
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.45	0.50
1:C:365:GLU:N	1:C:366:PRO:HD2	2.26	0.50
1:D:323:HIS:O	1:D:326:ILE:HB	2.11	0.50
1:D:324:GLU:OE2	1:D:443:ARG:HD2	2.11	0.50
1:D:461:THR:C	1:D:463:MET:H	2.14	0.50
1:C:220:ASP:O	1:C:221:SER:C	2.50	0.50
1:C:271:GLN:HE22	1:C:277:VAL:H	1.58	0.50
1:B:291:GLU:O	1:B:293:VAL:N	2.45	0.50
1:B:322:VAL:CG1	1:B:323:HIS:N	2.74	0.50
1:C:299:TYR:O	1:C:302:SER:HB3	2.11	0.50
1:D:368:PHE:O	1:D:369:GLU:C	2.50	0.50
1:A:251:ASP:OD1	1:A:252:MET:N	2.44	0.50
1:B:324:GLU:OE1	1:B:397:ARG:NH2	2.44	0.50
1:C:311:LEU:O	1:C:314:GLN:HB2	2.11	0.50
1:B:430:GLN:HE21	1:B:433:ALA:HB2	1.77	0.50
1:C:363:PHE:O	1:C:364:MET:HG2	2.11	0.50
1:A:350:ARG:HG3	1:A:368:PHE:CE1	2.46	0.50
1:A:421:LEU:HD12	1:A:432:PHE:HA	1.94	0.50
1:D:384:LEU:H	1:D:384:LEU:HD12	1.76	0.50
1:B:266:HIS:CG	1:B:267:ILE:N	2.79	0.50
1:B:287:PHE:C	1:B:287:PHE:HD1	2.15	0.50
1:B:289:SER:O	1:B:293:VAL:HG23	2.11	0.50
1:D:255:LEU:HG	1:D:256:MET:HE2	1.93	0.50
1:A:219:TYR:CD1	1:A:382:SER:HA	2.47	0.50
1:C:414:LEU:HB3	1:D:430:GLN:HG3	1.92	0.50
1:A:457:LYS:C	1:A:459:THR:H	2.14	0.50
1:B:312:ASN:ND2	1:B:312:ASN:H	2.06	0.50
1:B:330:LEU:C	1:B:330:LEU:HD23	2.32	0.50
1:C:386:ILE:O	1:C:390:VAL:HG23	2.12	0.50
1:D:377:LEU:HB2	1:D:379:LEU:HD22	1.94	0.50
1:B:266:HIS:CD2	1:B:267:ILE:HG22	2.47	0.49
1:C:443:ARG:O	1:C:446:VAL:HB	2.12	0.49
1:A:305:GLY:HA2	1:A:308:ASN:ND2	2.27	0.49
1:A:390:VAL:O	1:A:391:ILE:C	2.50	0.49
1:C:425:HIS:N	1:C:426:PRO:HD3	2.27	0.49
1:D:277:VAL:O	1:D:280:ARG:N	2.46	0.49
1:A:362:ASP:O	1:A:366:PRO:CD	2.60	0.49
1:B:447:THR:O	1:B:450:VAL:HG22	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:CG1	1:C:468:LEU:HD13	2.41	0.49
1:D:343:GLU:C	1:D:345:GLN:N	2.64	0.49
1:B:236:ILE:O	1:B:237:LEU:O	2.31	0.49
1:B:279:ILE:CD1	1:B:279:ILE:H	2.08	0.49
1:C:220:ASP:O	1:C:221:SER:O	2.31	0.49
1:C:401:LEU:HB2	1:C:402:ASN:OD1	2.12	0.49
1:D:316:THR:O	1:D:317:LEU:C	2.51	0.49
1:A:262:ILE:HG22	1:A:263:LYS:H	1.78	0.49
1:A:453:LEU:HD13	1:A:473:TYR:CZ	2.47	0.49
1:B:276:GLU:O	1:B:277:VAL:C	2.50	0.49
1:B:374:PHE:O	1:B:377:LEU:HG	2.13	0.49
1:B:430:GLN:NE2	1:B:430:GLN:HA	2.28	0.49
1:D:277:VAL:O	1:D:280:ARG:HB2	2.13	0.49
1:A:245:SER:HB3	1:A:246:PRO:HD2	1.94	0.49
1:A:222:TYR:HE2	1:A:381:ASP:OD1	1.95	0.49
1:A:438:LYS:O	1:A:441:ASP:HB2	2.12	0.49
1:A:468:LEU:O	1:A:472:ILE:HG12	2.12	0.49
1:B:220:ASP:O	1:B:224:LYS:HG2	2.12	0.49
1:B:287:PHE:C	1:B:287:PHE:CD1	2.86	0.49
1:C:251:ASP:C	1:C:251:ASP:OD1	2.50	0.49
1:A:276:GLU:OE1	1:A:278:ALA:N	2.45	0.49
1:A:289:SER:O	1:A:292:ALA:N	2.43	0.49
1:B:333:LEU:HD22	1:B:340:LEU:HD12	1.93	0.49
1:B:476:LEU:N	1:B:476:LEU:HD22	2.24	0.49
1:D:360:PHE:C	1:D:362:ASP:H	2.16	0.49
1:A:470:GLN:HE21	1:A:470:GLN:HA	1.78	0.49
1:B:448:GLU:O	1:B:452:LEU:HD13	2.13	0.49
1:C:335:ASN:O	1:C:336:LYS:C	2.51	0.49
1:C:360:PHE:O	1:C:363:PHE:N	2.34	0.49
1:C:405:PRO:HG2	1:C:406:ILE:H	1.77	0.49
1:D:275:LYS:HB3	1:D:280:ARG:HD2	1.94	0.49
1:D:466:HIS:N	1:D:467:PRO:CD	2.71	0.49
1:A:275:LYS:HG3	1:A:279:ILE:HG21	1.95	0.49
1:A:293:VAL:HG13	1:A:322:VAL:HG21	1.94	0.49
1:B:323:HIS:O	1:B:326:ILE:N	2.46	0.49
1:B:419:LEU:O	1:B:422:LYS:HB2	2.13	0.49
1:C:452:LEU:O	1:C:456:ILE:HD12	2.13	0.49
1:D:281:ILE:HG12	2:D:4:072:H3H	1.95	0.49
1:D:316:THR:O	1:D:319:LYS:N	2.45	0.49
1:C:453:LEU:O	1:C:453:LEU:HD23	2.12	0.48
1:A:331:ALA:C	1:A:333:LEU:H	2.16	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:SER:O	1:B:224:LYS:N	2.46	0.48
1:C:445:ILE:O	1:C:446:VAL:C	2.50	0.48
1:D:465:LEU:C	1:D:466:HIS:HD2	2.17	0.48
1:B:287:PHE:O	1:B:290:VAL:HB	2.13	0.48
1:B:429:SER:O	1:B:434:LYS:NZ	2.43	0.48
1:B:460:GLU:HG2	1:B:463:MET:CG	2.43	0.48
1:D:255:LEU:HD21	1:D:277:VAL:CG1	2.43	0.48
1:D:362:ASP:OD1	1:D:362:ASP:N	2.44	0.48
1:B:249:ILE:HD13	1:B:255:LEU:HD13	1.94	0.48
1:B:246:PRO:HB2	1:B:346:GLY:CA	2.43	0.48
1:B:348:MET:CG	1:B:353:LEU:HD21	2.44	0.48
1:C:390:VAL:HG13	1:C:410:GLN:HG3	1.95	0.48
1:D:374:PHE:O	1:D:377:LEU:HG	2.13	0.48
1:A:264:PHE:O	1:A:266:HIS:N	2.44	0.48
1:A:440:THR:HG23	1:A:441:ASP:N	2.28	0.48
1:B:256:MET:HE1	1:B:280:ARG:HH22	1.78	0.48
1:B:340:LEU:HB3	1:B:344:GLY:HA2	1.95	0.48
1:C:440:THR:HA	1:D:440:THR:HG22	1.94	0.48
1:D:418:GLU:HG3	1:D:422:LYS:HE3	1.96	0.48
1:A:210:ASP:O	1:A:213:ALA:HB3	2.14	0.48
1:A:440:THR:HG23	1:A:441:ASP:H	1.79	0.48
1:A:474:LYS:CB	1:A:474:LYS:HZ2	2.26	0.48
1:B:228:LEU:CD2	1:B:233:ALA:HB2	2.43	0.48
1:C:271:GLN:O	1:C:275:LYS:O	2.32	0.48
1:C:294:GLN:NE2	1:C:294:GLN:CA	2.74	0.48
1:C:404:LYS:N	1:C:405:PRO:CD	2.76	0.48
1:D:267:ILE:HD11	1:D:270:LEU:HD12	1.95	0.48
1:D:371:ALA:O	1:D:374:PHE:N	2.46	0.48
1:A:266:HIS:O	1:A:267:ILE:C	2.51	0.48
1:C:257:MET:O	1:C:260:ASP:HB3	2.13	0.48
1:C:444:GLN:NE2	1:C:444:GLN:N	2.62	0.48
1:C:319:LYS:NZ	1:C:471:GLU:O	2.47	0.48
1:C:334:MET:HE2	1:C:339:VAL:HB	1.95	0.48
1:D:335:ASN:O	1:D:337:ASP:N	2.47	0.48
1:A:442:LEU:HD12	1:A:442:LEU:H	1.78	0.48
1:B:222:TYR:O	1:B:226:PHE:HD1	1.96	0.48
1:C:207:GLU:HG2	1:C:209:ALA:HB3	1.94	0.48
1:D:321:GLY:O	1:D:322:VAL:C	2.52	0.48
1:A:320:TYR:CZ	1:A:398:PRO:HD2	2.48	0.48
1:A:364:MET:HG3	2:A:1:072:H2D1	1.95	0.48
1:C:456:ILE:HA	1:C:459:THR:OG1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:PHE:CZ	1:D:436:LEU:HD11	2.48	0.48
1:A:270:LEU:HD13	1:A:272:GLU:N	2.29	0.47
1:A:365:GLU:O	1:A:369:GLU:OE2	2.32	0.47
1:B:449:HIS:CE1	1:B:453:LEU:HD22	2.49	0.47
1:C:227:PRO:O	1:C:228:LEU:C	2.52	0.47
1:C:227:PRO:HD2	1:C:295:GLU:CD	2.34	0.47
1:C:363:PHE:CZ	1:C:449:HIS:HD2	2.31	0.47
1:D:248:VAL:HG12	1:D:249:ILE:N	2.29	0.47
1:D:311:LEU:C	1:D:313:ASP:H	2.16	0.47
1:D:452:LEU:O	1:D:456:ILE:N	2.47	0.47
1:C:236:ILE:H	1:C:236:ILE:HD12	1.79	0.47
1:C:274:SER:O	1:C:275:LYS:CB	2.60	0.47
1:C:330:LEU:O	1:C:333:LEU:HB2	2.14	0.47
1:D:461:THR:C	1:D:463:MET:N	2.68	0.47
1:A:271:GLN:O	1:A:276:GLU:CA	2.57	0.47
1:A:444:GLN:O	1:A:448:GLU:HG3	2.13	0.47
1:A:319:LYS:HG3	1:A:472:ILE:HA	1.96	0.47
1:C:258:GLY:O	1:C:262:ILE:HB	2.14	0.47
1:C:440:THR:HG23	1:C:441:ASP:OD1	2.13	0.47
1:A:377:LEU:HB3	1:A:431:LEU:HD11	1.95	0.47
1:B:277:VAL:HA	1:B:280:ARG:HH11	1.78	0.47
1:B:351:GLU:O	1:B:352:PHE:C	2.53	0.47
1:C:232:LYS:O	1:C:236:ILE:CD1	2.60	0.47
1:C:424:ASN:C	1:C:426:PRO:HD3	2.34	0.47
1:D:265:LYS:O	1:D:266:HIS:CB	2.62	0.47
1:D:442:LEU:O	1:D:446:VAL:HG23	2.15	0.47
1:B:288:ARG:HH21	2:B:2:072:H1C2	1.79	0.47
1:B:328:THR:O	1:B:331:ALA:HB3	2.14	0.47
1:B:339:VAL:N	1:B:347:PHE:CE1	2.83	0.47
1:B:446:VAL:O	1:B:450:VAL:HG13	2.15	0.47
1:C:244:LYS:NZ	1:C:244:LYS:HB2	2.30	0.47
1:C:277:VAL:CG1	1:C:278:ALA:N	2.78	0.47
1:C:444:GLN:NE2	1:C:444:GLN:H	2.12	0.47
1:D:250:TYR:HA	1:D:349:THR:HG21	1.96	0.47
1:B:207:GLU:O	1:B:211:LEU:HG	2.15	0.47
1:B:367:LYS:O	1:B:370:PHE:HB3	2.14	0.47
1:B:218:LEU:HD12	1:B:386:ILE:HG12	1.97	0.47
1:C:409:ILE:O	1:C:412:ASN:HB3	2.15	0.47
1:C:465:LEU:O	1:C:466:HIS:O	2.33	0.47
1:A:316:THR:O	1:A:320:TYR:HD1	1.98	0.47
1:A:475:ASP:O	1:A:476:LEU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:CD1	1:B:386:ILE:HG12	2.45	0.47
1:B:234:ARG:O	1:B:235:ALA:C	2.52	0.47
1:B:338:GLY:O	1:B:368:PHE:HE1	1.98	0.47
1:B:473:TYR:N	1:B:473:TYR:CD1	2.82	0.47
1:C:282:PHE:O	1:C:285:CYS:HB3	2.15	0.47
1:D:469:LEU:HD22	1:D:473:TYR:HE2	1.79	0.47
1:D:256:MET:HE3	1:D:280:ARG:NH2	2.30	0.47
1:A:331:ALA:C	1:A:333:LEU:N	2.68	0.47
1:C:281:ILE:HG12	2:C:3:072:C3H	2.45	0.47
1:A:374:PHE:HB2	1:A:438:LYS:HE2	1.95	0.47
1:C:465:LEU:HB3	1:C:470:GLN:HE22	1.80	0.47
1:D:402:ASN:CG	1:D:402:ASN:O	2.54	0.47
1:A:449:HIS:CE1	1:A:453:LEU:HD12	2.50	0.46
1:A:469:LEU:HA	1:A:472:ILE:CG1	2.45	0.46
1:B:472:ILE:HG22	1:B:472:ILE:O	2.14	0.46
1:D:259:GLU:HG2	1:D:262:ILE:CG2	2.46	0.46
1:A:320:TYR:CD1	1:A:320:TYR:N	2.83	0.46
1:B:393:LEU:HD22	1:B:393:LEU:N	2.29	0.46
1:B:317:LEU:HD21	1:B:406:ILE:CG2	2.45	0.46
1:B:418:GLU:HG3	1:B:432:PHE:CD2	2.50	0.46
1:A:220:ASP:O	1:A:224:LYS:HG3	2.16	0.46
1:A:262:ILE:HG22	1:A:263:LYS:N	2.30	0.46
1:A:277:VAL:CG1	1:A:278:ALA:N	2.77	0.46
1:B:409:ILE:O	1:B:412:ASN:N	2.49	0.46
1:B:456:ILE:HA	1:B:459:THR:HB	1.96	0.46
1:C:225:SER:O	1:C:227:PRO:HD3	2.15	0.46
1:C:470:GLN:HE21	1:C:470:GLN:HB2	1.48	0.46
1:A:228:LEU:HD11	1:A:343:GLU:O	2.16	0.46
1:A:282:PHE:C	1:A:284:GLY:N	2.69	0.46
1:B:234:ARG:NH2	1:B:332:SER:O	2.43	0.46
1:B:357:ARG:HD2	1:B:360:PHE:HE2	1.79	0.46
1:B:439:MET:O	1:B:443:ARG:HB2	2.14	0.46
1:B:476:LEU:CD2	1:B:476:LEU:H	2.21	0.46
1:D:364:MET:CA	1:D:367:LYS:HG2	2.42	0.46
1:A:442:LEU:O	1:A:446:VAL:HG23	2.15	0.46
1:B:246:PRO:HB2	1:B:346:GLY:HA2	1.98	0.46
1:B:305:GLY:O	1:B:308:ASN:HB2	2.15	0.46
1:B:352:PHE:O	1:B:355:SER:N	2.37	0.46
1:B:441:ASP:O	1:B:444:GLN:HB2	2.15	0.46
1:D:353:LEU:O	1:D:361:GLY:HA2	2.16	0.46
1:A:287:PHE:O	1:A:290:VAL:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASN:C	1:B:255:LEU:N	2.67	0.46
1:C:315:VAL:O	1:C:318:LEU:HB2	2.16	0.46
1:C:437:GLN:O	1:C:439:MET:N	2.49	0.46
1:A:434:LYS:O	1:A:437:GLN:HB2	2.15	0.46
1:B:322:VAL:O	1:B:325:ILE:HB	2.16	0.46
1:B:460:GLU:CG	1:B:463:MET:SD	3.03	0.46
1:C:348:MET:CE	1:C:352:PHE:HE2	2.29	0.46
1:A:291:GLU:O	1:A:294:GLN:HB2	2.16	0.46
1:B:324:GLU:HB2	1:B:391:ILE:HG21	1.98	0.46
1:D:391:ILE:O	1:D:394:SER:HB2	2.16	0.46
1:D:445:ILE:CA	1:D:448:GLU:HG3	2.45	0.46
1:A:222:TYR:CD1	1:A:226:PHE:CD2	3.04	0.46
1:A:277:VAL:HG22	1:A:281:ILE:CG1	2.44	0.46
1:A:336:LYS:HE2	1:A:372:VAL:HG21	1.98	0.46
1:A:466:HIS:CG	1:A:467:PRO:HD2	2.50	0.46
1:B:338:GLY:O	1:B:368:PHE:CE1	2.69	0.46
1:B:471:GLU:O	1:B:474:LYS:HG3	2.15	0.46
1:C:262:ILE:HG22	1:C:263:LYS:N	2.31	0.46
1:C:288:ARG:NE	2:C:3:072:O1D	2.47	0.46
1:C:316:THR:O	1:C:319:LYS:HB3	2.15	0.46
1:C:370:PHE:CZ	1:C:442:LEU:HD21	2.50	0.46
1:C:455:VAL:HG12	1:C:459:THR:CG2	2.44	0.46
1:D:240:LYS:C	1:D:242:THR:H	2.18	0.46
1:D:381:ASP:HA	1:D:384:LEU:HD13	1.98	0.46
1:C:319:LYS:O	1:C:322:VAL:HG12	2.16	0.46
1:C:434:LYS:HA	1:C:437:GLN:HG2	1.97	0.46
1:D:243:ASP:OD2	1:D:244:LYS:HE2	2.16	0.46
1:D:262:ILE:HD11	1:D:342:SER:HB3	1.97	0.46
1:D:476:LEU:N	1:D:476:LEU:CD2	2.78	0.46
1:A:360:PHE:O	1:A:363:PHE:HB2	2.16	0.45
1:A:458:LYS:CE	1:C:210:ASP:OD1	2.63	0.45
1:B:341:ILE:HG12	1:B:348:MET:CE	2.45	0.45
1:B:352:PHE:O	1:B:355:SER:OG	2.31	0.45
1:B:451:GLN:O	1:B:451:GLN:NE2	2.49	0.45
1:C:383:ASP:OD2	1:C:425:HIS:HE1	1.99	0.45
1:C:450:VAL:CG1	1:C:475:ASP:HA	2.46	0.45
1:D:421:LEU:HD12	1:D:432:PHE:HA	1.99	0.45
1:A:277:VAL:O	1:A:278:ALA:C	2.54	0.45
1:A:389:ALA:HB1	1:A:413:LEU:HD13	1.97	0.45
1:C:252:MET:HA	1:C:255:LEU:HB3	1.98	0.45
1:C:364:MET:HB3	1:C:368:PHE:CE1	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HD23	1:C:416:ALA:HB2	1.98	0.45
1:D:364:MET:O	1:D:367:LYS:HG2	2.16	0.45
1:A:406:ILE:HA	1:A:409:ILE:HD12	1.97	0.45
1:B:237:LEU:HD22	1:B:238:THR:H	1.82	0.45
1:D:265:LYS:HG3	1:D:265:LYS:O	2.17	0.45
1:D:264:PHE:CE2	1:D:266:HIS:HB3	2.50	0.45
1:A:364:MET:C	1:A:366:PRO:HD2	2.36	0.45
1:A:384:LEU:O	1:A:388:ILE:HG12	2.16	0.45
1:A:386:ILE:O	1:A:389:ALA:HB3	2.16	0.45
1:A:469:LEU:HG	1:A:473:TYR:CE2	2.50	0.45
1:B:317:LEU:HD21	1:B:406:ILE:HG21	1.98	0.45
1:B:334:MET:HG2	1:B:339:VAL:HG23	1.98	0.45
1:B:339:VAL:HG13	1:B:341:ILE:CD1	2.46	0.45
1:B:457:LYS:HD2	1:B:457:LYS:C	2.37	0.45
1:C:227:PRO:HD2	1:C:295:GLU:OE1	2.17	0.45
1:C:425:HIS:HB3	1:C:428:SER:CB	2.46	0.45
1:D:256:MET:CE	1:D:280:ARG:NH2	2.80	0.45
1:A:415:GLN:O	1:A:416:ALA:C	2.54	0.45
1:C:364:MET:O	1:C:368:PHE:HD1	1.98	0.45
1:D:234:ARG:NH2	1:D:334:MET:O	2.49	0.45
1:A:271:GLN:HB3	1:A:280:ARG:HH22	1.81	0.45
1:B:425:HIS:N	1:B:426:PRO:CD	2.79	0.45
1:C:221:SER:O	1:C:222:TYR:C	2.55	0.45
1:C:377:LEU:CB	1:C:379:LEU:HG	2.47	0.45
1:C:405:PRO:O	1:C:406:ILE:C	2.53	0.45
1:A:298:GLU:O	1:A:301:LYS:HB2	2.15	0.45
1:B:281:ILE:HG12	2:B:2:072:H3H	1.99	0.45
1:B:341:ILE:HG13	2:B:2:072:C1A	2.45	0.45
1:C:239:GLY:C	1:C:241:THR:N	2.70	0.45
1:D:278:ALA:O	1:D:279:ILE:C	2.54	0.45
1:D:465:LEU:O	1:D:466:HIS:CD2	2.60	0.45
1:D:470:GLN:HG2	1:D:470:GLN:O	2.15	0.45
1:A:248:VAL:HG22	1:A:347:PHE:HB3	1.99	0.45
1:A:397:ARG:O	1:A:400:LEU:HB2	2.16	0.45
1:B:311:LEU:H	1:B:311:LEU:CD1	2.01	0.45
1:D:325:ILE:CG2	1:D:388:ILE:HG23	2.47	0.45
1:D:356:LEU:O	1:D:357:ARG:O	2.35	0.45
1:A:319:LYS:O	1:A:322:VAL:HG12	2.17	0.45
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.47	0.45
1:A:474:LYS:HA	1:A:474:LYS:CE	2.46	0.45
1:B:472:ILE:HG22	1:B:473:TYR:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:LEU:CD1	1:C:435:LEU:HD22	2.47	0.45
1:C:410:GLN:O	1:C:411:ASP:C	2.55	0.45
1:A:357:ARG:O	1:A:358:LYS:C	2.56	0.44
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.98	0.44
1:B:275:LYS:HB3	1:B:280:ARG:HG3	1.99	0.44
1:B:291:GLU:C	1:B:293:VAL:N	2.69	0.44
1:C:270:LEU:HD13	1:C:271:GLN:N	2.31	0.44
1:D:256:MET:CE	1:D:280:ARG:HH22	2.30	0.44
1:D:452:LEU:HD12	1:D:452:LEU:H	1.81	0.44
1:A:207:GLU:HG2	1:A:210:ASP:OD2	2.18	0.44
1:A:340:LEU:HA	1:A:346:GLY:O	2.17	0.44
1:A:390:VAL:O	1:A:393:LEU:N	2.51	0.44
1:A:400:LEU:HD11	1:A:406:ILE:CD1	2.46	0.44
1:B:228:LEU:HD22	1:B:233:ALA:HB2	1.99	0.44
1:C:212:ARG:HD3	1:C:423:LEU:HD13	1.97	0.44
1:C:277:VAL:HA	1:C:280:ARG:HB3	1.99	0.44
1:C:360:PHE:O	1:C:361:GLY:C	2.54	0.44
1:C:384:LEU:O	1:C:387:PHE:N	2.50	0.44
1:C:434:LYS:HA	1:C:437:GLN:CG	2.48	0.44
1:C:444:GLN:O	1:C:447:THR:OG1	2.32	0.44
1:D:288:ARG:HH21	1:D:342:SER:CA	2.23	0.44
1:D:348:MET:HB2	1:D:348:MET:HE2	1.67	0.44
1:D:438:LYS:C	1:D:440:THR:N	2.71	0.44
1:A:216:LYS:H	1:A:216:LYS:CD	2.29	0.44
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.99	0.44
1:C:330:LEU:HA	1:C:333:LEU:HG	1.98	0.44
1:C:374:PHE:O	1:C:377:LEU:HG	2.17	0.44
1:C:469:LEU:HD12	1:C:469:LEU:H	1.82	0.44
1:A:451:GLN:HA	1:A:454:GLN:HB2	1.99	0.44
1:A:466:HIS:ND1	1:A:468:LEU:HG	2.32	0.44
1:C:317:LEU:HD23	1:C:317:LEU:N	2.31	0.44
1:C:325:ILE:O	1:C:328:THR:HB	2.17	0.44
1:C:411:ASP:O	1:C:415:GLN:HG3	2.17	0.44
1:D:289:SER:O	1:D:293:VAL:HG23	2.18	0.44
1:D:446:VAL:O	1:D:449:HIS:HB3	2.17	0.44
1:A:255:LEU:HD22	1:A:352:PHE:HZ	1.82	0.44
1:A:450:VAL:O	1:A:452:LEU:N	2.51	0.44
1:A:466:HIS:HA	1:A:467:PRO:HD3	1.83	0.44
1:A:475:ASP:O	1:A:476:LEU:CB	2.66	0.44
1:B:237:LEU:HD22	1:B:238:THR:HG23	1.99	0.44
1:A:432:PHE:HE2	1:B:433:ALA:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG23	1:C:466:HIS:CE1	2.52	0.44
1:D:207:GLU:HB3	1:D:210:ASP:OD1	2.18	0.44
1:D:464:SER:C	1:D:466:HIS:H	2.21	0.44
1:A:267:ILE:HB	1:A:280:ARG:HH11	1.82	0.44
1:B:253:ASN:O	1:B:255:LEU:N	2.51	0.44
1:B:430:GLN:O	1:B:434:LYS:N	2.49	0.44
1:B:462:ASP:HB3	1:D:423:LEU:HD13	1.99	0.44
1:C:311:LEU:O	1:C:312:ASN:C	2.56	0.44
1:D:243:ASP:OD2	1:D:244:LYS:HG2	2.17	0.44
1:D:321:GLY:O	1:D:323:HIS:N	2.51	0.44
1:D:421:LEU:HB3	1:D:431:LEU:HD23	1.99	0.44
1:D:465:LEU:C	1:D:466:HIS:CD2	2.91	0.44
1:A:214:LEU:O	1:A:215:ALA:O	2.35	0.44
1:B:405:PRO:HA	1:B:408:ASP:HB2	1.98	0.44
1:A:414:LEU:O	1:A:418:GLU:HB2	2.18	0.44
1:A:430:GLN:NE2	1:B:414:LEU:HB3	2.33	0.44
1:B:241:THR:HG22	1:B:243:ASP:OD2	2.18	0.44
1:B:271:GLN:NE2	1:B:271:GLN:HA	2.33	0.44
1:B:313:ASP:OD1	1:B:400:LEU:HA	2.18	0.44
1:D:234:ARG:HD3	1:D:234:ARG:HA	1.61	0.44
1:D:292:ALA:O	1:D:295:GLU:N	2.50	0.44
1:A:383:ASP:OD2	1:A:424:ASN:ND2	2.50	0.44
1:A:415:GLN:O	1:A:418:GLU:HB3	2.18	0.44
1:B:462:ASP:HA	1:D:212:ARG:NE	2.33	0.44
1:D:303:ILE:HG21	1:D:393:LEU:HD21	2.00	0.44
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.80	0.43
1:A:411:ASP:O	1:A:412:ASN:C	2.56	0.43
1:B:275:LYS:HD2	1:B:275:LYS:N	2.33	0.43
1:B:297:THR:O	1:B:301:LYS:HD3	2.18	0.43
1:C:297:THR:O	1:C:301:LYS:HD3	2.18	0.43
1:D:232:LYS:HD2	1:D:232:LYS:HA	1.83	0.43
1:D:232:LYS:HE2	1:D:244:LYS:HE3	2.00	0.43
1:D:349:THR:OG1	1:D:352:PHE:CB	2.66	0.43
1:D:364:MET:HA	1:D:367:LYS:HG3	1.97	0.43
1:D:460:GLU:O	1:D:460:GLU:CD	2.56	0.43
1:A:251:ASP:OD1	1:A:251:ASP:C	2.57	0.43
1:B:431:LEU:HD12	1:B:431:LEU:HA	1.90	0.43
1:C:394:SER:OG	1:C:397:ARG:HG3	2.19	0.43
1:C:447:THR:HA	1:C:450:VAL:HB	1.99	0.43
1:D:348:MET:SD	1:D:353:LEU:HD21	2.58	0.43
1:D:391:ILE:O	1:D:392:ILE:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:SER:O	1:D:396:ASP:N	2.50	0.43
1:B:214:LEU:O	1:B:218:LEU:HG	2.18	0.43
1:B:243:ASP:OD1	1:B:244:LYS:N	2.51	0.43
1:B:248:VAL:HG12	1:B:249:ILE:N	2.33	0.43
1:B:325:ILE:HG23	1:B:388:ILE:HG23	2.00	0.43
1:B:453:LEU:O	1:B:454:GLN:C	2.57	0.43
1:C:219:TYR:O	1:C:222:TYR:HB3	2.17	0.43
1:C:299:TYR:O	1:C:300:ALA:C	2.55	0.43
1:C:338:GLY:HA2	1:C:368:PHE:HE2	1.82	0.43
1:C:430:GLN:C	1:C:432:PHE:N	2.71	0.43
1:D:291:GLU:O	1:D:292:ALA:C	2.55	0.43
1:D:335:ASN:C	1:D:337:ASP:N	2.72	0.43
1:D:364:MET:O	1:D:365:GLU:C	2.56	0.43
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.85	0.43
1:C:212:ARG:NH2	1:C:216:LYS:HE3	2.24	0.43
1:D:303:ILE:HG23	1:D:304:PRO:HD2	2.00	0.43
1:D:438:LYS:C	1:D:440:THR:H	2.21	0.43
1:D:476:LEU:N	1:D:476:LEU:HD23	2.19	0.43
1:A:393:LEU:N	1:A:393:LEU:HD22	2.33	0.43
1:A:403:VAL:C	1:A:405:PRO:CD	2.86	0.43
1:A:404:LYS:N	1:A:405:PRO:CD	2.81	0.43
1:B:462:ASP:C	1:B:464:SER:H	2.22	0.43
1:D:360:PHE:O	1:D:362:ASP:N	2.50	0.43
1:D:370:PHE:CE1	1:D:441:ASP:HB2	2.53	0.43
1:A:358:LYS:HB2	1:A:359:PRO:HD3	2.00	0.43
1:A:365:GLU:N	1:A:366:PRO:CD	2.80	0.43
1:B:207:GLU:HB3	1:B:210:ASP:HB2	2.00	0.43
1:B:306:PHE:C	1:B:308:ASN:N	2.72	0.43
1:C:299:TYR:O	1:C:302:SER:N	2.51	0.43
1:D:245:SER:HA	1:D:246:PRO:HD3	1.75	0.43
1:D:292:ALA:O	1:D:293:VAL:C	2.57	0.43
1:A:379:LEU:HD21	1:A:435:LEU:CD2	2.44	0.43
1:B:249:ILE:HD12	1:B:348:MET:HE1	2.01	0.43
1:C:290:VAL:CG1	1:C:291:GLU:N	2.81	0.43
1:C:326:ILE:HG22	1:C:327:TYR:N	2.33	0.43
1:C:325:ILE:HG23	1:C:388:ILE:HG23	2.01	0.43
1:A:314:GLN:HA	1:A:317:LEU:HD12	2.00	0.43
1:A:342:SER:O	1:A:345:GLN:HB2	2.18	0.43
1:B:463:MET:O	1:B:466:HIS:CD2	2.72	0.43
1:B:472:ILE:HG22	1:B:473:TYR:CE1	2.54	0.43
1:C:288:ARG:NH1	1:C:289:SER:HA	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:TYR:CE2	1:C:398:PRO:HD2	2.54	0.43
1:C:466:HIS:CE1	1:C:468:LEU:H	2.35	0.43
1:D:380:ASP:O	1:D:383:ASP:HB2	2.18	0.43
1:A:293:VAL:HG13	1:A:322:VAL:CG2	2.49	0.43
1:A:373:LYS:O	1:A:376:ALA:HB3	2.18	0.43
1:B:240:LYS:HG2	1:B:241:THR:N	2.34	0.43
1:B:404:LYS:N	1:B:405:PRO:CD	2.82	0.43
1:D:256:MET:SD	1:D:271:GLN:HB2	2.59	0.43
1:D:297:THR:HG23	1:D:318:LEU:CD2	2.48	0.43
1:D:380:ASP:O	1:D:383:ASP:N	2.50	0.43
1:D:222:TYR:HE2	1:D:388:ILE:CD1	2.31	0.43
1:A:270:LEU:CD1	1:A:272:GLU:N	2.82	0.43
1:A:360:PHE:CD1	1:A:360:PHE:N	2.75	0.43
1:A:382:SER:OG	1:A:383:ASP:OD1	2.36	0.43
1:B:264:PHE:CE2	1:B:266:HIS:HB3	2.53	0.43
1:B:279:ILE:O	1:B:283:GLN:HG3	2.19	0.43
1:B:323:HIS:O	1:B:324:GLU:C	2.57	0.43
1:B:430:GLN:O	1:B:431:LEU:C	2.57	0.43
1:C:311:LEU:O	1:C:314:GLN:N	2.52	0.43
1:C:407:GLU:O	1:C:411:ASP:OD2	2.37	0.43
1:D:219:TYR:O	1:D:220:ASP:C	2.56	0.43
1:A:281:ILE:HG22	2:A:1:072:H2F1	2.01	0.42
1:B:317:LEU:HD22	1:B:393:LEU:HD13	2.01	0.42
1:B:462:ASP:OD1	1:B:463:MET:N	2.52	0.42
1:C:232:LYS:O	1:C:235:ALA:HB3	2.19	0.42
1:C:367:LYS:HD3	1:C:367:LYS:H	1.83	0.42
1:C:384:LEU:O	1:C:385:ALA:C	2.57	0.42
1:C:391:ILE:O	1:C:392:ILE:C	2.57	0.42
1:D:348:MET:HG2	1:D:353:LEU:CG	2.49	0.42
1:D:349:THR:OG1	1:D:352:PHE:HB3	2.19	0.42
1:A:297:THR:O	1:A:300:ALA:HB3	2.18	0.42
1:A:306:PHE:C	1:A:308:ASN:H	2.21	0.42
1:C:249:ILE:HG21	1:C:255:LEU:CD1	2.47	0.42
1:C:258:GLY:HA3	1:C:264:PHE:CE2	2.54	0.42
1:D:370:PHE:HA	1:D:373:LYS:HE2	2.01	0.42
1:D:418:GLU:CG	1:D:422:LYS:HE3	2.49	0.42
1:B:405:PRO:HG2	1:B:406:ILE:H	1.84	0.42
1:C:207:GLU:O	1:C:211:LEU:HG	2.19	0.42
1:C:288:ARG:HD2	1:C:292:ALA:HB2	2.00	0.42
1:C:293:VAL:O	1:C:294:GLN:C	2.58	0.42
1:C:466:HIS:HE1	1:C:468:LEU:HG	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:LEU:HD21	1:D:435:LEU:HD23	2.00	0.42
1:A:214:LEU:O	1:A:215:ALA:C	2.58	0.42
1:A:327:TYR:OH	1:A:449:HIS:CD2	2.72	0.42
1:B:436:LEU:C	1:B:438:LYS:N	2.73	0.42
1:B:465:LEU:C	1:B:467:PRO:HD2	2.39	0.42
1:C:258:GLY:C	1:C:260:ASP:H	2.23	0.42
1:C:387:PHE:HZ	1:C:439:MET:HG3	1.84	0.42
1:C:449:HIS:CD2	1:C:453:LEU:HD12	2.53	0.42
1:A:359:PRO:O	1:A:362:ASP:OD1	2.36	0.42
1:A:417:LEU:O	1:A:420:GLN:HB3	2.19	0.42
1:A:457:LYS:C	1:A:459:THR:N	2.73	0.42
1:B:337:ASP:OD1	1:B:337:ASP:N	2.53	0.42
1:C:218:LEU:HD11	1:C:413:LEU:CD2	2.50	0.42
1:C:261:LYS:HE3	1:C:261:LYS:HB3	1.92	0.42
1:C:294:GLN:HB2	1:C:295:GLU:H	1.72	0.42
1:C:214:LEU:HD23	1:C:416:ALA:CB	2.49	0.42
1:D:336:LYS:O	1:D:350:ARG:CD	2.67	0.42
1:A:444:GLN:O	1:A:447:THR:HB	2.18	0.42
1:B:330:LEU:HD23	1:B:334:MET:HG3	2.01	0.42
1:C:259:GLU:HG2	1:C:264:PHE:HD2	1.83	0.42
1:C:267:ILE:HD12	1:C:275:LYS:HB3	2.01	0.42
1:A:270:LEU:HD22	1:A:271:GLN:N	2.21	0.42
1:A:325:ILE:HG13	1:A:391:ILE:HG21	2.00	0.42
1:A:438:LYS:HA	1:A:441:ASP:OD2	2.19	0.42
1:B:334:MET:HG2	1:B:339:VAL:CG2	2.50	0.42
1:B:410:GLN:HE21	1:B:410:GLN:HB3	1.49	0.42
1:B:475:ASP:OD2	1:B:476:LEU:HD13	2.20	0.42
1:C:303:ILE:HG21	1:C:413:LEU:HD11	2.02	0.42
1:C:386:ILE:HD12	1:C:420:GLN:HG2	2.00	0.42
1:C:319:LYS:HD2	1:C:472:ILE:HA	2.00	0.42
1:D:285:CYS:O	1:D:286:GLN:C	2.57	0.42
1:D:297:THR:HG23	1:D:318:LEU:HD21	2.01	0.42
1:D:357:ARG:HB3	1:D:360:PHE:CD2	2.48	0.42
1:B:333:LEU:CD2	1:B:340:LEU:HD12	2.49	0.42
1:C:351:GLU:HA	1:C:354:LYS:HB3	2.01	0.42
1:D:232:LYS:O	1:D:235:ALA:N	2.53	0.42
1:D:285:CYS:O	1:D:288:ARG:N	2.52	0.42
1:A:212:ARG:NH1	1:A:423:LEU:HD12	2.34	0.42
1:C:237:LEU:CD2	1:C:340:LEU:HD21	2.50	0.42
1:C:377:LEU:CD1	1:C:435:LEU:HD13	2.50	0.42
1:C:436:LEU:HA	1:C:439:MET:SD	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:HB3	1:A:216:LYS:HZ2	1.83	0.42
1:A:443:ARG:O	1:A:446:VAL:N	2.53	0.42
1:B:237:LEU:C	1:B:239:GLY:N	2.73	0.42
1:C:374:PHE:O	1:C:375:ASN:C	2.55	0.42
1:C:325:ILE:HG23	1:C:388:ILE:HD12	2.01	0.42
1:C:390:VAL:CG1	1:C:410:GLN:OE1	2.68	0.42
1:D:289:SER:HB3	1:D:326:ILE:HD13	2.01	0.42
1:D:336:LYS:O	1:D:350:ARG:HD2	2.20	0.42
1:A:288:ARG:CD	1:A:289:SER:N	2.83	0.41
1:A:330:LEU:HA	1:A:333:LEU:HD23	2.02	0.41
1:A:363:PHE:O	1:A:367:LYS:HE3	2.20	0.41
1:A:393:LEU:HG	1:A:409:ILE:CG2	2.50	0.41
1:B:271:GLN:CA	1:B:271:GLN:HE21	2.28	0.41
1:A:430:GLN:CG	1:B:414:LEU:HD12	2.45	0.41
1:C:235:ALA:O	1:C:236:ILE:C	2.58	0.41
1:D:216:LYS:HE3	1:D:220:ASP:OD1	2.19	0.41
1:D:287:PHE:C	1:D:287:PHE:CD1	2.94	0.41
1:D:457:LYS:HD2	1:D:461:THR:CG2	2.50	0.41
1:D:464:SER:O	1:D:467:PRO:HD2	2.19	0.41
1:A:322:VAL:O	1:A:326:ILE:HD12	2.20	0.41
1:B:277:VAL:N	1:B:280:ARG:HH11	2.18	0.41
1:C:384:LEU:O	1:C:386:ILE:N	2.53	0.41
1:C:397:ARG:HA	1:C:398:PRO:HD3	1.80	0.41
1:C:403:VAL:C	1:C:405:PRO:CD	2.87	0.41
1:C:465:LEU:O	1:C:466:HIS:C	2.59	0.41
1:D:237:LEU:CD2	1:D:238:THR:H	2.33	0.41
1:D:243:ASP:OD1	1:D:243:ASP:N	2.53	0.41
1:A:208:SER:OG	1:A:209:ALA:N	2.52	0.41
1:B:326:ILE:HG22	1:B:327:TYR:N	2.35	0.41
1:B:457:LYS:HG3	1:B:458:LYS:H	1.82	0.41
1:B:467:PRO:O	1:B:471:GLU:N	2.53	0.41
1:C:430:GLN:O	1:C:432:PHE:N	2.53	0.41
1:C:379:LEU:CD2	1:C:431:LEU:HD21	2.50	0.41
1:D:240:LYS:C	1:D:242:THR:N	2.73	0.41
1:D:288:ARG:NH2	1:D:342:SER:CA	2.73	0.41
1:A:215:ALA:O	1:A:217:HIS:N	2.54	0.41
1:A:263:LYS:O	1:A:264:PHE:HD1	2.03	0.41
1:A:285:CYS:SG	2:A:1:072:H2A	2.61	0.41
1:A:373:LYS:NZ	1:A:438:LYS:HE3	2.35	0.41
1:B:249:ILE:HD13	1:B:255:LEU:CD1	2.51	0.41
1:B:278:ALA:HB3	1:B:279:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:VAL:O	1:C:316:THR:C	2.59	0.41
1:C:383:ASP:OD2	1:C:425:HIS:CE1	2.74	0.41
1:D:222:TYR:CE2	1:D:388:ILE:CD1	3.03	0.41
1:D:288:ARG:NH2	1:D:343:GLU:H	2.17	0.41
1:D:451:GLN:NE2	1:D:455:VAL:HG21	2.34	0.41
1:B:233:ALA:O	1:B:234:ARG:C	2.59	0.41
1:B:235:ALA:O	1:B:239:GLY:O	2.39	0.41
1:B:277:VAL:HG12	1:B:278:ALA:N	2.35	0.41
1:B:292:ALA:O	1:B:296:ILE:HG13	2.20	0.41
1:C:279:ILE:O	1:C:283:GLN:HG3	2.20	0.41
1:C:321:GLY:N	1:C:397:ARG:NH1	2.68	0.41
1:D:348:MET:HG2	1:D:353:LEU:HD21	2.01	0.41
1:D:390:VAL:HG22	1:D:413:LEU:HB3	2.03	0.41
1:D:471:GLU:C	1:D:473:TYR:N	2.72	0.41
1:A:220:ASP:HB2	1:A:224:LYS:CE	2.51	0.41
1:A:270:LEU:HD13	1:A:271:GLN:H	1.85	0.41
1:A:320:TYR:O	1:A:322:VAL:N	2.53	0.41
1:B:365:GLU:O	1:B:369:GLU:HG3	2.21	0.41
1:B:466:HIS:C	1:B:470:GLN:HB2	2.41	0.41
1:B:475:ASP:O	1:B:476:LEU:O	2.39	0.41
1:C:255:LEU:HD22	1:C:352:PHE:HZ	1.84	0.41
1:D:300:ALA:HB1	1:D:306:PHE:CE1	2.56	0.41
1:D:335:ASN:C	1:D:337:ASP:H	2.24	0.41
1:C:414:LEU:HB2	1:D:430:GLN:HG2	2.02	0.41
1:A:450:VAL:C	1:A:452:LEU:N	2.72	0.41
1:C:400:LEU:HB3	1:C:403:VAL:HG22	2.02	0.41
1:D:277:VAL:CG1	1:D:281:ILE:HD11	2.51	0.41
1:D:363:PHE:HB2	1:D:452:LEU:HD21	2.03	0.41
1:D:403:VAL:O	1:D:404:LYS:C	2.58	0.41
1:A:256:MET:CA	1:A:259:GLU:HG3	2.41	0.41
1:A:288:ARG:CZ	1:A:289:SER:CA	2.98	0.41
1:A:330:LEU:CA	1:A:333:LEU:HD23	2.51	0.41
1:A:430:GLN:NE2	1:B:414:LEU:CB	2.83	0.41
1:B:462:ASP:HB3	1:D:423:LEU:CB	2.35	0.41
1:C:293:VAL:CB	1:C:468:LEU:HD13	2.50	0.41
1:A:403:VAL:O	1:A:404:LYS:C	2.59	0.41
1:B:475:ASP:OD1	1:B:476:LEU:CD2	2.65	0.41
1:C:325:ILE:HG22	1:C:329:MET:HG3	2.03	0.41
1:D:207:GLU:O	1:D:210:ASP:HB2	2.21	0.41
1:D:241:THR:O	1:D:241:THR:HG22	2.21	0.41
1:D:310:ASP:OD2	1:D:312:ASN:ND2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD12	1:A:432:PHE:CA	2.51	0.41
1:A:425:HIS:HB3	1:A:428:SER:CB	2.42	0.41
1:B:299:TYR:O	1:B:302:SER:N	2.54	0.41
1:C:237:LEU:HD21	1:C:340:LEU:HG	2.02	0.41
1:C:295:GLU:O	1:C:298:GLU:HB3	2.21	0.41
1:C:319:LYS:HZ1	1:C:474:LYS:HZ2	1.69	0.41
1:C:397:ARG:H	1:C:400:LEU:CD1	2.33	0.41
1:C:474:LYS:HE3	1:C:474:LYS:HA	2.03	0.41
1:D:469:LEU:C	1:D:471:GLU:H	2.24	0.41
1:A:207:GLU:O	1:A:210:ASP:N	2.54	0.41
1:A:259:GLU:HA	1:A:264:PHE:CD2	2.55	0.41
1:B:350:ARG:HG3	1:B:368:PHE:CD2	2.56	0.41
1:B:473:TYR:N	1:B:473:TYR:HD1	2.19	0.41
1:B:323:HIS:CE1	1:B:476:LEU:HD12	2.56	0.41
1:C:377:LEU:HB3	1:C:379:LEU:HG	2.02	0.41
1:C:455:VAL:O	1:C:457:LYS:N	2.54	0.41
1:A:271:GLN:NE2	1:A:272:GLU:N	2.69	0.40
1:A:473:TYR:C	1:A:474:LYS:HZ1	2.22	0.40
1:B:338:GLY:O	1:B:339:VAL:HB	2.21	0.40
1:B:454:GLN:O	1:B:457:LYS:HB3	2.21	0.40
1:C:264:PHE:C	1:C:266:HIS:N	2.74	0.40
1:C:359:PRO:HG2	1:C:360:PHE:CD2	2.56	0.40
1:C:360:PHE:HA	1:C:363:PHE:HB2	2.02	0.40
1:B:212:ARG:HB3	1:B:212:ARG:CZ	2.51	0.40
1:C:221:SER:O	1:C:224:LYS:N	2.54	0.40
1:C:288:ARG:HD2	1:C:289:SER:HA	2.02	0.40
1:C:473:TYR:O	1:C:474:LYS:NZ	2.50	0.40
1:D:348:MET:HG2	1:D:353:LEU:HG	2.03	0.40
1:A:287:PHE:CD2	1:A:288:ARG:N	2.89	0.40
1:A:438:LYS:O	1:A:442:LEU:CD1	2.66	0.40
1:B:234:ARG:NH1	1:B:237:LEU:HB3	2.37	0.40
1:B:349:THR:OG1	1:B:352:PHE:HB3	2.20	0.40
1:B:352:PHE:O	1:B:353:LEU:C	2.60	0.40
1:B:380:ASP:OD1	1:B:382:SER:N	2.50	0.40
1:B:405:PRO:HG2	1:B:406:ILE:N	2.37	0.40
1:B:431:LEU:O	1:B:434:LYS:N	2.53	0.40
1:C:333:LEU:HD11	2:C:3:072:H5B2	2.04	0.40
1:D:321:GLY:O	1:D:324:GLU:N	2.52	0.40
1:D:371:ALA:C	1:D:375:ASN:ND2	2.74	0.40
1:D:469:LEU:O	1:D:473:TYR:HD2	2.05	0.40
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:HA	1:A:373:LYS:HZ2	1.86	0.40
1:B:335:ASN:HD21	1:B:337:ASP:HB2	1.86	0.40
1:B:448:GLU:O	1:B:449:HIS:C	2.58	0.40
1:C:276:GLU:OE2	1:C:279:ILE:HG12	2.21	0.40
1:C:428:SER:CB	1:C:431:LEU:HD22	2.52	0.40
1:C:440:THR:CA	1:D:440:THR:HG22	2.51	0.40
1:B:380:ASP:C	1:B:384:LEU:HD12	2.41	0.40
1:B:421:LEU:CD1	1:B:432:PHE:HA	2.45	0.40
1:B:460:GLU:OE2	1:B:466:HIS:CE1	2.74	0.40
1:A:458:LYS:HE3	1:C:210:ASP:CG	2.42	0.40
1:C:249:ILE:HG23	1:C:255:LEU:CA	2.51	0.40
1:D:456:ILE:O	1:D:457:LYS:C	2.60	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:D:245:SER:OG	1:D:245:SER:OG[2_756]	1.79	0.41

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	268/270 (99%)	195 (73%)	46 (17%)	27 (10%)	0 1
1	B	268/270 (99%)	182 (68%)	56 (21%)	30 (11%)	0 1
1	C	268/270 (99%)	164 (61%)	68 (25%)	36 (13%)	0 0
1	D	268/270 (99%)	175 (65%)	70 (26%)	23 (9%)	1 2
All	All	1072/1080 (99%)	716 (67%)	240 (22%)	116 (11%)	0 1

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ALA
1	A	240	LYS
1	A	267	ILE
1	A	269	PRO
1	A	272	GLU
1	A	309	LEU
1	A	330	LEU
1	A	359	PRO
1	A	428	SER
1	A	456	ILE
1	B	231	ALA
1	B	237	LEU
1	B	240	LYS
1	B	277	VAL
1	B	467	PRO
1	C	227	PRO
1	C	243	ASP
1	C	269	PRO
1	C	273	GLN
1	C	294	GLN
1	C	356	LEU
1	C	394	SER
1	C	428	SER
1	C	455	VAL
1	C	475	ASP
1	D	242	THR
1	D	266	HIS
1	D	277	VAL
1	D	322	VAL
1	D	357	ARG
1	D	370	PHE
1	D	371	ALA
1	D	372	VAL
1	D	428	SER
1	D	467	PRO
1	A	216	LYS
1	A	265	LYS
1	A	270	LEU
1	A	391	ILE
1	A	455	VAL
1	B	227	PRO
1	B	238	THR
1	B	242	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	266	HIS
1	B	275	LYS
1	B	278	ALA
1	B	307	VAL
1	B	475	ASP
1	C	221	SER
1	C	265	LYS
1	C	275	LYS
1	C	345	GLN
1	C	359	PRO
1	C	361	GLY
1	C	446	VAL
1	C	466	HIS
1	D	336	LYS
1	D	378	GLU
1	D	395	GLY
1	D	458	LYS
1	D	460	GLU
1	B	208	SER
1	B	265	LYS
1	B	292	ALA
1	B	306	PHE
1	B	464	SER
1	C	274	SER
1	C	311	LEU
1	C	336	LYS
1	C	358	LYS
1	C	385	ALA
1	C	438	LYS
1	C	467	PRO
1	D	361	GLY
1	D	466	HIS
1	D	468	LEU
1	A	307	VAL
1	A	321	GLY
1	A	332	SER
1	A	382	SER
1	A	416	ALA
1	B	272	GLU
1	B	342	SER
1	B	422	LYS
1	B	459	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	346	GLY
1	D	304	PRO
1	D	392	ILE
1	D	474	LYS
1	A	227	PRO
1	A	289	SER
1	A	360	PHE
1	B	274	SER
1	B	339	VAL
1	B	352	PHE
1	B	463	MET
1	C	251	ASP
1	C	264	PHE
1	C	364	MET
1	C	391	ILE
1	C	395	GLY
1	C	456	ILE
1	B	252	MET
1	B	437	GLN
1	C	267	ILE
1	C	268	THR
1	D	237	LEU
1	D	292	ALA
1	A	304	PRO
1	A	358	LYS
1	A	390	VAL
1	C	236	ILE
1	A	296	ILE
1	B	361	GLY
1	C	405	PRO
1	B	372	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/243 (100%)	212 (87%)	31 (13%)	4	13
1	B	243/243 (100%)	217 (89%)	26 (11%)	6	20
1	C	243/243 (100%)	221 (91%)	22 (9%)	9	28
1	D	243/243 (100%)	220 (90%)	23 (10%)	8	26
All	All	972/972 (100%)	870 (90%)	102 (10%)	7	21

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	220	ASP
1	A	241	THR
1	A	253	ASN
1	A	271	GLN
1	A	287	PHE
1	A	288	ARG
1	A	304	PRO
1	A	309	LEU
1	A	326	ILE
1	A	337	ASP
1	A	345	GLN
1	A	358	LYS
1	A	360	PHE
1	A	381	ASP
1	A	383	ASP
1	A	396	ASP
1	A	400	LEU
1	A	401	LEU
1	A	407	GLU
1	A	410	GLN
1	A	412	ASN
1	A	415	GLN
1	A	427	GLU
1	A	440	THR
1	A	453	LEU
1	A	454	GLN
1	A	458	LYS
1	A	460	GLU
1	A	474	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	476	LEU
1	B	207	GLU
1	B	210	ASP
1	B	212	ARG
1	B	223	ILE
1	B	237	LEU
1	B	266	HIS
1	B	287	PHE
1	B	294	GLN
1	B	311	LEU
1	B	312	ASN
1	B	316	THR
1	B	337	ASP
1	B	351	GLU
1	B	379	LEU
1	B	380	ASP
1	B	393	LEU
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN
1	B	440	THR
1	B	443	ARG
1	B	451	GLN
1	B	457	LYS
1	B	458	LYS
1	B	467	PRO
1	B	469	LEU
1	C	216	LYS
1	C	217	HIS
1	C	220	ASP
1	C	261	LYS
1	C	265	LYS
1	C	271	GLN
1	C	285	CYS
1	C	288	ARG
1	C	294	GLN
1	C	302	SER
1	C	310	ASP
1	C	337	ASP
1	C	351	GLU
1	C	380	ASP
1	C	409	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	423	LEU
1	C	427	GLU
1	C	458	LYS
1	C	467	PRO
1	C	470	GLN
1	C	474	LYS
1	C	475	ASP
1	D	214	LEU
1	D	216	LYS
1	D	228	LEU
1	D	237	LEU
1	D	253	ASN
1	D	257	MET
1	D	259	GLU
1	D	282	PHE
1	D	287	PHE
1	D	301	LYS
1	D	309	LEU
1	D	343	GLU
1	D	379	LEU
1	D	381	ASP
1	D	412	ASN
1	D	443	ARG
1	D	451	GLN
1	D	460	GLU
1	D	461	THR
1	D	467	PRO
1	D	470	GLN
1	D	475	ASP
1	D	476	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	283	GLN
1	A	308	ASN
1	A	314	GLN
1	A	402	ASN
1	A	410	GLN
1	A	412	ASN
1	A	430	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	449	HIS
1	A	451	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	266	HIS
1	B	271	GLN
1	B	308	ASN
1	B	312	ASN
1	B	345	GLN
1	B	410	GLN
1	B	412	ASN
1	B	420	GLN
1	B	424	ASN
1	B	430	GLN
1	B	437	GLN
1	B	444	GLN
1	B	449	HIS
1	B	451	GLN
1	B	454	GLN
1	B	466	HIS
1	B	470	GLN
1	C	253	ASN
1	C	271	GLN
1	C	294	GLN
1	C	345	GLN
1	C	375	ASN
1	C	425	HIS
1	C	444	GLN
1	C	449	HIS
1	C	451	GLN
1	C	466	HIS
1	C	470	GLN
1	D	271	GLN
1	D	294	GLN
1	D	308	ASN
1	D	375	ASN
1	D	410	GLN
1	D	412	ASN
1	D	415	GLN
1	D	444	GLN
1	D	451	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	470	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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$
2	072	C	3	-	43,47,47	3.78	31 (72%)	50,61,61	2.87	12 (24%)
2	072	D	4	-	43,47,47	3.92	32 (74%)	50,61,61	2.65	16 (32%)
2	072	A	1	-	43,47,47	3.99	31 (72%)	50,61,61	3.44	14 (28%)
2	072	B	2	-	43,47,47	3.83	32 (74%)	50,61,61	2.63	14 (28%)

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	072	C	3	-	-	14/30/50/50	0/4/4/4
2	072	D	4	-	-	7/30/50/50	0/4/4/4
2	072	A	1	-	-	10/30/50/50	0/4/4/4
2	072	B	2	-	-	7/30/50/50	0/4/4/4

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	072	C4B-N4A	10.20	1.62	1.46
2	A	1	072	C4B-N4A	9.54	1.61	1.46
2	B	2	072	C3B-N3A	8.56	1.61	1.46
2	D	4	072	C3B-N3A	8.32	1.60	1.46
2	B	2	072	C1C-C1D	8.11	1.66	1.51
2	C	3	072	C4B-C4C	8.08	1.65	1.51
2	B	2	072	C5B-N4A	7.84	1.59	1.46
2	D	4	072	C4B-N4A	7.75	1.58	1.46
2	D	4	072	C5B-N4A	7.74	1.58	1.46
2	A	1	072	C3B-N3A	7.74	1.59	1.46
2	C	3	072	C5B-N4A	7.68	1.58	1.46
2	A	1	072	C5B-N4A	7.62	1.58	1.46
2	C	3	072	C3B-N3A	7.57	1.59	1.46
2	B	2	072	C4B-N4A	7.30	1.58	1.46
2	D	4	072	C1C-C1D	7.04	1.64	1.51
2	D	4	072	C4B-C4C	6.79	1.63	1.51
2	A	1	072	C1C-C1D	6.73	1.64	1.51
2	A	1	072	C4B-C4C	5.99	1.62	1.51
2	A	1	072	C1D-N4A	5.89	1.47	1.35
2	D	4	072	C5B-C5C	5.86	1.62	1.51
2	B	2	072	C1D-N4A	5.69	1.46	1.35
2	A	1	072	C5D-C5C	5.49	1.50	1.38
2	C	3	072	C1C-C1D	5.36	1.61	1.51
2	D	4	072	C1D-N4A	5.09	1.45	1.35
2	B	2	072	C4B-C4C	5.06	1.60	1.51
2	B	2	072	C5B-C5C	4.95	1.60	1.51
2	A	1	072	C5B-C5C	4.92	1.60	1.51
2	A	1	072	C4E-C4C	4.66	1.48	1.38
2	C	3	072	C1D-N4A	4.60	1.44	1.35
2	D	4	072	C3J-C3H	4.57	1.47	1.38
2	A	1	072	C2A-S1B	-4.55	1.76	1.83
2	A	1	072	C3G-C3F	4.53	1.48	1.38
2	C	3	072	C4E-C4C	4.46	1.48	1.38
2	D	4	072	C3G-C3F	4.46	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	072	C3J-C3K	4.41	1.48	1.39
2	B	2	072	C3G-C3F	4.38	1.48	1.38
2	D	4	072	C1A-N3A	4.38	1.41	1.35
2	A	1	072	C2B-C2A	4.28	1.62	1.52
2	B	2	072	C1A-N3A	4.27	1.41	1.35
2	A	1	072	C1A-N3A	4.20	1.41	1.35
2	B	2	072	C5E-C5C	4.14	1.47	1.38
2	B	2	072	C3H-C3F	4.14	1.47	1.38
2	C	3	072	C1A-N3A	4.09	1.40	1.35
2	C	3	072	C5B-C5C	4.04	1.58	1.51
2	D	4	072	C4E-C4C	4.03	1.47	1.38
2	B	2	072	C3I-C3G	4.02	1.46	1.38
2	D	4	072	C3I-C3G	4.00	1.46	1.38
2	D	4	072	C4D-C4C	3.97	1.47	1.38
2	A	1	072	C3I-C3G	3.88	1.45	1.38
2	B	2	072	C5D-C5C	3.87	1.47	1.38
2	B	2	072	C3J-C3K	3.85	1.47	1.39
2	C	3	072	C3G-C3F	3.82	1.47	1.38
2	B	2	072	C3J-C3H	3.82	1.45	1.38
2	C	3	072	C3H-C3F	3.80	1.47	1.38
2	A	1	072	C4D-C4C	3.79	1.47	1.38
2	A	1	072	C5E-C5C	3.78	1.47	1.38
2	C	3	072	C3E-C3F	3.78	1.62	1.51
2	B	2	072	C4D-C4C	3.78	1.47	1.38
2	A	1	072	C5H-C5G	3.76	1.48	1.38
2	D	4	072	C3H-C3F	3.69	1.46	1.38
2	D	4	072	C5E-C5C	3.63	1.46	1.38
2	D	4	072	C5D-C5C	3.63	1.46	1.38
2	D	4	072	C4G-C4E	3.61	1.46	1.38
2	C	3	072	C4D-C4C	3.60	1.46	1.38
2	D	4	072	C3I-C3K	3.58	1.47	1.39
2	A	1	072	C3H-C3F	3.56	1.46	1.38
2	D	4	072	C2B-C2A	3.56	1.60	1.52
2	C	3	072	C5E-C5C	3.53	1.46	1.38
2	B	2	072	C4E-C4C	3.52	1.46	1.38
2	A	1	072	C3E-C3F	3.51	1.61	1.51
2	C	3	072	C3I-C3K	3.50	1.46	1.39
2	A	1	072	C3J-C3K	3.49	1.46	1.39
2	C	3	072	C4G-C4E	3.44	1.46	1.38
2	B	2	072	C1B-S1B	3.42	1.89	1.80
2	A	1	072	C5F-C5D	3.38	1.46	1.38
2	B	2	072	C3I-C3K	3.35	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	072	C3J-C3K	3.32	1.46	1.39
2	C	3	072	C3I-C3G	3.30	1.44	1.38
2	B	2	072	C4G-C4E	3.29	1.45	1.38
2	D	4	072	C5F-C5D	3.25	1.45	1.38
2	A	1	072	C3I-C3K	3.22	1.46	1.39
2	B	2	072	C3E-C3F	3.21	1.61	1.51
2	B	2	072	C2B-C2A	3.20	1.59	1.52
2	D	4	072	C5H-C5F	3.18	1.46	1.38
2	A	1	072	C5G-C5E	3.17	1.45	1.38
2	C	3	072	C3J-C3H	3.17	1.44	1.38
2	D	4	072	C4F-C4D	3.10	1.45	1.38
2	D	4	072	C3E-C3F	3.06	1.60	1.51
2	A	1	072	C4G-C4E	2.99	1.45	1.38
2	C	3	072	C5D-C5C	2.96	1.45	1.38
2	D	4	072	C5G-C5E	2.95	1.45	1.38
2	C	3	072	C5G-C5E	2.91	1.45	1.38
2	D	4	072	O1A-C1A	2.85	1.27	1.22
2	B	2	072	C4F-C4D	2.84	1.44	1.38
2	C	3	072	C4F-C4D	2.83	1.44	1.38
2	C	3	072	C3K-C3L	2.77	1.50	1.47
2	A	1	072	C1B-S1B	-2.75	1.73	1.80
2	D	4	072	C5H-C5G	2.72	1.45	1.38
2	B	2	072	C5F-C5D	2.71	1.44	1.38
2	B	2	072	O1A-C1A	2.71	1.27	1.22
2	C	3	072	C2B-C2A	2.69	1.58	1.52
2	C	3	072	C5H-C5F	2.62	1.45	1.38
2	A	1	072	O1A-C1A	2.60	1.27	1.22
2	B	2	072	C5H-C5F	2.56	1.44	1.38
2	D	4	072	C1C-C1B	2.54	1.61	1.52
2	D	4	072	C4H-C4G	2.49	1.44	1.38
2	B	2	072	C1C-C1B	2.43	1.60	1.52
2	C	3	072	C4H-C4G	2.40	1.44	1.38
2	B	2	072	C2C-C2B	2.38	1.62	1.52
2	A	1	072	C4H-C4G	2.38	1.44	1.38
2	C	3	072	C5H-C5G	2.38	1.44	1.38
2	D	4	072	C4H-C4F	2.35	1.44	1.38
2	A	1	072	C3J-C3H	2.33	1.43	1.38
2	A	1	072	C3C-C3B	2.32	1.61	1.51
2	C	3	072	C2A-S1B	-2.30	1.79	1.83
2	A	1	072	C5H-C5F	2.29	1.44	1.38
2	B	2	072	C3C-C3B	2.28	1.61	1.51
2	C	3	072	C2C-C2B	2.23	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	072	C4H-C4F	2.21	1.43	1.38
2	D	4	072	C3C-C3B	2.20	1.60	1.51
2	D	4	072	C3D-C3E	2.20	1.62	1.52
2	A	1	072	C4F-C4D	2.19	1.43	1.38
2	B	2	072	C3D-C3E	2.18	1.62	1.52
2	B	2	072	C5G-C5E	2.09	1.43	1.38
2	B	2	072	C5H-C5G	2.09	1.43	1.38
2	C	3	072	C5F-C5D	2.02	1.43	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	072	C4C-C4B-N4A	12.53	133.27	113.13
2	A	1	072	C4C-C4B-N4A	11.59	131.75	113.13
2	A	1	072	C2A-S1B-C1B	10.02	101.34	94.12
2	A	1	072	C1C-C1B-C1A	9.60	126.18	111.08
2	D	4	072	C3C-C3B-N3A	8.77	126.86	113.31
2	B	2	072	C3C-C3B-N3A	8.45	126.37	113.31
2	A	1	072	C5C-C5B-N4A	7.69	125.49	113.13
2	B	2	072	O1D-C1D-C1C	-7.36	108.93	122.20
2	B	2	072	C1C-C1D-N4A	6.67	131.41	118.52
2	D	4	072	C1C-C1D-N4A	6.51	131.10	118.52
2	C	3	072	O1D-C1D-C1C	-6.42	110.61	122.20
2	A	1	072	O1D-C1D-C1C	-6.22	110.99	122.20
2	C	3	072	C2A-S1B-C1B	6.13	98.54	94.12
2	A	1	072	C3C-C3B-N3A	5.95	122.50	113.31
2	D	4	072	O1D-C1D-C1C	-5.94	111.49	122.20
2	B	2	072	C1A-C1B-S1B	5.89	107.99	105.19
2	C	3	072	C5C-C5B-N4A	5.81	122.48	113.13
2	D	4	072	C1A-C1B-S1B	5.71	107.91	105.19
2	C	3	072	C1C-C1D-N4A	5.63	129.41	118.52
2	D	4	072	C4C-C4B-N4A	5.57	122.09	113.13
2	B	2	072	C2A-S1B-C1B	-5.56	90.12	94.12
2	A	1	072	C1C-C1D-N4A	5.52	129.19	118.52
2	C	3	072	C1A-C1B-S1B	-5.07	102.78	105.19
2	D	4	072	C1C-C1B-C1A	4.75	118.56	111.08
2	A	1	072	C1C-C1B-S1B	-4.66	105.11	115.10
2	C	3	072	C1C-C1B-C1A	4.46	118.10	111.08
2	C	3	072	C3C-C3B-N3A	4.05	119.57	113.31
2	A	1	072	C1A-C1B-S1B	-3.99	103.30	105.19
2	D	4	072	C3D-C3E-C3F	3.98	128.67	113.68
2	B	2	072	C2C-C2B-C2A	3.97	124.76	113.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	072	C4C-C4B-N4A	3.94	119.47	113.13
2	B	2	072	C3B-N3A-C1A	-3.81	117.81	122.28
2	B	2	072	C1C-C1B-C1A	3.80	117.06	111.08
2	D	4	072	C5C-C5B-N4A	3.75	119.16	113.13
2	A	1	072	C3C-C3D-C3E	3.30	126.61	113.76
2	D	4	072	C3C-C3D-C3E	3.15	126.03	113.76
2	C	3	072	C2D-C2C-C2B	3.07	124.49	113.62
2	A	1	072	C2E-C2D-C2C	3.01	129.72	114.42
2	A	1	072	C3D-C3E-C3F	2.99	124.92	113.68
2	D	4	072	C1C-C1B-S1B	-2.96	108.76	115.10
2	A	1	072	C2C-C2B-C2A	2.80	121.36	113.22
2	D	4	072	C3D-C3C-C3B	2.71	125.72	113.21
2	B	2	072	C3D-C3E-C3F	2.66	123.70	113.68
2	B	2	072	C2D-C2C-C2B	2.64	122.96	113.62
2	D	4	072	C2D-C2C-C2B	2.62	122.90	113.62
2	B	2	072	C3D-C3C-C3B	2.62	125.29	113.21
2	D	4	072	C2C-C2B-C2A	2.50	120.50	113.22
2	B	2	072	C3C-C3D-C3E	2.49	123.45	113.76
2	D	4	072	O1D-C1D-N4A	-2.39	117.39	122.05
2	A	1	072	C2D-C2C-C2B	2.35	121.94	113.62
2	C	3	072	C2F-C2E-C2D	2.32	126.19	114.42
2	D	4	072	C2A-S1B-C1B	-2.31	92.46	94.12
2	C	3	072	C2C-C2B-C2A	2.18	119.55	113.22
2	D	4	072	C3B-N3A-C1A	-2.16	119.74	122.28
2	C	3	072	C2E-C2D-C2C	2.02	124.70	114.42
2	B	2	072	C2E-C2D-C2C	2.01	124.64	114.42

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	072	S1B-C1B-C1C-C1D
2	C	3	072	C1A-C1B-C1C-C1D
2	C	3	072	S1B-C2A-C2B-C2C
2	C	3	072	N3A-C2A-C2B-C2C
2	C	3	072	C4C-C4B-N4A-C1D
2	D	4	072	S1B-C2A-C2B-C2C
2	D	4	072	N3A-C2A-C2B-C2C
2	A	1	072	S1B-C2A-C2B-C2C
2	A	1	072	N3A-C2A-C2B-C2C
2	A	1	072	C4C-C4B-N4A-C1D
2	A	1	072	C2C-C2D-C2E-C2F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1	072	N3A-C3B-C3C-C3D
2	B	2	072	C3C-C3D-C3E-C3F
2	D	4	072	C3C-C3D-C3E-C3F
2	C	3	072	C4C-C4B-N4A-C5B
2	B	2	072	C2A-C2B-C2C-C2D
2	D	4	072	N3A-C3B-C3C-C3D
2	D	4	072	O1D-C1D-N4A-C4B
2	A	1	072	C2A-C2B-C2C-C2D
2	C	3	072	O1D-C1D-N4A-C4B
2	C	3	072	C1C-C1D-N4A-C4B
2	D	4	072	C1C-C1D-N4A-C4B
2	A	1	072	C1C-C1D-N4A-C4B
2	A	1	072	C4C-C4B-N4A-C5B
2	C	3	072	C2A-C2B-C2C-C2D
2	B	2	072	C2E-C2F-C2G-C2H
2	C	3	072	O1D-C1D-N4A-C5B
2	C	3	072	C1C-C1D-N4A-C5B
2	B	2	072	C1A-C1B-C1C-C1D
2	A	1	072	C1A-C1B-C1C-C1D
2	A	1	072	O1D-C1D-N4A-C4B
2	C	3	072	C2C-C2D-C2E-C2F
2	C	3	072	C1B-C1C-C1D-O1D
2	B	2	072	C1B-C1C-C1D-O1D
2	C	3	072	N3A-C3B-C3C-C3D
2	D	4	072	C2E-C2F-C2G-C2H
2	B	2	072	S1B-C2A-C2B-C2C
2	B	2	072	C2C-C2D-C2E-C2F

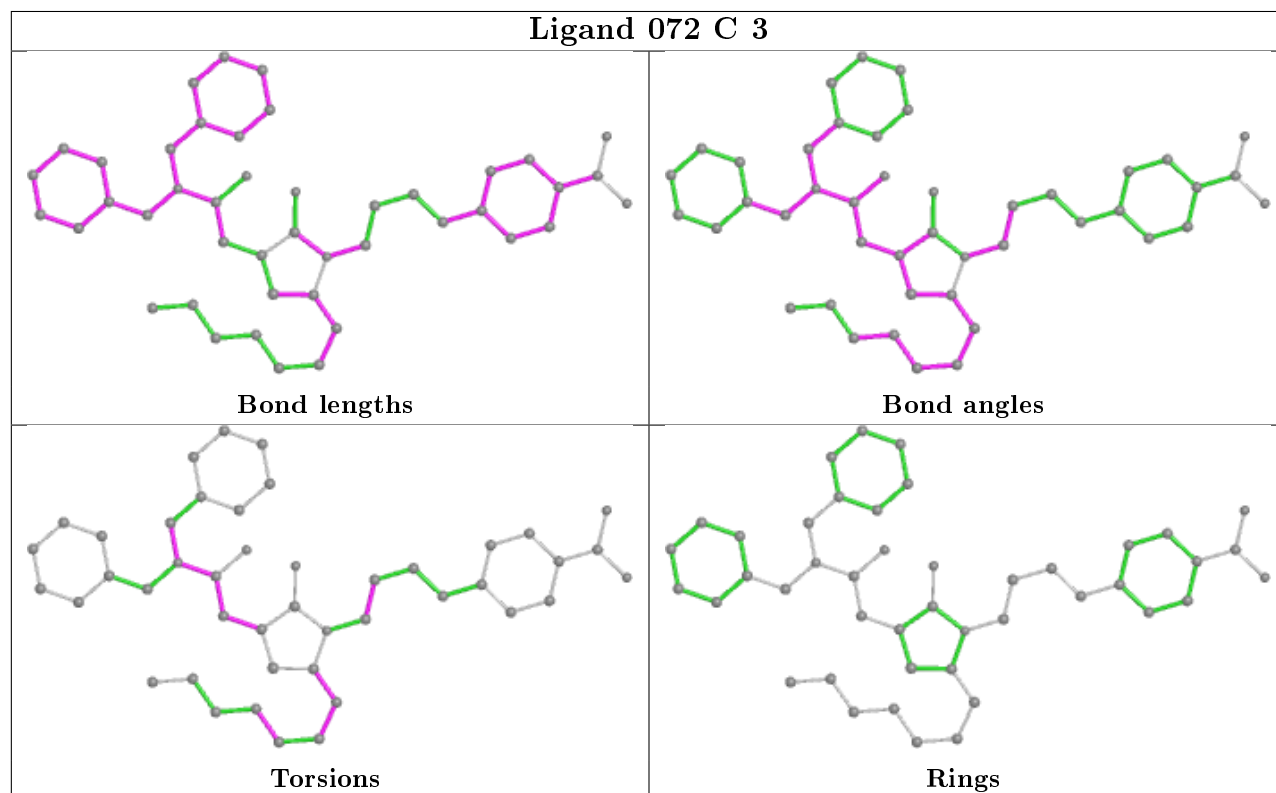
There are no ring outliers.

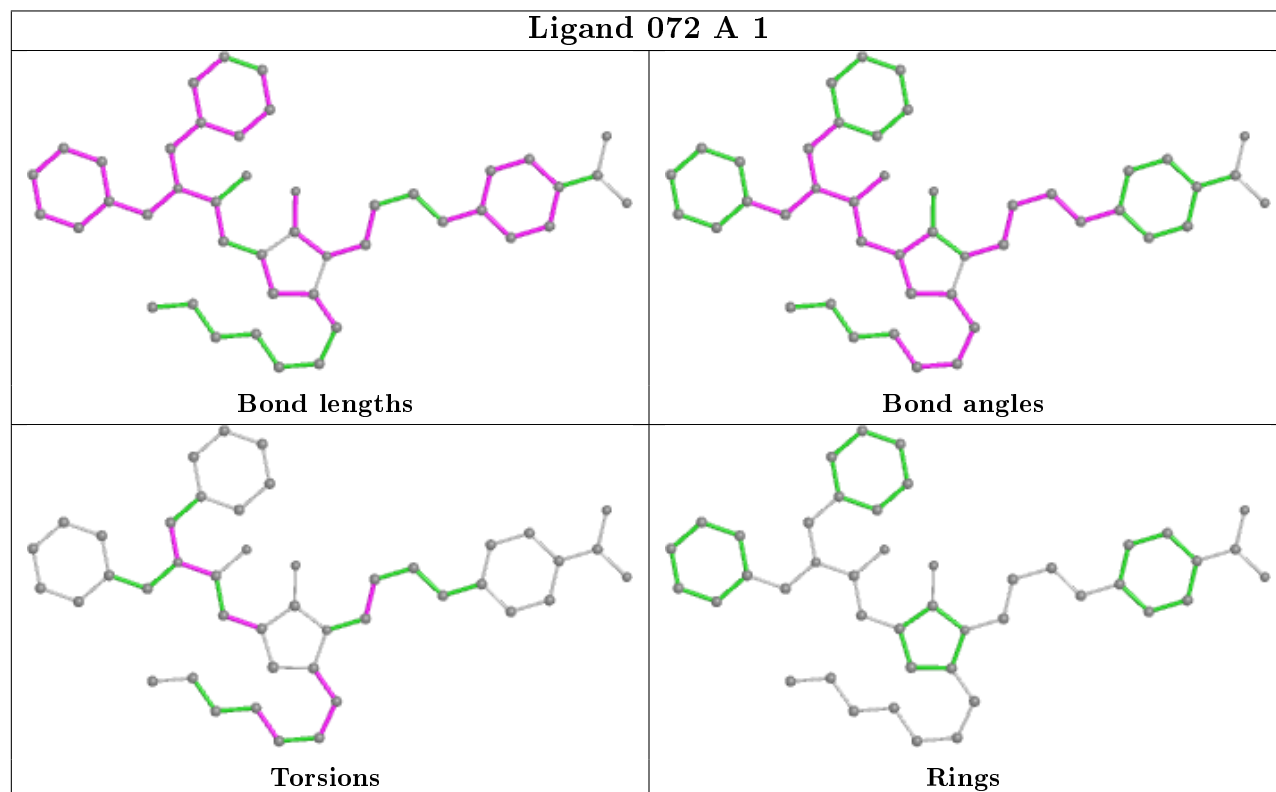
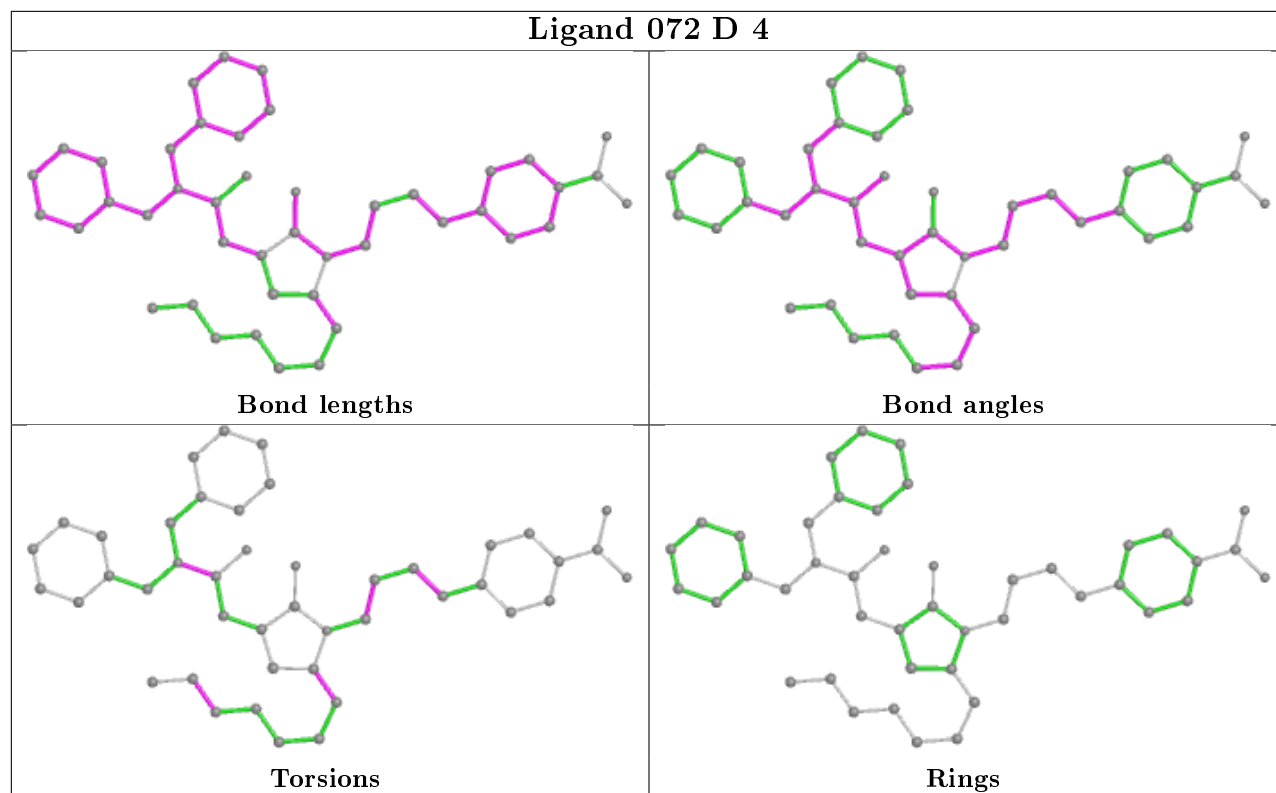
4 monomers are involved in 15 short contacts:

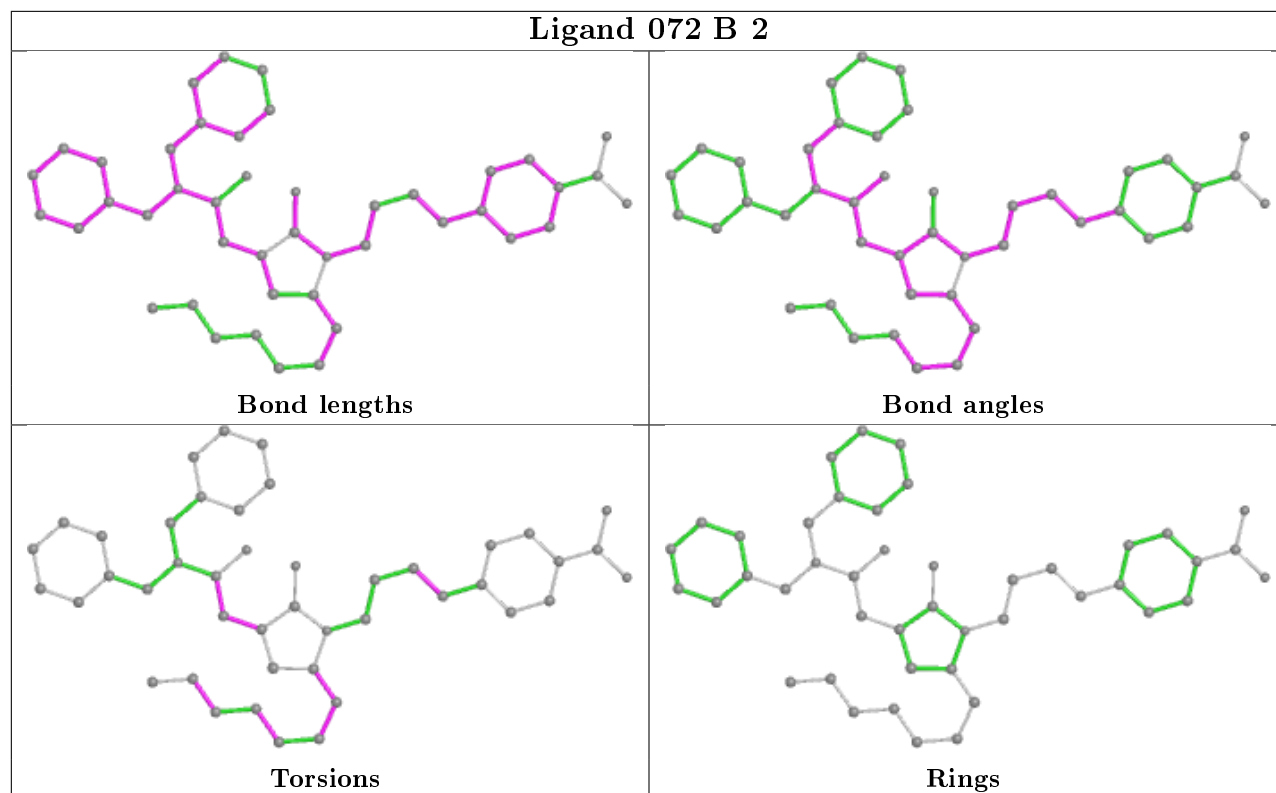
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	072	4	0
2	D	4	072	1	0
2	A	1	072	6	0
2	B	2	072	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

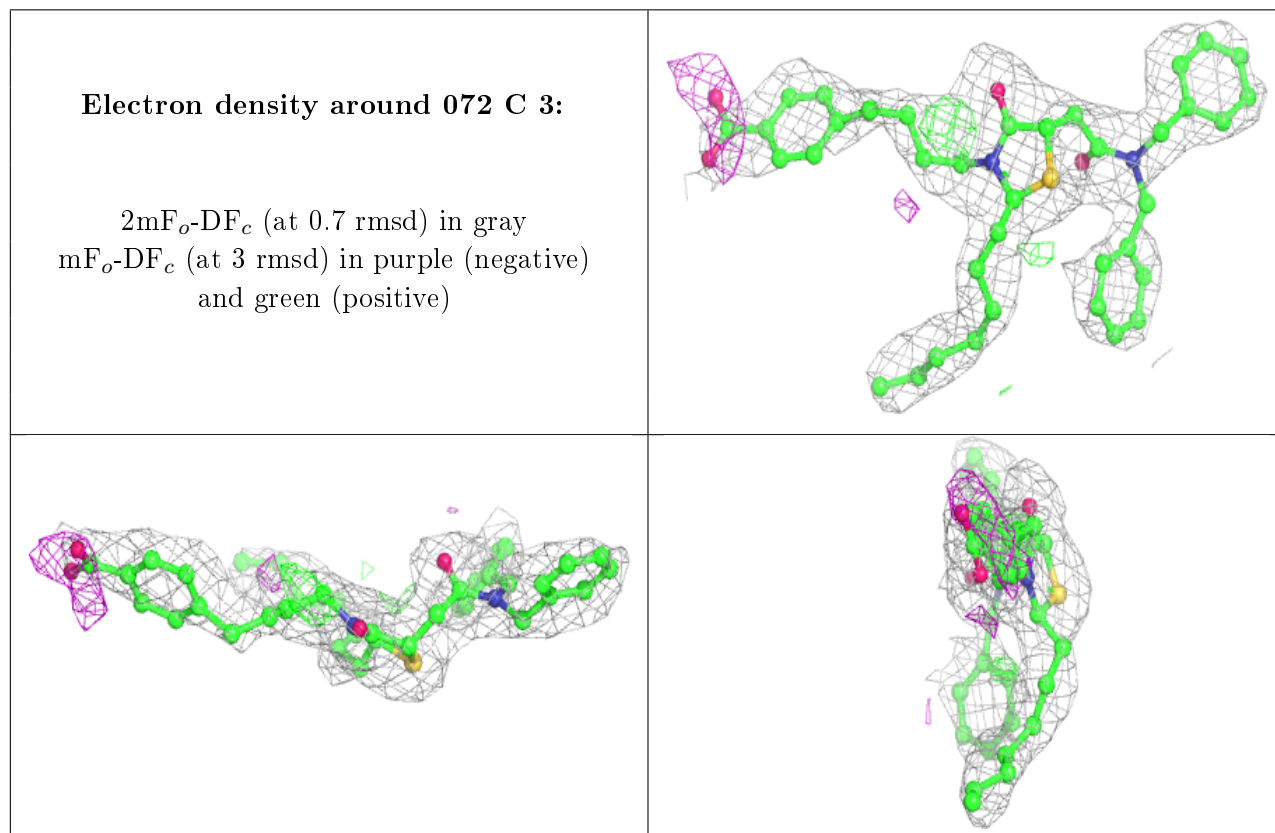
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

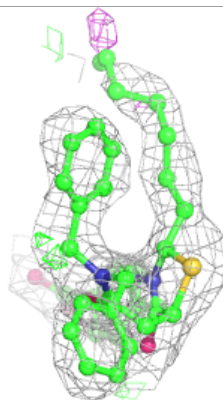
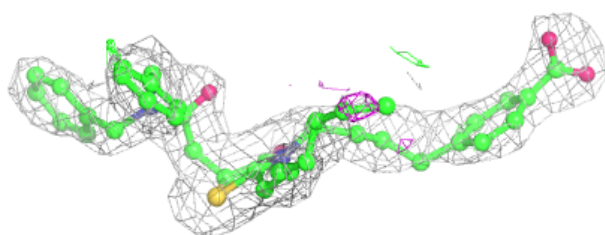
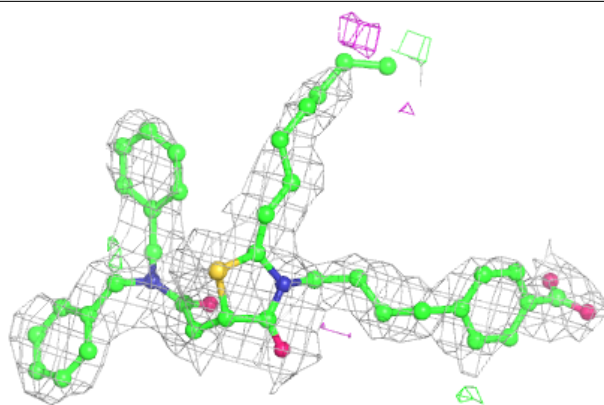
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

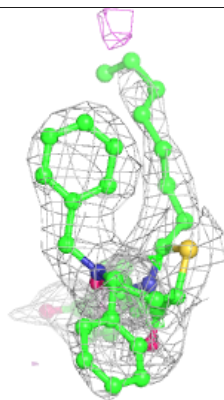
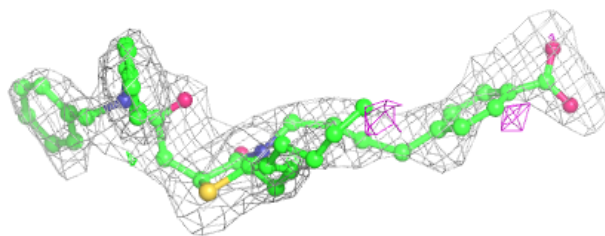
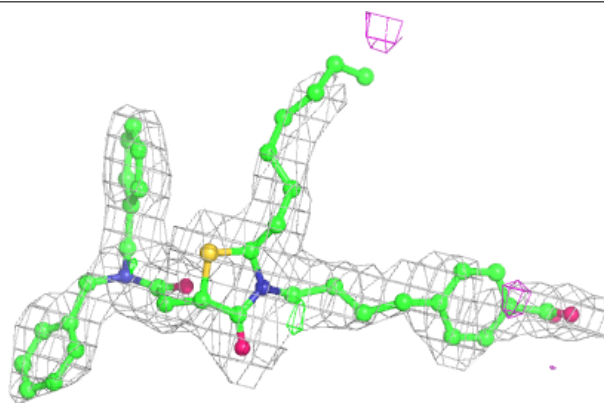


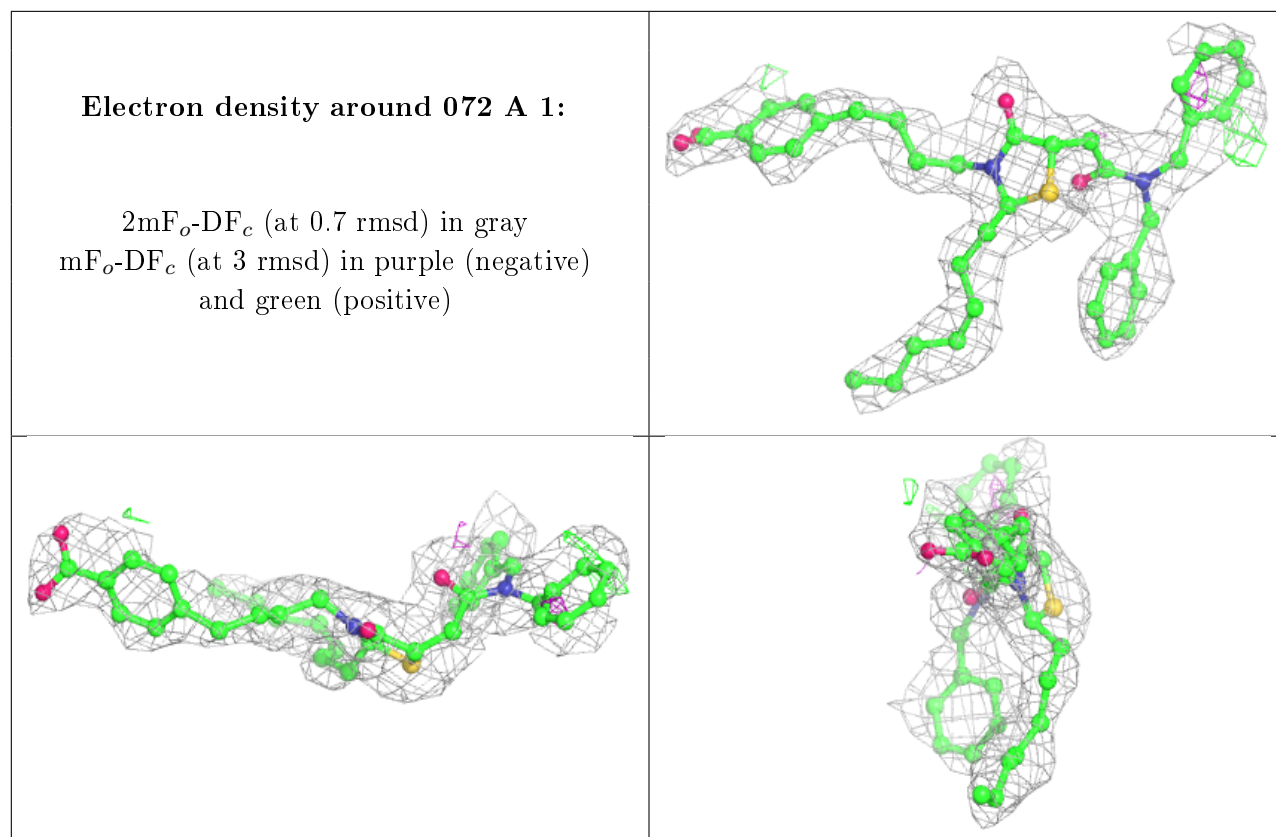
Electron density around 072 B 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 072 D 4:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.