



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:28 pm BST

PDB ID : 3NDM
Title : Crystal structure of Rho-Associated Protein Kinase (ROCK1) with a potent isoquinolone derivative
Authors : Li, X.
Deposited on : 2010-06-07
Resolution : 3.30 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

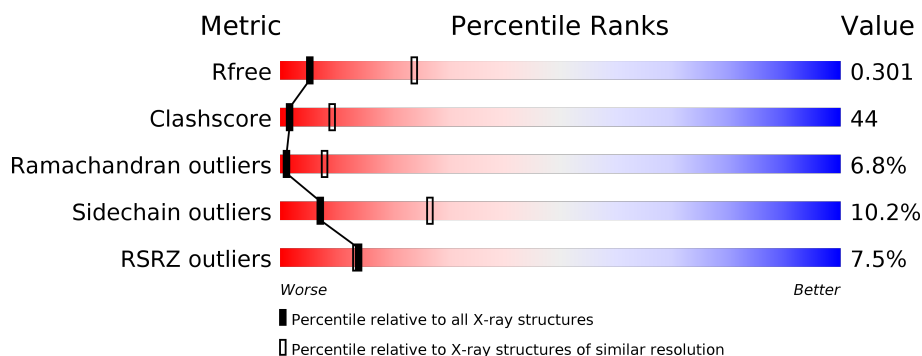
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 $\leq 5\%$. 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	415	
1	B	415	
1	C	415	
1	D	415	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12746 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.

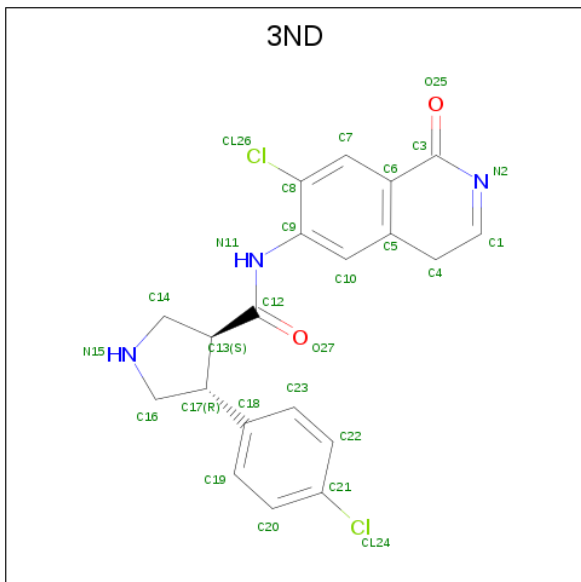
- Molecule 1 is a protein called Rho-Associated Protein Kinase (ROCK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3128	2005	517	584	22			
1	B	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			
1	C	371	Total	C	N	O	S	0	0	0
			3028	1944	493	569	22			
1	D	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q13464
A	2	SER	-	EXPRESSION TAG	UNP Q13464
A	3	LEU	-	EXPRESSION TAG	UNP Q13464
A	4	HIS	-	EXPRESSION TAG	UNP Q13464
A	5	MET	-	EXPRESSION TAG	UNP Q13464
B	1	GLY	-	EXPRESSION TAG	UNP Q13464
B	2	SER	-	EXPRESSION TAG	UNP Q13464
B	3	LEU	-	EXPRESSION TAG	UNP Q13464
B	4	HIS	-	EXPRESSION TAG	UNP Q13464
B	5	MET	-	EXPRESSION TAG	UNP Q13464
C	1	GLY	-	EXPRESSION TAG	UNP Q13464
C	2	SER	-	EXPRESSION TAG	UNP Q13464
C	3	LEU	-	EXPRESSION TAG	UNP Q13464
C	4	HIS	-	EXPRESSION TAG	UNP Q13464
C	5	MET	-	EXPRESSION TAG	UNP Q13464
D	1	GLY	-	EXPRESSION TAG	UNP Q13464
D	2	SER	-	EXPRESSION TAG	UNP Q13464
D	3	LEU	-	EXPRESSION TAG	UNP Q13464
D	4	HIS	-	EXPRESSION TAG	UNP Q13464
D	5	MET	-	EXPRESSION TAG	UNP Q13464

- Molecule 2 is (3S,4R)-N-(7-chloro-1-oxo-1,4-dihydroisoquinolin-6-yl)-4-(4-chlorophenyl)pyrrolidine-3-carboxamide (three-letter code: 3ND) (formula: C₂₀H₁₇Cl₂N₃O₂).



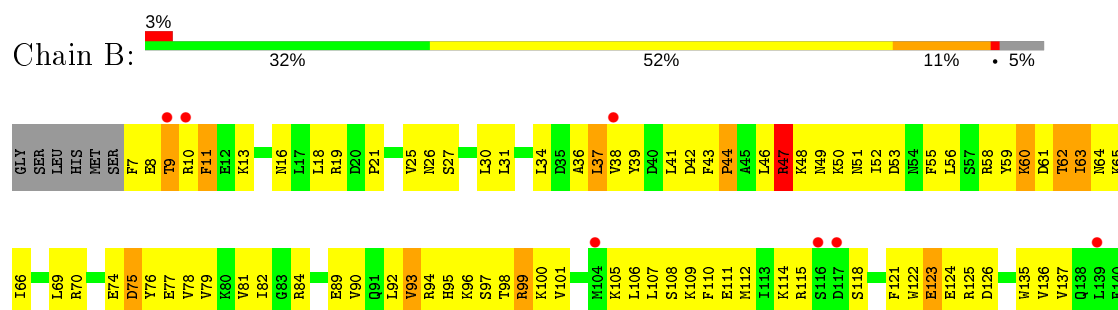
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	D	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		

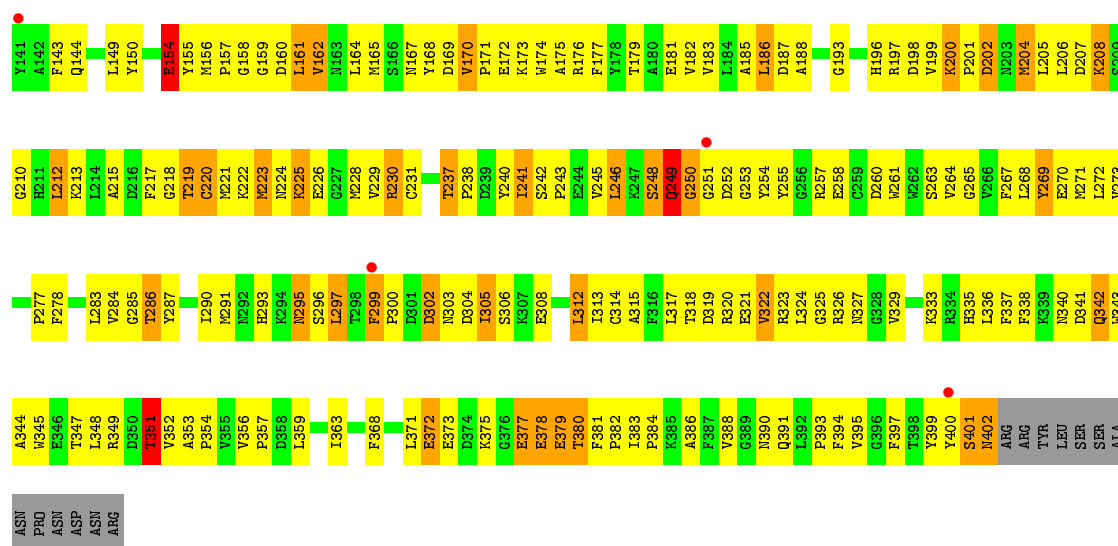
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	16	Total	O	0	0
			16	16		
3	C	15	Total	O	0	0
			15	15		
3	D	14	Total	O	0	0
			14	14		

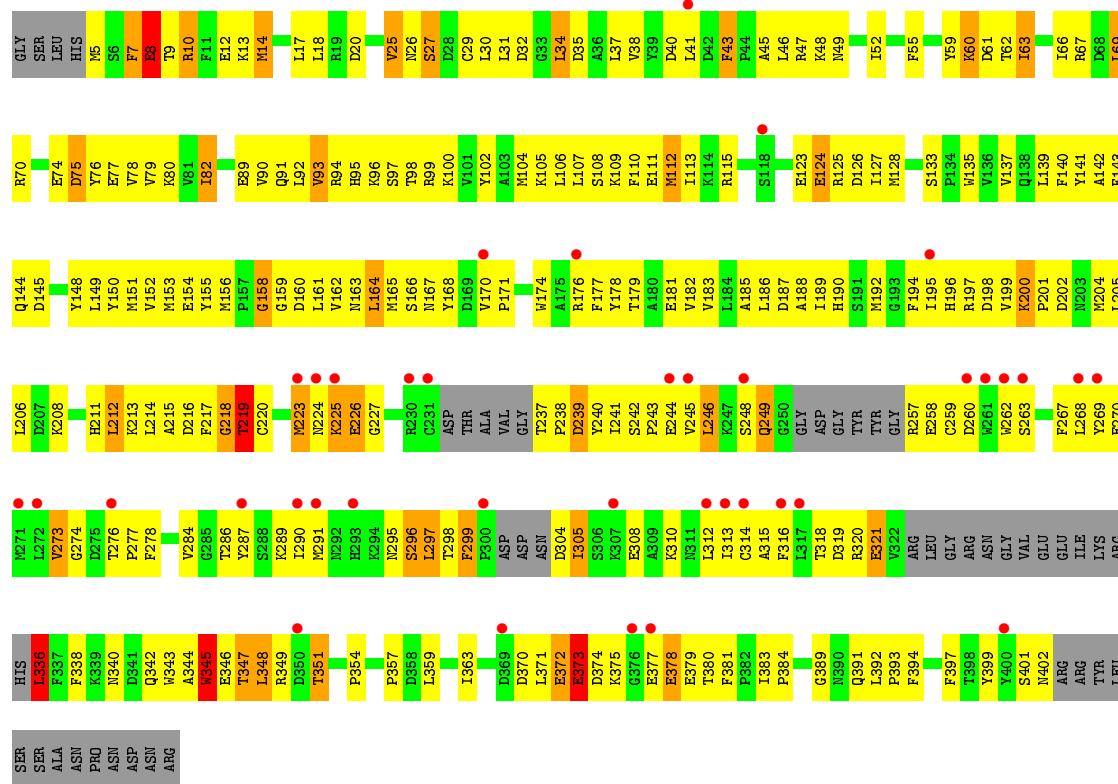
i

- Molecule 1: Rho-Associated Protein Kinase (ROCK1)

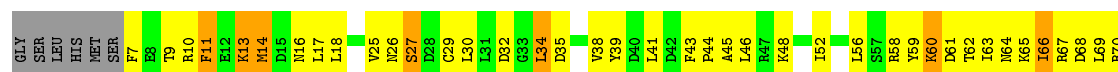




● Molecule 1: Rho-Associated Protein Kinase (ROCK1)



● Molecule 1: Rho-Associated Protein Kinase (ROCK1)



ASN	D341	L268	P201	Q138	W71
PRO	Q342	Y269	D202	L139	K72
ASN	W343	E270	N203	F140	
ASP	A344	M271	N204		D75
ASN	W345	L272	L205	F143	Y76
ASN	E346	V273	L206	G144	
ARG	T347		D207	D145	
	L348	P277	K208	D146	V79
	R349	F278	S209	R147	K80
	D350		G210	Y148	V81
	T351	D281	H211		I82
		L212		V152	G83
	P354	S282		M153	R84
	V355	L283	D216	E154	
	V356	V284	F217	Y155	E89
	P357	T286	G218	M156	V90
		Y287	T219	P157	Q91
	D362	S288	C220	G158	L92
	I363	K289	N221	G159	V93
	D364	I290	K222	D160	R94
	T365		M223	L161	H95
		K294	N224	V162	A96
	F368	N295	K225	N163	S97
	D369	S296	E226	L164	T98
	D370	L297	G227	M165	R99
	L371	T298	K228	S166	K100
	E372	F299	V229		V101
	E373	P300	R230	M167	
	D374		C231	Y168	M104
		N303		D169	K105
	E377	D304	V235	V170	L406
	E378	I305	G236	P171	L107
	E379	S306	T237	E172	S108
	T380	K307	P238	A173	K109
	F381		D239	W174	F110
	P382	L312	Y240	A175	E111
	I383	I313	I241	R176	M112
	P384	G314	S242	F177	I113
	K385	A315	F243	Y178	K114
	A386	F316	E244	T179	K115
	F387	L317	V245	A180	S116
	V388	T318	V245	E181	D117
	G389	K247	L246	V182	S118
	N390	V222	K247	V183	A119
	Q391	K323	S248	L184	F120
	L392	L324	Q249	A185	F121
	P393	G325	G250	L186	F122
		R326	G251	D187	W123
		N327	D252	A188	E124
	F397	G328	G253	I189	R125
		V329		H190	D126
	Y400	E330	R257	S191	I127
	N402	E331		M192	M128
	ARG	I332	D260	G193	A129
	ARG	K333	W261	F194	F130
	TYR		W262	I195	
	LEU	F337	S263	H196	S133
	SER	F338	V264	R197	F134
	SER	K339	G265	D198	W135
	ALA	N340	V266	V199	V136
			F267	K200	V137

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.78 Å 83.55 Å 177.96 Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	42.53 – 3.30 44.72 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.53-3.30) 99.6 (44.72-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.32 Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.241 , 0.310 0.232 , 0.301	Depositor DCC
R_{free} test set	1402 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	129.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 160.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12746	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: 3ND

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	0.39	0/3199	0.57	0/4314
1	B	0.55	0/3299	0.67	0/4457
1	C	0.49	0/3098	0.62	1/4180 (0.0%)
1	D	0.56	0/3299	0.67	0/4457
All	All	0.50	0/12895	0.63	1/17408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	LEU	CA-CB-CG	-5.52	102.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3128	0	3048	269	0
1	B	3222	0	3120	282	0
1	C	3028	0	2943	304	0
1	D	3222	0	3120	292	0
2	B	27	0	17	7	0
2	C	27	0	17	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	17	5	0
3	A	20	0	0	5	0
3	B	16	0	0	3	0
3	C	15	0	0	5	0
3	D	14	0	0	1	0
All	All	12746	0	12282	1105	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 44.

All (1105) 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:66:ILE:HD11	1:B:25:VAL:HG21	1.35	1.08
1:A:399:TYR:CE2	1:A:401:SER:HB2	1.91	1.04
1:A:230:ARG:HH21	1:A:254:TYR:HB2	1.23	1.02
1:C:78:VAL:HA	1:C:93:VAL:HG12	1.42	1.00
1:B:38:VAL:HG21	1:B:63:ILE:HG13	1.41	0.99
1:D:161:LEU:HD23	1:D:267:PHE:HZ	1.27	0.99
1:D:34:LEU:HD12	1:D:63:ILE:HD11	1.48	0.96
1:B:159:GLY:HA2	1:B:368:PHE:HE2	1.31	0.96
1:B:149:LEU:HD22	1:B:397:PHE:CD2	2.01	0.95
1:A:381:PHE:HD2	1:A:382:PRO:HD2	1.27	0.95
1:B:159:GLY:HA2	1:B:368:PHE:CE2	2.03	0.94
1:C:141:TYR:HH	1:D:7:PHE:HZ	0.97	0.92
1:C:90:VAL:HG22	1:C:105:LYS:HB2	1.48	0.91
1:D:105:LYS:HE2	1:D:107:LEU:HD21	1.51	0.90
1:D:289:LYS:HD3	1:D:296:SER:OG	1.72	0.90
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.52	0.89
1:A:149:LEU:HD22	1:A:397:PHE:CD2	2.07	0.89
1:D:190:HIS:HB3	1:D:257:ARG:HH12	1.35	0.88
1:D:261:TRP:O	1:D:264:VAL:HB	1.73	0.88
1:B:225:LYS:HG3	1:C:379:GLU:HG2	1.56	0.88
1:A:78:VAL:HA	1:A:93:VAL:HG12	1.54	0.87
1:A:324:LEU:HG	1:A:332:ILE:HG12	1.57	0.86
1:C:187:ASP:HA	1:C:190:HIS:HD2	1.40	0.86
1:D:165:MET:HE1	1:D:271:MET:HA	1.58	0.86
1:A:87:PHE:HE1	1:A:115:ARG:HG3	1.40	0.85
1:C:139:LEU:HD11	1:C:141:TYR:O	1.76	0.85
1:B:181:GLU:HG2	1:B:348:LEU:HD21	1.57	0.85
1:D:190:HIS:HB3	1:D:257:ARG:NH1	1.92	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PHE:CD2	1:A:382:PRO:HD2	2.13	0.84
1:D:181:GLU:HB3	1:D:212:LEU:HD22	1.59	0.84
1:B:41:LEU:HD22	1:B:52:ILE:HD13	1.59	0.84
1:B:399:TYR:CZ	1:B:401:SER:HB3	2.14	0.83
1:B:268:LEU:HD23	1:B:313:ILE:HG13	1.61	0.82
1:A:304:ASP:N	1:A:310:LYS:HZ1	1.78	0.82
1:C:225:LYS:HD3	1:C:225:LYS:H	1.43	0.82
1:C:38:VAL:HG21	1:C:63:ILE:HG13	1.60	0.82
1:A:196:HIS:HE1	1:A:216:ASP:O	1.62	0.82
1:C:43:PHE:CD1	1:C:384:PRO:HD2	2.13	0.82
1:D:159:GLY:HA2	1:D:368:PHE:HE2	1.43	0.82
1:B:174:TRP:CD1	1:B:354:PRO:HB3	2.15	0.81
1:A:144:GLN:HB3	1:A:149:LEU:HD23	1.62	0.81
1:C:305:ILE:HD13	1:C:305:ILE:H	1.44	0.81
1:C:8:GLU:H	1:C:8:GLU:CD	1.84	0.81
1:B:215:ALA:HB1	2:B:900:3ND:H4A	1.62	0.81
1:C:25:VAL:HG23	1:C:25:VAL:O	1.81	0.81
1:D:184:LEU:HD21	1:D:333:LYS:NZ	1.96	0.81
1:A:261:TRP:HE3	1:A:264:VAL:HG21	1.46	0.81
1:D:184:LEU:HD21	1:D:333:LYS:HZ1	1.46	0.81
1:C:158:GLY:HA3	1:C:206:LEU:O	1.81	0.80
1:A:241:ILE:HG12	1:A:246:LEU:HD13	1.62	0.80
1:B:258:GLU:HG3	1:B:320:ARG:HG3	1.63	0.80
1:B:399:TYR:OH	1:B:401:SER:HB3	1.81	0.80
1:C:171:PRO:HD2	1:C:174:TRP:CE3	2.17	0.80
1:D:159:GLY:HA2	1:D:368:PHE:CE2	2.16	0.80
1:A:179:THR:O	1:A:183:VAL:HG23	1.82	0.79
1:C:13:LYS:O	1:C:17:LEU:HD13	1.83	0.78
1:D:362:ASP:OD2	1:D:363:ILE:HG23	1.83	0.78
1:A:159:GLY:HA2	1:A:368:PHE:CZ	2.17	0.78
1:A:47:ARG:HH11	1:A:47:ARG:HG2	1.46	0.78
1:B:105:LYS:HE2	1:B:107:LEU:HD21	1.65	0.78
1:B:137:VAL:HG11	2:B:900:3ND:H1	1.64	0.78
1:B:246:LEU:HG	1:B:287:TYR:CE1	2.18	0.78
1:C:393:PRO:HA	1:D:58:ARG:HH22	1.48	0.78
1:C:393:PRO:HA	1:D:58:ARG:NH2	1.99	0.78
1:B:160:ASP:OD2	1:B:162:VAL:HG12	1.84	0.77
1:D:217:PHE:HB3	1:D:220:CYS:SG	2.24	0.77
1:C:200:LYS:HE3	1:C:202:ASP:HB2	1.66	0.77
1:B:177:PHE:CE2	1:B:354:PRO:HD2	2.20	0.76
1:A:392:LEU:HD22	1:B:55:PHE:CD1	2.19	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD12	1:B:63:ILE:HD11	1.67	0.76
1:D:182:VAL:HG21	1:D:267:PHE:HE2	1.50	0.76
1:C:215:ALA:HB1	2:C:900:3ND:H4A	1.67	0.76
1:D:218:GLY:O	1:D:219:THR:HG23	1.86	0.76
1:B:246:LEU:HG	1:B:287:TYR:HE1	1.49	0.76
1:D:286:THR:O	1:D:290:ILE:HG13	1.86	0.76
1:D:200:LYS:HE2	1:D:202:ASP:HB2	1.68	0.76
1:A:25:VAL:HG23	1:A:25:VAL:O	1.84	0.76
1:A:268:LEU:HD22	1:A:312:LEU:HD13	1.66	0.76
1:C:179:THR:O	1:C:183:VAL:HG23	1.86	0.76
1:A:39:TYR:CE1	1:A:146:ASP:HB3	2.21	0.75
1:B:81:VAL:HG21	1:B:373:GLU:HA	1.66	0.75
1:B:181:GLU:HG2	1:B:348:LEU:CD2	2.16	0.75
1:C:170:VAL:HG13	1:C:174:TRP:HB2	1.66	0.75
1:A:136:VAL:HG12	1:A:137:VAL:O	1.87	0.75
1:B:158:GLY:HA3	1:B:206:LEU:HB2	1.66	0.75
1:A:262:TRP:HB2	1:A:323:ARG:NH1	2.01	0.74
1:B:322:VAL:HG22	1:B:322:VAL:O	1.86	0.74
1:C:41:LEU:HD22	1:C:52:ILE:HD13	1.67	0.74
1:D:204:MET:C	1:D:205:LEU:HD23	2.07	0.74
1:A:261:TRP:CE3	1:A:264:VAL:HG21	2.23	0.74
1:C:241:ILE:HD11	1:C:245:VAL:HG11	1.69	0.74
1:C:69:LEU:O	1:D:10:ARG:HD2	1.87	0.74
1:A:31:LEU:HG	1:B:30:LEU:HD13	1.69	0.74
1:B:245:VAL:O	1:B:248:SER:HB2	1.88	0.73
1:C:66:ILE:O	1:C:70:ARG:HG3	1.87	0.73
1:B:400:TYR:O	1:B:401:SER:HB2	1.88	0.73
1:D:212:LEU:O	1:D:212:LEU:HD23	1.87	0.73
1:D:261:TRP:HE3	1:D:264:VAL:HG21	1.54	0.73
1:A:78:VAL:HA	1:A:93:VAL:CG1	2.18	0.73
1:B:161:LEU:HD11	1:B:206:LEU:HD21	1.71	0.73
1:C:69:LEU:HD12	1:D:14:MET:SD	2.28	0.73
1:D:41:LEU:HD22	1:D:52:ILE:HD13	1.69	0.73
1:B:66:ILE:O	1:B:70:ARG:HG3	1.89	0.73
1:C:115:ARG:HG2	1:C:115:ARG:HH21	1.54	0.72
1:A:156:MET:SD	1:A:213:LYS:HD2	2.28	0.72
1:B:202:ASP:O	2:B:900:3ND:H14A	1.89	0.72
1:D:161:LEU:O	1:D:165:MET:HG3	1.88	0.72
1:C:29:CYS:O	1:C:32:ASP:HB2	1.89	0.72
1:C:299:PHE:CZ	1:C:310:LYS:HG2	2.24	0.72
1:C:90:VAL:HA	1:C:105:LYS:HA	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLU:OE2	1:C:213:LYS:HE3	1.90	0.72
1:D:161:LEU:HD23	1:D:267:PHE:CZ	2.18	0.71
1:B:92:LEU:HD13	1:B:155:TYR:CD1	2.25	0.71
1:D:177:PHE:CE2	1:D:354:PRO:HD2	2.26	0.71
1:D:392:LEU:N	1:D:393:PRO:HD2	2.05	0.71
1:D:111:GLU:HB3	1:D:115:ARG:NH2	2.05	0.71
1:B:246:LEU:C	1:B:248:SER:H	1.90	0.71
1:B:84:ARG:NH2	1:B:372:GLU:HG3	2.05	0.71
1:A:321:GLU:H	1:A:321:GLU:CD	1.94	0.71
1:B:212:LEU:HG	1:B:213:LYS:N	2.02	0.71
1:B:161:LEU:CD1	1:B:206:LEU:HD21	2.21	0.71
1:C:141:TYR:HB2	1:C:152:VAL:HB	1.73	0.70
1:D:241:ILE:HD11	1:D:245:VAL:HB	1.73	0.70
1:A:66:ILE:O	1:A:70:ARG:HG3	1.92	0.70
1:A:137:VAL:HG23	1:A:214:LEU:O	1.91	0.70
1:B:381:PHE:HD2	1:B:382:PRO:HD2	1.57	0.70
1:C:34:LEU:O	1:C:38:VAL:HG23	1.92	0.70
1:A:158:GLY:HA3	1:A:206:LEU:O	1.91	0.70
1:B:84:ARG:HH22	1:B:372:GLU:HG3	1.56	0.70
1:D:41:LEU:HD13	1:D:52:ILE:HG23	1.72	0.70
1:A:38:VAL:HG21	1:A:63:ILE:HG13	1.72	0.70
1:C:343:TRP:HB3	1:C:351:THR:HG21	1.73	0.70
1:A:69:LEU:HD22	1:B:10:ARG:HB3	1.72	0.70
1:B:149:LEU:HD22	1:B:397:PHE:HD2	1.55	0.70
1:C:199:VAL:O	1:C:200:LYS:HB3	1.91	0.70
1:D:189:ILE:HA	1:D:192:MET:CE	2.22	0.70
1:A:109:LYS:HB3	1:A:394:PHE:HE1	1.57	0.69
1:D:343:TRP:CD2	1:D:348:LEU:HD13	2.26	0.69
1:C:269:TYR:CZ	1:C:273:VAL:HG21	2.27	0.69
1:A:58:ARG:HH22	1:B:393:PRO:HA	1.55	0.69
1:D:333:LYS:HB3	1:D:345:TRP:NE1	2.07	0.69
1:C:18:LEU:HD22	1:D:27:SER:HB3	1.73	0.69
1:A:230:ARG:NH2	1:A:254:TYR:HB2	2.04	0.69
1:D:266:VAL:HG13	1:D:277:PRO:HD2	1.75	0.69
1:B:225:LYS:HG3	1:C:379:GLU:CG	2.23	0.69
1:C:123:GLU:O	1:C:127:ILE:HG13	1.92	0.69
1:D:237:THR:HG22	1:D:238:PRO:HD2	1.75	0.69
1:C:217:PHE:HB3	1:C:220:CYS:SG	2.33	0.69
1:C:79:VAL:HG11	1:C:92:LEU:HD23	1.74	0.69
1:D:104:MET:HG3	1:D:152:VAL:HG22	1.76	0.68
1:C:373:GLU:O	1:C:373:GLU:HG3	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:93:VAL:HG13	1.93	0.68
1:D:84:ARG:HD3	1:D:89:GLU:HB3	1.74	0.68
1:A:226:GLU:O	1:A:228:MET:HG2	1.93	0.68
1:C:262:TRP:CZ2	1:C:290:ILE:HG23	2.28	0.68
1:A:14:MET:SD	1:B:69:LEU:HB2	2.34	0.67
1:C:76:TYR:HE2	1:C:152:VAL:HG21	1.59	0.67
1:A:229:VAL:O	1:A:254:TYR:HD1	1.76	0.67
1:B:108:SER:HB3	1:B:111:GLU:HB2	1.76	0.67
1:B:136:VAL:HG12	1:B:137:VAL:O	1.94	0.67
1:D:225:LYS:HD3	1:D:225:LYS:H	1.59	0.67
1:A:8:GLU:H	1:A:8:GLU:CD	1.97	0.67
1:D:109:LYS:NZ	1:D:145:ASP:O	2.23	0.67
1:A:308:GLU:HB3	1:A:337:PHE:HA	1.76	0.67
1:C:189:ILE:HA	1:C:192:MET:HE2	1.77	0.67
1:C:304:ASP:N	3:C:419:HOH:O	2.27	0.67
1:A:330:GLU:OE2	1:A:333:LYS:HD2	1.95	0.67
1:B:59:TYR:O	1:B:60:LYS:C	2.32	0.66
1:D:82:ILE:HB	1:D:368:PHE:HD1	1.60	0.66
1:C:345:TRP:CE3	1:C:345:TRP:HA	2.29	0.66
1:C:345:TRP:HA	1:C:345:TRP:HE3	1.60	0.66
1:D:123:GLU:O	1:D:127:ILE:HG13	1.96	0.66
1:A:115:ARG:HH21	1:A:115:ARG:HG2	1.60	0.66
1:A:176:ARG:HD3	1:A:338:PHE:HA	1.77	0.66
1:A:328:GLY:O	1:A:331:GLU:HG2	1.96	0.66
1:B:225:LYS:CG	1:C:379:GLU:HG2	2.25	0.66
1:D:35:ASP:OD1	1:D:67:ARG:NE	2.28	0.66
1:C:8:GLU:CD	1:C:8:GLU:N	2.49	0.66
1:B:179:THR:O	1:B:183:VAL:HG23	1.96	0.66
1:C:343:TRP:CB	1:C:351:THR:HG21	2.25	0.66
1:C:93:VAL:HB	3:C:423:HOH:O	1.95	0.66
1:C:9:THR:O	1:C:12:GLU:N	2.28	0.66
1:B:38:VAL:HG11	1:B:63:ILE:HG21	1.78	0.66
1:C:142:ALA:HB3	1:C:399:TYR:HB3	1.78	0.66
1:C:140:PHE:O	1:C:141:TYR:CD1	2.49	0.66
1:D:322:VAL:HB	1:D:326:ARG:HH21	1.60	0.66
1:A:6:SER:O	1:A:9:THR:HB	1.94	0.65
1:B:277:PRO:HG2	1:B:278:PHE:CD2	2.31	0.65
1:C:187:ASP:HA	1:C:190:HIS:CD2	2.26	0.65
1:C:199:VAL:HB	1:C:263:SER:HB3	1.78	0.65
1:D:238:PRO:O	1:D:241:ILE:HG22	1.96	0.65
1:D:392:LEU:N	1:D:393:PRO:CD	2.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:O	1:A:17:LEU:HD13	1.97	0.65
1:B:174:TRP:NE1	1:B:354:PRO:HB3	2.11	0.65
1:C:205:LEU:O	1:C:212:LEU:HA	1.96	0.65
1:C:258:GLU:HG3	1:C:320:ARG:HG3	1.79	0.65
1:C:78:VAL:HA	1:C:93:VAL:CG1	2.21	0.65
1:B:182:VAL:HG21	1:B:204:MET:HE2	1.79	0.65
1:C:204:MET:HB3	1:C:212:LEU:HD12	1.79	0.65
1:D:182:VAL:HG22	1:D:212:LEU:HD11	1.79	0.65
1:D:286:THR:HA	1:D:289:LYS:HB2	1.77	0.65
1:A:127:ILE:HD11	1:A:194:PHE:CD2	2.32	0.65
1:A:225:LYS:H	1:A:225:LYS:HD3	1.62	0.65
1:A:312:LEU:HD12	1:A:337:PHE:CD2	2.32	0.65
1:B:308:GLU:HB3	1:B:337:PHE:HA	1.79	0.65
1:D:158:GLY:HA3	1:D:206:LEU:O	1.97	0.65
1:D:277:PRO:C	1:D:278:PHE:CD2	2.70	0.64
1:A:186:LEU:HD22	1:A:190:HIS:NE2	2.12	0.64
1:B:55:PHE:HD2	1:B:56:LEU:HD23	1.62	0.64
1:C:170:VAL:HG22	1:C:174:TRP:HE3	1.61	0.64
1:D:38:VAL:HG21	1:D:63:ILE:HG13	1.79	0.64
1:D:82:ILE:HB	1:D:368:PHE:CD1	2.33	0.64
1:B:401:SER:HA	1:B:402:ASN:C	2.18	0.64
1:A:43:PHE:CD1	1:A:384:PRO:HD2	2.33	0.64
1:D:391:GLN:C	1:D:393:PRO:HD2	2.18	0.64
1:B:193:GLY:O	1:B:222:LYS:HG3	1.98	0.64
1:D:154:GLU:HG3	1:D:154:GLU:O	1.97	0.64
1:C:45:ALA:O	1:C:48:LYS:HD3	1.98	0.63
1:C:63:ILE:HD13	1:C:66:ILE:HD12	1.80	0.63
1:C:75:ASP:C	1:C:76:TYR:HD1	2.02	0.63
1:D:189:ILE:HA	1:D:192:MET:HE2	1.78	0.63
1:D:363:ILE:O	1:D:363:ILE:HG13	1.98	0.63
1:D:66:ILE:O	1:D:70:ARG:HG3	1.99	0.63
1:A:269:TYR:CE2	1:A:273:VAL:HG21	2.33	0.63
1:A:278:PHE:O	1:A:286:THR:HG23	1.98	0.63
1:A:268:LEU:CD2	1:A:312:LEU:HD13	2.28	0.63
1:A:224:ASN:HB2	1:A:225:LYS:HZ2	1.64	0.63
1:B:196:HIS:O	1:B:197:ARG:HB2	1.96	0.63
1:A:34:LEU:HD12	1:A:63:ILE:HD11	1.81	0.63
1:C:27:SER:HB3	1:D:18:LEU:HD22	1.79	0.63
1:D:262:TRP:HZ2	1:D:290:ILE:CG2	2.10	0.63
1:D:333:LYS:HE2	1:D:345:TRP:CE2	2.34	0.63
1:C:208:LYS:C	1:C:357:PRO:HG2	2.18	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:HG2	3:A:424:HOH:O	1.99	0.62
1:C:204:MET:C	1:C:205:LEU:HD23	2.19	0.62
1:D:165:MET:CE	1:D:271:MET:HA	2.28	0.62
1:A:47:ARG:CG	1:A:47:ARG:HH11	2.11	0.62
1:A:395:VAL:O	1:B:58:ARG:NH1	2.33	0.62
1:A:32:ASP:OD2	1:A:398:THR:HB	1.99	0.62
1:B:156:MET:HE1	1:B:207:ASP:HB3	1.81	0.62
1:C:76:TYR:CE2	1:C:152:VAL:HG21	2.33	0.62
1:D:262:TRP:HZ2	1:D:290:ILE:HG23	1.65	0.62
1:D:164:LEU:HD11	1:D:178:TYR:OH	1.98	0.62
1:D:46:LEU:HD21	1:D:386:ALA:HA	1.81	0.62
1:A:77:GLU:O	1:A:93:VAL:HG12	2.00	0.62
1:B:31:LEU:HB3	1:B:70:ARG:NH1	2.13	0.62
1:D:146:ASP:N	1:D:146:ASP:OD1	2.25	0.62
1:A:161:LEU:HD23	1:A:267:PHE:CZ	2.34	0.62
1:A:161:LEU:HD23	1:A:267:PHE:HZ	1.63	0.62
1:A:47:ARG:NH1	1:A:47:ARG:HG2	2.11	0.62
1:D:138:GLN:HG2	1:D:140:PHE:CE2	2.35	0.62
1:D:333:LYS:HE2	1:D:345:TRP:CD2	2.35	0.62
1:C:128:MET:CE	1:C:153:MET:SD	2.88	0.61
1:B:295:ASN:O	1:B:297:LEU:N	2.33	0.61
1:D:269:TYR:CE2	1:D:273:VAL:HG21	2.35	0.61
1:A:226:GLU:HG3	1:A:228:MET:HG3	1.82	0.61
1:B:381:PHE:CD2	1:B:382:PRO:HD2	2.36	0.61
1:C:92:LEU:O	1:C:93:VAL:HG13	2.01	0.61
1:A:224:ASN:HB2	1:A:225:LYS:NZ	2.14	0.61
1:B:167:ASN:O	1:B:168:TYR:CD1	2.53	0.61
1:C:41:LEU:HD22	1:C:52:ILE:CD1	2.29	0.61
1:D:307:LYS:NZ	1:D:307:LYS:HB3	2.15	0.61
1:B:165:MET:CE	1:B:271:MET:HA	2.30	0.61
1:C:224:ASN:OD1	1:C:226:GLU:HG2	2.01	0.61
1:D:59:TYR:O	1:D:60:LYS:C	2.38	0.61
1:D:211:HIS:HB3	1:D:349:ARG:HH21	1.64	0.61
1:B:230:ARG:NH1	1:B:230:ARG:HB3	2.16	0.61
1:C:94:ARG:N	3:C:423:HOH:O	2.33	0.61
1:C:108:SER:O	1:C:112:MET:HB2	2.01	0.60
1:C:111:GLU:OE1	1:C:115:ARG:NH2	2.30	0.60
1:C:297:LEU:HD21	1:C:314:CYS:SG	2.40	0.60
1:C:76:TYR:HE2	1:C:152:VAL:CG2	2.14	0.60
1:A:330:GLU:HA	1:A:330:GLU:OE2	2.01	0.60
1:C:244:GLU:CD	1:C:320:ARG:HB2	2.21	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:HA	1:B:308:GLU:OE1	2.01	0.60
1:B:321:GLU:O	1:B:326:ARG:CZ	2.50	0.60
1:B:144:GLN:NE2	1:B:394:PHE:O	2.31	0.60
1:D:174:TRP:CD1	1:D:354:PRO:HB3	2.37	0.60
1:C:113:ILE:HG13	1:C:381:PHE:HZ	1.65	0.60
1:C:278:PHE:O	1:C:286:THR:HG23	2.01	0.60
1:D:108:SER:O	1:D:112:MET:HE2	2.01	0.60
1:D:81:VAL:HG21	1:D:373:GLU:HA	1.83	0.60
1:A:196:HIS:CE1	1:A:216:ASP:O	2.51	0.60
1:B:165:MET:HE2	1:B:271:MET:HA	1.84	0.60
1:A:135:TRP:HA	1:A:135:TRP:CE3	2.37	0.60
1:A:237:THR:HG23	1:A:238:PRO:HD2	1.83	0.60
1:B:109:LYS:HE2	1:B:394:PHE:CD1	2.37	0.60
1:B:110:PHE:CG	1:B:379:GLU:HB3	2.37	0.60
1:C:156:MET:HG3	1:C:205:LEU:HD12	1.84	0.60
1:A:135:TRP:CH2	1:A:181:GLU:HG2	2.36	0.59
1:B:265:GLY:HA3	1:B:317:LEU:CD1	2.32	0.59
1:D:181:GLU:HB3	1:D:212:LEU:CD2	2.31	0.59
1:B:164:LEU:HD23	1:B:164:LEU:O	2.01	0.59
1:C:135:TRP:CH2	1:C:181:GLU:HG2	2.37	0.59
1:C:40:ASP:OD2	1:C:391:GLN:HB2	2.02	0.59
1:B:225:LYS:H	1:B:225:LYS:HD3	1.67	0.59
1:C:223:MET:HE3	1:C:227:GLY:HA2	1.83	0.59
1:D:243:PRO:HD3	1:D:262:TRP:CE2	2.37	0.59
1:B:224:ASN:HD21	1:B:228:MET:HB2	1.68	0.59
1:B:7:PHE:C	1:B:9:THR:H	2.06	0.59
1:C:299:PHE:CE2	1:C:305:ILE:HD11	2.37	0.59
1:C:66:ILE:HD11	1:D:25:VAL:HG11	1.84	0.59
1:B:114:LYS:HE2	1:B:115:ARG:NH1	2.18	0.59
1:A:14:MET:HE1	1:B:69:LEU:HD12	1.84	0.59
1:B:230:ARG:HD2	1:C:380:THR:HG21	1.85	0.59
1:C:262:TRP:HZ2	1:C:290:ILE:HG23	1.68	0.59
1:D:160:ASP:OD2	1:D:162:VAL:HG12	2.02	0.59
1:A:11:PHE:O	1:A:15:ASP:OD2	2.21	0.59
1:A:208:LYS:C	1:A:357:PRO:HG2	2.23	0.59
1:B:204:MET:HB3	1:B:212:LEU:HD12	1.85	0.58
1:C:139:LEU:HD12	1:C:152:VAL:O	2.03	0.58
1:C:392:LEU:N	1:C:393:PRO:CD	2.66	0.58
1:D:44:PRO:HD3	3:D:417:HOH:O	2.03	0.58
1:A:308:GLU:OE1	1:A:336:LEU:HB3	2.02	0.58
1:C:249:GLN:CD	1:C:249:GLN:H	2.06	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:MET:HE1	1:C:270:GLU:HG2	1.85	0.58
1:C:176:ARG:HD3	1:C:340:ASN:HD22	1.69	0.58
1:D:277:PRO:O	1:D:278:PHE:CD2	2.56	0.58
1:A:321:GLU:N	1:A:321:GLU:CD	2.56	0.58
1:A:14:MET:CE	1:B:69:LEU:HD12	2.33	0.58
1:D:179:THR:O	1:D:183:VAL:HG23	2.03	0.58
1:B:379:GLU:HA	1:B:379:GLU:OE1	2.04	0.58
1:C:161:LEU:HD11	1:C:206:LEU:HD21	1.86	0.58
1:B:42:ASP:O	1:B:42:ASP:OD1	2.22	0.58
1:D:136:VAL:HG12	1:D:137:VAL:O	2.04	0.58
1:D:324:LEU:HG	1:D:332:ILE:HG12	1.86	0.57
1:B:41:LEU:HD22	1:B:52:ILE:CD1	2.33	0.57
1:A:190:HIS:CE1	1:A:257:ARG:HB2	2.39	0.57
1:B:175:ALA:CB	1:B:272:LEU:HD21	2.34	0.57
1:C:164:LEU:O	1:C:168:TYR:HB2	2.04	0.57
1:B:246:LEU:C	1:B:248:SER:N	2.58	0.57
1:C:242:SER:HB3	1:C:262:TRP:CG	2.40	0.57
1:D:110:PHE:CD2	1:D:110:PHE:C	2.77	0.57
1:D:195:ILE:HD12	1:D:229:VAL:CG1	2.34	0.57
1:B:241:ILE:HG13	1:B:242:SER:N	2.18	0.57
1:D:211:HIS:HB3	1:D:349:ARG:NH2	2.19	0.57
1:A:149:LEU:HB3	1:A:397:PHE:CE2	2.40	0.57
1:A:95:HIS:CE1	1:A:97:SER:HB3	2.40	0.57
1:C:59:TYR:O	1:C:60:LYS:C	2.43	0.57
1:D:238:PRO:HG3	1:D:283:LEU:HD13	1.86	0.57
1:B:223:MET:HA	1:B:229:VAL:HG12	1.86	0.57
1:B:84:ARG:HA	1:B:89:GLU:HA	1.86	0.57
1:C:344:ALA:O	1:C:345:TRP:C	2.43	0.57
1:D:137:VAL:HG11	2:D:900:3ND:H1	1.86	0.57
1:A:59:TYR:O	1:A:60:LYS:C	2.43	0.57
1:C:174:TRP:O	1:C:177:PHE:HB3	2.05	0.57
1:D:225:LYS:H	1:D:225:LYS:CD	2.15	0.56
1:D:295:ASN:O	1:D:297:LEU:N	2.38	0.56
1:A:196:HIS:HD2	1:A:198:ASP:N	2.04	0.56
1:A:269:TYR:CZ	1:A:273:VAL:HG21	2.41	0.56
1:B:43:PHE:CD1	1:B:384:PRO:HD2	2.40	0.56
1:C:156:MET:HE1	1:C:213:LYS:HE3	1.88	0.56
1:A:205:LEU:O	1:A:212:LEU:HA	2.05	0.56
1:A:399:TYR:CE2	1:A:401:SER:CB	2.79	0.56
1:B:59:TYR:O	1:B:61:ASP:N	2.38	0.56
1:B:77:GLU:HB2	1:B:96:LYS:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:HD13	1:D:155:TYR:CD1	2.40	0.56
1:C:375:LYS:HB3	1:C:377:GLU:HG3	1.87	0.56
1:C:242:SER:HB2	1:C:243:PRO:CD	2.36	0.56
1:C:59:TYR:O	1:C:61:ASP:N	2.39	0.56
1:B:186:LEU:HD21	1:B:260:ASP:HB3	1.86	0.56
1:A:58:ARG:NH2	1:B:393:PRO:HA	2.21	0.56
1:C:25:VAL:O	1:C:25:VAL:CG2	2.53	0.56
1:D:242:SER:HB2	1:D:243:PRO:HD2	1.86	0.56
1:A:78:VAL:CA	1:A:93:VAL:HG12	2.32	0.56
1:D:289:LYS:HD3	1:D:296:SER:HG	1.70	0.56
1:A:229:VAL:O	1:A:254:TYR:HA	2.06	0.56
1:C:9:THR:O	1:C:10:ARG:C	2.45	0.55
1:D:114:LYS:HG2	1:D:115:ARG:HD3	1.87	0.55
1:D:199:VAL:O	1:D:200:LYS:HB3	2.06	0.55
1:D:125:ARG:NE	1:D:397:PHE:O	2.40	0.55
1:A:133:SER:OG	1:A:135:TRP:HB2	2.06	0.55
1:A:37:LEU:HD21	1:B:37:LEU:HD21	1.88	0.55
1:B:357:PRO:HB3	1:B:359:LEU:HD21	1.87	0.55
1:C:108:SER:O	1:C:112:MET:HE2	2.06	0.55
1:C:43:PHE:HE1	1:C:384:PRO:HG2	1.70	0.55
1:A:381:PHE:HD2	1:A:382:PRO:CD	2.10	0.55
1:A:6:SER:HB3	1:A:9:THR:OG1	2.06	0.55
1:B:55:PHE:CD2	1:B:56:LEU:HD23	2.42	0.55
1:D:257:ARG:CZ	1:D:257:ARG:HB3	2.36	0.55
1:D:305:ILE:N	1:D:305:ILE:HD13	2.21	0.55
1:B:261:TRP:O	1:B:264:VAL:HB	2.06	0.55
1:B:313:ILE:HG22	1:B:314:CYS:N	2.21	0.55
1:D:268:LEU:HD23	1:D:313:ILE:HG12	1.89	0.55
1:D:333:LYS:HB3	1:D:345:TRP:CE2	2.41	0.55
1:D:127:ILE:HD11	1:D:194:PHE:CD2	2.42	0.55
1:A:181:GLU:HB3	1:A:212:LEU:HD22	1.88	0.55
1:A:135:TRP:HH2	1:A:181:GLU:HG2	1.71	0.55
1:B:13:LYS:HA	1:B:16:ASN:ND2	2.22	0.55
1:D:237:THR:CG2	1:D:238:PRO:HD2	2.36	0.55
1:A:162:VAL:HB	1:A:201:PRO:HB2	1.89	0.54
1:D:224:ASN:HB2	1:D:225:LYS:NZ	2.22	0.54
1:B:124:GLU:HG3	1:B:217:PHE:HB2	1.89	0.54
1:C:239:ASP:HB3	1:C:276:THR:HG21	1.88	0.54
1:D:184:LEU:CD2	1:D:333:LYS:NZ	2.68	0.54
1:A:157:PRO:HB2	1:A:359:LEU:HD21	1.88	0.54
1:D:299:PHE:HD2	1:D:300:PRO:CD	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASN:HA	1:C:166:SER:OG	2.07	0.54
1:C:208:LYS:O	1:C:357:PRO:HG2	2.06	0.54
1:C:346:GLU:H	1:C:346:GLU:CD	2.10	0.54
1:A:61:ASP:CG	1:C:372:GLU:HG2	2.28	0.54
1:C:98:THR:O	1:C:100:LYS:N	2.40	0.54
1:C:389:GLY:HA3	1:C:392:LEU:HD12	1.88	0.54
1:D:98:THR:O	1:D:100:LYS:N	2.40	0.54
1:A:229:VAL:N	1:A:255:TYR:O	2.38	0.54
1:A:210:GLY:HA3	1:A:355:VAL:O	2.07	0.54
1:C:242:SER:HB3	1:C:262:TRP:CD1	2.42	0.54
1:D:56:LEU:O	1:D:60:LYS:HB2	2.07	0.54
1:A:381:PHE:CZ	1:A:390:ASN:HB3	2.42	0.54
1:A:70:ARG:NH1	3:A:416:HOH:O	2.26	0.54
1:B:377:GLU:HG3	1:B:378:GLU:N	2.23	0.54
1:C:107:LEU:HB2	1:C:149:LEU:HB2	1.88	0.54
1:C:399:TYR:CZ	1:C:401:SER:HB3	2.43	0.54
1:A:217:PHE:HB3	1:A:220:CYS:SG	2.48	0.54
1:A:242:SER:OG	1:A:245:VAL:HG23	2.07	0.54
1:A:262:TRP:O	1:A:266:VAL:HG23	2.06	0.54
1:D:225:LYS:N	1:D:225:LYS:HD3	2.22	0.54
1:A:186:LEU:CD2	1:A:190:HIS:NE2	2.71	0.54
1:A:306:SER:O	1:A:310:LYS:HG3	2.08	0.54
1:A:46:LEU:O	1:A:48:LYS:N	2.40	0.54
1:C:161:LEU:HD23	1:C:267:PHE:HZ	1.73	0.54
1:A:204:MET:HB3	1:A:212:LEU:HD12	1.90	0.54
1:D:182:VAL:CG2	1:D:212:LEU:HD11	2.37	0.54
1:D:218:GLY:O	1:D:219:THR:CG2	2.56	0.54
1:B:286:THR:O	1:B:290:ILE:HG13	2.08	0.53
1:D:59:TYR:O	1:D:61:ASP:N	2.41	0.53
1:A:377:GLU:N	1:A:378:GLU:HA	2.21	0.53
1:A:110:PHE:CZ	1:A:379:GLU:HB3	2.42	0.53
1:C:176:ARG:CD	1:C:340:ASN:HD22	2.21	0.53
1:D:65:LYS:O	1:D:68:ASP:HB2	2.08	0.53
1:A:160:ASP:HA	1:A:204:MET:O	2.07	0.53
1:D:135:TRP:HZ3	1:D:181:GLU:OE2	1.92	0.53
1:D:346:GLU:CD	1:D:346:GLU:H	2.11	0.53
1:A:54:ASN:HA	3:A:422:HOH:O	2.07	0.53
1:B:187:ASP:OD1	1:B:329:VAL:HG11	2.09	0.53
1:B:314:CYS:O	1:B:318:THR:CG2	2.57	0.53
1:C:212:LEU:HD23	1:C:212:LEU:O	2.08	0.53
1:D:196:HIS:O	1:D:197:ARG:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HB	1:A:92:LEU:O	2.09	0.53
1:B:106:LEU:HG	1:B:150:TYR:CD2	2.44	0.53
1:B:161:LEU:HD23	1:B:267:PHE:HZ	1.72	0.53
1:C:150:TYR:CD1	1:C:150:TYR:N	2.77	0.53
1:C:295:ASN:O	1:C:297:LEU:N	2.42	0.53
1:D:147:ARG:HB2	1:D:148:TYR:CD1	2.44	0.53
1:D:230:ARG:NH2	1:D:253:GLY:O	2.42	0.53
1:A:244:GLU:CG	1:A:320:ARG:HD3	2.38	0.53
1:A:59:TYR:O	1:A:61:ASP:N	2.42	0.53
1:C:109:LYS:HE2	1:C:394:PHE:CD1	2.43	0.53
1:A:367:ASN:OD1	1:A:367:ASN:N	2.41	0.53
1:C:30:LEU:HB3	1:D:30:LEU:CB	2.33	0.53
1:C:43:PHE:CE1	1:C:384:PRO:HD2	2.44	0.53
1:D:400:TYR:O	1:D:401:SER:HB2	2.08	0.53
1:A:61:ASP:OD2	1:C:372:GLU:HG2	2.08	0.53
1:B:173:LYS:HG2	1:B:176:ARG:HH12	1.74	0.53
1:C:128:MET:HE1	1:C:153:MET:SD	2.49	0.53
1:C:160:ASP:OD2	1:C:162:VAL:HG12	2.08	0.53
1:C:161:LEU:CD1	1:C:206:LEU:HD21	2.38	0.53
1:C:5:MET:O	1:C:5:MET:CG	2.57	0.53
1:A:135:TRP:HE3	1:A:135:TRP:HA	1.73	0.52
1:B:186:LEU:CD2	1:B:260:ASP:HB3	2.40	0.52
1:C:269:TYR:CE1	1:C:273:VAL:HG21	2.43	0.52
1:D:182:VAL:HG21	1:D:267:PHE:CE2	2.37	0.52
1:D:231:CYS:O	1:D:253:GLY:HA3	2.09	0.52
1:D:46:LEU:HD21	1:D:386:ALA:CA	2.38	0.52
1:A:46:LEU:C	1:A:48:LYS:H	2.12	0.52
1:B:382:PRO:O	1:B:384:PRO:HD3	2.09	0.52
1:B:46:LEU:CD2	1:B:386:ALA:HA	2.39	0.52
1:D:177:PHE:CD2	1:D:354:PRO:HG2	2.44	0.52
1:D:189:ILE:HA	1:D:192:MET:HE3	1.92	0.52
1:A:177:PHE:CD1	1:A:348:LEU:HD11	2.45	0.52
1:C:189:ILE:HG23	1:C:194:PHE:HB2	1.91	0.52
1:D:69:LEU:HD23	1:D:69:LEU:N	2.23	0.52
1:D:89:GLU:HA	2:D:900:3ND:H22	1.91	0.52
1:B:225:LYS:CD	1:B:225:LYS:H	2.16	0.52
1:B:340:ASN:HB2	1:B:342:GLN:OE1	2.10	0.52
1:C:289:LYS:HD3	1:C:296:SER:OG	2.10	0.52
1:C:299:PHE:HE2	1:C:305:ILE:HD11	1.74	0.52
1:D:177:PHE:CE2	1:D:354:PRO:CD	2.92	0.52
1:A:344:ALA:O	1:A:345:TRP:C	2.46	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:HA	2:C:900:3ND:H22	1.92	0.52
1:C:94:ARG:C	3:C:423:HOH:O	2.47	0.52
1:A:110:PHE:CD2	1:A:110:PHE:C	2.83	0.52
1:A:262:TRP:C	1:A:262:TRP:CD1	2.82	0.52
1:A:343:TRP:HB3	1:A:351:THR:HG21	1.92	0.52
1:C:338:PHE:CD1	1:C:345:TRP:CH2	2.98	0.52
1:B:308:GLU:OE1	1:B:336:LEU:HB2	2.10	0.52
1:D:195:ILE:HD12	1:D:229:VAL:HG11	1.92	0.52
1:B:155:TYR:CD2	1:B:157:PRO:HD3	2.45	0.51
1:C:199:VAL:HB	1:C:263:SER:CB	2.40	0.51
1:C:79:VAL:HG23	1:C:93:VAL:HA	1.91	0.51
1:D:299:PHE:HD2	1:D:300:PRO:HD2	1.75	0.51
1:B:277:PRO:HG2	1:B:278:PHE:CE2	2.45	0.51
1:B:308:GLU:HG3	1:B:336:LEU:HB3	1.91	0.51
1:B:82:ILE:HG21	1:B:92:LEU:HB2	1.91	0.51
1:D:94:ARG:HA	1:D:100:LYS:O	2.10	0.51
1:D:230:ARG:NH1	1:D:230:ARG:HB3	2.25	0.51
1:A:286:THR:HA	1:A:289:LYS:HG3	1.92	0.51
1:A:388:VAL:HG23	1:A:389:GLY:N	2.26	0.51
1:D:46:LEU:C	1:D:48:LYS:H	2.14	0.51
1:A:92:LEU:HD12	1:A:102:TYR:O	2.10	0.51
1:B:172:GLU:OE2	1:B:306:SER:HB2	2.10	0.51
1:A:10:ARG:NH1	1:B:75:ASP:OD1	2.44	0.51
1:C:14:MET:HE1	1:D:69:LEU:HB2	1.93	0.51
1:C:74:GLU:C	1:C:76:TYR:H	2.13	0.51
1:D:211:HIS:CB	1:D:349:ARG:NH2	2.73	0.51
1:D:261:TRP:CE3	1:D:264:VAL:HG21	2.41	0.51
1:D:344:ALA:O	1:D:345:TRP:C	2.49	0.51
1:A:90:VAL:HA	1:A:105:LYS:HA	1.93	0.51
1:B:156:MET:HE1	1:B:213:LYS:HE3	1.92	0.51
1:B:225:LYS:N	1:B:225:LYS:HD3	2.26	0.51
1:C:241:ILE:HD11	1:C:245:VAL:CG1	2.40	0.51
1:B:60:LYS:HE3	1:B:64:ASN:HD21	1.74	0.51
1:C:168:TYR:HE2	1:C:174:TRP:HH2	1.58	0.51
1:C:49:ASN:C	1:C:49:ASN:OD1	2.49	0.51
1:A:13:LYS:HA	1:A:16:ASN:HD21	1.75	0.51
1:C:177:PHE:CD1	1:C:348:LEU:HD11	2.46	0.51
1:D:109:LYS:O	1:D:113:ILE:HG12	2.10	0.51
1:D:262:TRP:CZ2	1:D:290:ILE:CG2	2.91	0.51
1:A:117:ASP:HB3	3:A:419:HOH:O	2.11	0.51
1:A:295:ASN:O	1:A:297:LEU:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:C	1:B:248:SER:HB2	2.30	0.51
1:D:105:LYS:HE3	2:D:900:3ND:CL24	2.47	0.51
1:B:223:MET:HE1	1:B:257:ARG:HH22	1.76	0.50
1:C:375:LYS:HD2	1:C:377:GLU:OE1	2.09	0.50
1:A:230:ARG:HG2	1:A:254:TYR:CE1	2.47	0.50
1:B:98:THR:O	1:B:100:LYS:N	2.44	0.50
1:C:305:ILE:N	1:C:305:ILE:HD13	2.22	0.50
1:C:74:GLU:O	1:C:76:TYR:N	2.44	0.50
1:D:212:LEU:HD23	1:D:212:LEU:C	2.31	0.50
1:D:184:LEU:CD2	1:D:333:LYS:HZ2	2.24	0.50
1:A:164:LEU:CD2	1:A:178:TYR:HE1	2.25	0.50
1:A:199:VAL:HB	1:A:263:SER:HB3	1.93	0.50
1:D:223:MET:SD	1:D:257:ARG:NH2	2.84	0.50
1:B:156:MET:CE	1:B:207:ASP:HB3	2.40	0.50
1:C:110:PHE:C	1:C:110:PHE:CD2	2.85	0.50
1:C:135:TRP:HA	1:C:135:TRP:CE3	2.47	0.50
1:D:120:PHE:O	1:D:123:GLU:HG2	2.11	0.50
1:D:242:SER:HA	1:D:262:TRP:NE1	2.26	0.50
1:A:316:PHE:C	1:A:318:THR:H	2.14	0.50
1:A:321:GLU:O	1:A:326:ARG:HD3	2.11	0.50
1:B:199:VAL:O	1:B:200:LYS:HB3	2.12	0.50
1:D:205:LEU:N	1:D:205:LEU:HD23	2.27	0.50
1:A:200:LYS:HB2	1:A:201:PRO:HD2	1.93	0.50
1:B:74:GLU:C	1:B:76:TYR:H	2.15	0.50
1:C:195:ILE:HG23	1:C:260:ASP:OD2	2.12	0.50
1:A:225:LYS:CD	1:A:225:LYS:H	2.24	0.50
1:C:392:LEU:N	1:C:393:PRO:HD2	2.26	0.50
1:D:240:TYR:O	1:D:241:ILE:C	2.50	0.50
1:A:125:ARG:HH21	1:A:399:TYR:HB2	1.77	0.50
1:A:333:LYS:HD3	1:A:345:TRP:CD1	2.47	0.50
1:D:205:LEU:O	1:D:212:LEU:HA	2.11	0.50
1:B:199:VAL:HB	1:B:263:SER:CB	2.41	0.50
1:B:63:ILE:HG22	1:B:64:ASN:N	2.25	0.50
1:C:43:PHE:CE1	1:C:384:PRO:HG2	2.47	0.50
1:D:224:ASN:OD1	1:D:226:GLU:HG2	2.10	0.50
1:D:61:ASP:O	1:D:64:ASN:HB2	2.12	0.50
1:B:135:TRP:CH2	1:B:349:ARG:HD2	2.47	0.49
1:B:229:VAL:HG22	1:B:255:TYR:O	2.12	0.49
1:C:286:THR:O	1:C:289:LYS:HB2	2.12	0.49
1:C:174:TRP:CG	1:C:354:PRO:HB3	2.47	0.49
1:C:26:ASN:O	1:C:27:SER:C	2.49	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:GLY:O	1:D:331:GLU:HG2	2.12	0.49
1:D:90:VAL:HA	1:D:105:LYS:HA	1.93	0.49
1:B:34:LEU:O	1:B:38:VAL:HG23	2.13	0.49
1:B:46:LEU:HD21	1:B:386:ALA:HA	1.93	0.49
1:C:156:MET:HE1	1:C:213:LYS:CE	2.42	0.49
1:C:137:VAL:HG11	2:C:900:3ND:H1	1.93	0.49
1:A:333:LYS:HA	1:A:345:TRP:CZ2	2.47	0.49
1:B:174:TRP:CE2	1:B:354:PRO:HB3	2.47	0.49
1:C:63:ILE:HA	1:C:66:ILE:HD12	1.93	0.49
1:A:238:PRO:O	1:A:241:ILE:HG22	2.12	0.49
1:D:46:LEU:C	1:D:48:LYS:N	2.65	0.49
1:B:135:TRP:HA	1:B:135:TRP:CE3	2.48	0.49
1:B:228:MET:HB3	1:B:254:TYR:CE1	2.48	0.49
1:B:323:ARG:O	1:B:324:LEU:C	2.51	0.49
1:C:177:PHE:CE2	1:C:354:PRO:HD2	2.46	0.49
1:C:46:LEU:C	1:C:48:LYS:H	2.15	0.49
1:A:165:MET:HE1	1:A:270:GLU:O	2.13	0.49
1:A:217:PHE:O	1:A:219:THR:N	2.43	0.49
1:A:109:LYS:CB	1:A:394:PHE:HE1	2.24	0.49
1:A:46:LEU:C	1:A:48:LYS:N	2.65	0.49
1:B:185:ALA:O	1:B:188:ALA:HB3	2.12	0.49
1:C:242:SER:HB2	1:C:243:PRO:HD2	1.94	0.49
1:C:244:GLU:OE2	1:C:320:ARG:HB2	2.11	0.49
1:D:17:LEU:N	1:D:17:LEU:HD12	2.28	0.49
1:A:295:ASN:N	1:A:295:ASN:HD22	2.10	0.49
1:A:297:LEU:HD13	1:A:317:LEU:HD23	1.95	0.49
1:B:193:GLY:HA2	1:B:223:MET:CE	2.43	0.49
1:C:246:LEU:C	1:C:248:SER:H	2.17	0.49
1:C:26:ASN:ND2	1:C:29:CYS:SG	2.86	0.49
1:C:319:ASP:OD1	1:C:321:GLU:HG2	2.13	0.49
1:A:279:TYR:CD2	1:A:280:ALA:N	2.81	0.49
1:B:240:TYR:O	1:B:241:ILE:C	2.51	0.49
1:B:110:PHE:CD1	1:B:379:GLU:HB3	2.48	0.49
1:B:46:LEU:C	1:B:48:LYS:N	2.65	0.49
1:C:225:LYS:CD	1:C:225:LYS:H	2.11	0.49
1:C:277:PRO:O	1:C:278:PHE:CG	2.66	0.49
1:D:105:LYS:CE	1:D:107:LEU:HD21	2.35	0.49
1:B:312:LEU:O	1:B:315:ALA:HB3	2.13	0.48
1:B:343:TRP:CD2	1:B:348:LEU:HD13	2.48	0.48
1:B:351:THR:OG1	1:B:352:VAL:N	2.43	0.48
1:C:371:LEU:HG	1:C:372:GLU:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLU:HB3	1:D:115:ARG:HH22	1.77	0.48
1:D:217:PHE:HB3	1:D:220:CYS:HG	1.78	0.48
1:D:304:ASP:N	1:D:305:ILE:HD13	2.27	0.48
1:A:61:ASP:OD1	1:C:372:GLU:HG2	2.13	0.48
1:D:219:THR:O	1:D:220:CYS:C	2.51	0.48
1:A:278:PHE:HD1	1:A:289:LYS:HB3	1.78	0.48
1:A:343:TRP:CD2	1:A:348:LEU:HD13	2.48	0.48
1:B:171:PRO:HD2	1:B:174:TRP:CE3	2.49	0.48
1:B:78:VAL:HG21	1:B:375:LYS:NZ	2.28	0.48
1:B:49:ASN:OD1	1:B:51:ASN:HB2	2.13	0.48
1:C:164:LEU:CD2	1:C:178:TYR:HE1	2.26	0.48
1:C:158:GLY:CA	1:C:206:LEU:O	2.57	0.48
1:C:316:PHE:C	1:C:318:THR:H	2.17	0.48
1:D:217:PHE:C	1:D:220:CYS:HG	2.16	0.48
1:A:47:ARG:NH1	1:A:53:ASP:OD1	2.46	0.48
1:C:115:ARG:NH2	1:C:115:ARG:HG2	2.26	0.48
1:C:170:VAL:HG13	1:C:174:TRP:CB	2.39	0.48
1:B:135:TRP:HB3	1:B:185:ALA:HA	1.93	0.48
1:B:94:ARG:HD2	1:B:99:ARG:CZ	2.42	0.48
1:C:182:VAL:HG21	1:C:267:PHE:CE2	2.48	0.48
1:C:259:CYS:SG	1:C:260:ASP:N	2.87	0.48
1:C:62:THR:HG22	1:C:63:ILE:N	2.28	0.48
1:D:307:LYS:HB3	1:D:307:LYS:HZ3	1.79	0.48
1:A:199:VAL:O	1:A:200:LYS:HB3	2.14	0.48
1:A:393:PRO:HG2	1:A:394:PHE:CE2	2.48	0.48
1:B:177:PHE:CE2	1:B:354:PRO:CD	2.95	0.48
1:B:265:GLY:HA3	1:B:317:LEU:HD13	1.95	0.48
1:C:154:GLU:O	1:C:154:GLU:HG3	2.13	0.48
1:A:34:LEU:O	1:A:38:VAL:HG23	2.14	0.48
1:A:399:TYR:CZ	1:A:401:SER:HB2	2.46	0.48
1:C:109:LYS:NZ	1:C:145:ASP:O	2.43	0.48
1:C:181:GLU:HG3	1:C:348:LEU:HD21	1.95	0.48
1:C:269:TYR:CD2	1:C:277:PRO:HD3	2.49	0.48
1:C:35:ASP:OD1	1:C:67:ARG:NE	2.46	0.48
1:A:322:VAL:HG22	1:A:322:VAL:O	2.14	0.48
1:B:109:LYS:NZ	1:B:144:GLN:OE1	2.44	0.48
1:B:226:GLU:OE1	1:C:380:THR:O	2.32	0.48
1:B:248:SER:O	1:B:249:GLN:C	2.52	0.48
1:C:143:PHE:CE1	1:C:150:TYR:CG	3.01	0.48
1:C:128:MET:HE2	1:C:153:MET:SD	2.52	0.48
1:C:338:PHE:CD1	1:C:345:TRP:HH2	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:TRP:CD1	1:C:354:PRO:HB3	2.49	0.48
1:D:322:VAL:CB	1:D:326:ARG:HH21	2.27	0.48
1:D:70:ARG:HB3	1:D:400:TYR:OH	2.14	0.48
1:B:11:PHE:CG	3:B:419:HOH:O	2.66	0.48
1:B:322:VAL:CG2	1:B:322:VAL:O	2.58	0.48
1:C:211:HIS:CE1	1:C:349:ARG:O	2.66	0.48
1:C:7:PHE:HA	1:C:10:ARG:HD2	1.95	0.48
1:C:77:GLU:O	1:C:93:VAL:HG12	2.14	0.48
1:D:80:LYS:HE3	1:D:370:ASP:OD2	2.14	0.48
1:B:250:GLY:HA2	1:B:251:GLY:HA2	1.67	0.47
1:C:217:PHE:O	1:C:219:THR:N	2.46	0.47
1:C:273:VAL:HG12	1:C:274:GLY:N	2.28	0.47
1:D:164:LEU:HD21	1:D:178:TYR:HE1	1.78	0.47
1:D:17:LEU:H	1:D:17:LEU:HD12	1.77	0.47
1:C:393:PRO:CA	1:D:58:ARG:HH22	2.24	0.47
1:A:115:ARG:NH2	1:A:115:ARG:HG2	2.26	0.47
1:A:240:TYR:O	1:A:241:ILE:C	2.52	0.47
1:A:308:GLU:HB3	1:A:337:PHE:CA	2.43	0.47
1:B:46:LEU:C	1:B:48:LYS:H	2.16	0.47
1:B:93:VAL:O	1:B:101:VAL:HA	2.15	0.47
1:A:297:LEU:HD21	1:A:314:CYS:SG	2.54	0.47
1:B:78:VAL:HG21	1:B:375:LYS:HZ1	1.79	0.47
1:B:49:ASN:O	1:B:50:LYS:C	2.52	0.47
1:C:344:ALA:HB3	1:C:347:THR:HG22	1.94	0.47
1:A:277:PRO:O	1:A:278:PHE:CG	2.68	0.47
1:A:340:ASN:HB2	1:A:342:GLN:OE1	2.13	0.47
1:B:112:MET:O	1:B:118:SER:HB3	2.14	0.47
1:B:181:GLU:HB3	1:B:212:LEU:HD22	1.96	0.47
1:C:76:TYR:CD1	1:C:76:TYR:N	2.81	0.47
1:D:210:GLY:HA3	1:D:355:VAL:O	2.13	0.47
1:A:98:THR:O	1:A:100:LYS:N	2.47	0.47
1:A:333:LYS:HA	1:A:345:TRP:HZ2	1.79	0.47
1:D:128:MET:HB3	1:D:139:LEU:HB2	1.96	0.47
1:B:144:GLN:HB3	1:B:149:LEU:HD23	1.97	0.47
1:B:74:GLU:O	1:B:76:TYR:N	2.47	0.47
1:B:205:LEU:HD11	2:B:900:3ND:C7	2.44	0.47
1:C:17:LEU:HD12	1:C:17:LEU:N	2.28	0.47
1:C:8:GLU:OE1	1:C:8:GLU:N	2.47	0.47
1:D:176:ARG:HD3	1:D:338:PHE:HA	1.95	0.47
1:C:338:PHE:CG	1:C:345:TRP:CH2	3.03	0.47
1:D:230:ARG:HB3	1:D:230:ARG:HH11	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:OD1	1:A:226:GLU:HG2	2.15	0.47
1:A:241:ILE:HD11	1:A:245:VAL:CG1	2.45	0.47
1:A:110:PHE:CE1	1:A:379:GLU:HB3	2.50	0.47
1:B:156:MET:CE	1:B:213:LYS:HD2	2.45	0.47
1:D:268:LEU:HG	1:D:313:ILE:HD11	1.96	0.47
1:D:325:GLY:O	1:D:326:ARG:C	2.53	0.47
1:D:343:TRP:CB	1:D:351:THR:HG21	2.45	0.47
1:A:394:PHE:N	1:A:394:PHE:CD2	2.83	0.47
1:B:13:LYS:HA	1:B:16:ASN:HD21	1.79	0.47
1:C:102:TYR:HB3	1:C:153:MET:O	2.15	0.47
1:D:169:ASP:O	1:D:170:VAL:C	2.53	0.47
1:A:7:PHE:HB2	1:B:97:SER:CB	2.45	0.47
1:B:343:TRP:CE3	1:B:348:LEU:HD13	2.49	0.47
1:B:348:LEU:O	1:B:351:THR:HG23	2.14	0.47
1:B:62:THR:O	1:B:65:LYS:N	2.46	0.47
1:C:160:ASP:HA	1:C:204:MET:O	2.15	0.47
1:C:269:TYR:CE2	1:C:273:VAL:HG21	2.50	0.47
1:C:296:SER:O	1:C:298:THR:HG23	2.14	0.47
1:D:158:GLY:HA3	1:D:206:LEU:HB2	1.96	0.47
1:D:257:ARG:HB3	1:D:257:ARG:NH1	2.30	0.47
1:A:8:GLU:O	1:A:12:GLU:HG3	2.15	0.47
1:D:14:MET:HA	1:D:14:MET:CE	2.45	0.47
1:D:316:PHE:C	1:D:318:THR:H	2.18	0.47
1:D:45:ALA:O	1:D:48:LYS:HD3	2.15	0.47
1:A:196:HIS:O	1:A:197:ARG:HB2	2.15	0.46
1:A:238:PRO:C	1:A:240:TYR:H	2.18	0.46
1:B:143:PHE:CE1	1:B:150:TYR:HB2	2.50	0.46
1:C:224:ASN:HB2	1:C:225:LYS:NZ	2.30	0.46
1:C:338:PHE:CG	1:C:345:TRP:HH2	2.32	0.46
1:C:80:LYS:HD2	1:C:370:ASP:HB3	1.97	0.46
1:D:13:LYS:HA	1:D:16:ASN:ND2	2.30	0.46
1:D:378:GLU:OE2	1:D:378:GLU:HA	2.15	0.46
1:D:46:LEU:CD2	1:D:386:ALA:HA	2.43	0.46
1:A:222:LYS:HB2	1:A:222:LYS:HE3	1.33	0.46
1:C:79:VAL:HG12	1:C:80:LYS:N	2.30	0.46
1:B:36:ALA:O	1:B:39:TYR:HB2	2.15	0.46
1:C:104:MET:CE	1:C:106:LEU:HD11	2.46	0.46
1:C:168:TYR:HD2	1:C:174:TRP:HZ3	1.64	0.46
1:D:238:PRO:HG3	1:D:283:LEU:CD1	2.45	0.46
1:A:306:SER:HB2	1:A:309:ALA:CB	2.45	0.46
1:A:316:PHE:CE2	1:A:324:LEU:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:PHE:HZ	1:C:310:LYS:HG2	1.75	0.46
1:C:371:LEU:CG	1:C:372:GLU:H	2.28	0.46
1:D:48:LYS:NZ	1:D:48:LYS:HB3	2.31	0.46
2:D:900:3ND:H19	2:D:900:3ND:H13	1.58	0.46
1:A:195:ILE:O	1:A:197:ARG:HG3	2.15	0.46
1:A:304:ASP:N	1:A:310:LYS:NZ	2.58	0.46
1:C:30:LEU:HD13	1:D:30:LEU:HB2	1.97	0.46
1:D:283:LEU:O	1:D:284:VAL:C	2.54	0.46
1:B:79:VAL:HB	1:B:92:LEU:O	2.15	0.46
1:C:200:LYS:HE3	1:C:202:ASP:CB	2.43	0.46
1:D:401:SER:HA	1:D:402:ASN:HA	1.69	0.46
1:A:212:LEU:HG	1:A:213:LYS:N	2.30	0.46
1:B:197:ARG:NH2	1:B:221:MET:HE3	2.30	0.46
1:B:395:VAL:HG12	1:B:395:VAL:O	2.15	0.46
1:C:217:PHE:HB3	1:C:220:CYS:HG	1.80	0.46
1:C:357:PRO:HB3	1:C:359:LEU:HD21	1.98	0.46
1:D:223:MET:CE	1:D:227:GLY:HA2	2.46	0.46
1:A:199:VAL:HB	1:A:263:SER:CB	2.46	0.46
1:A:218:GLY:O	1:A:219:THR:HG23	2.16	0.46
1:B:176:ARG:HD3	1:B:338:PHE:HA	1.97	0.46
1:B:329:VAL:O	1:B:333:LYS:HG3	2.16	0.46
1:B:208:LYS:C	1:B:357:PRO:HG2	2.36	0.46
1:A:139:LEU:HD11	1:A:141:TYR:O	2.15	0.46
1:A:25:VAL:HG11	1:B:66:ILE:HD11	1.97	0.46
1:B:156:MET:HB3	1:B:206:LEU:O	2.16	0.46
1:D:177:PHE:CZ	1:D:181:GLU:OE1	2.68	0.46
1:D:90:VAL:HG12	1:D:91:GLN:N	2.31	0.46
1:B:325:GLY:O	1:B:326:ARG:C	2.54	0.45
1:C:125:ARG:HD2	1:C:397:PHE:CD1	2.52	0.45
1:D:135:TRP:HB3	1:D:185:ALA:HA	1.99	0.45
1:D:187:ASP:OD2	1:D:187:ASP:O	2.34	0.45
1:D:383:ILE:HG23	1:D:384:PRO:HD2	1.98	0.45
1:A:10:ARG:NH2	1:B:75:ASP:OD2	2.49	0.45
2:B:900:3ND:H13	2:B:900:3ND:H19	1.65	0.45
1:C:162:VAL:HB	1:C:201:PRO:HB2	1.97	0.45
1:D:80:LYS:HZ3	1:D:80:LYS:HB3	1.80	0.45
1:A:306:SER:HB2	1:A:309:ALA:HB2	1.98	0.45
1:A:392:LEU:N	1:A:393:PRO:CD	2.79	0.45
1:C:156:MET:SD	1:C:213:LYS:HD2	2.56	0.45
1:C:149:LEU:HD22	1:C:397:PHE:CD2	2.51	0.45
1:D:267:PHE:O	1:D:271:MET:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:TRP:HA	1:A:345:TRP:CE3	2.50	0.45
1:B:193:GLY:HA2	1:B:223:MET:HE2	1.98	0.45
1:B:258:GLU:HG3	1:B:320:ARG:CG	2.42	0.45
1:B:7:PHE:O	1:B:9:THR:N	2.45	0.45
1:D:34:LEU:O	1:D:38:VAL:HG23	2.16	0.45
1:A:295:ASN:ND2	1:A:295:ASN:N	2.64	0.45
1:B:245:VAL:O	1:B:245:VAL:HG12	2.15	0.45
1:C:159:GLY:O	1:C:205:LEU:HA	2.16	0.45
1:D:224:ASN:HB2	1:D:225:LYS:HZ3	1.79	0.45
1:D:208:LYS:C	1:D:357:PRO:HG2	2.37	0.45
1:A:135:TRP:HB3	1:A:185:ALA:HA	1.99	0.45
1:B:43:PHE:HA	1:B:44:PRO:HD2	1.67	0.45
1:C:168:TYR:CE2	1:C:174:TRP:HH2	2.34	0.45
1:D:10:ARG:O	1:D:13:LYS:N	2.50	0.45
1:D:267:PHE:CZ	1:D:271:MET:HE1	2.52	0.45
1:D:282:SER:O	1:D:283:LEU:C	2.55	0.45
1:D:338:PHE:CD1	1:D:345:TRP:HZ2	2.34	0.45
1:A:308:GLU:CD	1:A:336:LEU:HB3	2.37	0.45
1:C:115:ARG:CG	1:C:115:ARG:HH21	2.25	0.45
1:C:135:TRP:HB3	1:C:185:ALA:HA	1.98	0.45
1:D:34:LEU:HA	1:D:34:LEU:HD22	1.51	0.45
1:B:344:ALA:O	1:B:345:TRP:C	2.54	0.45
1:C:149:LEU:HB3	1:C:397:PHE:CE2	2.52	0.45
1:D:294:LYS:HB2	1:D:294:LYS:HE2	1.74	0.45
1:D:388:VAL:HG21	1:D:390:ASN:ND2	2.32	0.45
1:A:277:PRO:O	1:A:278:PHE:CD2	2.69	0.45
1:C:240:TYR:O	1:C:241:ILE:C	2.53	0.45
1:D:199:VAL:HB	1:D:263:SER:CB	2.46	0.45
1:D:25:VAL:O	1:D:30:LEU:HD11	2.16	0.45
1:A:125:ARG:NE	1:A:397:PHE:O	2.50	0.45
1:A:19:ARG:O	1:A:21:PRO:HD3	2.16	0.45
1:A:34:LEU:HA	1:A:34:LEU:HD22	1.62	0.45
1:A:31:LEU:HD22	1:A:66:ILE:HG21	1.99	0.45
1:B:246:LEU:HA	1:B:246:LEU:HD12	1.66	0.45
1:C:195:ILE:O	1:C:197:ARG:HG3	2.17	0.45
1:C:200:LYS:HG3	1:C:202:ASP:H	1.82	0.45
1:C:204:MET:O	1:C:205:LEU:HD23	2.17	0.45
1:C:75:ASP:OD2	1:D:10:ARG:NH2	2.49	0.45
1:D:200:LYS:HE2	1:D:202:ASP:CB	2.43	0.45
1:D:26:ASN:O	1:D:27:SER:C	2.54	0.45
1:D:383:ILE:HA	1:D:384:PRO:HD3	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HG12	1:A:246:LEU:CD1	2.38	0.44
1:B:231:CYS:HB3	1:B:255:TYR:OH	2.17	0.44
1:B:321:GLU:O	1:B:326:ARG:NE	2.50	0.44
1:B:65:LYS:HB3	1:B:65:LYS:NZ	2.31	0.44
1:B:90:VAL:HA	1:B:105:LYS:HA	1.98	0.44
1:C:177:PHE:HD2	1:C:178:TYR:CD2	2.34	0.44
1:C:258:GLU:CG	1:C:320:ARG:HG3	2.45	0.44
1:D:110:PHE:CE1	1:D:380:THR:C	2.90	0.44
1:A:111:GLU:OE1	1:A:115:ARG:NH2	2.38	0.44
1:A:56:LEU:O	1:A:60:LYS:HB3	2.17	0.44
1:B:229:VAL:HG21	1:B:255:TYR:CE2	2.53	0.44
1:B:388:VAL:HG21	1:B:390:ASN:ND2	2.31	0.44
1:C:17:LEU:CD1	1:C:17:LEU:N	2.80	0.44
1:C:215:ALA:CB	2:C:900:3ND:H4A	2.43	0.44
1:D:322:VAL:HB	1:D:326:ARG:NH2	2.28	0.44
1:A:185:ALA:O	1:A:188:ALA:HB3	2.17	0.44
1:A:330:GLU:O	1:A:333:LYS:HB2	2.17	0.44
1:A:176:ARG:NE	1:A:337:PHE:O	2.48	0.44
1:B:154:GLU:O	1:B:154:GLU:HG2	2.16	0.44
1:B:377:GLU:HG3	1:B:378:GLU:H	1.82	0.44
1:B:65:LYS:O	1:B:69:LEU:HG	2.17	0.44
1:C:82:ILE:HG21	1:C:92:LEU:HB2	1.99	0.44
1:D:197:ARG:CZ	1:D:235:VAL:HG21	2.47	0.44
1:A:262:TRP:HH2	1:A:293:HIS:HB3	1.82	0.44
1:A:348:LEU:O	1:A:351:THR:HG23	2.18	0.44
1:A:37:LEU:HD22	1:A:41:LEU:HD11	1.98	0.44
1:B:242:SER:HB2	1:B:243:PRO:HD2	1.99	0.44
1:B:322:VAL:HA	1:B:326:ARG:HH21	1.82	0.44
1:B:210:GLY:O	1:B:353:ALA:CB	2.65	0.44
1:C:135:TRP:HH2	1:C:181:GLU:HG2	1.80	0.44
1:C:74:GLU:C	1:C:76:TYR:N	2.71	0.44
1:D:162:VAL:HB	1:D:201:PRO:HB2	1.99	0.44
1:C:141:TYR:OH	1:D:7:PHE:HZ	1.78	0.44
1:A:208:LYS:O	1:A:357:PRO:HG2	2.17	0.44
1:B:302:ASP:O	1:B:304:ASP:N	2.50	0.44
1:A:24:GLU:OE2	1:B:58:ARG:HG3	2.17	0.44
1:B:69:LEU:N	1:B:69:LEU:HD23	2.33	0.44
1:C:186:LEU:O	1:C:190:HIS:CD2	2.70	0.44
1:C:402:ASN:C	1:D:11:PHE:CE2	2.91	0.44
1:C:43:PHE:CD2	1:C:43:PHE:N	2.82	0.44
1:D:93:VAL:O	1:D:101:VAL:HG13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:TYR:CZ	1:B:401:SER:CB	2.94	0.44
1:B:47:ARG:NH2	1:B:56:LEU:HB2	2.31	0.44
1:C:34:LEU:HD12	1:C:63:ILE:HD11	2.00	0.44
1:D:241:ILE:HD11	1:D:245:VAL:CB	2.45	0.44
1:A:239:ASP:HB3	1:A:276:THR:HG21	1.98	0.44
1:A:6:SER:N	1:A:9:THR:HB	2.33	0.44
1:C:196:HIS:HD2	1:C:198:ASP:H	1.66	0.44
1:C:37:LEU:HD22	1:C:41:LEU:HD11	2.00	0.44
1:C:401:SER:HA	1:C:402:ASN:HA	1.60	0.44
1:D:110:PHE:CE1	1:D:381:PHE:HA	2.53	0.44
1:A:346:GLU:CD	1:A:346:GLU:H	2.20	0.44
1:A:349:ARG:HH11	1:A:349:ARG:HG2	1.82	0.44
1:C:171:PRO:HD2	1:C:174:TRP:CD2	2.51	0.44
1:D:176:ARG:HD3	1:D:337:PHE:O	2.17	0.44
1:D:383:ILE:HG23	1:D:384:PRO:CD	2.48	0.44
1:D:82:ILE:HD11	1:D:90:VAL:HG12	1.98	0.44
1:A:69:LEU:HD22	1:B:10:ARG:CB	2.43	0.44
1:B:200:LYS:HD3	1:B:237:THR:OG1	2.18	0.44
1:C:137:VAL:HG23	1:C:214:LEU:O	2.18	0.44
1:D:79:VAL:HG23	1:D:93:VAL:HA	2.00	0.44
1:B:169:ASP:O	1:B:170:VAL:C	2.55	0.43
1:B:287:TYR:O	1:B:291:MET:HG2	2.18	0.43
1:D:307:LYS:NZ	1:D:307:LYS:CB	2.80	0.43
1:A:158:GLY:HA3	1:A:206:LEU:HB2	1.99	0.43
1:A:238:PRO:O	1:A:240:TYR:N	2.51	0.43
1:A:88:GLY:O	1:A:89:GLU:HB3	2.18	0.43
1:B:154:GLU:O	1:B:154:GLU:CG	2.66	0.43
1:B:356:VAL:HG13	1:B:357:PRO:HD2	1.98	0.43
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.57	0.43
1:B:74:GLU:C	1:B:76:TYR:N	2.71	0.43
1:D:171:PRO:HD2	1:D:174:TRP:CE3	2.53	0.43
1:D:312:LEU:HD12	1:D:337:PHE:CD2	2.53	0.43
1:D:342:GLN:HB3	1:D:342:GLN:HE21	1.58	0.43
1:D:202:ASP:O	2:D:900:3ND:H14A	2.18	0.43
1:A:312:LEU:HD21	1:A:316:PHE:CE1	2.53	0.43
1:A:57:SER:N	3:A:427:HOH:O	2.51	0.43
1:D:167:ASN:O	1:D:168:TYR:CG	2.71	0.43
1:B:269:TYR:O	1:B:270:GLU:C	2.57	0.43
1:B:205:LEU:CD1	2:B:900:3ND:C6	2.97	0.43
1:A:104:MET:HA	1:A:151:MET:O	2.18	0.43
1:A:239:ASP:CB	1:A:276:THR:HG21	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.86	0.43
1:B:135:TRP:O	1:B:213:LYS:HA	2.19	0.43
1:B:353:ALA:N	3:B:427:HOH:O	2.40	0.43
1:C:115:ARG:CG	1:C:115:ARG:NH2	2.81	0.43
1:C:315:ALA:HA	1:C:318:THR:CG2	2.48	0.43
1:D:164:LEU:CD1	1:D:178:TYR:OH	2.67	0.43
1:A:129:ALA:HB2	1:A:139:LEU:HD23	2.00	0.43
1:B:110:PHE:C	1:B:110:PHE:CD2	2.92	0.43
1:C:155:TYR:CD1	1:C:156:MET:N	2.86	0.43
1:C:158:GLY:HA3	1:C:206:LEU:HB2	1.99	0.43
1:C:170:VAL:HG22	1:C:174:TRP:CE3	2.47	0.43
1:D:283:LEU:O	1:D:286:THR:N	2.52	0.43
1:A:54:ASN:O	1:A:57:SER:HB2	2.19	0.43
1:B:165:MET:HE3	1:B:271:MET:HA	2.00	0.43
1:B:109:LYS:NZ	1:B:391:GLN:OE1	2.49	0.43
1:C:113:ILE:HG13	1:C:381:PHE:CZ	2.51	0.43
1:C:124:GLU:HG2	1:C:151:MET:CE	2.48	0.43
1:C:223:MET:HE3	1:C:257:ARG:NH2	2.34	0.43
1:D:277:PRO:O	1:D:278:PHE:CG	2.72	0.43
1:A:161:LEU:HB2	1:A:204:MET:HB2	2.01	0.43
1:A:172:GLU:CD	1:A:337:PHE:HE1	2.21	0.43
1:B:125:ARG:O	1:B:126:ASP:C	2.56	0.43
1:B:162:VAL:HB	1:B:201:PRO:HB2	2.01	0.43
1:B:228:MET:HB3	1:B:254:TYR:HE1	1.84	0.43
1:B:304:ASP:N	1:B:305:ILE:HD13	2.33	0.43
1:B:325:GLY:C	1:B:327:ASN:N	2.71	0.43
1:B:43:PHE:CD2	1:B:43:PHE:N	2.85	0.43
1:C:137:VAL:HG13	1:C:154:GLU:HG2	2.00	0.43
1:C:305:ILE:HD13	3:C:419:HOH:O	2.17	0.43
1:C:76:TYR:HD1	1:C:76:TYR:N	2.15	0.43
1:C:78:VAL:HG23	1:C:91:GLN:HE21	1.84	0.43
1:D:126:ASP:O	1:D:130:PHE:CD1	2.72	0.43
1:D:138:GLN:H	1:D:154:GLU:HG2	1.84	0.43
1:D:185:ALA:O	1:D:188:ALA:HB3	2.19	0.43
1:D:347:THR:O	1:D:349:ARG:N	2.52	0.43
1:D:110:PHE:CD1	1:D:381:PHE:N	2.86	0.43
1:A:189:ILE:HG22	1:A:194:PHE:O	2.19	0.43
1:A:324:LEU:O	1:A:332:ILE:HD11	2.18	0.43
1:B:121:PHE:CD1	1:B:122:TRP:N	2.87	0.43
1:B:252:ASP:O	1:B:253:GLY:C	2.58	0.43
1:C:241:ILE:O	1:C:290:ILE:HD13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:O	1:D:371:LEU:HD22	2.19	0.43
1:A:94:ARG:HA	1:A:100:LYS:O	2.19	0.42
1:B:19:ARG:O	1:B:21:PRO:HD3	2.19	0.42
1:D:347:THR:O	1:D:348:LEU:C	2.57	0.42
1:D:59:TYR:O	1:D:62:THR:N	2.52	0.42
1:D:80:LYS:HZ3	1:D:80:LYS:CB	2.32	0.42
1:D:7:PHE:N	1:D:9:THR:HG1	2.17	0.42
1:B:135:TRP:CZ3	1:B:349:ARG:HD2	2.54	0.42
1:B:175:ALA:HB1	1:B:272:LEU:HD21	1.98	0.42
1:B:314:CYS:O	1:B:318:THR:HG22	2.19	0.42
1:B:320:ARG:C	1:B:322:VAL:H	2.22	0.42
1:C:164:LEU:HD21	1:C:178:TYR:HE1	1.82	0.42
1:C:278:PHE:HB3	1:C:289:LYS:HB3	2.01	0.42
1:D:110:PHE:HD2	1:D:110:PHE:C	2.22	0.42
1:B:135:TRP:HE3	1:B:135:TRP:HA	1.84	0.42
1:A:244:GLU:HG3	1:A:320:ARG:HD3	2.01	0.42
1:A:333:LYS:HG2	1:A:345:TRP:CZ2	2.54	0.42
1:B:181:GLU:HG2	1:B:348:LEU:HD23	2.00	0.42
1:C:223:MET:CE	1:C:227:GLY:HA2	2.46	0.42
1:D:305:ILE:H	1:D:305:ILE:HD13	1.84	0.42
1:D:29:CYS:O	1:D:32:ASP:HB2	2.18	0.42
1:A:143:PHE:CD2	1:A:143:PHE:N	2.87	0.42
1:A:46:LEU:HD21	1:A:386:ALA:HA	2.02	0.42
1:A:40:ASP:OD2	1:A:391:GLN:HB2	2.20	0.42
1:C:109:LYS:NZ	1:C:144:GLN:HB2	2.34	0.42
1:C:148:TYR:HB2	1:C:150:TYR:CZ	2.54	0.42
1:C:371:LEU:HG	1:C:372:GLU:HG3	2.00	0.42
1:B:94:ARG:HD2	1:B:99:ARG:NH2	2.34	0.42
1:C:20:ASP:C	1:C:20:ASP:OD1	2.57	0.42
1:C:59:TYR:O	1:C:62:THR:N	2.52	0.42
1:D:112:MET:O	1:D:118:SER:HB3	2.19	0.42
1:A:261:TRP:HA	1:A:261:TRP:CE3	2.54	0.42
1:A:299:PHE:HA	1:A:300:PRO:HD3	1.93	0.42
1:A:59:TYR:O	1:A:62:THR:N	2.52	0.42
1:A:79:VAL:HG23	1:A:93:VAL:HA	2.00	0.42
1:B:237:THR:O	1:B:238:PRO:C	2.56	0.42
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.85	0.42
1:C:167:ASN:O	1:C:168:TYR:CD1	2.73	0.42
1:C:170:VAL:HA	1:C:171:PRO:HD2	1.78	0.42
1:D:165:MET:HE1	1:D:271:MET:CA	2.39	0.42
1:A:34:LEU:HD13	1:A:34:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PHE:O	1:B:219:THR:N	2.44	0.42
1:B:46:LEU:O	1:B:48:LYS:N	2.52	0.42
1:B:81:VAL:HG21	1:B:373:GLU:CA	2.44	0.42
1:C:109:LYS:HD2	1:C:145:ASP:O	2.19	0.42
1:D:156:MET:HE1	1:D:207:ASP:HB3	2.00	0.42
1:A:159:GLY:O	1:A:205:LEU:HA	2.19	0.42
1:A:241:ILE:HD11	1:A:245:VAL:HG12	2.02	0.42
1:B:335:HIS:CD2	1:B:337:PHE:H	2.37	0.42
1:B:383:ILE:HA	1:B:384:PRO:HD3	1.85	0.42
1:C:345:TRP:CE3	1:C:345:TRP:CA	3.00	0.42
1:B:242:SER:HB2	1:B:243:PRO:CD	2.49	0.42
1:C:286:THR:HA	1:C:289:LYS:HB2	2.02	0.42
1:D:242:SER:OG	1:D:245:VAL:HG23	2.20	0.42
1:A:107:LEU:HB3	1:A:112:MET:CE	2.50	0.41
1:A:269:TYR:CD1	1:A:277:PRO:HB3	2.54	0.41
1:A:279:TYR:C	1:A:279:TYR:CD2	2.92	0.41
1:B:11:PHE:CD2	3:B:419:HOH:O	2.57	0.41
1:B:210:GLY:O	1:B:353:ALA:HB1	2.20	0.41
1:C:204:MET:HG2	1:C:212:LEU:HD11	2.02	0.41
1:C:46:LEU:C	1:C:48:LYS:N	2.73	0.41
1:D:39:TYR:O	1:D:43:PHE:CZ	2.73	0.41
1:A:133:SER:OG	1:A:134:PRO:HD2	2.20	0.41
1:B:237:THR:O	1:B:241:ILE:HG22	2.19	0.41
1:C:241:ILE:HG21	1:C:246:LEU:HD11	2.01	0.41
1:C:268:LEU:HD23	1:C:313:ILE:CG1	2.51	0.41
1:C:372:GLU:HG3	1:C:372:GLU:H	1.52	0.41
1:A:189:ILE:HG23	1:A:194:PHE:HB2	2.03	0.41
1:A:343:TRP:CB	1:A:351:THR:HG21	2.51	0.41
1:A:9:THR:HG22	1:A:10:ARG:N	2.35	0.41
1:B:219:THR:O	1:B:220:CYS:C	2.58	0.41
1:C:200:LYS:CE	1:C:202:ASP:HB2	2.42	0.41
1:D:161:LEU:HD12	1:D:161:LEU:HA	1.69	0.41
1:D:193:GLY:O	1:D:222:LYS:HA	2.20	0.41
1:D:194:PHE:CE1	1:D:222:LYS:HE3	2.55	0.41
1:A:283:LEU:O	1:A:286:THR:N	2.54	0.41
1:A:6:SER:O	1:A:9:THR:N	2.53	0.41
1:B:26:ASN:O	1:B:27:SER:C	2.59	0.41
1:B:285:GLY:C	1:B:287:TYR:N	2.74	0.41
1:B:43:PHE:CE1	1:B:384:PRO:HD2	2.55	0.41
1:C:14:MET:O	1:C:17:LEU:HB2	2.19	0.41
1:C:75:ASP:O	1:C:96:LYS:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TRP:HA	1:D:135:TRP:CE3	2.56	0.41
1:D:160:ASP:HA	1:D:204:MET:O	2.20	0.41
1:D:98:THR:O	1:D:100:LYS:HG2	2.21	0.41
1:A:212:LEU:HD23	1:A:212:LEU:O	2.21	0.41
1:A:293:HIS:O	1:A:297:LEU:HB2	2.21	0.41
1:B:305:ILE:HD13	1:B:305:ILE:N	2.35	0.41
1:B:77:GLU:O	1:B:93:VAL:HG12	2.20	0.41
1:C:182:VAL:HG21	1:C:204:MET:HE1	2.02	0.41
1:C:268:LEU:HD23	1:C:313:ILE:HG13	2.02	0.41
1:C:343:TRP:HZ3	1:C:345:TRP:CE3	2.39	0.41
1:D:13:LYS:O	1:D:17:LEU:HD13	2.20	0.41
1:D:199:VAL:HB	1:D:263:SER:HB2	2.01	0.41
1:A:138:GLN:HG2	1:A:139:LEU:N	2.35	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.84	0.41
1:B:106:LEU:HD21	1:B:150:TYR:HE2	1.84	0.41
1:B:62:THR:O	1:B:63:ILE:C	2.59	0.41
1:C:287:TYR:O	1:C:291:MET:HG2	2.20	0.41
1:C:343:TRP:CZ3	1:C:345:TRP:CZ3	3.08	0.41
1:D:343:TRP:HB3	1:D:351:THR:HG21	2.02	0.41
1:D:44:PRO:O	1:D:48:LYS:HG3	2.20	0.41
1:A:221:MET:HE3	1:A:221:MET:HB2	1.87	0.41
1:B:199:VAL:HB	1:B:263:SER:HB2	2.03	0.41
1:B:230:ARG:CZ	1:B:230:ARG:HB3	2.50	0.41
1:B:293:HIS:O	1:B:297:LEU:HB2	2.21	0.41
1:B:299:PHE:HD2	1:B:300:PRO:HD2	1.85	0.41
1:B:308:GLU:CD	1:B:336:LEU:HB3	2.40	0.41
1:C:185:ALA:O	1:C:188:ALA:HB3	2.21	0.41
1:C:245:VAL:O	1:C:248:SER:HB2	2.20	0.41
1:D:111:GLU:OE1	1:D:115:ARG:NH2	2.49	0.41
1:D:242:SER:HB2	1:D:243:PRO:CD	2.49	0.41
1:D:378:GLU:OE2	1:D:378:GLU:CA	2.67	0.41
1:A:43:PHE:HA	1:A:44:PRO:HD2	1.58	0.41
1:C:237:THR:HG23	1:C:238:PRO:HD2	2.03	0.41
1:C:383:ILE:HA	1:C:384:PRO:HD3	1.73	0.41
1:C:69:LEU:HB3	1:D:14:MET:SD	2.61	0.41
1:D:340:ASN:HB2	1:D:342:GLN:OE1	2.20	0.41
1:A:261:TRP:O	1:A:264:VAL:N	2.54	0.41
1:B:92:LEU:HD11	1:B:101:VAL:CG1	2.50	0.41
1:B:196:HIS:N	1:B:260:ASP:OD2	2.46	0.41
1:A:74:GLU:O	1:A:76:TYR:N	2.54	0.41
1:B:171:PRO:HD2	1:B:174:TRP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:HE1	1:B:380:THR:O	2.03	0.41
1:D:139:LEU:HD12	1:D:152:VAL:O	2.21	0.41
1:D:170:VAL:HA	1:D:171:PRO:HD2	1.99	0.41
1:D:172:GLU:OE2	1:D:306:SER:HB2	2.21	0.41
1:A:142:ALA:HB3	1:A:399:TYR:HB3	2.03	0.40
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.84	0.40
1:B:114:LYS:HE2	1:B:115:ARG:CZ	2.51	0.40
1:B:240:TYR:CD2	1:B:240:TYR:N	2.89	0.40
1:C:109:LYS:HA	1:C:112:MET:HE3	2.04	0.40
1:C:308:GLU:OE1	1:C:336:LEU:HB3	2.21	0.40
1:D:143:PHE:CD2	1:D:143:PHE:N	2.88	0.40
1:A:325:GLY:O	1:A:326:ARG:C	2.59	0.40
1:B:78:VAL:O	1:B:78:VAL:HG13	2.21	0.40
1:C:43:PHE:CE1	1:C:384:PRO:CD	3.04	0.40
1:C:75:ASP:O	1:C:76:TYR:HD1	2.03	0.40
1:D:159:GLY:O	1:D:205:LEU:HA	2.21	0.40
1:D:196:HIS:CD2	1:D:196:HIS:C	2.94	0.40
1:D:313:ILE:C	1:D:315:ALA:H	2.24	0.40
1:D:98:THR:OG1	1:D:100:LYS:HG2	2.21	0.40
1:A:128:MET:HE3	1:A:137:VAL:HB	2.03	0.40
1:A:22:LYS:HG2	1:A:130:PHE:CE1	2.57	0.40
1:A:84:ARG:HH22	1:A:372:GLU:C	2.23	0.40
1:B:283:LEU:O	1:B:286:THR:N	2.55	0.40
1:B:38:VAL:CG2	1:B:63:ILE:HG13	2.31	0.40
1:B:94:ARG:HA	1:B:100:LYS:O	2.22	0.40
1:C:196:HIS:HD2	1:C:198:ASP:N	2.19	0.40
1:C:363:ILE:HD13	1:C:363:ILE:HG21	1.81	0.40
1:C:55:PHE:HB2	1:D:392:LEU:HB3	2.02	0.40
1:D:127:ILE:HG22	1:D:128:MET:N	2.36	0.40
1:D:158:GLY:HA3	1:D:206:LEU:C	2.41	0.40
1:D:268:LEU:CD2	1:D:313:ILE:HG12	2.51	0.40
1:A:261:TRP:O	1:A:264:VAL:HB	2.21	0.40
1:A:305:ILE:HG22	1:A:306:SER:N	2.36	0.40
1:B:123:GLU:H	1:B:123:GLU:HG2	1.45	0.40
1:B:161:LEU:HD23	1:B:267:PHE:CZ	2.55	0.40
1:B:205:LEU:HD11	2:B:900:3ND:C6	2.52	0.40
1:B:61:ASP:O	1:B:62:THR:C	2.57	0.40
1:B:77:GLU:HB2	1:B:96:LYS:CG	2.51	0.40
1:C:189:ILE:HG22	1:C:194:PHE:O	2.22	0.40
1:C:218:GLY:O	1:C:219:THR:HG23	2.21	0.40
1:D:121:PHE:HE1	1:D:122:TRP:CE2	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:PHE:CD2	1:D:354:PRO:CD	3.05	0.40
1:D:16:ASN:HB2	1:D:17:LEU:HD12	2.02	0.40
1:D:43:PHE:HA	1:D:44:PRO:HD2	1.73	0.40
1:A:258:GLU:HG3	1:A:320:ARG:HG3	2.03	0.40
1:A:62:THR:HG21	1:B:25:VAL:HG13	2.03	0.40
1:C:168:TYR:CE2	1:C:174:TRP:CH2	3.09	0.40
1:C:378:GLU:O	1:C:379:GLU:C	2.60	0.40
1:D:247:LYS:HB3	1:D:247:LYS:HE2	1.79	0.40
1:D:196:HIS:N	1:D:260:ASP:OD2	2.52	0.40
1:D:299:PHE:HD2	1:D:300:PRO:HD3	1.86	0.40
1:D:48:LYS:CB	1:D:48:LYS:NZ	2.85	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	373/415 (90%)	282 (76%)	65 (17%)	26 (7%)	1	7
1	B	394/415 (95%)	294 (75%)	70 (18%)	30 (8%)	1	6
1	C	361/415 (87%)	268 (74%)	67 (19%)	26 (7%)	1	7
1	D	394/415 (95%)	286 (73%)	86 (22%)	22 (6%)	2	11
All	All	1522/1660 (92%)	1130 (74%)	288 (19%)	104 (7%)	1	8

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	99	ARG
1	A	273	VAL
1	A	351	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	60	LYS
1	B	99	ARG
1	B	296	SER
1	B	347	THR
1	B	378	GLU
1	C	7	PHE
1	C	60	LYS
1	C	99	ARG
1	C	273	VAL
1	D	60	LYS
1	D	99	ARG
1	D	296	SER
1	D	297	LEU
1	D	347	THR
1	D	378	GLU
1	A	296	SER
1	A	297	LEU
1	A	347	THR
1	A	379	GLU
1	B	8	GLU
1	B	218	GLY
1	B	249	GLN
1	B	250	GLY
1	B	273	VAL
1	B	284	VAL
1	B	297	LEU
1	B	303	ASN
1	B	322	VAL
1	B	401	SER
1	C	47	ARG
1	C	75	ASP
1	C	95	HIS
1	C	296	SER
1	C	297	LEU
1	C	347	THR
1	C	351	THR
1	C	373	GLU
1	C	378	GLU
1	D	75	ASP
1	D	250	GLY
1	D	273	VAL
1	D	351	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	9	THR
1	A	47	ARG
1	A	198	ASP
1	A	219	THR
1	B	75	ASP
1	B	220	CYS
1	B	269	TYR
1	B	351	THR
1	C	124	GLU
1	C	219	THR
1	D	198	ASP
1	D	249	GLN
1	A	97	SER
1	A	124	GLU
1	A	220	CYS
1	B	44	PRO
1	B	47	ARG
1	B	198	ASP
1	B	200	LYS
1	B	202	ASP
1	B	208	LYS
1	B	295	ASN
1	C	8	GLU
1	C	345	TRP
1	C	348	LEU
1	D	124	GLU
1	D	170	VAL
1	D	200	LYS
1	D	219	THR
1	D	303	ASN
1	D	348	LEU
1	A	44	PRO
1	A	75	ASP
1	A	317	LEU
1	B	154	GLU
1	B	286	THR
1	C	97	SER
1	C	321	GLU
1	D	11	PHE
1	C	27	SER
1	C	200	LYS
1	C	239	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	97	SER
1	D	208	LYS
1	A	218	GLY
1	A	313	ILE
1	A	328	GLY
1	C	158	GLY
1	A	127	ILE
1	B	63	ILE
1	C	218	GLY
1	C	284	VAL
1	A	241	ILE
1	A	274	GLY
1	A	322	VAL
1	B	170	VAL
1	A	158	GLY
1	D	253	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/369 (93%)	307 (90%)	36 (10%)	7	25
1	B	352/369 (95%)	312 (89%)	40 (11%)	5	22
1	C	334/369 (90%)	302 (90%)	32 (10%)	8	29
1	D	352/369 (95%)	319 (91%)	33 (9%)	8	30
All	All	1381/1476 (94%)	1240 (90%)	141 (10%)	7	27

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	ARG
1	A	11	PHE
1	A	16	ASN
1	A	20	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	GLU
1	A	25	VAL
1	A	47	ARG
1	A	58	ARG
1	A	93	VAL
1	A	95	HIS
1	A	126	ASP
1	A	135	TRP
1	A	164	LEU
1	A	186	LEU
1	A	212	LEU
1	A	219	THR
1	A	223	MET
1	A	225	LYS
1	A	239	ASP
1	A	241	ILE
1	A	246	LEU
1	A	254	TYR
1	A	319	ASP
1	A	321	GLU
1	A	336	LEU
1	A	341	ASP
1	A	342	GLN
1	A	351	THR
1	A	367	ASN
1	A	369	ASP
1	A	370	ASP
1	A	371	LEU
1	A	372	GLU
1	A	381	PHE
1	A	394	PHE
1	B	9	THR
1	B	11	PHE
1	B	18	LEU
1	B	37	LEU
1	B	47	ARG
1	B	53	ASP
1	B	62	THR
1	B	93	VAL
1	B	95	HIS
1	B	123	GLU
1	B	154	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	161	LEU
1	B	162	VAL
1	B	186	LEU
1	B	204	MET
1	B	212	LEU
1	B	219	THR
1	B	223	MET
1	B	225	LYS
1	B	230	ARG
1	B	237	THR
1	B	241	ILE
1	B	246	LEU
1	B	248	SER
1	B	249	GLN
1	B	299	PHE
1	B	302	ASP
1	B	305	ILE
1	B	312	LEU
1	B	319	ASP
1	B	341	ASP
1	B	342	GLN
1	B	351	THR
1	B	363	ILE
1	B	371	LEU
1	B	372	GLU
1	B	377	GLU
1	B	379	GLU
1	B	380	THR
1	B	402	ASN
1	C	8	GLU
1	C	10	ARG
1	C	14	MET
1	C	25	VAL
1	C	31	LEU
1	C	34	LEU
1	C	43	PHE
1	C	63	ILE
1	C	69	LEU
1	C	82	ILE
1	C	93	VAL
1	C	112	MET
1	C	126	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	133	SER
1	C	164	LEU
1	C	212	LEU
1	C	216	ASP
1	C	219	THR
1	C	223	MET
1	C	225	LYS
1	C	226	GLU
1	C	246	LEU
1	C	249	GLN
1	C	299	PHE
1	C	305	ILE
1	C	312	LEU
1	C	336	LEU
1	C	342	GLN
1	C	345	TRP
1	C	372	GLU
1	C	373	GLU
1	C	374	ASP
1	D	13	LYS
1	D	14	MET
1	D	27	SER
1	D	34	LEU
1	D	66	ILE
1	D	72	LYS
1	D	95	HIS
1	D	123	GLU
1	D	126	ASP
1	D	133	SER
1	D	145	ASP
1	D	146	ASP
1	D	153	MET
1	D	189	ILE
1	D	212	LEU
1	D	216	ASP
1	D	223	MET
1	D	225	LYS
1	D	230	ARG
1	D	239	ASP
1	D	248	SER
1	D	281	ASP
1	D	288	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	299	PHE
1	D	305	ILE
1	D	312	LEU
1	D	329	VAL
1	D	342	GLN
1	D	349	ARG
1	D	351	THR
1	D	365	THR
1	D	374	ASP
1	D	377	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	196	HIS
1	A	293	HIS
1	A	295	ASN
1	A	311	ASN
1	A	390	ASN
1	B	16	ASN
1	B	51	ASN
1	B	64	ASN
1	B	138	GLN
1	B	190	HIS
1	B	211	HIS
1	B	292	ASN
1	B	295	ASN
1	B	335	HIS
1	B	390	ASN
1	C	26	ASN
1	C	138	GLN
1	C	190	HIS
1	C	196	HIS
1	C	211	HIS
1	C	292	ASN
1	C	295	ASN
1	C	311	ASN
1	C	340	ASN
1	C	342	GLN
1	D	16	ASN
1	D	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	138	GLN
1	D	196	HIS
1	D	292	ASN
1	D	295	ASN
1	D	311	ASN
1	D	327	ASN
1	D	342	GLN
1	D	390	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	3ND	C	900	-	28,30,30	1.10	2 (7%)	38,43,43	1.88	8 (21%)
2	3ND	D	900	-	28,30,30	1.09	2 (7%)	38,43,43	1.92	8 (21%)
2	3ND	B	900	-	28,30,30	1.16	3 (10%)	38,43,43	1.95	8 (21%)

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	3ND	C	900	-	-	3/12/32/32	0/3/4/4
2	3ND	D	900	-	-	2/12/32/32	0/3/4/4
2	3ND	B	900	-	-	2/12/32/32	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	3ND	C1-N2	3.36	1.36	1.28
2	B	900	3ND	C1-N2	3.36	1.36	1.28
2	C	900	3ND	C1-N2	3.02	1.35	1.28
2	C	900	3ND	C3-N2	-2.65	1.33	1.38
2	B	900	3ND	C18-C17	-2.48	1.48	1.51
2	D	900	3ND	C3-N2	-2.33	1.34	1.38
2	B	900	3ND	C3-N2	-2.27	1.34	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	3ND	C18-C17-C13	-6.49	100.92	114.64
2	D	900	3ND	C18-C17-C13	-6.18	101.57	114.64
2	C	900	3ND	C18-C17-C13	-5.67	102.64	114.64
2	D	900	3ND	C13-C12-N11	5.43	121.18	114.50
2	C	900	3ND	C13-C12-N11	5.13	120.82	114.50
2	B	900	3ND	C13-C12-N11	5.10	120.77	114.50
2	C	900	3ND	C5-C6-C3	-3.66	118.25	120.91
2	D	900	3ND	C5-C6-C3	-3.58	118.31	120.91
2	B	900	3ND	C5-C6-C3	-3.39	118.45	120.91
2	B	900	3ND	C22-C23-C18	-3.26	117.92	121.20
2	D	900	3ND	O27-C12-C13	-3.18	117.89	121.73
2	B	900	3ND	C23-C18-C19	3.09	122.15	118.29
2	D	900	3ND	C22-C23-C18	-3.03	118.14	121.20
2	C	900	3ND	C9-C8-CL26	-3.00	116.13	119.54
2	B	900	3ND	O27-C12-C13	-2.95	118.18	121.73
2	C	900	3ND	C23-C18-C19	2.52	121.44	118.29
2	D	900	3ND	C23-C18-C19	2.47	121.38	118.29
2	D	900	3ND	C9-C8-CL26	-2.47	116.73	119.54
2	C	900	3ND	O27-C12-C13	-2.38	118.86	121.73
2	B	900	3ND	C16-C17-C18	-2.31	111.97	115.03
2	C	900	3ND	O25-C3-N2	-2.13	117.78	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	3ND	C6-C3-N2	2.11	120.82	117.88
2	D	900	3ND	C9-N11-C12	-2.07	121.24	126.92
2	B	900	3ND	C7-C8-C9	2.03	123.38	121.72

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	900	3ND	O27-C12-C13-C17
2	D	900	3ND	O27-C12-C13-C17
2	B	900	3ND	O27-C12-C13-C17
2	C	900	3ND	N11-C12-C13-C17
2	D	900	3ND	N11-C12-C13-C17
2	B	900	3ND	N11-C12-C13-C17
2	C	900	3ND	C8-C9-N11-C12

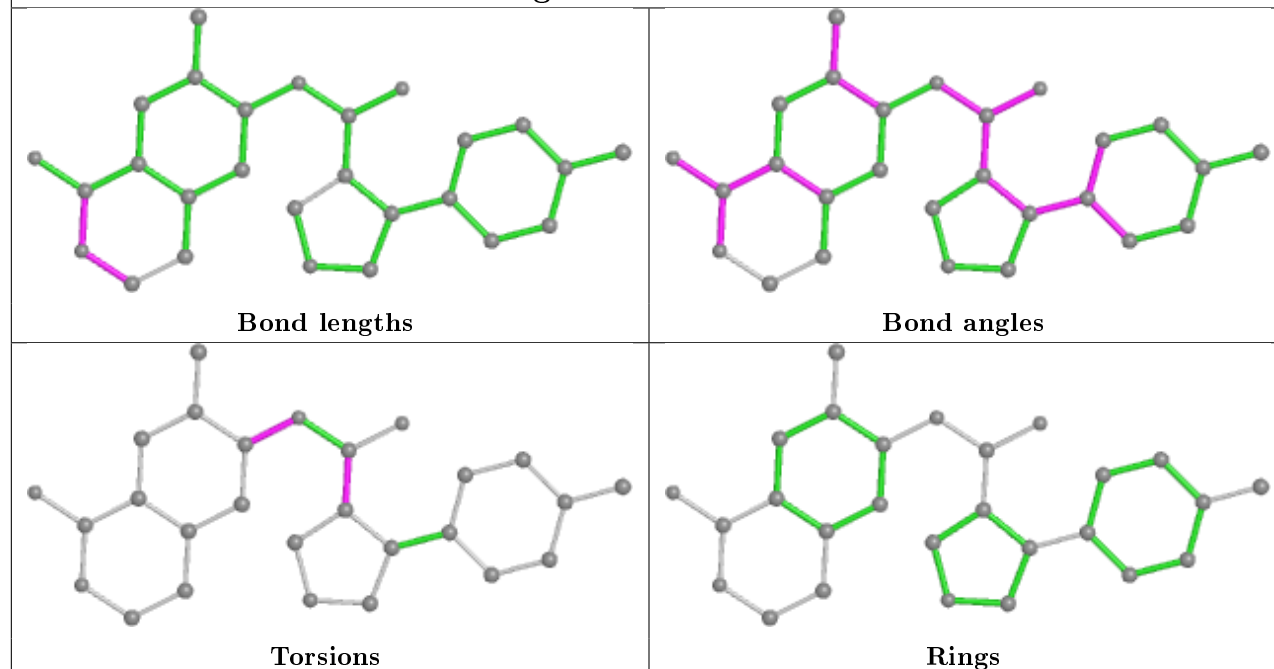
There are no ring outliers.

3 monomers are involved in 16 short contacts:

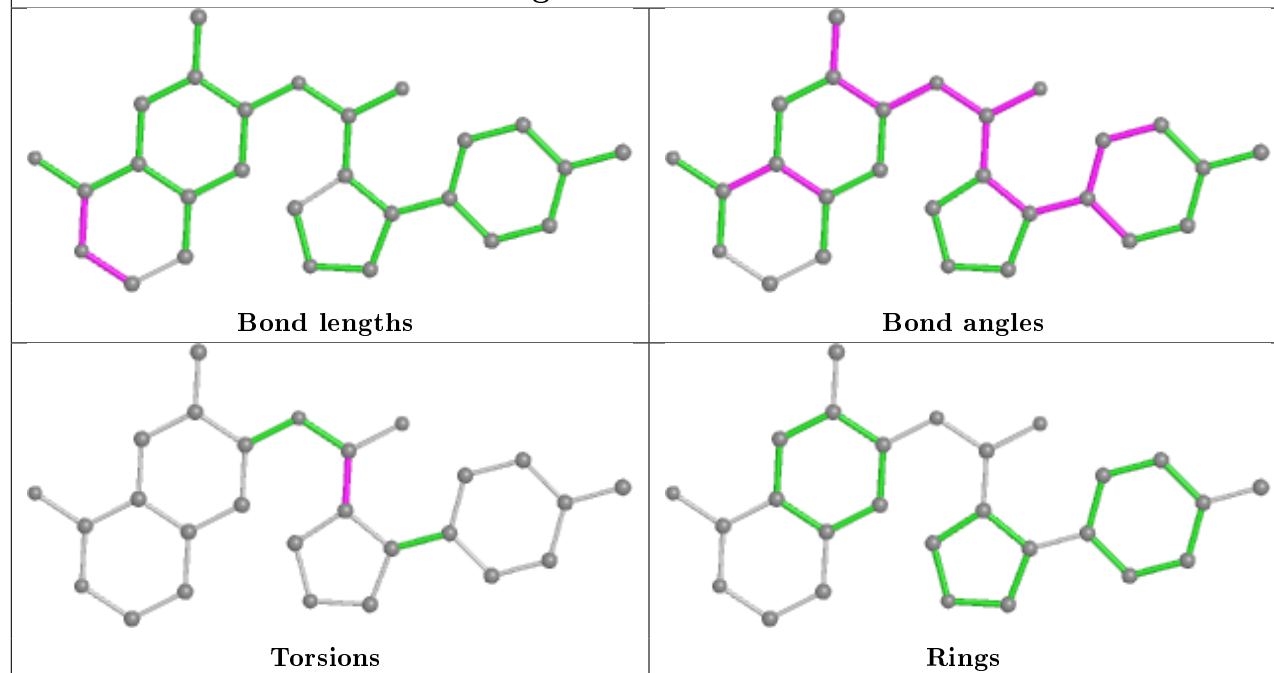
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	3ND	4	0
2	D	900	3ND	5	0
2	B	900	3ND	7	0

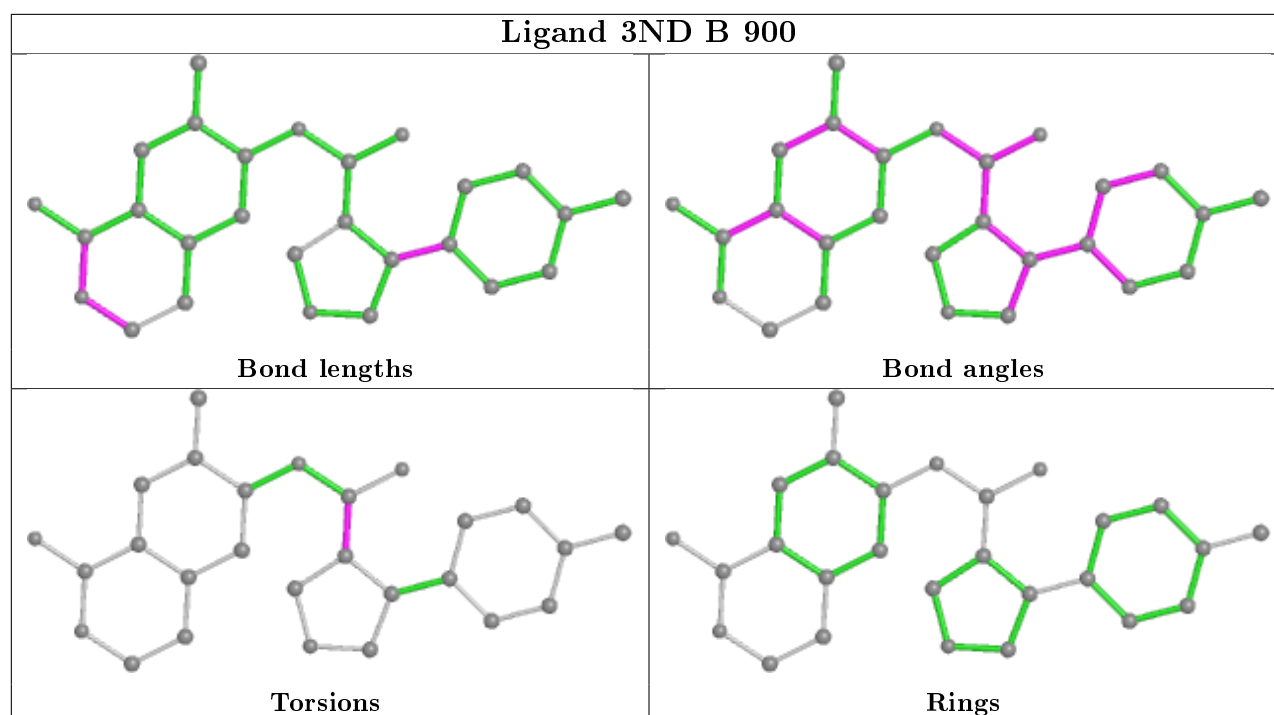
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 3ND C 900



Ligand 3ND D 900





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/415 (92%)	0.74	59 (15%) 2 2	102, 200, 300, 366	0
1	B	396/415 (95%)	0.16	11 (2%) 53 51	83, 143, 237, 329	0
1	C	371/415 (89%)	0.44	38 (10%) 6 6	88, 168, 274, 403	0
1	D	396/415 (95%)	0.18	8 (2%) 65 64	82, 153, 232, 336	0
All	All	1546/1660 (93%)	0.38	116 (7%) 14 13	82, 164, 271, 403	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	TYR	6.8
1	A	245	VAL	5.0
1	C	260	ASP	4.9
1	A	336	LEU	4.7
1	A	353	ALA	4.7
1	A	203	ASN	4.5
1	C	245	VAL	4.3
1	C	377	GLU	4.2
1	A	231	CYS	4.1
1	A	268	LEU	4.1
1	C	291	MET	4.1
1	A	76	TYR	4.0
1	A	104	MET	4.0
1	A	327	ASN	4.0
1	A	272	LEU	4.0
1	A	299	PHE	4.0
1	C	317	LEU	4.0
1	A	107	LEU	3.9
1	A	244	GLU	3.8
1	A	338	PHE	3.8
1	C	293	HIS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	7	PHE	3.7
1	D	80	LYS	3.7
1	C	290	ILE	3.6
1	A	359	LEU	3.6
1	A	290	ILE	3.5
1	D	251	GLY	3.4
1	C	313	ILE	3.4
1	C	276	THR	3.3
1	C	248	SER	3.3
1	A	84	ARG	3.3
1	C	262	TRP	3.3
1	C	268	LEU	3.2
1	B	38	VAL	3.2
1	D	226	GLU	3.2
1	C	230	ARG	3.1
1	A	317	LEU	3.1
1	A	402	ASN	3.0
1	A	371	LEU	3.0
1	A	297	LEU	3.0
1	C	376	GLY	2.9
1	B	9	THR	2.9
1	D	326	ARG	2.9
1	C	312	LEU	2.8
1	B	116	SER	2.8
1	A	365	THR	2.8
1	A	199	VAL	2.7
1	A	324	LEU	2.7
1	A	346	GLU	2.7
1	A	87	PHE	2.6
1	A	277	PRO	2.6
1	C	314	CYS	2.6
1	A	357	PRO	2.6
1	C	41	LEU	2.6
1	C	170	VAL	2.6
1	A	132	ASN	2.6
1	A	157	PRO	2.6
1	C	307	LYS	2.5
1	C	176	ARG	2.5
1	A	312	LEU	2.5
1	C	287	TYR	2.5
1	A	316	PHE	2.4
1	C	300	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	118	SER	2.4
1	A	304	ASP	2.4
1	C	231	CYS	2.4
1	C	195	ILE	2.4
1	A	400	TYR	2.4
1	C	225	LYS	2.4
1	A	300	PRO	2.4
1	A	287	TYR	2.4
1	C	263	SER	2.4
1	D	332	ILE	2.4
1	A	337	PHE	2.3
1	C	223	MET	2.3
1	A	235	VAL	2.3
1	A	82	ILE	2.3
1	A	332	ILE	2.3
1	B	139	LEU	2.3
1	A	395	VAL	2.3
1	A	161	LEU	2.3
1	A	81	VAL	2.3
1	A	267	PHE	2.3
1	A	91	GLN	2.3
1	C	244	GLU	2.3
1	A	307	LYS	2.3
1	C	224	ASN	2.2
1	A	155	TYR	2.2
1	A	291	MET	2.2
1	C	271	MET	2.2
1	A	181	GLU	2.2
1	B	251	GLY	2.2
1	A	121	PHE	2.2
1	D	117	ASP	2.2
1	A	355	VAL	2.1
1	A	271	MET	2.1
1	C	272	LEU	2.1
1	C	400	TYR	2.1
1	B	104	MET	2.1
1	A	392	LEU	2.1
1	A	10	ARG	2.1
1	B	117	ASP	2.1
1	C	269	TYR	2.1
1	A	381	PHE	2.1
1	B	10	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	368	PHE	2.1
1	C	350	ASP	2.1
1	D	118	SER	2.0
1	B	299	PHE	2.0
1	C	316	PHE	2.0
1	C	261	TRP	2.0
1	C	369	ASP	2.0
1	A	232	ASP	2.0
1	A	309	ALA	2.0
1	B	141	TYR	2.0
1	D	76	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

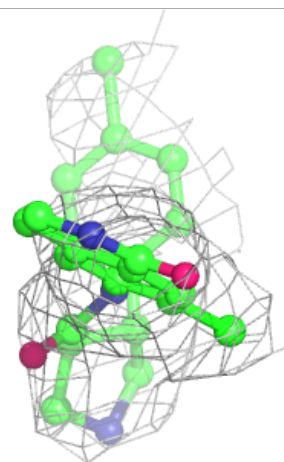
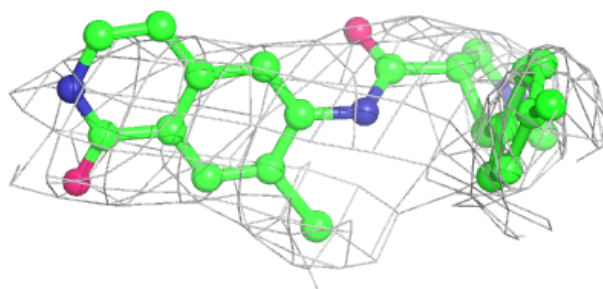
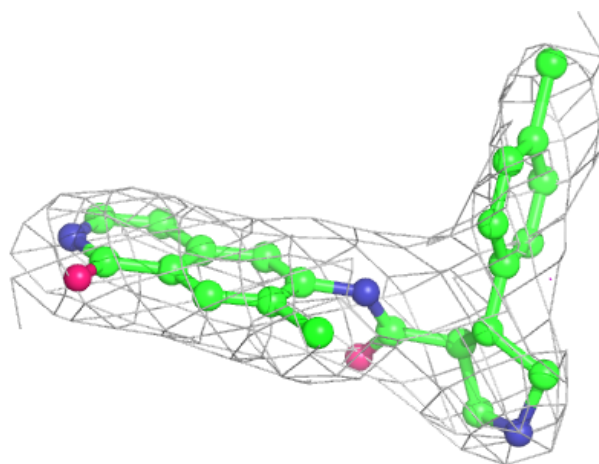
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	3ND	D	900	27/27	0.88	0.33	150,150,150,150	0
2	3ND	B	900	27/27	0.90	0.28	142,142,142,142	0
2	3ND	C	900	27/27	0.92	0.25	138,138,138,138	0

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.

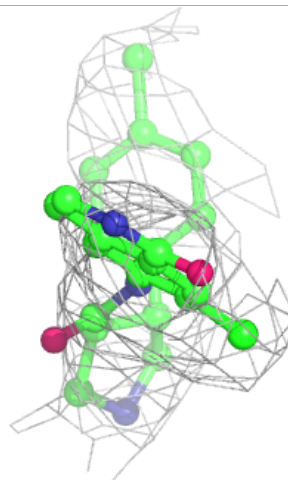
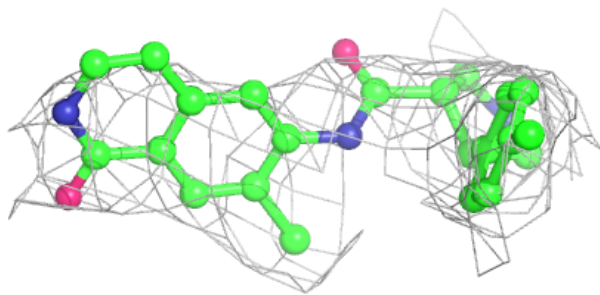
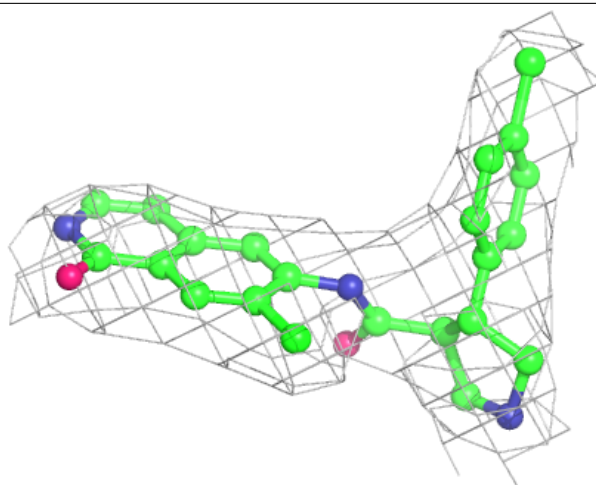
Electron density around 3ND D 900:

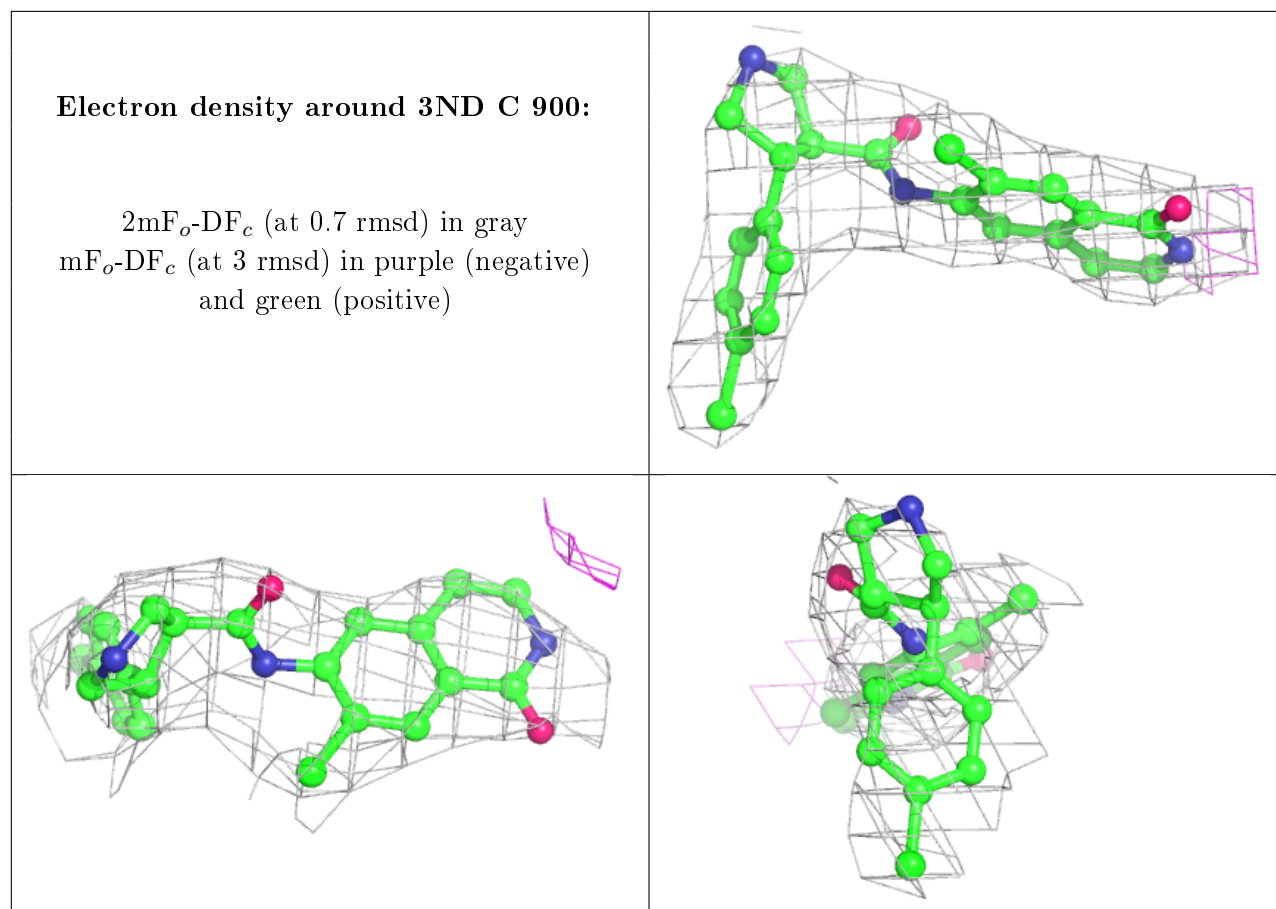
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3ND B 900:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.