



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:53 PM UTC

PDB ID : 4PWX / pdb_00004pwx
Title : Crystal structure of an ATP-bound Get3-Get4-Get5 complex from *S.cerevisiae*
Authors : Gristick, H.B.; Clemons Jr., W.M.
Deposited on : 2014-03-21
Resolution : 5.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

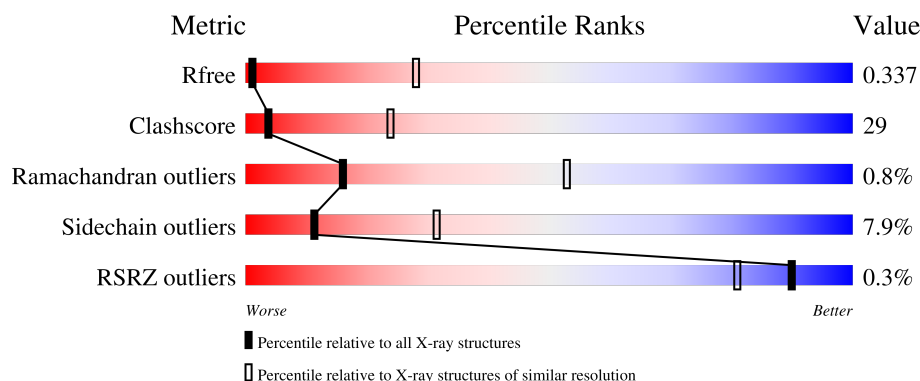
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.40 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}	180053	1060 (6.80-4.00)
Clashscore	190562	1117 (6.80-4.00)
Ramachandran outliers	187476	1020 (6.80-3.96)
Sidechain outliers	187428	1019 (6.86-3.94)
RSRZ outliers	180081	1053 (6.80-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	356	% 38% 38% 5% 17%
1	B	356	40% 39% 5% 16%
2	C	288	% 51% 42% . .
2	E	288	51% 43% . .
3	D	54	61% 30% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	54	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (57%), yellow (31%), and orange (7%). A small grey dot is at the end of the bar.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10159 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2319	1475	382	446	16			
1	B	299	Total	C	N	O	S	0	0	0
			2358	1497	388	456	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q12154
A	0	VAL	-	expression tag	UNP Q12154
A	1	ASP	-	expression tag	UNP Q12154
A	57	VAL	ASP	engineered mutation	UNP Q12154
B	-1	SER	-	expression tag	UNP Q12154
B	0	VAL	-	expression tag	UNP Q12154
B	1	ASP	-	expression tag	UNP Q12154
B	57	VAL	ASP	engineered mutation	UNP Q12154

- Molecule 2 is a protein called Golgi to ER traffic protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	277	Total	C	N	O	S	0	0	0
			2301	1498	362	436	5			
2	C	276	Total	C	N	O	S	0	0	0
			2296	1495	361	435	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	MET	-	expression tag	UNP Q12125
E	10	GLY	-	expression tag	UNP Q12125
E	258	ALA	LYS	engineered mutation	UNP Q12125
E	260	ALA	LYS	engineered mutation	UNP Q12125

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	291	GLU	-	expression tag	UNP Q12125
E	292	ASN	-	expression tag	UNP Q12125
E	293	LEU	-	expression tag	UNP Q12125
E	294	TYR	-	expression tag	UNP Q12125
E	295	PHE	-	expression tag	UNP Q12125
E	296	GLN	-	expression tag	UNP Q12125
C	9	MET	-	expression tag	UNP Q12125
C	10	GLY	-	expression tag	UNP Q12125
C	258	ALA	LYS	engineered mutation	UNP Q12125
C	260	ALA	LYS	engineered mutation	UNP Q12125
C	291	GLU	-	expression tag	UNP Q12125
C	292	ASN	-	expression tag	UNP Q12125
C	293	LEU	-	expression tag	UNP Q12125
C	294	TYR	-	expression tag	UNP Q12125
C	295	PHE	-	expression tag	UNP Q12125
C	296	GLN	-	expression tag	UNP Q12125

- | Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|-------|
| 3 | F | 52 | Total
410 | C
270 | N
64 | O
76 | 0 | 0 | 0 |
| 3 | D | 52 | Total
410 | C
270 | N
64 | O
76 | 0 | 0 | 0 |

- # ATP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

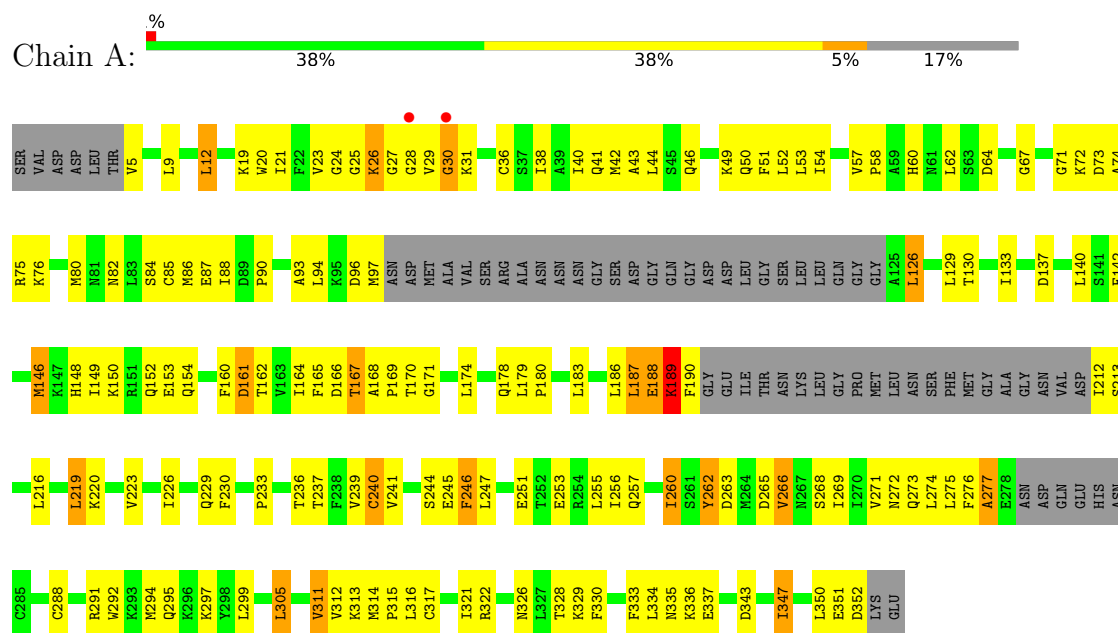
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

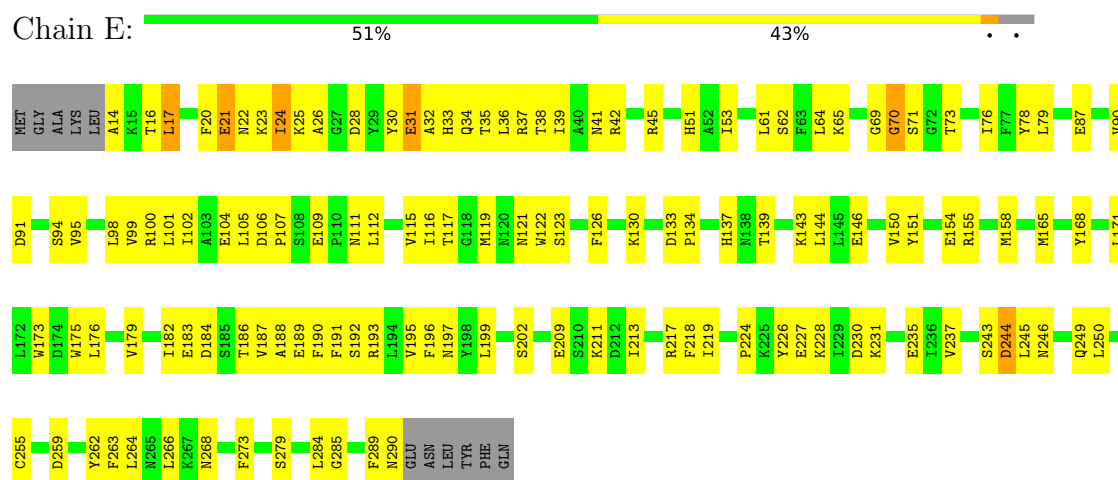
3 Residue-property plots

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

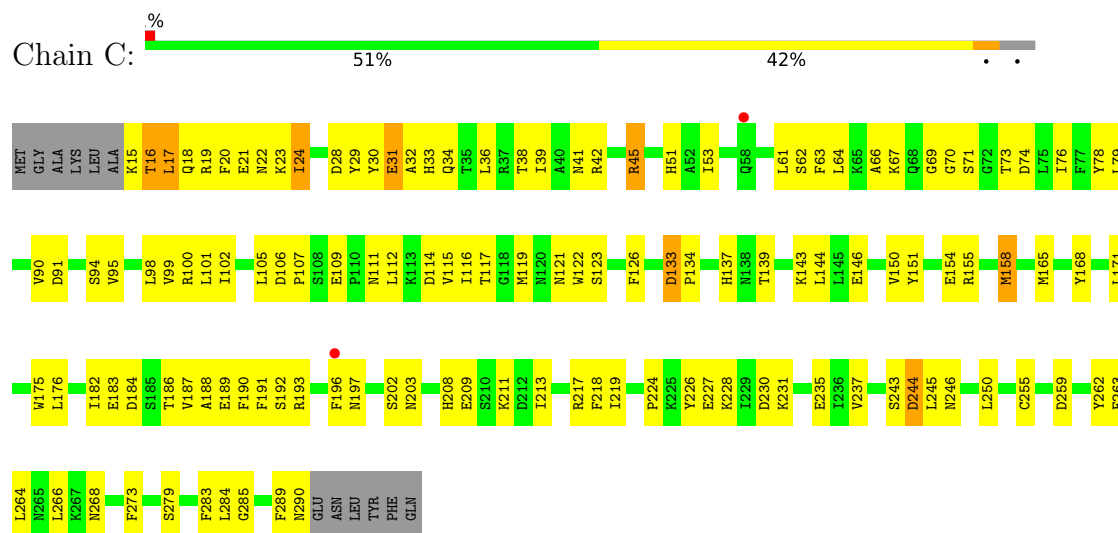
• Molecule 1: ATPase GET3



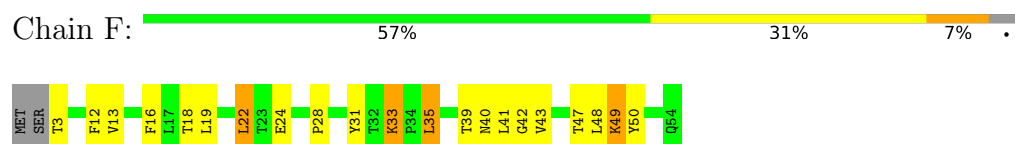
- Molecule 2: Golgi to ER traffic protein 4



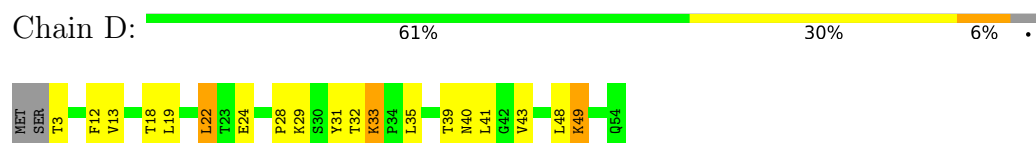
- Molecule 2: Golgi to ER traffic protein 4



- Molecule 3: Ubiquitin-like protein MDY2



- Molecule 3: Ubiquitin-like protein MDY2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.34Å 134.50Å 84.06Å 90.00° 113.37° 90.00°	Depositor
Resolution (Å)	30.00 – 5.40 30.00 – 5.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-5.40) 93.4 (30.00-5.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 5.34Å)	Xtriage
Refinement program	REFMAC v6.3, CNS 1.2	Depositor
R, R_{free}	0.270 , 0.328 0.280 , 0.337	Depositor DCC
R_{free} test set	538 reflections (9.09%)	wwPDB-VP
Wilson B-factor (Å ²)	355.6	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 314.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10159	wwPDB-VP
Average B, all atoms (Å ²)	347.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, MG

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	0.28	0/2357	0.76	3/3177 (0.1%)
1	B	0.27	0/2396	0.76	2/3230 (0.1%)
2	C	0.27	0/2353	0.74	3/3179 (0.1%)
2	E	0.27	0/2358	0.74	2/3186 (0.1%)
3	D	0.32	0/421	0.76	0/572
3	F	0.33	0/421	0.75	0/572
All	All	0.28	0/10306	0.75	10/13916 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	22	ASN	N-CA-C	-5.96	104.36	111.69
1	B	46	GLN	CA-C-N	5.20	126.33	119.84
1	B	46	GLN	C-N-CA	5.20	126.33	119.84
2	E	133	ASP	CA-C-N	5.17	124.62	119.24
2	E	133	ASP	C-N-CA	5.17	124.62	119.24
2	C	133	ASP	CA-C-N	5.16	124.60	119.24
2	C	133	ASP	C-N-CA	5.16	124.60	119.24
1	A	46	GLN	CA-C-N	5.09	126.20	119.84
1	A	46	GLN	C-N-CA	5.09	126.20	119.84
1	A	262	TYR	N-CA-C	-5.04	107.13	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2319	0	2324	174	0
1	B	2358	0	2356	173	0
2	C	2296	0	2218	124	0
2	E	2301	0	2223	131	0
3	D	410	0	433	23	0
3	F	410	0	433	25	2
4	A	31	0	12	5	0
4	B	31	0	12	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
All	All	10159	0	10011	581	2

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 29.

All (581) 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:305:LEU:HG	2:C:42:ARG:HH22	1.17	1.06
1:A:28:GLY:HA3	1:B:28:GLY:HA3	1.44	0.98
1:A:305:LEU:HG	2:C:42:ARG:NH2	1.81	0.94
1:A:12:LEU:HD21	1:A:237:THR:HG21	1.48	0.93
2:E:158:MET:SD	2:E:197:ASN:HB3	2.11	0.91
1:A:247:LEU:HD11	1:B:322:ARG:HD2	1.52	0.90
1:B:12:LEU:HD21	1:B:237:THR:HG21	1.54	0.90
1:A:41:GLN:HE22	1:A:335:ASN:HD22	1.19	0.88
1:A:21:ILE:HD13	1:A:42:MET:HE1	1.56	0.87
1:A:305:LEU:CG	2:C:42:ARG:HH22	1.89	0.85
2:E:250:LEU:HD11	3:F:13:VAL:HG22	1.55	0.85
1:B:187:LEU:HD21	1:B:219:LEU:HD22	1.59	0.84
1:B:21:ILE:HD13	1:B:42:MET:HE1	1.58	0.83
1:A:30:GLY:HA2	4:A:401:ATP:O1A	1.79	0.83
1:B:41:GLN:HE22	1:B:335:ASN:HD22	1.25	0.82
2:E:24:ILE:HG12	2:E:32:ALA:CB	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:GLU:HA	2:E:24:ILE:HG13	1.59	0.82
2:C:24:ILE:HG12	2:C:32:ALA:CB	2.08	0.82
2:E:155:ARG:HE	3:F:41:LEU:HD13	1.43	0.81
2:E:250:LEU:HD21	3:F:13:VAL:HG13	1.62	0.80
2:C:155:ARG:HE	3:D:41:LEU:HD13	1.46	0.80
2:C:16:THR:HG22	2:C:19:ARG:NH1	1.97	0.80
2:C:250:LEU:HD11	3:D:13:VAL:HG22	1.63	0.78
1:A:64:ASP:HB3	1:B:247:LEU:HG	1.66	0.78
1:A:322:ARG:HD2	1:B:247:LEU:HD11	1.66	0.77
2:C:158:MET:SD	2:C:197:ASN:HB3	2.25	0.77
1:B:54:ILE:HG13	1:B:86:MET:HB3	1.65	0.76
2:C:279:SER:HB2	3:D:43:VAL:HG11	1.68	0.76
1:B:230:PHE:HD1	1:B:236:THR:HG21	1.50	0.75
2:E:61:LEU:HD21	2:E:100:ARG:CZ	2.17	0.74
1:A:26:LYS:HG2	1:A:27:GLY:H	1.50	0.74
2:C:61:LEU:HD21	2:C:100:ARG:CZ	2.16	0.74
1:A:67:GLY:O	2:E:30:TYR:HB2	1.88	0.73
1:A:187:LEU:HD21	1:A:219:LEU:HD12	1.69	0.73
2:C:183:GLU:HG3	2:C:184:ASP:N	2.02	0.73
1:A:244:SER:HB3	1:A:295:GLN:HG2	1.70	0.73
2:C:98:LEU:HD13	2:C:119:MET:HB3	1.70	0.72
1:B:58:PRO:HG3	1:B:137:ASP:CG	2.13	0.72
1:B:244:SER:HB3	1:B:295:GLN:HG2	1.72	0.72
2:E:17:LEU:HD22	2:E:39:ILE:HD13	1.72	0.72
1:B:57:VAL:HG23	1:B:166:ASP:O	1.89	0.71
1:A:129:LEU:HD21	1:B:186:LEU:HD21	1.72	0.71
1:B:246:PHE:C	1:B:246:PHE:CD2	2.67	0.71
2:E:285:GLY:HA2	2:E:289:PHE:HD2	1.55	0.71
2:C:285:GLY:HA2	2:C:289:PHE:HD2	1.54	0.70
1:A:53:LEU:HD13	1:A:164:ILE:HB	1.74	0.70
2:E:73:THR:HG21	2:E:111:ASN:ND2	2.07	0.70
1:B:53:LEU:HD13	1:B:164:ILE:HB	1.72	0.70
2:E:23:LYS:HD2	2:E:31:GLU:HG2	1.73	0.70
1:A:58:PRO:HG3	1:A:137:ASP:CG	2.18	0.69
1:B:26:LYS:HG2	1:B:27:GLY:H	1.57	0.69
3:F:49:LYS:H	3:F:49:LYS:HD2	1.58	0.69
1:B:71:GLY:H	1:B:75:ARG:NH1	1.90	0.69
2:E:183:GLU:HG3	2:E:184:ASP:N	2.07	0.69
1:A:54:ILE:HG13	1:A:86:MET:HB3	1.73	0.69
1:A:57:VAL:HG23	1:A:166:ASP:O	1.93	0.69
1:A:186:LEU:HD21	1:B:129:LEU:HD21	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:401:ATP:H5'1	1:B:247:LEU:HD22	1.75	0.68
2:E:279:SER:HB2	3:F:43:VAL:HG11	1.76	0.68
1:A:60:HIS:HB3	1:A:87:GLU:CD	2.18	0.68
1:B:228:GLN:HA	1:B:231:THR:HG22	1.75	0.68
2:C:73:THR:HG21	2:C:111:ASN:ND2	2.09	0.68
2:E:24:ILE:HG12	2:E:32:ALA:HB2	1.75	0.67
1:A:246:PHE:C	1:A:246:PHE:CD2	2.73	0.67
1:A:257:GLN:CD	2:C:41:ASN:ND2	2.53	0.66
2:E:155:ARG:O	2:E:158:MET:HB2	1.95	0.66
1:B:170:THR:HG22	1:B:255:LEU:HD22	1.77	0.65
1:B:23:VAL:HB	1:B:165:PHE:O	1.96	0.65
1:B:60:HIS:HB3	1:B:87:GLU:CD	2.19	0.65
2:C:219:ILE:HD11	2:C:237:VAL:HG11	1.78	0.65
2:E:154:GLU:HG3	2:E:168:TYR:CE1	2.32	0.65
2:C:155:ARG:HH21	3:D:41:LEU:HD12	1.61	0.65
3:D:49:LYS:H	3:D:49:LYS:HD2	1.61	0.65
1:A:229:GLN:O	1:A:236:THR:HG23	1.97	0.65
1:A:247:LEU:HD12	1:A:247:LEU:H	1.62	0.65
2:E:188:ALA:HB2	2:E:244:ASP:HB3	1.78	0.64
1:A:41:GLN:NE2	1:A:335:ASN:HD22	1.94	0.64
2:C:213:ILE:O	2:C:217:ARG:HG3	1.97	0.64
2:E:213:ILE:O	2:E:217:ARG:HG3	1.97	0.64
2:C:28:ASP:HB3	2:C:31:GLU:HB2	1.79	0.64
2:C:17:LEU:HA	2:C:20:PHE:CE2	2.33	0.64
3:F:19:LEU:HA	3:F:22:LEU:HD21	1.80	0.63
1:A:23:VAL:HB	1:A:165:PHE:O	1.97	0.63
2:C:250:LEU:HD21	3:D:13:VAL:HG13	1.80	0.63
1:A:253:GLU:O	1:A:257:GLN:HG3	1.98	0.63
2:E:219:ILE:HD11	2:E:237:VAL:HG11	1.81	0.63
2:C:188:ALA:HB2	2:C:244:ASP:HB3	1.80	0.63
1:A:247:LEU:HG	1:B:64:ASP:HB3	1.81	0.63
1:B:272:ASN:ND2	1:B:273:GLN:HG3	2.14	0.63
2:E:150:VAL:HG13	2:E:151:TYR:H	1.64	0.63
2:E:98:LEU:HD13	2:E:119:MET:HB3	1.80	0.63
1:A:71:GLY:H	1:A:75:ARG:NH1	1.97	0.62
2:E:90:VAL:HG23	2:E:126:PHE:HB2	1.80	0.62
2:C:90:VAL:HG23	2:C:126:PHE:HB2	1.82	0.62
1:B:244:SER:O	1:B:245:GLU:HG3	1.99	0.62
1:A:51:PHE:CD1	1:A:162:THR:HB	2.35	0.62
1:A:26:LYS:HG2	1:A:27:GLY:N	2.14	0.61
2:C:183:GLU:HG3	2:C:184:ASP:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:SER:O	1:A:245:GLU:HG3	2.01	0.61
1:B:314:MET:HE3	1:B:330:PHE:CZ	2.36	0.61
2:E:150:VAL:HG23	2:E:171:LEU:HD21	1.83	0.61
1:B:90:PRO:HA	1:B:140:LEU:CD1	2.31	0.60
1:A:41:GLN:HE22	1:A:335:ASN:ND2	1.95	0.60
1:A:272:ASN:ND2	1:A:273:GLN:HG3	2.17	0.60
2:C:154:GLU:HG3	2:C:168:TYR:CE1	2.36	0.60
1:A:247:LEU:HD22	4:B:401:ATP:H5'1	1.84	0.60
2:C:285:GLY:HA2	2:C:289:PHE:CD2	2.37	0.60
1:B:51:PHE:CD1	1:B:162:THR:HB	2.37	0.60
1:B:253:GLU:O	1:B:257:GLN:HG3	2.02	0.59
1:A:43:ALA:HB3	1:A:80:MET:HE3	1.84	0.59
1:A:21:ILE:HD12	1:A:162:THR:HG21	1.84	0.59
1:A:38:ILE:O	1:A:42:MET:HG3	2.02	0.59
1:A:53:LEU:HB3	1:A:85:CYS:SG	2.42	0.59
1:A:90:PRO:HA	1:A:140:LEU:CD1	2.33	0.59
2:C:150:VAL:HG23	2:C:171:LEU:HD21	1.84	0.59
1:B:69:LYS:HE2	2:C:74:ASP:OD2	2.03	0.59
2:E:99:VAL:HG13	2:E:139:THR:HG21	1.84	0.59
2:C:105:LEU:HD11	2:C:115:VAL:HG11	1.85	0.59
1:B:71:GLY:N	1:B:75:ARG:NH1	2.51	0.59
2:E:28:ASP:HB3	2:E:31:GLU:HB2	1.84	0.59
2:E:150:VAL:HG13	2:E:151:TYR:N	2.17	0.59
2:C:94:SER:HB3	2:C:122:TRP:CH2	2.38	0.59
2:E:34:GLN:NE2	2:E:34:GLN:HA	2.17	0.58
2:C:150:VAL:HG13	2:C:151:TYR:H	1.66	0.58
1:B:253:GLU:HG2	2:E:38:THR:HG22	1.86	0.58
2:C:20:PHE:HB2	2:C:32:ALA:HA	1.85	0.58
2:E:191:PHE:CZ	2:E:211:LYS:HG3	2.38	0.58
1:A:351:GLU:HG2	1:A:352:ASP:H	1.68	0.58
3:D:49:LYS:HD2	3:D:49:LYS:N	2.19	0.58
1:A:146:MET:SD	1:A:223:VAL:HG22	2.44	0.58
2:E:24:ILE:C	2:E:26:ALA:H	2.12	0.58
1:A:54:ILE:HD11	1:A:88:ILE:HD11	1.84	0.58
1:A:314:MET:HE3	1:A:330:PHE:CZ	2.38	0.58
1:A:305:LEU:CD1	2:C:42:ARG:HH22	2.17	0.58
1:A:230:PHE:HD1	1:A:236:THR:HG21	1.69	0.58
2:C:150:VAL:HG13	2:C:151:TYR:N	2.17	0.58
1:B:351:GLU:HG2	1:B:352:ASP:H	1.69	0.57
2:E:14:ALA:O	2:E:17:LEU:HD23	2.03	0.57
2:E:95:VAL:O	2:E:99:VAL:HG23	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:116:ILE:HG12	2:C:144:LEU:HD21	1.86	0.57
1:A:142:PHE:HB2	1:A:179:LEU:HD23	1.86	0.57
1:B:233:PRO:HA	1:B:265:ASP:HB2	1.87	0.57
2:C:191:PHE:CZ	2:C:211:LYS:HG3	2.39	0.57
1:A:51:PHE:CE1	1:A:162:THR:HB	2.40	0.57
2:E:99:VAL:HA	2:E:102:ILE:HD12	1.87	0.57
1:A:170:THR:HG22	1:A:255:LEU:HD22	1.87	0.57
1:A:317:CYS:SG	1:A:321:ILE:HD11	2.44	0.57
1:B:183:LEU:O	1:B:187:LEU:HB2	2.05	0.57
2:E:285:GLY:HA2	2:E:289:PHE:CD2	2.38	0.57
1:B:40:ILE:HA	1:B:80:MET:CE	2.35	0.57
1:B:51:PHE:CE1	1:B:162:THR:HB	2.40	0.57
2:C:16:THR:HA	2:C:19:ARG:HH11	1.70	0.56
2:C:95:VAL:O	2:C:99:VAL:HG23	2.05	0.56
1:A:29:VAL:HG23	1:A:30:GLY:H	1.69	0.56
3:F:49:LYS:HD2	3:F:49:LYS:N	2.20	0.56
1:A:54:ILE:HD11	1:A:88:ILE:CD1	2.34	0.56
1:B:317:CYS:SG	1:B:321:ILE:HD11	2.45	0.56
2:C:117:THR:HG22	2:C:121:ASN:ND2	2.21	0.56
4:A:401:ATP:O3'	1:B:247:LEU:HD13	2.05	0.56
2:C:90:VAL:HG21	2:C:123:SER:HA	1.87	0.56
1:B:38:ILE:O	1:B:42:MET:HG3	2.05	0.56
2:C:76:ILE:HG12	2:C:101:LEU:HD13	1.87	0.56
2:C:98:LEU:O	2:C:102:ILE:HG13	2.06	0.56
2:C:99:VAL:HA	2:C:102:ILE:HD12	1.88	0.56
3:D:24:GLU:CD	3:D:24:GLU:H	2.14	0.56
1:B:351:GLU:HG2	1:B:352:ASP:N	2.21	0.56
1:A:351:GLU:HG2	1:A:352:ASP:N	2.20	0.56
1:B:40:ILE:HA	1:B:80:MET:HE2	1.88	0.56
1:A:129:LEU:HD11	1:B:186:LEU:HG	1.88	0.55
1:A:187:LEU:O	1:A:190:PHE:HB2	2.06	0.55
1:B:41:GLN:HE22	1:B:335:ASN:ND2	1.99	0.55
2:E:20:PHE:HB3	2:E:35:THR:HG21	1.88	0.55
1:B:26:LYS:HG2	1:B:27:GLY:N	2.20	0.55
1:A:19:LYS:O	1:A:162:THR:HA	2.06	0.55
1:A:183:LEU:O	1:A:187:LEU:HB2	2.06	0.55
1:B:31:LYS:HZ2	1:B:169:PRO:HA	1.71	0.55
2:C:102:ILE:O	2:C:143:LYS:HD3	2.07	0.55
2:E:102:ILE:O	2:E:143:LYS:HD3	2.06	0.55
2:E:165:MET:HE1	2:E:209:GLU:CD	2.31	0.55
1:B:314:MET:HE3	1:B:330:PHE:CE2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:HIS:O	1:B:152:GLN:HG3	2.07	0.55
1:B:41:GLN:NE2	1:B:335:ASN:HD22	2.02	0.55
2:E:33:HIS:CE1	2:E:37:ARG:HD2	2.42	0.55
2:E:266:LEU:HA	3:F:12:PHE:HZ	1.71	0.55
1:A:246:PHE:HE1	1:B:322:ARG:HE	1.54	0.55
2:E:90:VAL:HG21	2:E:123:SER:HA	1.89	0.55
1:A:186:LEU:HG	1:B:129:LEU:HD11	1.89	0.54
1:A:233:PRO:HA	1:A:265:ASP:HB2	1.89	0.54
1:B:21:ILE:HD12	1:B:162:THR:HG21	1.89	0.54
1:A:219:LEU:O	1:A:223:VAL:HG23	2.08	0.54
1:B:19:LYS:O	1:B:162:THR:HA	2.06	0.54
3:F:24:GLU:CD	3:F:24:GLU:H	2.15	0.54
2:C:165:MET:HE1	2:C:209:GLU:CD	2.32	0.54
2:E:155:ARG:HH21	3:F:41:LEU:HD12	1.71	0.54
2:C:175:TRP:CZ3	3:D:48:LEU:HD12	2.42	0.54
1:A:40:ILE:HA	1:A:80:MET:HE2	1.88	0.54
1:A:24:GLY:O	1:A:240:CYS:HA	2.07	0.54
1:B:237:THR:HA	1:B:265:ASP:HB3	1.89	0.54
1:B:187:LEU:O	1:B:190:PHE:HB2	2.09	0.54
1:A:246:PHE:HE1	1:B:322:ARG:NE	2.06	0.53
1:A:322:ARG:HE	1:B:246:PHE:HE1	1.55	0.53
1:A:188:GLU:O	1:A:190:PHE:N	2.42	0.53
2:E:105:LEU:HD11	2:E:115:VAL:HG11	1.90	0.53
1:A:20:TRP:O	1:A:236:THR:HA	2.09	0.53
1:B:20:TRP:O	1:B:236:THR:HA	2.09	0.53
1:B:142:PHE:HB2	1:B:179:LEU:HD23	1.91	0.53
2:E:24:ILE:HD11	2:E:32:ALA:HB1	1.89	0.53
1:A:52:LEU:HB2	1:A:160:PHE:CG	2.43	0.53
2:E:34:GLN:HE22	2:E:37:ARG:HD3	1.74	0.53
1:A:40:ILE:O	1:A:44:LEU:HG	2.09	0.53
1:A:322:ARG:NE	1:B:246:PHE:HE1	2.06	0.53
2:E:61:LEU:HD21	2:E:100:ARG:NH2	2.24	0.53
2:C:99:VAL:HG13	2:C:139:THR:HG21	1.90	0.53
1:A:322:ARG:NE	1:B:246:PHE:CE1	2.77	0.52
1:B:40:ILE:O	1:B:44:LEU:HG	2.09	0.52
2:E:187:VAL:HG12	2:E:245:LEU:HD11	1.91	0.52
2:E:94:SER:HB3	2:E:122:TRP:CH2	2.44	0.52
1:B:43:ALA:HB3	1:B:80:MET:HE3	1.91	0.52
3:D:49:LYS:H	3:D:49:LYS:CD	2.18	0.52
1:A:322:ARG:HD2	1:B:247:LEU:CD1	2.36	0.52
1:B:25:GLY:O	1:B:169:PRO:HA	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:CG	1:B:273:GLN:N	2.66	0.52
2:E:20:PHE:HA	2:E:23:LYS:HG3	1.90	0.52
1:A:148:HIS:O	1:A:152:GLN:HG3	2.09	0.52
1:B:174:LEU:O	1:B:178:GLN:HG3	2.10	0.52
1:B:247:LEU:H	1:B:247:LEU:HD12	1.75	0.52
1:A:29:VAL:HG23	1:A:30:GLY:N	2.24	0.52
1:A:41:GLN:NE2	1:A:335:ASN:ND2	2.57	0.52
1:A:60:HIS:CG	1:A:87:GLU:HB3	2.44	0.52
1:B:52:LEU:HB2	1:B:160:PHE:CG	2.44	0.52
1:A:129:LEU:CD2	1:B:186:LEU:HD21	2.39	0.52
2:C:61:LEU:HD21	2:C:100:ARG:NH2	2.25	0.52
1:A:237:THR:HA	1:A:265:ASP:HB3	1.92	0.51
2:C:24:ILE:HD11	2:C:63:PHE:CE1	2.45	0.51
1:A:71:GLY:N	1:A:75:ARG:NH1	2.58	0.51
1:B:60:HIS:CG	1:B:87:GLU:HB3	2.45	0.51
2:C:155:ARG:O	2:C:158:MET:HB2	2.10	0.51
3:F:49:LYS:H	3:F:49:LYS:CD	2.18	0.51
1:A:74:ALA:HB2	1:A:86:MET:HE3	1.93	0.51
1:B:24:GLY:O	1:B:240:CYS:HA	2.11	0.51
2:C:53:ILE:HG23	2:C:79:LEU:HD11	1.93	0.51
1:A:62:LEU:HB2	1:A:87:GLU:OE2	2.11	0.51
1:A:57:VAL:CG2	1:A:167:THR:C	2.84	0.51
2:E:243:SER:HB2	2:E:273:PHE:HZ	1.76	0.51
2:E:262:TYR:HB3	3:F:16:PHE:CZ	2.45	0.51
2:C:150:VAL:CG2	2:C:171:LEU:HD21	2.40	0.51
1:A:174:LEU:O	1:A:178:GLN:HG3	2.11	0.51
1:A:246:PHE:CE1	1:B:322:ARG:NE	2.79	0.51
1:B:336:LYS:O	1:B:336:LYS:HG3	2.11	0.51
1:B:30:GLY:HA2	4:B:401:ATP:O1A	2.11	0.51
1:A:31:LYS:HZ2	1:A:169:PRO:HA	1.76	0.51
2:E:23:LYS:HB3	2:E:28:ASP:HB2	1.93	0.51
1:A:28:GLY:CA	1:B:28:GLY:HA3	2.30	0.50
1:B:210:VAL:C	1:B:212:ILE:H	2.19	0.50
2:E:150:VAL:CG2	2:E:171:LEU:HD21	2.40	0.50
1:B:212:ILE:HD12	1:B:212:ILE:C	2.37	0.50
2:E:151:TYR:OH	3:F:47:THR:HG23	2.11	0.50
2:C:106:ASP:HB3	2:C:109:GLU:HG2	1.93	0.50
1:A:43:ALA:HB3	1:A:80:MET:CE	2.41	0.50
1:B:142:PHE:CE1	1:B:180:PRO:HG3	2.46	0.50
2:E:231:LYS:HG2	3:F:18:THR:OG1	2.12	0.50
1:A:311:VAL:CG2	1:A:313:LYS:HE2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:ILE:CD1	2:E:32:ALA:HB1	2.42	0.50
2:E:36:LEU:C	2:E:36:LEU:HD23	2.37	0.50
2:E:227:GLU:O	2:E:227:GLU:HG3	2.12	0.50
1:B:276:PHE:O	1:B:277:ALA:C	2.55	0.50
2:E:243:SER:HA	2:E:246:ASN:HD22	1.75	0.50
2:C:155:ARG:HH21	3:D:41:LEU:CD1	2.23	0.50
2:E:183:GLU:HG3	2:E:184:ASP:H	1.74	0.50
1:A:168:ALA:HB1	1:A:169:PRO:HD2	1.94	0.49
1:A:126:LEU:N	1:A:126:LEU:HD22	2.26	0.49
2:C:34:GLN:HA	2:C:34:GLN:NE2	2.26	0.49
1:A:40:ILE:HA	1:A:80:MET:CE	2.42	0.49
2:E:187:VAL:HG11	2:E:245:LEU:HD21	1.93	0.49
1:A:168:ALA:HB1	1:A:169:PRO:CD	2.43	0.49
1:B:31:LYS:HE3	1:B:168:ALA:C	2.38	0.49
1:B:168:ALA:HB1	1:B:169:PRO:HD2	1.95	0.49
1:A:272:ASN:CG	1:A:273:GLN:N	2.71	0.49
1:A:336:LYS:O	1:A:336:LYS:HG3	2.13	0.49
1:B:188:GLU:O	1:B:190:PHE:N	2.43	0.49
2:E:243:SER:HA	2:E:246:ASN:ND2	2.26	0.49
1:A:31:LYS:HE3	1:A:168:ALA:C	2.37	0.49
1:B:71:GLY:H	1:B:75:ARG:HH11	1.60	0.49
2:E:23:LYS:HD2	2:E:31:GLU:CG	2.41	0.49
2:E:33:HIS:O	2:E:37:ARG:HG3	2.12	0.49
2:E:76:ILE:HG12	2:E:101:LEU:HD13	1.94	0.49
2:E:255:CYS:SG	2:E:284:LEU:HD22	2.51	0.49
2:C:33:HIS:CD2	2:C:71:SER:HB3	2.48	0.49
1:A:86:MET:O	1:A:87:GLU:HB2	2.12	0.49
2:C:255:CYS:SG	2:C:284:LEU:HD22	2.53	0.49
2:C:24:ILE:HG12	2:C:32:ALA:HB2	1.94	0.49
1:A:60:HIS:HB3	1:A:87:GLU:OE1	2.12	0.48
1:B:29:VAL:HG23	1:B:30:GLY:H	1.77	0.48
2:E:33:HIS:CD2	2:E:71:SER:HB3	2.48	0.48
2:E:115:VAL:O	2:E:119:MET:HG2	2.13	0.48
1:A:314:MET:HE3	1:A:330:PHE:CE2	2.49	0.48
1:A:314:MET:HE2	1:A:334:LEU:HG	1.95	0.48
2:E:117:THR:HG22	2:E:121:ASN:ND2	2.28	0.48
1:A:314:MET:HE1	1:A:333:PHE:HB2	1.94	0.48
1:B:50:GLN:NE2	1:B:82:ASN:HA	2.29	0.48
1:B:168:ALA:HB1	1:B:169:PRO:CD	2.43	0.48
2:C:230:ASP:OD1	2:C:235:GLU:HB2	2.14	0.48
2:E:53:ILE:HG23	2:E:79:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:LEU:HG	2:E:116:ILE:HD13	1.95	0.48
2:E:189:GLU:HB3	3:F:48:LEU:CD2	2.44	0.48
1:B:52:LEU:HA	1:B:84:SER:O	2.13	0.48
2:E:23:LYS:CD	2:E:31:GLU:HG2	2.42	0.48
2:E:61:LEU:HD21	2:E:100:ARG:NE	2.28	0.48
2:C:243:SER:HB2	2:C:273:PHE:HZ	1.78	0.48
1:A:170:THR:HG21	1:A:251:GLU:HG2	1.96	0.48
1:A:276:PHE:O	1:A:277:ALA:C	2.55	0.48
1:B:126:LEU:N	1:B:126:LEU:HD22	2.29	0.48
2:E:183:GLU:H	2:E:186:THR:HB	1.78	0.48
1:B:29:VAL:HB	1:B:241:VAL:HG12	1.96	0.48
1:B:311:VAL:CG2	1:B:313:LYS:HE2	2.44	0.48
2:C:243:SER:HA	2:C:246:ASN:ND2	2.28	0.48
1:A:58:PRO:HB2	1:B:171:GLY:HA3	1.95	0.48
2:C:227:GLU:HG3	2:C:227:GLU:O	2.13	0.48
1:A:25:GLY:O	1:A:169:PRO:HA	2.14	0.48
1:B:53:LEU:HB3	1:B:85:CYS:SG	2.53	0.48
1:B:86:MET:O	1:B:87:GLU:HB2	2.14	0.47
2:E:175:TRP:CZ3	3:F:48:LEU:HD12	2.49	0.47
2:E:64:LEU:HD11	2:E:76:ILE:HD11	1.95	0.47
2:C:203:ASN:CG	3:D:32:THR:HG23	2.39	0.47
1:B:7:PRO:HA	1:B:311:VAL:O	2.14	0.47
3:F:28:PRO:HG2	3:F:31:TYR:HB2	1.97	0.47
2:C:91:ASP:H	2:C:94:SER:HB2	1.79	0.47
1:A:223:VAL:O	1:A:226:ILE:HB	2.15	0.47
1:A:247:LEU:HD12	1:A:247:LEU:N	2.28	0.47
2:C:183:GLU:H	2:C:186:THR:HB	1.80	0.47
2:E:259:ASP:HB3	2:E:262:TYR:CD2	2.50	0.47
2:C:61:LEU:HD21	2:C:100:ARG:NE	2.29	0.47
1:A:315:PRO:HB2	1:A:347:ILE:HD11	1.96	0.47
1:B:29:VAL:HG23	1:B:30:GLY:N	2.30	0.47
1:B:268:SER:C	1:B:269:ILE:HD12	2.39	0.47
2:E:24:ILE:CG1	2:E:32:ALA:CB	2.89	0.47
2:E:228:LYS:HD3	2:E:235:GLU:CD	2.40	0.47
2:C:39:ILE:O	2:C:42:ARG:HB3	2.14	0.47
2:C:263:PHE:HB2	2:C:289:PHE:CZ	2.49	0.47
1:A:50:GLN:HA	1:A:82:ASN:HB2	1.96	0.47
1:A:62:LEU:HB2	1:A:87:GLU:CD	2.39	0.47
1:B:53:LEU:HD12	1:B:164:ILE:O	2.14	0.47
2:C:208:HIS:CE1	3:D:29:LYS:HE3	2.49	0.47
1:B:50:GLN:HA	1:B:82:ASN:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:224:PRO:O	2:C:226:TYR:HD1	1.97	0.47
1:B:315:PRO:HB2	1:B:347:ILE:HD11	1.96	0.46
2:E:98:LEU:O	2:E:102:ILE:HG13	2.15	0.46
2:C:36:LEU:HD23	2:C:36:LEU:C	2.40	0.46
2:C:243:SER:HA	2:C:246:ASN:HD22	1.79	0.46
1:A:299:LEU:HD11	1:A:313:LYS:CD	2.46	0.46
2:C:112:LEU:HG	2:C:116:ILE:HD13	1.97	0.46
1:A:52:LEU:HA	1:A:84:SER:O	2.15	0.46
1:B:9:LEU:HG	1:B:312:VAL:HG21	1.97	0.46
1:B:57:VAL:CG2	1:B:167:THR:C	2.88	0.46
1:A:20:TRP:HB2	1:A:236:THR:HG22	1.98	0.46
1:B:50:GLN:HE22	1:B:82:ASN:HA	1.81	0.46
1:B:73:ASP:O	1:B:75:ARG:HG3	2.15	0.46
1:B:314:MET:HE1	1:B:333:PHE:HB2	1.97	0.46
1:A:142:PHE:CE1	1:A:180:PRO:HG3	2.50	0.46
1:B:62:LEU:HB2	1:B:87:GLU:CD	2.41	0.46
2:E:192:SER:HB2	2:E:196:PHE:CE2	2.51	0.46
2:C:69:GLY:HA3	2:C:109:GLU:OE2	2.16	0.46
1:B:142:PHE:HE1	1:B:180:PRO:HG3	1.80	0.46
2:C:115:VAL:HG12	2:C:119:MET:HE3	1.98	0.46
2:C:228:LYS:HD3	2:C:235:GLU:CD	2.40	0.46
2:C:285:GLY:O	2:C:289:PHE:HB2	2.16	0.46
1:A:40:ILE:HG21	1:A:328:THR:OG1	2.16	0.46
1:B:40:ILE:HD13	1:B:324:LEU:HD12	1.98	0.46
2:E:182:ILE:HG22	2:E:183:GLU:N	2.31	0.46
2:E:191:PHE:CE1	2:E:211:LYS:HG3	2.51	0.46
2:C:73:THR:HG23	2:C:115:VAL:CG2	2.46	0.46
2:C:115:VAL:CG1	2:C:119:MET:HE3	2.46	0.46
1:B:40:ILE:HG21	1:B:328:THR:OG1	2.16	0.45
2:E:20:PHE:CD1	2:E:21:GLU:N	2.84	0.45
2:E:230:ASP:OD1	2:E:235:GLU:HB2	2.17	0.45
1:B:20:TRP:HB2	1:B:236:THR:HG22	1.97	0.45
2:E:243:SER:HB2	2:E:273:PHE:CZ	2.52	0.45
1:A:9:LEU:HG	1:A:312:VAL:HG21	1.99	0.45
1:B:5:VAL:HG23	1:B:5:VAL:O	2.16	0.45
2:E:69:GLY:HA3	2:E:109:GLU:OE2	2.16	0.45
2:E:73:THR:HG23	2:E:115:VAL:CG2	2.46	0.45
2:C:16:THR:HA	2:C:19:ARG:HD3	1.98	0.45
2:C:264:LEU:HG	2:C:268:ASN:HD21	1.80	0.45
1:A:50:GLN:NE2	1:A:82:ASN:HA	2.31	0.45
1:A:179:LEU:O	1:A:183:LEU: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:337:GLU:N	1:A:337:GLU:OE1	2.49	0.45
2:C:182:ILE:HG22	2:C:183:GLU:N	2.31	0.45
1:B:52:LEU:HB2	1:B:160:PHE:CD1	2.52	0.45
1:B:54:ILE:HD11	1:B:88:ILE:HD11	1.99	0.45
2:E:17:LEU:HD13	2:E:20:PHE:HE2	1.82	0.45
1:A:186:LEU:HD21	1:B:129:LEU:CD2	2.44	0.45
1:B:170:THR:HG21	1:B:251:GLU:HG2	1.99	0.45
1:B:275:LEU:HD12	1:B:292:TRP:N	2.31	0.45
1:B:314:MET:HE2	1:B:334:LEU:HG	1.97	0.45
3:F:40:ASN:ND2	3:F:42:GLY:H	2.14	0.45
2:C:191:PHE:CE1	2:C:211:LYS:HG3	2.51	0.45
2:C:208:HIS:NE2	3:D:29:LYS:HG2	2.31	0.45
2:E:189:GLU:O	2:E:193:ARG:HG3	2.17	0.45
2:C:19:ARG:O	2:C:23:LYS:HG3	2.16	0.45
1:A:253:GLU:HG2	2:C:38:THR:HG22	1.98	0.45
1:A:260:ILE:HD12	2:C:45:ARG:NH2	2.32	0.45
1:B:74:ALA:HB2	1:B:86:MET:HE3	1.98	0.45
2:E:224:PRO:O	2:E:226:TYR:HD1	2.00	0.45
2:C:23:LYS:O	2:C:28:ASP:N	2.45	0.45
2:C:219:ILE:HA	2:C:224:PRO:HD2	1.99	0.45
1:A:73:ASP:O	1:A:75:ARG:HG3	2.17	0.45
1:B:212:ILE:HD12	1:B:213:SER:N	2.32	0.45
2:E:219:ILE:HA	2:E:224:PRO:HD2	1.99	0.45
2:C:202:SER:HB2	3:D:33:LYS:HD2	1.99	0.45
1:A:5:VAL:HG23	1:A:5:VAL:O	2.17	0.44
1:B:41:GLN:NE2	1:B:335:ASN:ND2	2.63	0.44
1:B:57:VAL:CG2	1:B:166:ASP:O	2.62	0.44
1:B:90:PRO:HA	1:B:140:LEU:HD12	1.98	0.44
2:E:183:GLU:H	2:E:186:THR:CB	2.30	0.44
2:E:183:GLU:O	2:E:186:THR:HB	2.18	0.44
1:A:52:LEU:HD12	1:A:84:SER:O	2.17	0.44
2:C:187:VAL:HG11	2:C:245:LEU:HD21	2.00	0.44
1:B:43:ALA:HB3	1:B:80:MET:CE	2.47	0.44
3:D:39:THR:HG23	3:D:40:ASN:N	2.32	0.44
1:A:23:VAL:HA	1:A:239:VAL:O	2.18	0.44
2:C:187:VAL:HG12	2:C:245:LEU:HD11	2.00	0.44
1:A:188:GLU:OE2	1:A:189:LYS:HD3	2.18	0.44
2:C:133:ASP:HA	2:C:134:PRO:HD3	1.90	0.44
1:A:326:ASN:CB	1:A:350:LEU:HD22	2.48	0.44
1:B:67:GLY:O	2:C:30:TYR:HB2	2.18	0.44
1:B:256:ILE:HA	1:B:259:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:CYS:SG	1:B:350:LEU:HD12	2.57	0.44
3:F:39:THR:HG23	3:F:40:ASN:N	2.32	0.44
1:A:49:LYS:HE2	1:A:161:ASP:CG	2.43	0.44
1:A:50:GLN:HE22	1:A:82:ASN:HA	1.82	0.44
1:A:53:LEU:HD12	1:A:164:ILE:O	2.18	0.44
1:A:277:ALA:HB3	1:A:292:TRP:CD1	2.53	0.44
2:C:90:VAL:CG2	2:C:123:SER:HA	2.47	0.44
1:A:31:LYS:HA	1:A:241:VAL:HG21	1.99	0.44
1:A:329:LYS:HD2	1:A:350:LEU:CD2	2.48	0.44
1:B:31:LYS:HA	1:B:241:VAL:HG21	2.00	0.44
1:B:231:THR:O	1:B:233:PRO:HD3	2.18	0.44
2:E:116:ILE:HG12	2:E:144:LEU:HD21	1.99	0.44
2:C:24:ILE:HD13	2:C:29:TYR:HA	2.00	0.44
3:D:19:LEU:HA	3:D:22:LEU:HD21	2.00	0.44
1:B:32:THR:CG2	1:B:65:ALA:HB2	2.48	0.43
2:E:39:ILE:O	2:E:42:ARG:HB3	2.18	0.43
1:B:72:LYS:HB2	1:B:72:LYS:NZ	2.33	0.43
2:E:17:LEU:HA	2:E:20:PHE:CE2	2.52	0.43
2:E:87:GLU:HA	2:E:126:PHE:CZ	2.53	0.43
2:E:91:ASP:H	2:E:94:SER:HB2	1.81	0.43
2:E:106:ASP:HB3	2:E:109:GLU:HG2	1.99	0.43
2:E:263:PHE:HB2	2:E:289:PHE:CZ	2.53	0.43
2:C:266:LEU:HA	3:D:12:PHE:HZ	1.82	0.43
2:C:283:PHE:HE1	3:D:40:ASN:HD21	1.63	0.43
1:A:212:ILE:C	1:A:212:ILE:HD12	2.44	0.43
1:B:266:VAL:HG13	1:B:266:VAL:O	2.19	0.43
3:D:28:PRO:HG2	3:D:31:TYR:HB2	2.00	0.43
1:A:275:LEU:HD12	1:A:292:TRP:N	2.33	0.43
1:B:52:LEU:HD12	1:B:84:SER:O	2.19	0.43
1:B:54:ILE:HD11	1:B:88:ILE:CD1	2.48	0.43
1:B:256:ILE:HG23	1:B:266:VAL:HG21	2.01	0.43
2:E:202:SER:HB2	3:F:33:LYS:HD2	2.00	0.43
2:E:17:LEU:HA	2:E:20:PHE:CD2	2.54	0.43
2:E:24:ILE:C	2:E:26:ALA:N	2.76	0.43
2:C:176:LEU:HD13	2:C:190:PHE:CD2	2.53	0.43
3:D:24:GLU:CD	3:D:24:GLU:N	2.76	0.43
1:B:62:LEU:HB2	1:B:87:GLU:OE2	2.18	0.43
2:E:245:LEU:O	2:E:249:GLN:HG3	2.18	0.43
2:C:259:ASP:HB3	2:C:262:TYR:CD2	2.53	0.43
1:B:96:ASP:OD1	2:C:114:ASP:OD1	2.37	0.43
1:B:228:GLN:HA	1:B:231:THR:CG2	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:LEU:HA	2:E:190:PHE:CZ	2.54	0.43
1:A:71:GLY:H	1:A:75:ARG:HH11	1.67	0.43
1:B:23:VAL:HA	1:B:239:VAL:O	2.18	0.43
2:E:30:TYR:CD2	2:E:31:GLU:N	2.86	0.43
2:E:195:VAL:HG12	2:E:199:LEU:HD12	2.01	0.43
2:C:41:ASN:HA	2:C:78:TYR:OH	2.18	0.43
2:C:64:LEU:HD11	2:C:76:ILE:HD11	2.01	0.43
2:C:218:PHE:CE2	2:C:224:PRO:HG3	2.53	0.43
1:A:174:LEU:HD22	1:A:262:TYR:CE2	2.54	0.43
1:A:220:LYS:HD2	1:A:220:LYS:O	2.19	0.43
2:E:107:PRO:CG	2:E:146:GLU:HB3	2.49	0.43
2:C:134:PRO:O	2:C:137:HIS:HB2	2.19	0.43
1:A:275:LEU:HD11	1:A:291:ARG:HB2	2.01	0.42
1:B:275:LEU:HD11	1:B:291:ARG:HB2	2.01	0.42
2:E:65:LYS:HG2	2:E:104:GLU:OE1	2.18	0.42
2:E:134:PRO:HG3	3:F:35:LEU:HD23	2.00	0.42
1:A:28:GLY:HA3	1:B:28:GLY:CA	2.31	0.42
1:A:52:LEU:HB2	1:A:160:PHE:CD1	2.53	0.42
1:B:210:VAL:C	1:B:212:ILE:N	2.77	0.42
1:B:267:ASN:O	1:B:310:HIS:HB2	2.19	0.42
2:E:24:ILE:CG1	2:E:32:ALA:HB1	2.48	0.42
2:C:73:THR:HG21	2:C:111:ASN:HD21	1.81	0.42
1:A:142:PHE:HE1	1:A:180:PRO:HG3	1.84	0.42
1:A:274:LEU:HD13	1:A:276:PHE:CZ	2.54	0.42
1:B:299:LEU:HD11	1:B:313:LYS:HD2	2.01	0.42
1:B:329:LYS:HD2	1:B:350:LEU:CD2	2.49	0.42
1:A:257:GLN:NE2	2:C:41:ASN:HB3	2.35	0.42
1:B:26:LYS:HD2	1:B:27:GLY:O	2.19	0.42
1:B:154:GLN:HB3	1:B:156:GLU:HG3	2.00	0.42
2:C:23:LYS:HD3	2:C:31:GLU:HG2	2.00	0.42
2:C:94:SER:HB3	2:C:122:TRP:HH2	1.84	0.42
2:C:189:GLU:O	2:C:193:ARG:HG3	2.18	0.42
2:E:23:LYS:HD2	2:E:31:GLU:HB3	2.01	0.42
2:E:176:LEU:HD13	2:E:190:PHE:CD2	2.54	0.42
3:F:24:GLU:CD	3:F:24:GLU:N	2.77	0.42
1:A:26:LYS:CG	1:A:27:GLY:N	2.82	0.42
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.88	0.42
1:B:326:ASN:CG	1:B:350:LEU:HD22	2.44	0.42
1:A:268:SER:C	1:A:269:ILE:HD12	2.44	0.42
1:A:299:LEU:HD11	1:A:313:LYS:HD2	2.02	0.42
2:E:130:LYS:O	2:E:130:LYS:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:O	1:B:100:MET:HB2	2.20	0.42
1:B:149:ILE:O	1:B:153:GLU:HG2	2.20	0.42
1:B:159:THR:HG23	1:B:160:PHE:CD2	2.54	0.42
1:B:238:PHE:N	1:B:265:ASP:O	2.52	0.42
2:E:41:ASN:HA	2:E:78:TYR:OH	2.20	0.42
2:C:115:VAL:O	2:C:119:MET:HG2	2.18	0.42
1:A:94:LEU:HD11	1:A:130:THR:HG22	2.01	0.42
1:A:275:LEU:HD11	1:A:291:ARG:CB	2.50	0.42
1:B:326:ASN:CB	1:B:350:LEU:HD22	2.49	0.42
2:C:192:SER:HB2	2:C:196:PHE:CE2	2.54	0.42
1:A:28:GLY:N	1:B:27:GLY:C	2.77	0.42
1:A:179:LEU:N	1:A:180:PRO:CD	2.83	0.42
1:A:247:LEU:CD1	1:B:322:ARG:HD2	2.38	0.42
1:B:174:LEU:HD22	1:B:262:TYR:CE2	2.55	0.42
2:E:90:VAL:CG2	2:E:123:SER:HA	2.48	0.42
2:C:107:PRO:CG	2:C:146:GLU:HB3	2.50	0.42
1:A:317:CYS:SG	1:A:350:LEU:HD12	2.60	0.41
1:B:62:LEU:HD12	1:B:87:GLU:HG2	2.01	0.41
1:B:228:GLN:CA	1:B:231:THR:HG22	2.49	0.41
2:E:24:ILE:HG12	2:E:32:ALA:HB1	1.95	0.41
2:C:183:GLU:H	2:C:186:THR:CB	2.32	0.41
1:A:27:GLY:C	1:A:29:VAL:H	2.28	0.41
1:A:53:LEU:CD1	1:A:164:ILE:HB	2.46	0.41
1:B:49:LYS:HE2	1:B:161:ASP:CG	2.45	0.41
2:E:102:ILE:HG21	2:E:139:THR:HG22	2.01	0.41
2:C:15:LYS:O	2:C:19:ARG:HD3	2.20	0.41
2:C:66:ALA:O	2:C:67:LYS:HB2	2.20	0.41
2:C:176:LEU:HA	2:C:190:PHE:CZ	2.55	0.41
2:C:231:LYS:HG2	3:D:18:THR:OG1	2.21	0.41
1:A:29:VAL:HB	1:A:241:VAL:HG12	2.03	0.41
1:A:93:ALA:O	1:A:97:MET:HE3	2.20	0.41
1:A:247:LEU:HD22	4:B:401:ATP:O2A	2.20	0.41
2:E:134:PRO:O	2:E:137:HIS:HB2	2.20	0.41
2:E:285:GLY:O	2:E:289:PHE:HB2	2.20	0.41
1:B:179:LEU:O	1:B:183:LEU:HB2	2.21	0.41
2:E:173:TRP:CH2	2:E:218:PHE:HA	2.56	0.41
2:C:24:ILE:HD13	2:C:24:ILE:HA	1.90	0.41
1:A:27:GLY:C	1:B:28:GLY:N	2.78	0.41
1:A:294:MET:O	1:A:297:LYS:HB3	2.21	0.41
1:B:246:PHE:CD1	1:B:247:LEU:HD12	2.56	0.41
1:B:295:GLN:O	1:B:299:LEU:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:189:GLU:OE2	3:F:49:LYS:HD3	2.20	0.41
1:A:142:PHE:CE2	1:A:183:LEU:HD23	2.55	0.41
1:A:126:LEU:HD22	1:A:126:LEU:H	1.86	0.41
2:C:119:MET:HG2	2:C:119:MET:H	1.63	0.41
2:C:189:GLU:HB3	3:D:48:LEU:CD2	2.51	0.41
1:A:52:LEU:HB2	1:A:160:PHE:CD2	2.56	0.41
1:A:64:ASP:HA	1:B:246:PHE:HZ	1.86	0.41
1:A:311:VAL:HG21	1:A:313:LYS:HE2	2.03	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.84	0.41
1:B:311:VAL:HG21	1:B:313:LYS:HE2	2.03	0.41
2:E:20:PHE:C	2:E:22:ASN:N	2.73	0.41
2:E:70:GLY:O	2:E:71:SER:C	2.64	0.41
2:E:211:LYS:HE2	2:E:211:LYS:HB3	1.93	0.41
2:C:243:SER:HB2	2:C:273:PHE:CZ	2.55	0.41
1:A:149:ILE:O	1:A:153:GLU:HG2	2.21	0.41
2:E:73:THR:HG21	2:E:111:ASN:HD21	1.82	0.41
2:E:179:VAL:HG22	3:F:50:TYR:CD1	2.56	0.41
2:E:264:LEU:HG	2:E:268:ASN:HD21	1.86	0.41
1:A:21:ILE:HG12	1:A:237:THR:HG22	2.02	0.40
1:A:230:PHE:CD1	1:A:236:THR:HG21	2.54	0.40
1:A:326:ASN:HB3	1:A:350:LEU:HD22	2.02	0.40
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.89	0.40
1:B:277:ALA:HB3	1:B:292:TRP:CD1	2.57	0.40
2:C:183:GLU:O	2:C:186:THR:HB	2.21	0.40
1:A:129:LEU:O	1:A:133:ILE:HG13	2.21	0.40
1:A:256:ILE:HG23	1:A:266:VAL:HG21	2.04	0.40
1:B:60:HIS:HB3	1:B:87:GLU:OE2	2.20	0.40
1:A:316:LEU:HD12	4:A:401:ATP:C2	2.56	0.40
4:A:401:ATP:O2G	1:B:27:GLY:HA3	2.21	0.40
1:B:230:PHE:CD1	1:B:236:THR:HG21	2.42	0.40
2:E:189:GLU:OE1	3:F:49:LYS:HD3	2.21	0.40
2:C:45:ARG:NH1	2:C:45:ARG:HG2	2.36	0.40

All (2) 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)
3:F:22:LEU:CD2	3:F:22:LEU:CD2[2_855]	2.10	0.10
3:F:22:LEU:CD1	3:F:22:LEU:CD1[2_855]	2.14	0.06

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	286/356 (80%)	250 (87%)	32 (11%)	4 (1%)	9	38
1	B	291/356 (82%)	252 (87%)	36 (12%)	3 (1%)	12	47
2	C	274/288 (95%)	257 (94%)	16 (6%)	1 (0%)	30	67
2	E	275/288 (96%)	257 (94%)	16 (6%)	2 (1%)	18	55
3	D	50/54 (93%)	46 (92%)	4 (8%)	0	100	100
3	F	50/54 (93%)	45 (90%)	5 (10%)	0	100	100
All	All	1226/1396 (88%)	1107 (90%)	109 (9%)	10 (1%)	16	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	171	GLY
1	A	189	LYS
1	B	277	ALA
2	E	70	GLY
2	C	70	GLY
1	A	277	ALA
1	B	189	LYS
2	E	25	LYS
1	A	30	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/311 (84%)	233 (89%)	29 (11%)	6	19
1	B	267/311 (86%)	239 (90%)	28 (10%)	6	21
2	C	249/258 (96%)	237 (95%)	12 (5%)	23	44
2	E	249/258 (96%)	239 (96%)	10 (4%)	28	48
3	D	48/50 (96%)	43 (90%)	5 (10%)	7	22
3	F	48/50 (96%)	43 (90%)	5 (10%)	7	22
All	All	1123/1238 (91%)	1034 (92%)	89 (8%)	11	31

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	26	LYS
1	A	36	CYS
1	A	72	LYS
1	A	76	LYS
1	A	96	ASP
1	A	126	LEU
1	A	146	MET
1	A	150	LYS
1	A	154	GLN
1	A	161	ASP
1	A	167	THR
1	A	187	LEU
1	A	188	GLU
1	A	189	LYS
1	A	213	SER
1	A	216	LEU
1	A	219	LEU
1	A	240	CYS
1	A	246	PHE
1	A	260	ILE
1	A	263	ASP
1	A	266	VAL
1	A	271	VAL
1	A	288	CYS
1	A	305	LEU
1	A	311	VAL
1	A	343	ASP
1	A	347	ILE
1	B	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	LYS
1	B	36	CYS
1	B	72	LYS
1	B	76	LYS
1	B	100	MET
1	B	126	LEU
1	B	146	MET
1	B	150	LYS
1	B	154	GLN
1	B	161	ASP
1	B	167	THR
1	B	187	LEU
1	B	188	GLU
1	B	189	LYS
1	B	211	ASP
1	B	219	LEU
1	B	240	CYS
1	B	246	PHE
1	B	260	ILE
1	B	263	ASP
1	B	266	VAL
1	B	271	VAL
1	B	288	CYS
1	B	305	LEU
1	B	311	VAL
1	B	343	ASP
1	B	347	ILE
2	E	16	THR
2	E	17	LEU
2	E	21	GLU
2	E	24	ILE
2	E	31	GLU
2	E	45	ARG
2	E	51	HIS
2	E	62	SER
2	E	244	ASP
2	E	290	ASN
3	F	3	THR
3	F	22	LEU
3	F	33	LYS
3	F	35	LEU
3	F	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	16	THR
2	C	17	LEU
2	C	18	GLN
2	C	21	GLU
2	C	24	ILE
2	C	31	GLU
2	C	45	ARG
2	C	51	HIS
2	C	62	SER
2	C	158	MET
2	C	244	ASP
2	C	290	ASN
3	D	3	THR
3	D	22	LEU
3	D	33	LYS
3	D	35	LEU
3	D	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	41	GLN
1	A	50	GLN
1	A	152	GLN
1	A	154	GLN
1	A	172	HIS
1	A	217	ASN
1	A	289	GLN
1	A	301	GLN
1	A	310	HIS
1	A	325	ASN
1	A	326	ASN
1	A	339	ASN
1	B	18	HIS
1	B	41	GLN
1	B	50	GLN
1	B	152	GLN
1	B	154	GLN
1	B	172	HIS
1	B	217	ASN
1	B	222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	289	GLN
1	B	301	GLN
1	B	310	HIS
1	B	325	ASN
1	B	326	ASN
1	B	339	ASN
2	E	33	HIS
2	E	34	GLN
2	E	41	ASN
2	E	51	HIS
2	E	121	ASN
2	E	178	GLN
2	E	232	ASN
2	E	268	ASN
2	E	269	HIS
2	E	275	GLN
3	F	40	ASN
2	C	33	HIS
2	C	34	GLN
2	C	41	ASN
2	C	51	HIS
2	C	138	ASN
2	C	232	ASN
2	C	268	ASN
2	C	269	HIS
2	C	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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
4	ATP	A	401	5	32,33,33	1.30	3 (9%)	48,52,52	2.27	16 (33%)
4	ATP	B	401	5	32,33,33	1.26	3 (9%)	48,52,52	2.24	13 (27%)

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
4	ATP	A	401	5	-	1/22/38/38	0/3/3/3
4	ATP	B	401	5	-	1/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ATP	PA-O3A	3.59	1.63	1.59
4	B	401	ATP	PA-O3A	2.84	1.62	1.59
4	B	401	ATP	PB-O3B	2.72	1.62	1.59
4	A	401	ATP	PB-O3B	2.44	1.62	1.59
4	A	401	ATP	O4'-C1'	2.09	1.46	1.42
4	B	401	ATP	O4'-C1'	2.03	1.46	1.42

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ATP	O5'-PA-O1A	-6.27	84.08	108.94
4	A	401	ATP	O5'-PA-O1A	-6.15	84.56	108.94
4	B	401	ATP	C5-C4-N3	-5.22	119.53	126.72
4	A	401	ATP	C5-C4-N3	-5.11	119.68	126.72
4	B	401	ATP	O2A-PA-O5'	-4.97	85.05	107.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ATP	O2A-PA-O5'	-4.90	85.34	107.57
4	B	401	ATP	N3-C2-N1	-4.79	121.33	128.58
4	A	401	ATP	N3-C2-N1	-4.62	121.59	128.58
4	B	401	ATP	N3-C4-N9	4.34	134.56	127.17
4	A	401	ATP	N3-C4-N9	4.24	134.38	127.17
4	B	401	ATP	C5-N7-C8	3.84	109.48	103.45
4	B	401	ATP	C2-N3-C4	3.82	121.15	111.83
4	A	401	ATP	C2-N3-C4	3.76	121.02	111.83
4	A	401	ATP	C5-N7-C8	3.73	109.32	103.45
4	A	401	ATP	O2A-PA-O3A	3.35	116.34	107.27
4	B	401	ATP	O2A-PA-O3A	3.03	115.46	107.27
4	B	401	ATP	C4-C5-N7	-2.95	107.21	110.58
4	A	401	ATP	C4-C5-N7	-2.93	107.23	110.58
4	B	401	ATP	O2A-PA-O1A	2.82	125.54	112.44
4	A	401	ATP	O3'-C3'-C4'	-2.67	103.42	111.08
4	A	401	ATP	O2A-PA-O1A	2.61	124.59	112.44
4	B	401	ATP	N9-C8-N7	-2.61	110.23	113.94
4	A	401	ATP	N9-C8-N7	-2.56	110.30	113.94
4	B	401	ATP	C3'-C2'-C1'	2.55	106.28	101.46
4	A	401	ATP	C3'-C2'-C1'	2.46	106.12	101.46
4	A	401	ATP	C2'-C1'-N9	-2.46	107.20	113.30
4	B	401	ATP	O4'-C1'-N9	2.17	112.26	108.09
4	A	401	ATP	O4'-C1'-N9	2.15	112.21	108.09
4	A	401	ATP	C2'-C3'-C4'	2.14	106.74	102.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	C5'-O5'-PA-O1A
4	B	401	ATP	C5'-O5'-PA-O1A

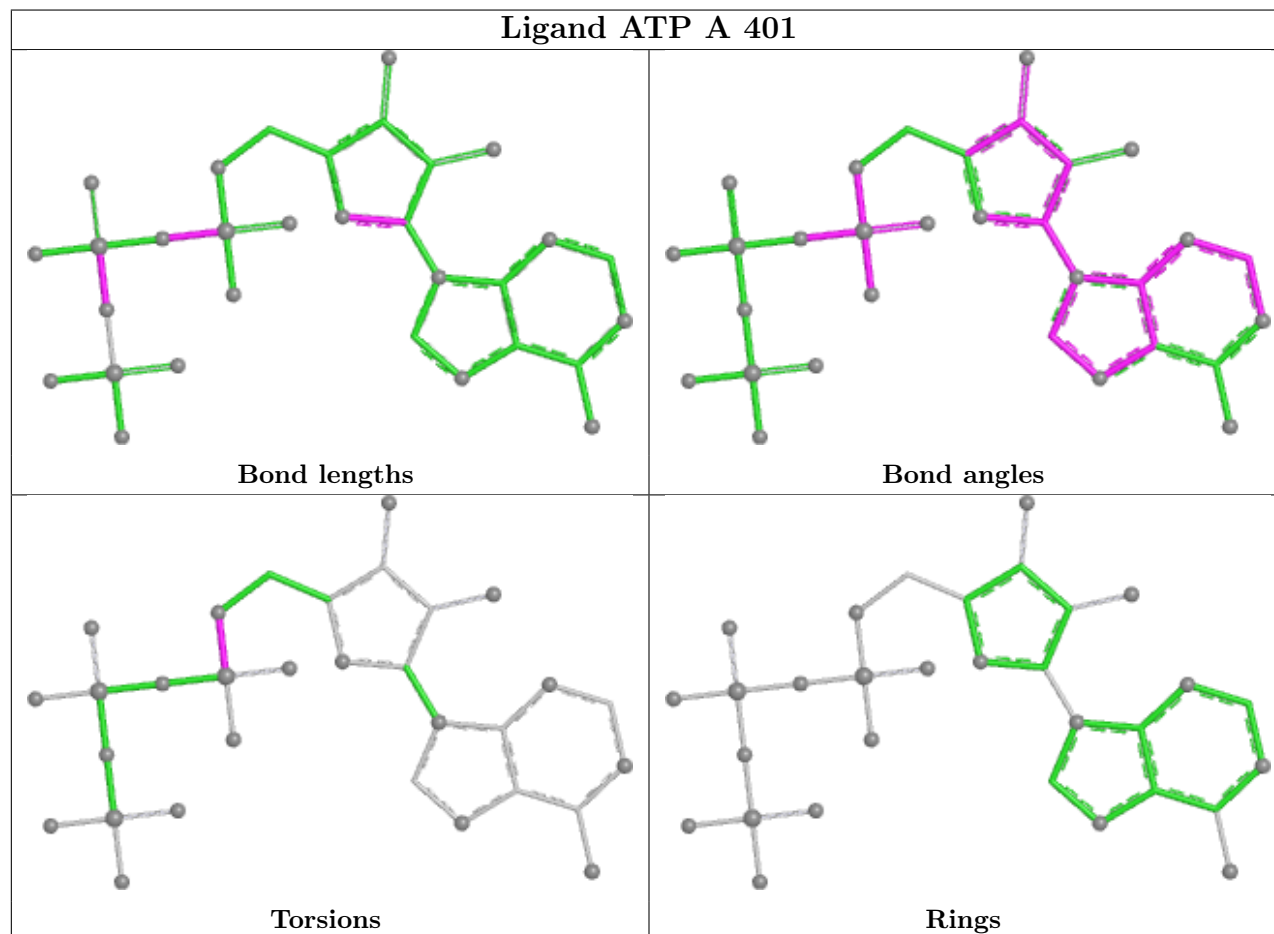
There are no ring outliers.

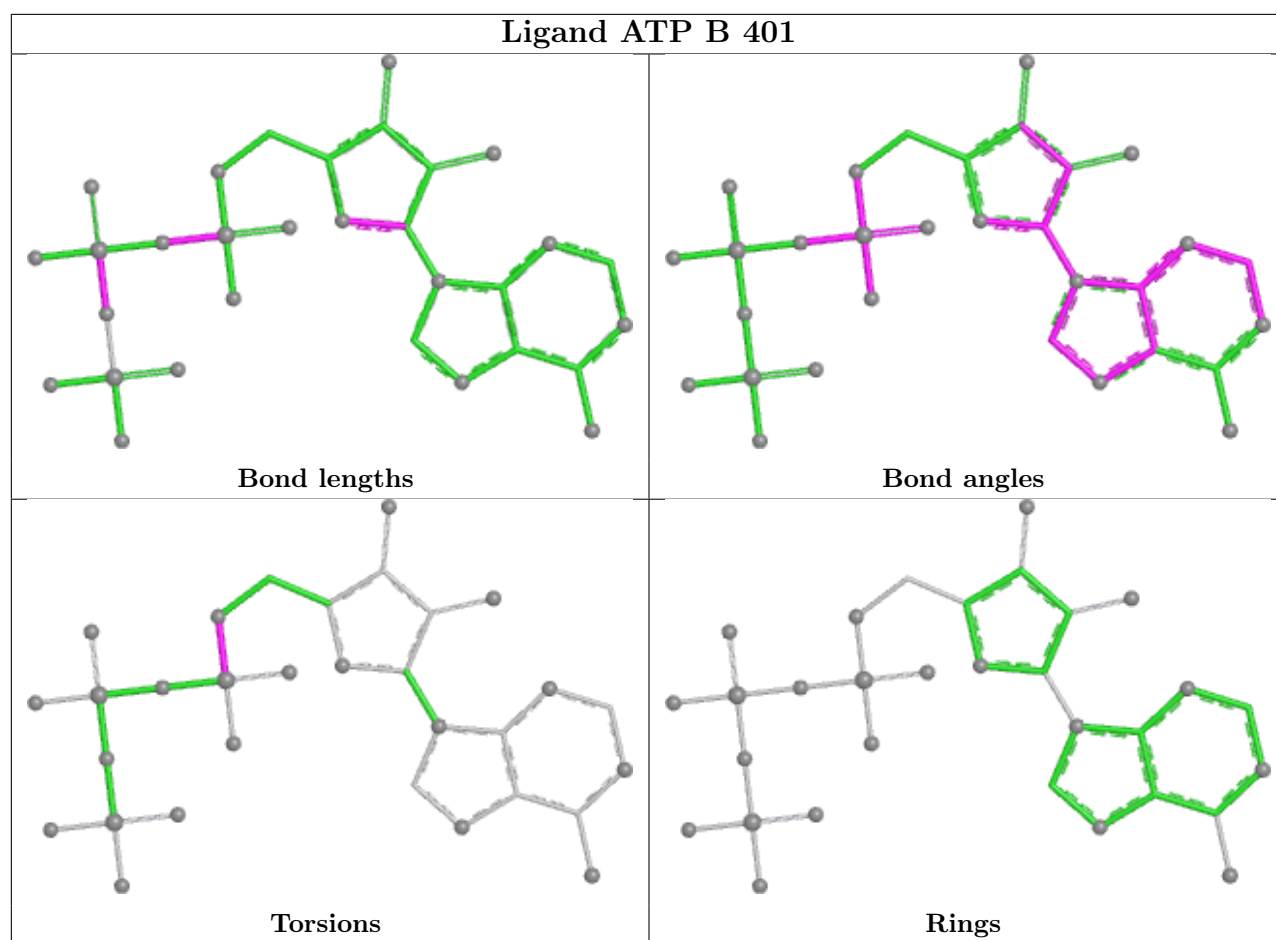
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	ATP	5	0
4	B	401	ATP	3	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](#)

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	294/356 (82%)	-0.48	2 (0%) 84 72	193, 339, 374, 396	0
1	B	299/356 (83%)	-0.45	0 100 100	193, 339, 378, 396	0
2	C	276/288 (95%)	-0.41	2 (0%) 84 72	280, 349, 386, 429	0
2	E	277/288 (96%)	-0.48	0 100 100	280, 349, 387, 429	0
3	D	52/54 (96%)	-0.45	0 100 100	333, 345, 405, 419	0
3	F	52/54 (96%)	-0.32	0 100 100	333, 345, 406, 419	0
All	All	1250/1396 (89%)	-0.45	4 (0%) 90 81	193, 344, 382, 429	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	58	GLN	3.0
1	A	28	GLY	2.6
1	A	30	GLY	2.2
2	C	196	PHE	2.1

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 oligosaccharides 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,

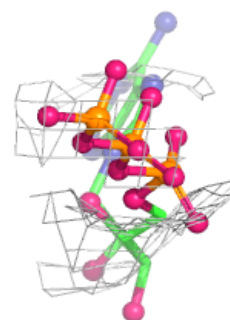
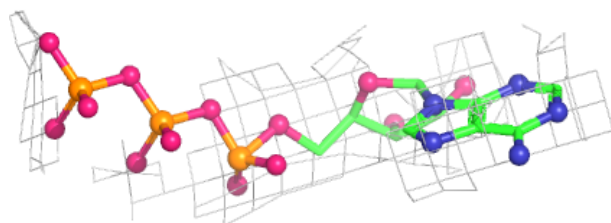
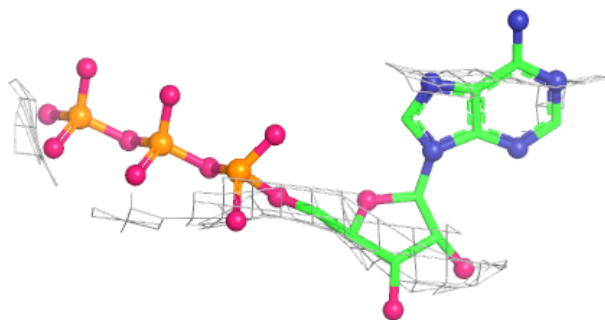
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

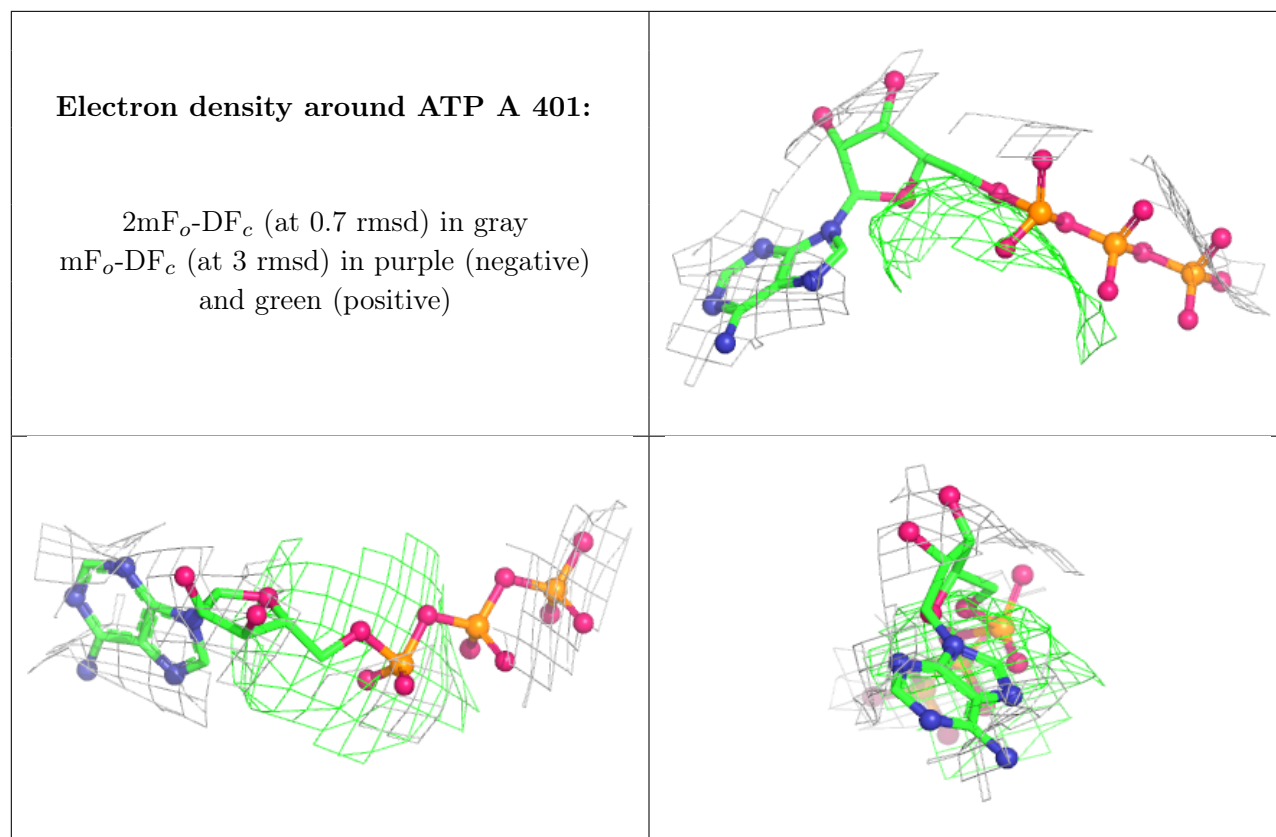
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ATP	B	401	31/31	0.83	0.09	316,321,324,324	0
5	MG	B	402	1/1	0.83	0.12	327,327,327,327	0
4	ATP	A	401	31/31	0.84	0.09	309,312,314,315	0
5	MG	A	402	1/1	0.86	0.13	327,327,327,327	0
6	ZN	A	403	1/1	0.89	0.05	327,327,327,327	0

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 ATP B 401:

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](#)

There are no such residues in this entry.