



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:32 AM EDT

PDB ID : 2OOY / pdb_00002ooy
Title : Crystal structure of the adenylate sensor from AMP-activated protein kinase complexed with ATP
Authors : Townley, R.; Shapiro, L.
Deposited on : 2007-01-26
Resolution : 2.88 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

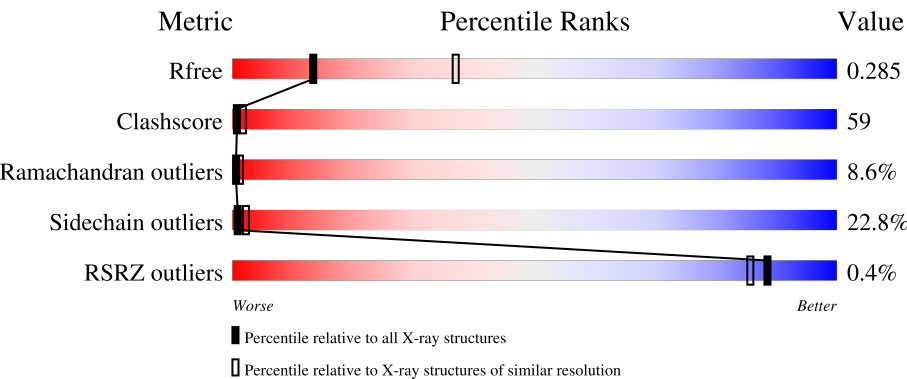
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	137	% 24% 47% 20% • 6%
1	C	137	19% 45% 15% • 16%
2	B	97	21% 39% 25% 10% 5%
2	D	97	% 31% 40% 15% 7% 6%
3	E	333	23% 52% 21% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	333	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	E	401	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9010 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1020	652	178	180	10			
1	C	115	Total	C	N	O	S	0	0	0
			915	594	150	162	9			

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	1	0
			714	455	125	132	2			
2	D	91	Total	C	N	O	S	0	0	0
			708	453	122	131	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	cloning artifact	UNP P78789
D	202	MET	-	cloning artifact	UNP P78789

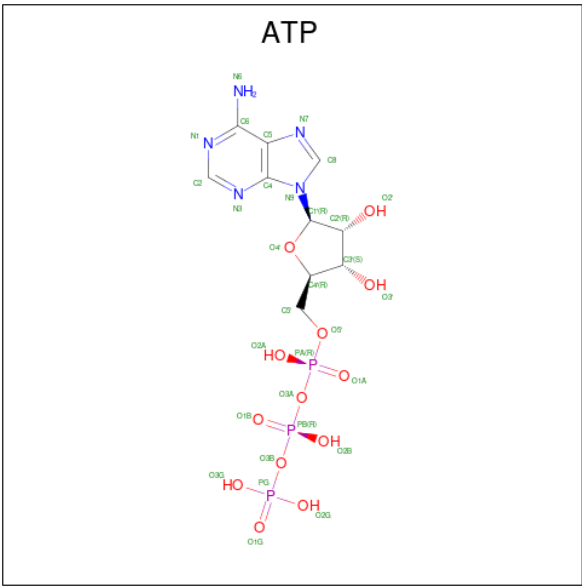
- Molecule 3 is a protein called Hypothetical protein C1556.08c in chromosome I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	324	Total	C	N	O	S	0	1	0
			2544	1627	421	481	15			
3	E	333	Total	C	N	O	S	0	0	0
			2606	1663	432	496	15			

There are 2 discrepancies between the modelled and reference sequences:

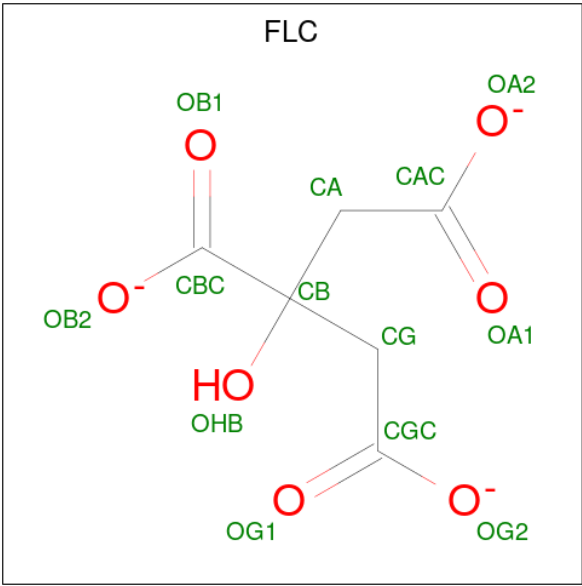
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	MET	-	cloning artifact	UNP Q10343
G	2	MET	-	cloning artifact	UNP Q10343

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			13	6	7		

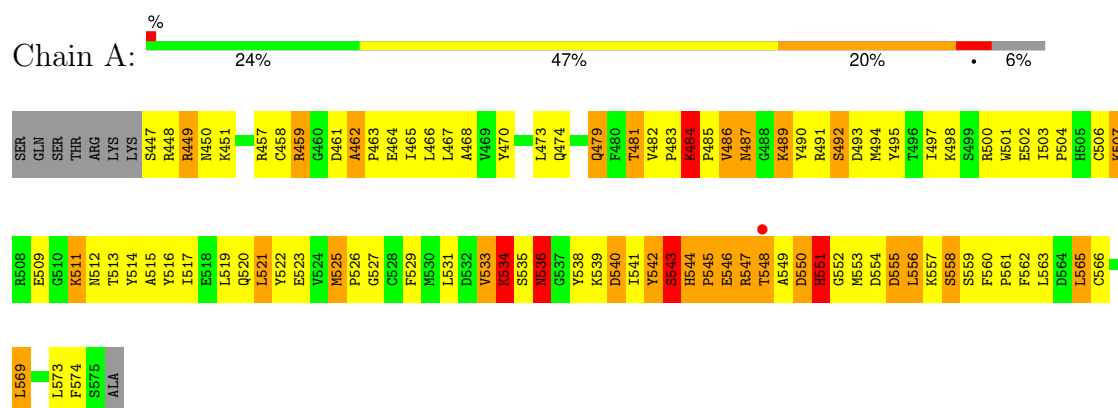
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total 50	O 50	0	0
6	B	41	Total 41	O 41	0	0
6	G	126	Total 126	O 126	0	0
6	C	50	Total 50	O 50	0	0
6	D	36	Total 36	O 36	0	0
6	E	125	Total 125	O 125	0	0

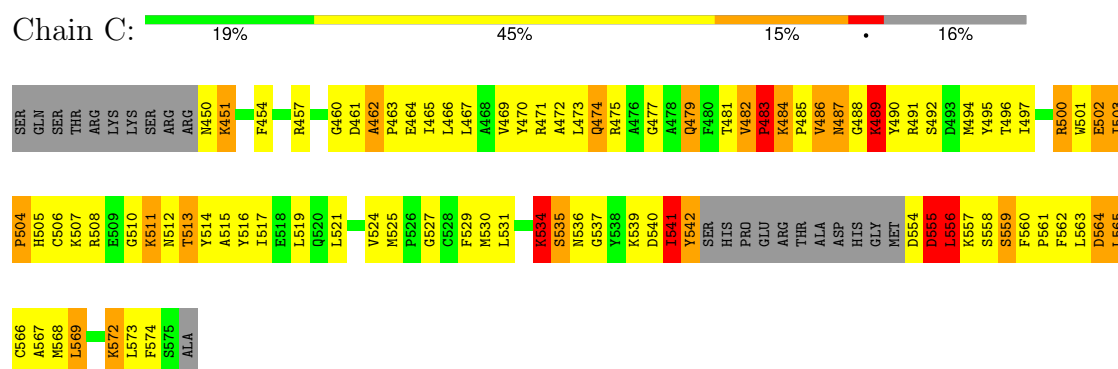
3 Residue-property plots

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.

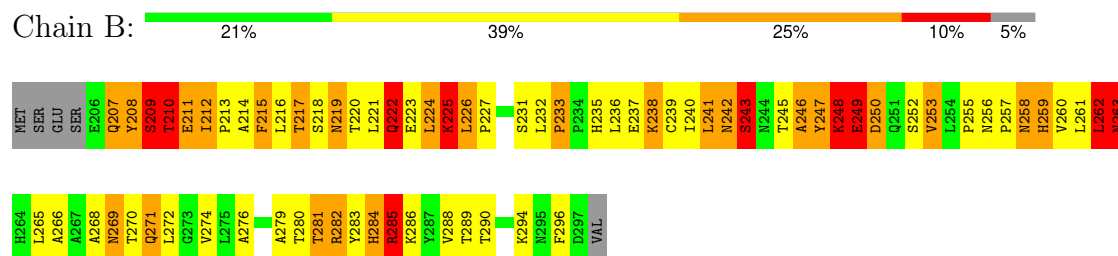
- Molecule 1: SNF1-like protein kinase ssp2



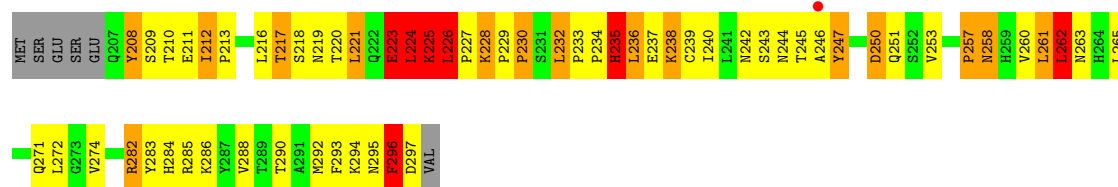
- Molecule 1: SNF1-like protein kinase ssp2



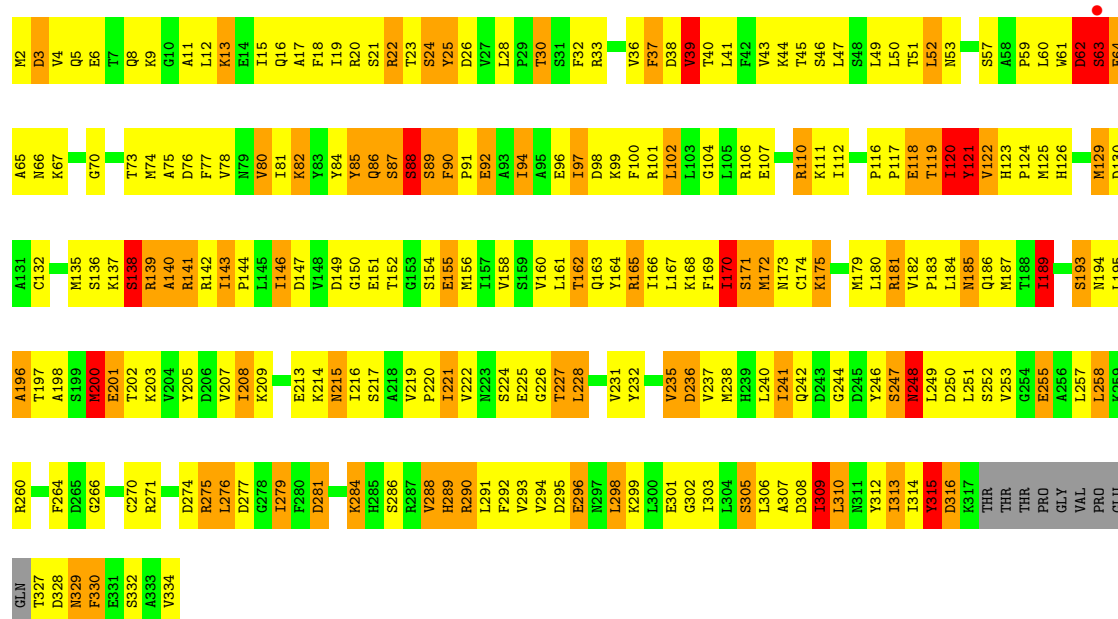
- Molecule 2: SPCC1919.03c protein



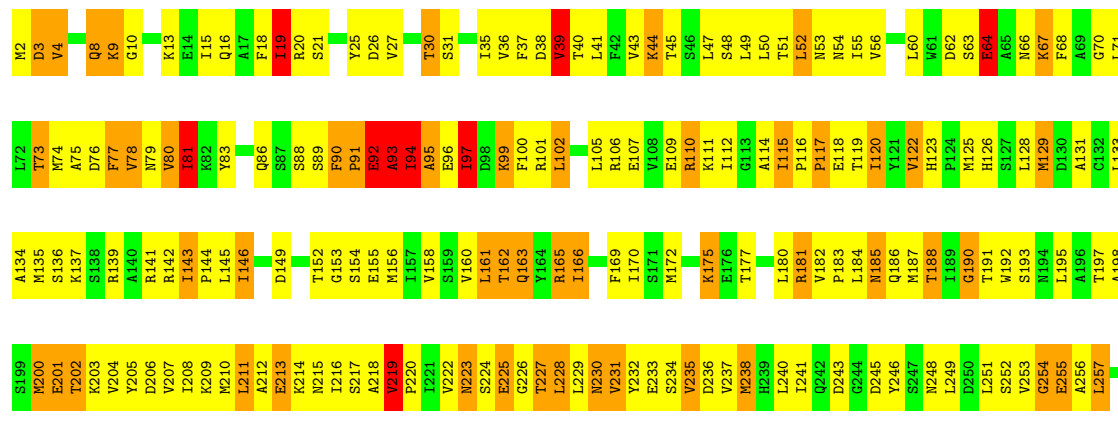
- Molecule 2: SPCC1919.03c protein



• Molecule 3: Hypothetical protein C1556.08c in chromosome I



• Molecule 3: Hypothetical protein C1556.08c in chromosome I





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.90Å 77.67Å 107.58Å 90.00° 123.99° 90.00°	Depositor
Resolution (Å)	50.00 – 2.88 50.00 – 2.88	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.88) 96.2 (50.00-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.298 0.187 , 0.285	Depositor DCC
R_{free} test set	1265 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: FLC, ATP

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	1.28	3/1047 (0.3%)	1.43	12/1415 (0.8%)
1	C	1.26	1/939 (0.1%)	1.46	15/1269 (1.2%)
2	B	1.23	1/735 (0.1%)	1.57	17/1006 (1.7%)
2	D	1.35	3/726 (0.4%)	1.53	15/994 (1.5%)
3	E	1.34	13/2651 (0.5%)	1.48	33/3596 (0.9%)
3	G	1.38	13/2590 (0.5%)	1.47	24/3509 (0.7%)
All	All	1.33	34/8688 (0.4%)	1.48	116/11789 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	1
2	B	0	6
2	D	0	2
3	E	0	3
3	G	0	4
All	All	0	21

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	286	LYS	C-N	-15.34	1.13	1.33
2	B	286	LYS	C-N	-9.68	1.20	1.33
1	A	479	GLN	CA-C	-7.22	1.43	1.52
3	E	93	ALA	CA-C	-7.09	1.43	1.52
3	G	189	ILE	N-CA	7.01	1.53	1.46
2	D	288	VAL	CA-CB	-6.65	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	267	VAL	CA-CB	-6.56	1.46	1.54
3	G	4	VAL	CA-CB	6.42	1.61	1.54
3	G	88	SER	N-CA	6.38	1.54	1.46
3	E	4	VAL	CA-CB	6.17	1.61	1.54
3	E	81	ILE	CA-CB	6.15	1.61	1.54
3	E	202	THR	CA-CB	-6.13	1.44	1.53
3	E	170	ILE	CA-CB	-6.08	1.47	1.54
3	G	208	ILE	N-CA	-5.97	1.39	1.46
2	D	246	ALA	C-N	5.97	1.40	1.33
3	E	320	THR	CA-CB	5.81	1.62	1.53
3	G	39	VAL	CA-CB	-5.68	1.46	1.54
3	G	309	ILE	CA-CB	-5.66	1.48	1.54
1	C	451	LYS	CA-C	5.66	1.59	1.53
3	G	244	GLY	C-N	-5.60	1.25	1.33
3	E	40	THR	CA-CB	5.51	1.62	1.53
3	G	119	THR	CA-CB	5.47	1.61	1.53
3	G	17	ALA	CA-CB	-5.43	1.44	1.53
3	E	158	VAL	CA-CB	-5.43	1.49	1.55
3	E	41	LEU	CA-C	-5.40	1.45	1.52
3	G	37	PHE	CA-C	5.38	1.59	1.52
3	G	290	ARG	CA-C	5.36	1.60	1.53
1	A	533	VAL	CA-C	-5.35	1.48	1.52
3	G	196	ALA	CA-CB	-5.31	1.46	1.53
3	E	307	ALA	CA-CB	-5.31	1.45	1.53
3	E	319	THR	CA-CB	5.21	1.62	1.53
3	E	19	ILE	CA-CB	-5.05	1.48	1.54
1	A	486	VAL	CA-CB	5.04	1.59	1.54
3	G	139	ARG	N-CA	5.02	1.52	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	315	TYR	N-CA-C	10.20	126.25	114.62
3	G	290	ARG	N-CA-C	9.97	123.69	110.53
1	C	451	LYS	N-CA-C	9.91	120.97	108.19
3	G	122	VAL	N-CA-C	9.56	129.24	109.34
2	D	286	LYS	O-C-N	-9.19	110.06	122.74
2	B	209	SER	N-CA-C	9.16	130.32	110.80
3	E	79	ASN	N-CA-C	8.96	120.73	110.97
3	E	94	ILE	N-CA-C	-8.80	91.04	109.34
3	E	92	GLU	N-CA-C	-8.66	97.67	110.23
3	E	307	ALA	N-CA-C	-8.38	101.73	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	ALA	CA-C-N	-8.12	110.58	119.19
1	C	462	ALA	C-N-CA	-8.12	110.58	119.19
3	G	247	SER	N-CA-C	-8.08	103.22	113.23
2	B	258	ASN	N-CA-C	7.80	121.24	108.52
3	G	288	VAL	N-CA-C	7.79	117.89	110.42
3	E	280	PHE	CA-C-N	-7.75	110.06	122.23
3	E	280	PHE	C-N-CA	-7.75	110.06	122.23
2	B	263	ASN	N-CA-C	7.73	122.67	110.70
3	G	147	ASP	N-CA-C	-7.63	98.34	109.18
2	B	233	PRO	CA-C-N	7.61	128.29	119.47
2	B	233	PRO	C-N-CA	7.61	128.29	119.47
1	C	513	THR	N-CA-C	7.58	123.20	113.88
3	G	171	SER	N-CA-C	-7.56	103.02	111.71
1	C	556	LEU	N-CA-C	7.54	121.60	110.30
3	G	90	PHE	CA-C-N	7.24	126.94	119.56
3	G	90	PHE	C-N-CA	7.24	126.94	119.56
3	G	208	ILE	N-CA-C	-7.23	103.25	110.62
2	B	208	TYR	N-CA-C	7.20	121.39	109.95
1	A	543	SER	CA-C-N	7.18	134.62	121.70
1	A	543	SER	C-N-CA	7.18	134.62	121.70
3	E	77	PHE	N-CA-C	7.14	118.85	111.14
2	B	221	LEU	N-CA-C	-7.05	103.64	111.82
2	D	286	LYS	CA-C-N	7.05	132.67	122.44
2	D	286	LYS	C-N-CA	7.05	132.67	122.44
2	B	257	PRO	CA-C-N	-6.96	113.31	123.05
2	B	257	PRO	C-N-CA	-6.96	113.31	123.05
2	D	251	GLN	N-CA-C	-6.88	104.87	113.20
2	B	285	ARG	CA-C-N	6.61	132.91	122.21
2	B	285	ARG	C-N-CA	6.61	132.91	122.21
3	G	121	TYR	N-CA-C	6.50	124.63	110.80
3	G	330	PHE	N-CA-C	6.49	120.28	109.95
3	E	267	VAL	N-CA-CB	-6.45	103.67	111.21
3	E	322	GLY	N-CA-C	-6.45	97.91	113.18
3	E	45	THR	N-CA-C	-6.42	104.28	111.28
3	E	267	VAL	CA-C-N	-6.40	114.02	123.11
3	E	267	VAL	C-N-CA	-6.40	114.02	123.11
3	E	111	LYS	N-CA-C	6.36	119.89	111.75
3	G	313	ILE	CB-CA-C	-6.27	103.83	112.04
3	E	90	PHE	CA-C-N	6.24	127.64	119.84
3	E	90	PHE	C-N-CA	6.24	127.64	119.84
3	G	24	SER	N-CA-C	-6.23	103.64	111.11
2	D	208	TYR	N-CA-C	6.20	119.59	107.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	163	GLN	N-CA-C	-6.17	104.45	112.23
1	A	486	VAL	N-CA-C	-6.12	101.65	109.30
3	E	219	VAL	CA-C-N	6.02	125.78	119.76
3	E	219	VAL	C-N-CA	6.02	125.78	119.76
2	B	210	THR	N-CA-C	5.96	123.50	110.80
3	E	81	ILE	CB-CA-C	5.92	119.55	111.97
2	D	257	PRO	CA-C-N	-5.92	113.14	121.72
2	D	257	PRO	C-N-CA	-5.92	113.14	121.72
1	C	574	PHE	N-CA-C	5.91	120.48	113.16
2	B	215	PHE	N-CA-C	-5.86	100.63	109.60
2	D	236	LEU	CA-C-N	-5.82	116.15	126.45
2	D	236	LEU	C-N-CA	-5.82	116.15	126.45
2	B	284	HIS	CA-C-N	-5.76	114.59	123.17
2	B	284	HIS	C-N-CA	-5.76	114.59	123.17
2	B	249	GLU	N-CA-C	-5.73	94.95	111.00
3	G	116	PRO	O-C-N	5.70	123.93	121.31
2	D	233	PRO	O-C-N	5.67	123.81	121.15
1	A	484	LYS	CA-C-N	-5.66	114.14	120.14
1	A	484	LYS	C-N-CA	-5.66	114.14	120.14
2	D	296	PHE	N-CA-C	-5.63	105.14	111.28
3	E	265	ASP	CA-C-N	-5.60	113.66	121.67
3	E	265	ASP	C-N-CA	-5.60	113.66	121.67
1	C	486	VAL	CB-CA-C	5.54	118.03	111.32
3	E	304	LEU	N-CA-C	-5.54	100.65	109.96
1	C	482	VAL	CA-C-N	5.53	126.76	119.84
1	C	482	VAL	C-N-CA	5.53	126.76	119.84
3	G	170	ILE	N-CA-C	-5.51	97.89	109.34
3	G	160	VAL	CA-C-N	-5.49	115.14	122.72
3	G	160	VAL	C-N-CA	-5.49	115.14	122.72
1	A	490	TYR	N-CA-C	5.48	118.33	109.79
1	C	510	GLY	N-CA-C	5.46	116.70	111.67
3	E	78	VAL	CB-CA-C	-5.44	104.92	111.88
1	A	533	VAL	N-CA-C	-5.43	101.97	109.46
3	E	314	ILE	N-CA-C	5.36	120.49	109.34
3	E	165	ARG	N-CA-C	-5.36	105.54	111.71
1	A	487	ASN	N-CA-C	5.34	122.18	110.80
1	A	539	LYS	N-CA-C	5.34	116.90	107.61
3	E	200	MET	N-CA-C	-5.34	106.61	113.02
3	E	50	LEU	N-CA-C	-5.33	105.63	111.82
3	E	201	GLU	N-CA-C	-5.31	106.18	113.30
1	A	555	ASP	N-CA-C	5.29	122.07	110.80
1	A	556	LEU	N-CA-C	5.28	122.05	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	250	ASP	N-CA-C	5.26	119.33	113.01
2	D	235	HIS	N-CA-C	5.26	117.76	111.71
2	D	224	LEU	N-CA-C	5.26	122.00	110.80
3	E	281	ASP	CB-CA-C	5.25	118.20	109.38
1	C	534	LYS	N-CA-C	5.23	116.92	108.34
2	B	212	ILE	CB-CA-C	-5.22	105.25	110.89
1	A	551	HIS	N-CA-C	5.22	121.91	110.80
1	C	525	MET	CA-C-N	-5.19	114.44	119.78
1	C	525	MET	C-N-CA	-5.19	114.44	119.78
3	E	288	VAL	CB-CA-C	-5.17	104.50	110.91
2	D	226	LEU	CA-C-N	-5.15	114.46	119.76
2	D	226	LEU	C-N-CA	-5.15	114.46	119.76
3	G	85	TYR	CA-C-N	-5.11	115.38	122.74
3	G	85	TYR	C-N-CA	-5.11	115.38	122.74
3	E	39	VAL	CB-CA-C	-5.11	102.92	111.29
3	G	219	VAL	CB-CA-C	-5.09	102.10	111.36
3	E	30	THR	N-CA-C	-5.08	106.60	112.89
3	G	30	THR	N-CA-C	-5.05	106.38	112.54
3	E	107	GLU	N-CA-C	-5.05	106.97	113.23
1	C	460	GLY	N-CA-C	5.04	117.66	111.45
1	C	517	ILE	CB-CA-C	-5.02	102.35	110.28
3	G	241	ILE	N-CA-C	5.01	116.98	111.77

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	ARG	Peptide
1	A	485	PRO	Peptide
1	A	536	ASN	Peptide
1	A	549	ALA	Peptide
1	A	550	ASP	Peptide
2	B	208	TYR	Peptide
2	B	209	SER	Peptide
2	B	242	ASN	Peptide
2	B	243	SER	Peptide
2	B	248	LYS	Peptide
2	B	250	ASP	Peptide
1	C	489	LYS	Peptide
2	D	219	ASN	Peptide
2	D	223	GLU	Peptide
3	E	266	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	E	318	THR	Peptide
3	E	321	PRO	Peptide
3	G	120	ILE	Peptide
3	G	121	TYR	Peptide
3	G	62	ASP	Peptide
3	G	63	SER	Peptide

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	1020	0	983	132	0
1	C	915	0	886	121	0
2	B	714	0	710	81	0
2	D	708	0	703	97	0
3	E	2606	0	2642	329	0
3	G	2544	0	2568	305	0
4	E	31	0	12	12	0
4	G	31	0	12	4	0
5	E	13	0	5	2	0
6	A	50	0	0	20	0
6	B	41	0	0	2	0
6	C	50	0	0	26	0
6	D	36	0	0	12	0
6	E	125	0	0	66	0
6	G	126	0	0	50	0
All	All	9010	0	8521	1015	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 59.

All (1015) 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)
3:G:99:LYS:HE3	6:G:478:HOH:O	1.19	1.28
6:G:415:HOH:O	2:D:271:GLN:HG2	1.29	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:162:THR:HG21	6:G:516:HOH:O	1.29	1.27
2:D:210:THR:HB	6:D:322:HOH:O	1.26	1.25
3:E:290:ARG:HA	6:E:520:HOH:O	1.37	1.24
3:E:73:THR:HG22	3:E:75:ALA:H	1.04	1.21
1:A:458:CYS:HA	6:E:453:HOH:O	1.42	1.19
3:E:303:ILE:HG22	6:E:490:HOH:O	1.40	1.18
3:E:308:ASP:OD2	6:E:527:HOH:O	1.60	1.16
1:A:569:LEU:O	6:A:241:HOH:O	1.61	1.15
2:B:282:ARG:CB	2:B:282:ARG:HH11	1.62	1.13
2:D:235:HIS:HE1	2:D:258:ASN:CB	1.60	1.13
2:D:235:HIS:HE1	2:D:258:ASN:HB2	1.01	1.12
3:E:181:ARG:HE	3:E:275:ARG:NH2	1.47	1.12
2:D:225:LYS:HG2	2:D:226:LEU:H	1.15	1.11
3:E:215:ASN:HD22	3:E:331:GLU:HA	0.98	1.11
2:D:225:LYS:HG2	2:D:227:PRO:HD3	1.31	1.09
3:E:215:ASN:ND2	3:E:331:GLU:HA	1.68	1.08
3:E:215:ASN:HD21	3:E:332:SER:N	1.49	1.08
3:G:253:VAL:HG12	3:G:257:LEU:HD21	1.35	1.08
1:C:474:GLN:HG3	6:C:205:HOH:O	1.55	1.07
3:E:223:ASN:ND2	6:E:431:HOH:O	1.88	1.06
2:B:248:LYS:CB	2:B:249:GLU:HA	1.87	1.05
1:C:503:ILE:HD12	1:C:514:TYR:H	1.20	1.05
2:D:235:HIS:CE1	2:D:258:ASN:HB2	1.92	1.05
3:G:141:ARG:HD3	6:G:503:HOH:O	1.58	1.04
1:A:494:MET:HE2	2:B:227:PRO:HG2	1.40	1.03
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.17	1.03
2:D:223:GLU:OE1	2:D:223:GLU:HA	1.51	1.03
3:G:182:VAL:O	3:G:187:MET:HE3	1.59	1.02
2:D:235:HIS:CE1	2:D:258:ASN:CB	2.43	1.02
2:D:236:LEU:O	2:D:237:GLU:HB3	1.58	1.02
3:E:129:MET:HE1	3:E:314:ILE:HG12	1.40	1.01
3:E:249:LEU:HB3	6:E:519:HOH:O	1.59	1.01
3:G:39:VAL:HG21	3:G:62:ASP:HB2	1.41	1.00
3:E:184:LEU:HD12	3:E:187:MET:HE1	1.44	1.00
4:E:401:ATP:C8	4:E:401:ATP:H5'1	1.95	1.00
3:G:43:VAL:HG12	6:G:485:HOH:O	1.61	0.99
2:B:249:GLU:OE2	3:G:165:ARG:HG2	1.62	0.98
2:B:282:ARG:NH1	2:B:282:ARG:HB2	1.78	0.97
2:D:282:ARG:HH11	2:D:282:ARG:HG3	1.28	0.97
3:G:220:PRO:O	6:G:482:HOH:O	1.83	0.96
1:C:482:VAL:HG13	2:D:213:PRO:HG3	1.46	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:ILE:HD13	1:C:503:ILE:N	1.79	0.96
3:G:139:ARG:O	3:G:141:ARG:N	1.98	0.95
3:E:215:ASN:ND2	3:E:332:SER:H	1.65	0.95
3:G:170:ILE:N	6:G:507:HOH:O	2.00	0.95
1:C:503:ILE:CD1	1:C:514:TYR:H	1.80	0.94
3:E:271:ARG:HH21	3:E:296:GLU:HA	1.32	0.94
2:B:282:ARG:CB	2:B:282:ARG:NH1	2.28	0.94
1:A:461:ASP:HB2	1:A:464:GLU:OE2	1.68	0.93
3:G:149:ASP:HB3	6:G:414:HOH:O	1.66	0.93
3:G:144:PRO:HB2	3:G:146:ILE:HD11	1.49	0.93
3:E:186:GLN:HB3	6:E:523:HOH:O	1.68	0.93
3:G:80:VAL:CG2	3:G:97:ILE:HD11	1.98	0.93
3:G:8:GLN:HE22	3:G:187:MET:HE2	1.33	0.92
3:G:80:VAL:HG22	3:G:97:ILE:HD11	1.52	0.92
3:G:169:PHE:O	3:G:170:ILE:HG13	1.69	0.92
3:G:221:ILE:HA	6:G:482:HOH:O	1.69	0.92
1:A:507:LYS:HD3	1:A:507:LYS:C	1.93	0.92
3:G:141:ARG:O	6:G:493:HOH:O	1.87	0.92
3:E:92:GLU:O	3:E:93:ALA:CB	2.18	0.92
3:E:274:ASP:HB2	6:E:524:HOH:O	1.68	0.91
4:E:401:ATP:H5'1	4:E:401:ATP:H8	1.27	0.91
1:C:502:GLU:HG2	1:C:502:GLU:O	1.70	0.91
3:G:164[B]:TYR:H	3:G:164[B]:TYR:HD1	1.04	0.91
3:G:215:ASN:HD21	3:G:332:SER:HB2	1.35	0.91
2:D:296:PHE:O	2:D:297:ASP:HB2	1.69	0.91
3:G:279:ILE:HD13	3:G:291:LEU:HD22	1.50	0.90
1:C:503:ILE:HD12	1:C:514:TYR:N	1.86	0.90
3:E:185:ASN:HD22	3:E:186:GLN:N	1.69	0.90
3:G:88:SER:HB3	6:G:468:HOH:O	1.69	0.90
1:C:503:ILE:CD1	1:C:503:ILE:H	1.84	0.90
3:G:195:LEU:HD22	3:G:303:ILE:HD12	1.52	0.90
3:E:184:LEU:HA	3:E:187:MET:CE	2.03	0.89
1:C:500:ARG:HG2	1:C:500:ARG:HH11	1.37	0.89
3:G:96:GLU:OE2	6:G:411:HOH:O	1.90	0.88
3:E:144:PRO:HB2	3:E:146:ILE:HD11	1.53	0.88
1:C:561:PRO:HB3	6:E:447:HOH:O	1.72	0.88
3:E:90:PHE:HA	6:E:453:HOH:O	1.74	0.87
1:C:559:SER:HB3	6:D:324:HOH:O	1.73	0.87
3:E:215:ASN:HD21	3:E:332:SER:H	0.90	0.87
1:C:511:LYS:CB	6:C:211:HOH:O	2.21	0.87
3:E:184:LEU:HA	3:E:187:MET:HE2	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:GLU:OE1	2:D:223:GLU:CA	2.23	0.86
3:E:163:GLN:O	3:E:166:ILE:HG22	1.74	0.86
3:G:240:LEU:HD13	6:G:499:HOH:O	1.74	0.86
3:E:73:THR:HG22	3:E:75:ALA:N	1.89	0.86
1:A:503:ILE:HD12	1:A:561:PRO:HG3	1.55	0.86
1:A:457:ARG:HD3	6:A:420:HOH:O	1.74	0.85
1:C:473:LEU:O	6:C:208:HOH:O	1.95	0.85
1:C:503:ILE:N	1:C:503:ILE:CD1	2.37	0.85
2:D:258:ASN:HD22	2:D:260:VAL:H	1.24	0.85
1:C:463:PRO:HD2	6:C:200:HOH:O	1.76	0.85
2:D:296:PHE:O	2:D:297:ASP:CB	2.24	0.85
3:E:230:ASN:OD1	6:E:483:HOH:O	1.95	0.85
1:A:447:SER:CB	6:A:418:HOH:O	2.25	0.84
2:B:248:LYS:CB	2:B:249:GLU:CA	2.56	0.84
1:A:561:PRO:O	1:A:565:LEU:HD22	1.78	0.84
3:G:260:ARG:NH1	6:G:513:HOH:O	1.87	0.84
1:A:501:TRP:HA	6:A:2:HOH:O	1.78	0.84
3:G:140:ALA:O	3:G:142:ARG:N	2.10	0.84
3:E:215:ASN:ND2	3:E:332:SER:N	2.23	0.83
1:C:450:ASN:O	1:C:451:LYS:HG2	1.78	0.83
3:E:66:ASN:HB3	3:E:154:SER:OG	1.77	0.83
3:E:241:ILE:HA	6:E:414:HOH:O	1.76	0.83
2:B:222:GLN:OE1	2:B:222:GLN:HA	1.78	0.83
3:G:185:ASN:ND2	3:G:186:GLN:HG3	1.95	0.82
2:D:225:LYS:CG	2:D:227:PRO:HD3	2.08	0.82
2:D:226:LEU:HD12	2:D:228:LYS:HE2	1.60	0.82
2:B:235:HIS:HA	6:B:317:HOH:O	1.80	0.82
3:E:77:PHE:O	3:E:81:ILE:HG22	1.80	0.82
6:G:469:HOH:O	1:C:450:ASN:CB	2.26	0.81
3:E:181:ARG:NE	3:E:275:ARG:NH2	2.28	0.81
3:E:328:ASP:OD2	6:E:468:HOH:O	1.99	0.81
1:A:498:LYS:HG3	6:A:336:HOH:O	1.79	0.81
3:E:129:MET:HE1	3:E:314:ILE:CG1	2.10	0.81
3:G:165:ARG:HD2	3:G:165:ARG:O	1.79	0.81
1:A:523:GLU:HA	1:A:529:PHE:CD2	2.14	0.81
1:C:479:GLN:OE1	1:C:500:ARG:NH1	2.11	0.81
3:E:10:GLY:HA2	3:E:13:LYS:HE2	1.59	0.81
3:E:237:VAL:O	3:E:240:LEU:N	2.14	0.81
3:E:305:SER:O	3:E:308:ASP:HB2	1.79	0.81
1:C:472:ALA:HB1	1:C:572:LYS:HB3	1.62	0.81
3:E:47:LEU:O	3:E:51:THR:HG22	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ASP:HB2	2:B:253:VAL:HG12	1.61	0.80
3:G:279:ILE:CD1	3:G:291:LEU:HD22	2.09	0.80
3:G:63:SER:N	3:G:65:ALA:H	1.79	0.80
1:A:462:ALA:HB3	1:A:463:PRO:HD3	1.64	0.80
3:G:253:VAL:O	3:G:257:LEU:CD2	2.29	0.80
3:G:270:CYS:HB2	3:G:274:ASP:OD1	1.81	0.80
3:G:12:LEU:HD23	3:G:180:LEU:CD2	2.12	0.80
4:E:401:ATP:C2'	6:E:527:HOH:O	2.30	0.79
3:G:61:TRP:NE1	3:G:63:SER:HB2	1.96	0.79
3:G:279:ILE:HD13	3:G:291:LEU:CD2	2.12	0.79
1:A:509:GLU:OE1	6:A:240:HOH:O	1.99	0.79
3:G:139:ARG:C	3:G:141:ARG:H	1.90	0.79
3:E:271:ARG:NH2	3:E:296:GLU:HA	1.97	0.79
3:G:185:ASN:HD22	3:G:186:GLN:N	1.80	0.78
1:C:471:ARG:NH2	6:C:316:HOH:O	2.15	0.78
3:E:110:ARG:HH11	3:E:117:PRO:HA	1.46	0.78
1:A:525:MET:HB2	1:A:526:PRO:HD2	1.65	0.78
3:E:92:GLU:O	3:E:93:ALA:HB2	1.82	0.78
3:G:52:LEU:HD22	3:G:52:LEU:H	1.48	0.78
3:G:2:MET:HB2	6:G:464:HOH:O	1.83	0.78
3:G:104:GLY:O	3:G:107:GLU:HB3	1.84	0.78
3:G:221:ILE:CD1	3:G:253:VAL:HG11	2.14	0.78
2:D:225:LYS:CG	2:D:226:LEU:H	1.94	0.77
3:E:215:ASN:HD22	3:E:331:GLU:CA	1.90	0.77
3:G:251:LEU:HB3	3:G:255:GLU:HG3	1.65	0.77
1:C:516:TYR:OH	6:C:52:HOH:O	2.03	0.77
2:B:261:LEU:O	2:B:262:LEU:O	2.03	0.77
3:G:99:LYS:HD3	2:D:297:ASP:O	1.85	0.77
1:A:574:PHE:O	6:A:93:HOH:O	2.03	0.76
3:G:195:LEU:HD22	3:G:303:ILE:CD1	2.14	0.76
6:C:205:HOH:O	2:D:212:ILE:HG22	1.85	0.76
3:E:129:MET:HA	3:E:129:MET:HE2	1.67	0.76
3:E:212:ALA:O	3:E:213:GLU:HB3	1.85	0.76
3:E:123:HIS:HB3	3:E:126:HIS:ND1	1.99	0.76
3:E:177:THR:HG21	3:E:280:PHE:CD2	2.21	0.76
3:G:253:VAL:O	3:G:257:LEU:HD22	1.84	0.76
1:C:500:ARG:HD2	1:C:514:TYR:CD2	2.21	0.76
2:D:225:LYS:HG2	2:D:227:PRO:CD	2.13	0.76
3:E:241:ILE:C	6:E:414:HOH:O	2.28	0.76
1:C:556:LEU:CD2	3:E:156:MET:SD	2.74	0.76
1:C:556:LEU:HD22	3:E:156:MET:SD	2.26	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:401:ATP:H2'	6:E:527:HOH:O	1.86	0.76
3:E:81:ILE:HD13	3:E:81:ILE:O	1.85	0.75
3:E:54:ASN:HA	6:E:515:HOH:O	1.86	0.75
1:A:573:LEU:N	6:A:241:HOH:O	1.76	0.75
3:E:290:ARG:HB3	6:E:442:HOH:O	1.87	0.75
1:C:521:LEU:HD12	2:D:229:PRO:HB3	1.68	0.75
3:E:204:VAL:HG11	3:E:240:LEU:CD2	2.16	0.75
2:D:225:LYS:HZ3	2:D:227:PRO:HD2	1.52	0.75
3:E:243:ASP:HB2	6:E:414:HOH:O	1.86	0.75
3:E:270:CYS:SG	6:E:524:HOH:O	2.43	0.75
3:E:200:MET:HE1	6:E:492:HOH:O	1.87	0.74
3:G:142:ARG:NE	3:G:334:VAL:O	2.19	0.74
1:C:503:ILE:HD11	6:C:212:HOH:O	1.88	0.74
3:E:62:ASP:OD2	3:E:64:GLU:HB2	1.87	0.73
3:E:73:THR:HG21	3:E:334:VAL:H	1.53	0.73
2:D:245:THR:N	6:D:302:HOH:O	2.22	0.73
3:G:61:TRP:HE1	3:G:63:SER:HB2	1.53	0.73
2:D:283:TYR:CE2	2:D:284:HIS:HD2	2.07	0.73
3:E:122:VAL:HG22	3:E:143:ILE:CD1	2.18	0.73
2:D:243:SER:OG	2:D:244:ASN:N	2.16	0.73
3:G:37:PHE:HB3	3:G:41:LEU:HD12	1.71	0.72
3:E:204:VAL:HG23	3:E:251:LEU:O	1.88	0.72
2:D:225:LYS:HG2	2:D:226:LEU:N	1.99	0.72
3:E:74:MET:HE2	3:E:238:MET:H	1.54	0.72
3:E:317:LYS:HE2	3:E:317:LYS:HA	1.72	0.72
3:E:2:MET:O	3:E:3:ASP:CB	2.38	0.72
3:G:21:SER:OG	3:G:22:ARG:NH1	2.22	0.72
3:G:221:ILE:HD13	3:G:253:VAL:HG11	1.70	0.72
3:G:61:TRP:CZ2	3:G:66:ASN:HA	2.25	0.72
3:G:6:GLU:CB	6:G:463:HOH:O	2.37	0.72
3:E:233:GLU:O	3:E:236:ASP:HB2	1.90	0.72
3:E:44:LYS:HD2	6:E:470:HOH:O	1.90	0.72
3:G:60:LEU:N	3:G:60:LEU:HD23	2.04	0.71
2:D:236:LEU:O	2:D:237:GLU:CB	2.36	0.71
3:E:163:GLN:OE1	6:E:444:HOH:O	2.08	0.71
3:E:205:TYR:HB3	6:E:519:HOH:O	1.90	0.71
3:E:310:LEU:O	3:E:314:ILE:HB	1.91	0.71
3:G:257:LEU:HD22	3:G:257:LEU:N	2.05	0.71
1:C:502:GLU:O	1:C:502:GLU:CG	2.38	0.71
3:E:184:LEU:HD12	3:E:187:MET:CE	2.20	0.71
3:G:162:THR:CG2	3:G:165:ARG:H	2.02	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:SER:CA	3:G:66:ASN:H	2.02	0.71
3:E:230:ASN:HB2	6:E:492:HOH:O	1.90	0.71
1:C:485:PRO:HG3	1:C:490:TYR:CE2	2.26	0.70
3:E:2:MET:O	3:E:3:ASP:HB3	1.89	0.70
4:E:401:ATP:O1A	4:E:401:ATP:O3G	2.08	0.70
3:G:162:THR:CG2	6:G:516:HOH:O	2.03	0.70
1:C:461:ASP:HB3	6:C:200:HOH:O	1.91	0.70
2:B:223:GLU:C	2:B:225:LYS:H	2.00	0.70
3:E:202:THR:O	3:E:253:VAL:HG23	1.90	0.70
3:E:94:ILE:HG23	3:E:95:ALA:H	1.55	0.70
2:D:283:TYR:CE2	2:D:284:HIS:CD2	2.80	0.70
3:E:128:LEU:HD21	3:E:166:ILE:HD11	1.74	0.69
3:G:295:ASP:OD2	3:G:299:LYS:HB3	1.92	0.69
2:B:226:LEU:HB3	2:B:227:PRO:HD2	1.73	0.69
3:G:213:GLU:OE2	6:G:495:HOH:O	2.10	0.69
2:D:225:LYS:O	2:D:226:LEU:HB2	1.91	0.69
3:E:122:VAL:HG22	3:E:143:ILE:HD13	1.73	0.69
3:E:215:ASN:ND2	3:E:331:GLU:CA	2.52	0.69
3:E:289:HIS:HD2	6:E:409:HOH:O	1.75	0.69
1:A:538:TYR:CE1	1:A:561:PRO:HD2	2.29	0.69
1:A:503:ILE:HD12	1:A:561:PRO:CG	2.22	0.68
2:B:249:GLU:HB2	3:G:168:LYS:HZ2	1.58	0.68
3:G:288:VAL:HG12	3:G:289:HIS:O	1.92	0.68
3:E:96:GLU:OE1	6:E:403:HOH:O	2.10	0.68
3:E:241:ILE:CA	6:E:414:HOH:O	2.36	0.68
1:A:544:HIS:CE1	1:A:545:PRO:HG2	2.29	0.68
3:E:19:ILE:HG21	3:E:129:MET:HE3	1.74	0.68
1:A:544:HIS:CG	1:A:545:PRO:HD2	2.28	0.68
3:G:328:ASP:HA	3:G:329:ASN:HB3	1.75	0.68
3:E:181:ARG:HB3	3:E:275:ARG:HH21	1.58	0.68
2:B:222:GLN:O	2:B:224:LEU:HG	1.94	0.68
1:C:484:LYS:NZ	1:C:484:LYS:HB3	2.08	0.68
2:B:237:GLU:O	6:B:338:HOH:O	2.11	0.68
3:E:204:VAL:O	3:E:208:ILE:HG12	1.94	0.67
1:A:483:PRO:HA	6:A:286:HOH:O	1.94	0.67
2:D:235:HIS:CE1	2:D:258:ASN:HB3	2.26	0.67
3:E:305:SER:HB3	6:E:527:HOH:O	1.93	0.67
3:E:324:PRO:HB2	6:E:436:HOH:O	1.95	0.67
3:G:142:ARG:HE	3:G:334:VAL:C	2.03	0.67
2:B:239:CYS:O	2:B:242:ASN:HB2	1.95	0.67
2:B:285:ARG:HG3	6:G:437:HOH:O	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:220:PRO:HB3	3:G:292:PHE:CE2	2.30	0.67
1:C:554:ASP:N	6:C:216:HOH:O	2.27	0.67
1:A:562:PHE:CE1	1:A:566:CYS:SG	2.88	0.66
3:G:63:SER:HA	3:G:66:ASN:H	1.60	0.66
3:E:181:ARG:HE	3:E:275:ARG:HH22	1.38	0.66
3:E:75:ALA:HB3	6:E:451:HOH:O	1.93	0.66
3:E:181:ARG:HB3	3:E:275:ARG:NH2	2.09	0.66
2:B:269:ASN:OD1	2:B:269:ASN:N	2.28	0.66
3:G:67:LYS:HA	3:G:155:GLU:HG3	1.77	0.66
1:C:457:ARG:NH2	6:C:400:HOH:O	2.08	0.66
3:E:245:ASP:OD1	3:E:245:ASP:C	2.35	0.66
2:B:249:GLU:O	2:B:249:GLU:OE1	2.13	0.66
1:C:531:LEU:HB2	6:C:352:HOH:O	1.95	0.66
1:A:533:VAL:HG12	1:A:534:LYS:H	1.61	0.66
3:G:12:LEU:CD2	3:G:180:LEU:CD2	2.73	0.66
3:G:135:MET:HE1	3:G:166:ILE:HD12	1.76	0.66
3:G:149:ASP:CB	6:G:414:HOH:O	2.35	0.66
3:E:110:ARG:NH1	3:E:117:PRO:HA	2.11	0.65
3:G:33:ARG:HD3	6:G:502:HOH:O	1.96	0.65
3:G:63:SER:O	3:G:66:ASN:OD1	2.14	0.65
3:E:62:ASP:OD2	3:E:62:ASP:C	2.39	0.65
3:E:73:THR:CG2	3:E:74:MET:N	2.58	0.65
3:E:81:ILE:HD13	3:E:81:ILE:C	2.20	0.65
3:E:289:HIS:CE1	6:E:491:HOH:O	2.48	0.65
3:G:86:GLN:HE22	3:G:327:THR:CB	2.09	0.65
1:A:547:ARG:O	1:A:548:THR:HB	1.96	0.65
3:G:63:SER:C	3:G:66:ASN:H	2.05	0.65
1:A:492:SER:O	1:A:494:MET:N	2.30	0.65
2:D:245:THR:CA	6:D:302:HOH:O	2.44	0.65
2:B:213:PRO:HB2	2:B:216:LEU:HD12	1.78	0.65
3:G:52:LEU:HD22	3:G:52:LEU:N	2.12	0.65
2:B:249:GLU:HB3	3:G:168:LYS:HZ3	1.62	0.65
3:G:152:THR:HG22	3:G:152:THR:O	1.96	0.65
3:E:197:THR:HG22	3:E:220:PRO:HG2	1.77	0.65
3:E:223:ASN:OD1	6:E:466:HOH:O	2.14	0.65
3:E:231:VAL:O	6:E:486:HOH:O	2.14	0.65
3:E:251:LEU:HB3	3:E:255:GLU:HG3	1.78	0.65
3:E:63:SER:O	3:E:64:GLU:C	2.40	0.64
1:A:491:ARG:HG2	1:A:492:SER:H	1.60	0.64
3:G:141:ARG:NH2	3:G:215:ASN:OD1	2.29	0.64
3:E:183:PRO:HA	3:E:274:ASP:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:HIS:NE2	1:A:545:PRO:HG2	2.12	0.64
2:D:240:ILE:HG23	6:D:307:HOH:O	1.97	0.64
3:E:231:VAL:HG12	3:E:267:VAL:HG22	1.79	0.64
3:G:12:LEU:HD23	3:G:180:LEU:HD21	1.79	0.64
3:G:166:ILE:O	3:G:169:PHE:O	2.14	0.64
6:C:42:HOH:O	3:E:156:MET:HE3	1.96	0.64
3:E:232:TYR:CD2	3:E:253:VAL:HG13	2.32	0.64
2:D:245:THR:CB	6:D:302:HOH:O	2.45	0.64
1:A:489:LYS:HA	6:A:91:HOH:O	1.97	0.64
3:G:81:ILE:HG12	3:G:94:ILE:HD11	1.80	0.64
3:E:81:ILE:C	3:E:81:ILE:CD1	2.71	0.64
3:E:232:TYR:HD2	3:E:253:VAL:HG13	1.62	0.64
3:G:87:SER:O	3:G:88:SER:HB3	1.98	0.64
3:E:141:ARG:O	3:E:163:GLN:HG3	1.98	0.64
3:G:8:GLN:HE22	3:G:187:MET:CE	2.07	0.64
3:E:223:ASN:O	3:E:226:GLY:N	2.22	0.64
3:E:319:THR:O	3:E:321:PRO:HD3	1.98	0.63
2:B:250:ASP:C	2:B:252:SER:H	2.04	0.63
4:E:401:ATP:O2B	4:E:401:ATP:O5'	2.16	0.63
3:G:87:SER:O	3:G:88:SER:CB	2.46	0.63
3:G:135:MET:HE1	3:G:166:ILE:CD1	2.28	0.63
2:B:271:GLN:N	2:B:271:GLN:OE1	2.31	0.63
3:E:166:ILE:C	3:E:166:ILE:HD13	2.22	0.63
3:G:111:LYS:HG3	3:G:111:LYS:O	1.97	0.63
3:E:144:PRO:HB2	3:E:146:ILE:CD1	2.27	0.63
2:D:230:PRO:HB2	6:D:317:HOH:O	1.99	0.63
3:G:168:LYS:O	3:G:172:MET:HG3	1.98	0.63
1:C:500:ARG:HD2	1:C:514:TYR:HD2	1.61	0.63
1:A:458:CYS:HB2	1:A:529:PHE:HB2	1.80	0.62
3:G:120:ILE:HG12	3:G:143:ILE:HG13	1.81	0.62
2:D:235:HIS:HB3	6:D:326:HOH:O	1.97	0.62
3:E:190:GLY:O	3:E:192:TRP:CD1	2.52	0.62
3:E:314:ILE:HG21	6:E:508:HOH:O	2.00	0.62
3:G:51:THR:HG21	3:G:242:GLN:OE1	1.99	0.62
1:C:556:LEU:HD23	3:E:156:MET:SD	2.39	0.62
3:E:110:ARG:HE	3:E:110:ARG:HA	1.64	0.62
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.65	0.62
3:G:96:GLU:OE1	6:G:410:HOH:O	2.16	0.62
3:G:5:GLN:HE21	3:G:9:LYS:HE2	1.64	0.62
1:A:523:GLU:HA	1:A:529:PHE:HD2	1.65	0.62
1:A:574:PHE:CD2	3:E:93:ALA:HB2	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:ARG:HG3	2:D:282:ARG:NH1	2.08	0.62
3:G:44:LYS:HZ1	2:D:272:LEU:HA	1.65	0.61
3:G:129:MET:HE1	3:G:314:ILE:HB	1.82	0.61
3:G:162:THR:HG23	3:G:165:ARG:H	1.64	0.61
3:E:165:ARG:HG3	6:E:489:HOH:O	1.99	0.61
3:G:80:VAL:HG21	3:G:97:ILE:HD11	1.80	0.61
1:A:520:GLN:HG2	1:A:522:TYR:CZ	2.35	0.61
3:E:94:ILE:HG23	3:E:95:ALA:N	2.15	0.61
3:G:156:MET:O	3:G:158:VAL:HG23	2.01	0.61
3:G:44:LYS:NZ	2:D:272:LEU:HA	2.15	0.61
3:G:78:VAL:N	6:G:477:HOH:O	2.06	0.61
3:E:185:ASN:HD22	3:E:185:ASN:C	2.06	0.61
1:A:466:LEU:CD1	1:A:497:ILE:HD11	2.31	0.61
3:G:8:GLN:NE2	3:G:187:MET:HE2	2.11	0.61
3:E:200:MET:HG3	3:E:254:GLY:HA2	1.82	0.61
3:G:197:THR:HG22	3:G:220:PRO:HG2	1.82	0.61
3:E:303:ILE:CG2	6:E:490:HOH:O	2.18	0.61
1:A:465:ILE:O	1:A:466:LEU:C	2.44	0.60
3:G:189:ILE:HD13	3:G:312:TYR:CD2	2.36	0.60
1:A:500:ARG:HD3	1:A:516:TYR:CE1	2.36	0.60
3:G:187:MET:SD	3:G:189:ILE:HD11	2.41	0.60
2:B:268:ALA:O	2:B:276:ALA:HB3	2.01	0.60
2:D:250:ASP:O	2:D:253:VAL:HG12	1.99	0.60
3:E:275:ARG:O	3:E:277:ASP:N	2.34	0.60
3:G:162:THR:HG23	3:G:164[B]:TYR:CD1	2.36	0.60
3:E:129:MET:CE	3:E:314:ILE:CG1	2.80	0.60
1:A:533:VAL:HG12	1:A:534:LYS:N	2.16	0.60
3:G:135:MET:O	3:G:138:SER:O	2.19	0.60
1:A:459:ARG:HA	1:A:527:GLY:O	2.01	0.60
2:B:249:GLU:CB	3:G:168:LYS:NZ	2.65	0.60
1:C:477:GLY:N	6:C:208:HOH:O	2.32	0.60
3:E:128:LEU:HD11	3:E:166:ILE:HG13	1.84	0.60
3:E:268:HIS:O	3:E:291:LEU:HD23	2.02	0.60
1:A:502:GLU:HG3	6:A:239:HOH:O	2.02	0.60
3:G:74:MET:SD	3:G:238:MET:HB2	2.41	0.60
1:A:494:MET:HE2	2:B:227:PRO:CG	2.24	0.60
3:E:66:ASN:ND2	6:E:447:HOH:O	2.34	0.60
3:G:63:SER:C	3:G:65:ALA:N	2.59	0.59
3:E:185:ASN:HD22	3:E:186:GLN:H	1.49	0.59
1:A:502:GLU:O	1:A:504:PRO:HD3	2.03	0.59
1:C:486:VAL:N	1:C:489:LYS:O	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:217:SER:OG	3:E:290:ARG:NH1	2.36	0.59
2:B:249:GLU:HB2	3:G:168:LYS:NZ	2.16	0.59
2:D:224:LEU:O	2:D:225:LYS:HB3	2.01	0.59
3:G:295:ASP:OD1	3:G:295:ASP:C	2.45	0.59
2:D:240:ILE:HG21	2:D:257:PRO:HA	1.82	0.59
3:E:131:ALA:O	3:E:135:MET:HG3	2.02	0.59
3:E:306:LEU:HB2	4:E:401:ATP:O1G	2.00	0.59
2:B:288:VAL:HG22	3:G:32:PHE:CZ	2.38	0.59
3:G:215:ASN:ND2	3:G:332:SER:HB2	2.13	0.59
1:A:574:PHE:CD2	3:E:93:ALA:CB	2.86	0.59
3:G:305:SER:O	3:G:308:ASP:HB2	2.03	0.59
2:D:292:MET:HE3	2:D:294:LYS:HB2	1.85	0.59
3:G:169:PHE:C	6:G:507:HOH:O	2.40	0.59
3:G:181:ARG:HA	3:G:275:ARG:HG3	1.84	0.59
1:C:558:SER:HB2	3:E:156:MET:SD	2.42	0.59
3:G:37:PHE:HB3	3:G:41:LEU:CD1	2.33	0.58
3:E:73:THR:HG22	3:E:74:MET:N	2.14	0.58
3:E:181:ARG:HH21	3:E:275:ARG:HH22	1.49	0.58
1:A:557:LYS:O	2:B:281:THR:HG21	2.03	0.58
3:E:193:SER:HA	6:E:463:HOH:O	2.02	0.58
2:B:270:THR:O	2:B:271:GLN:HB2	2.04	0.58
2:D:225:LYS:HZ3	2:D:227:PRO:CD	2.14	0.58
3:E:312:TYR:C	3:E:314:ILE:H	2.11	0.58
1:A:520:GLN:HG2	1:A:522:TYR:CE2	2.38	0.58
2:B:249:GLU:C	2:B:249:GLU:CD	2.71	0.58
3:G:12:LEU:CD2	3:G:180:LEU:HD22	2.33	0.58
3:E:255:GLU:O	3:E:256:ALA:C	2.43	0.58
2:B:249:GLU:O	2:B:249:GLU:CD	2.47	0.58
3:G:74:MET:HG3	3:G:235:VAL:HA	1.84	0.58
3:G:129:MET:HE1	3:G:314:ILE:CB	2.34	0.58
1:C:503:ILE:HD13	1:C:503:ILE:H	1.48	0.58
3:E:53:ASN:O	3:E:55:ILE:HG23	2.03	0.58
3:E:145:LEU:HD11	3:E:161:LEU:HD13	1.84	0.58
2:B:283:TYR:OH	3:G:124:PRO:HG2	2.04	0.58
3:G:88:SER:O	3:G:89:SER:HB2	2.03	0.58
3:G:144:PRO:HB2	3:G:146:ILE:CD1	2.27	0.58
2:D:282:ARG:HH11	2:D:282:ARG:CG	2.07	0.58
2:D:272:LEU:O	2:D:274:VAL:HG13	2.03	0.58
1:A:466:LEU:HD22	1:A:495:TYR:CD2	2.39	0.57
3:G:39:VAL:HG22	3:G:61:TRP:O	2.02	0.57
3:E:77:PHE:O	3:E:81:ILE:CG2	2.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:86:GLN:O	3:E:86:GLN:HG3	2.05	0.57
3:E:110:ARG:HA	3:E:110:ARG:NE	2.19	0.57
3:E:319:THR:C	3:E:321:PRO:HD3	2.29	0.57
1:A:459:ARG:HH21	3:E:91:PRO:HG2	1.69	0.57
2:B:209:SER:OG	2:B:210:THR:N	2.36	0.57
3:E:175:LYS:HD2	3:E:175:LYS:C	2.29	0.57
3:E:227:THR:HA	3:E:298:LEU:O	2.05	0.57
3:G:163:GLN:HE22	3:G:307:ALA:HB2	1.69	0.57
1:C:561:PRO:CB	6:E:447:HOH:O	2.42	0.57
3:E:191:THR:HG22	3:E:192:TRP:N	2.19	0.57
3:E:296:GLU:CB	6:E:488:HOH:O	2.53	0.57
1:A:574:PHE:CE2	3:E:93:ALA:HB2	2.39	0.57
3:E:94:ILE:O	3:E:97:ILE:N	2.28	0.57
3:E:275:ARG:HG3	3:E:277:ASP:OD2	2.05	0.57
3:G:214:LYS:NZ	6:G:426:HOH:O	2.36	0.57
1:C:513:THR:HA	1:C:540:ASP:HA	1.86	0.57
3:E:305:SER:HA	6:E:520:HOH:O	2.05	0.57
3:E:328:ASP:CG	3:E:328:ASP:O	2.48	0.57
2:B:240:ILE:HB	2:B:255:PRO:HG2	1.86	0.56
3:E:73:THR:HB	6:E:451:HOH:O	2.04	0.56
3:G:86:GLN:HB3	3:G:209:LYS:NZ	2.20	0.56
3:G:162:THR:HG22	3:G:165:ARG:H	1.70	0.56
3:G:236:ASP:OD2	3:G:260:ARG:HD3	2.06	0.56
1:C:472:ALA:CB	1:C:572:LYS:HB3	2.34	0.56
3:E:96:GLU:O	3:E:97:ILE:C	2.47	0.56
3:E:102:LEU:O	3:E:106:ARG:HG2	2.06	0.56
1:A:544:HIS:ND1	1:A:545:PRO:HD2	2.20	0.56
3:G:179:MET:HA	3:G:181:ARG:HD3	1.87	0.56
3:E:66:ASN:HB3	3:E:154:SER:HG	1.66	0.56
3:E:141:ARG:HB2	3:E:333:ALA:O	2.06	0.56
3:E:245:ASP:O	3:E:248:ASN:HB2	2.05	0.56
1:A:509:GLU:O	1:A:509:GLU:HG3	2.06	0.56
1:C:479:GLN:CD	1:C:500:ARG:HH12	2.07	0.56
1:C:568:MET:O	1:C:569:LEU:C	2.47	0.56
3:E:68:PHE:CE1	3:E:70:GLY:O	2.58	0.56
1:A:502:GLU:CG	6:A:239:HOH:O	2.53	0.56
3:G:162:THR:HA	6:G:493:HOH:O	2.04	0.56
3:G:183:PRO:HB2	3:G:185:ASN:HD21	1.71	0.56
1:C:505:HIS:CD2	3:E:66:ASN:HB2	2.40	0.56
1:C:560:PHE:HD2	1:C:564:ASP:OD2	1.87	0.56
3:G:90:PHE:CZ	1:C:573:LEU:HD22	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:92:GLU:HB3	6:C:400:HOH:O	2.05	0.56
1:A:500:ARG:HD3	1:A:516:TYR:HE1	1.70	0.56
3:G:295:ASP:OD2	3:G:299:LYS:CB	2.54	0.56
2:D:212:ILE:CG1	2:D:217:THR:HG22	2.36	0.56
3:E:8:GLN:NE2	3:E:182:VAL:HB	2.21	0.56
3:E:81:ILE:HG23	3:E:208:ILE:HG21	1.88	0.56
3:E:81:ILE:HG12	3:E:94:ILE:HD11	1.87	0.56
3:G:9:LYS:O	3:G:13:LYS:HG3	2.05	0.56
1:C:504:PRO:HG2	6:E:456:HOH:O	2.06	0.56
3:E:92:GLU:O	3:E:93:ALA:HB3	2.02	0.56
3:E:184:LEU:CA	3:E:187:MET:HE2	2.32	0.56
1:A:517:ILE:HG22	1:A:519:LEU:HD11	1.88	0.56
2:D:234:PRO:O	2:D:236:LEU:O	2.23	0.56
3:E:116:PRO:HB2	6:E:476:HOH:O	2.06	0.56
3:G:290:ARG:HE	4:G:401:ATP:PG	2.29	0.55
1:C:454:PHE:O	1:C:530:MET:HE2	2.07	0.55
3:E:25:TYR:O	3:E:27:VAL:N	2.40	0.55
3:E:71:LEU:HD22	3:E:144:PRO:HD3	1.89	0.55
1:C:481:THR:HG23	6:C:315:HOH:O	2.06	0.55
1:C:561:PRO:CA	6:E:447:HOH:O	2.53	0.55
2:D:296:PHE:O	2:D:297:ASP:CG	2.50	0.55
1:C:470:TYR:O	1:C:474:GLN:N	2.40	0.55
2:D:223:GLU:OE1	2:D:223:GLU:C	2.50	0.55
3:E:212:ALA:O	3:E:213:GLU:CB	2.51	0.55
3:G:39:VAL:HG21	3:G:62:ASP:CB	2.26	0.55
3:G:62:ASP:O	3:G:67:LYS:O	2.25	0.55
1:C:500:ARG:HH11	1:C:500:ARG:CG	2.16	0.55
1:C:511:LYS:CA	6:C:211:HOH:O	2.54	0.55
3:G:215:ASN:O	3:G:216:ILE:HD13	2.07	0.55
1:C:502:GLU:O	1:C:503:ILE:C	2.49	0.55
3:E:223:ASN:O	3:E:224:SER:C	2.50	0.55
1:C:464:GLU:O	1:C:467:LEU:HB3	2.07	0.55
1:C:475:ARG:HG3	1:C:572:LYS:HG3	1.89	0.55
2:D:237:GLU:O	2:D:237:GLU:HG2	2.07	0.55
2:D:293:PHE:CG	3:E:49:LEU:HD13	2.42	0.55
3:E:181:ARG:HH21	3:E:275:ARG:NH2	2.05	0.55
3:E:177:THR:O	3:E:180:LEU:HG	2.07	0.55
1:A:546:GLU:O	1:A:547:ARG:HB2	2.07	0.54
2:B:259[B]:HIS:CD2	2:B:259[B]:HIS:H	2.25	0.54
3:G:106:ARG:O	3:G:110:ARG:HB2	2.07	0.54
3:E:188:THR:N	6:E:462:HOH:O	2.33	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:255:GLU:O	3:E:257:LEU:N	2.41	0.54
3:G:257:LEU:CD1	6:G:513:HOH:O	2.56	0.54
3:E:265:ASP:OD1	3:E:287:ARG:HD3	2.07	0.54
3:G:169:PHE:O	3:G:170:ILE:CG1	2.49	0.54
2:D:284:HIS:NE2	3:E:125:MET:HE2	2.22	0.54
3:E:19:ILE:HG21	3:E:129:MET:CE	2.37	0.54
3:G:193:SER:O	3:G:194:ASN:HB2	2.07	0.54
3:G:291:LEU:HD12	3:G:291:LEU:N	2.23	0.54
1:C:500:ARG:CG	1:C:514:TYR:HD2	2.20	0.54
1:C:503:ILE:HG12	1:C:506:CYS:HB2	1.88	0.54
1:C:540:ASP:O	1:C:542:TYR:N	2.36	0.54
3:E:73:THR:CG2	3:E:334:VAL:H	2.20	0.54
3:E:94:ILE:CG2	3:E:95:ALA:H	2.19	0.54
3:E:252:SER:OG	3:E:255:GLU:HG2	2.06	0.54
3:E:311:ASN:HA	3:E:314:ILE:HG22	1.89	0.54
3:G:231:VAL:HG22	3:G:232:TYR:N	2.23	0.54
2:D:239:CYS:HB2	2:D:242:ASN:ND2	2.22	0.54
3:E:36:VAL:HG12	3:E:37:PHE:N	2.21	0.54
3:E:222:VAL:HG23	3:E:223:ASN:N	2.23	0.54
2:B:274:VAL:HB	2:B:294:LYS:O	2.08	0.53
6:C:205:HOH:O	2:D:212:ILE:CG2	2.50	0.53
3:E:192:TRP:CH2	3:E:293:VAL:HG11	2.44	0.53
1:A:544:HIS:C	1:A:546:GLU:H	2.17	0.53
1:A:574:PHE:CG	3:E:93:ALA:CB	2.92	0.53
1:C:500:ARG:CD	1:C:514:TYR:HD2	2.21	0.53
1:A:503:ILE:HG23	1:A:561:PRO:HG3	1.90	0.53
2:B:247:TYR:O	2:B:248:LYS:C	2.50	0.53
3:G:70:GLY:HA3	3:G:106:ARG:NH2	2.23	0.53
3:E:200:MET:HG3	3:E:254:GLY:CA	2.38	0.53
3:G:39:VAL:CG2	3:G:62:ASP:HB2	2.26	0.53
3:G:182:VAL:HB	3:G:187:MET:HE2	1.91	0.53
2:D:221:LEU:HB3	6:D:312:HOH:O	2.08	0.53
3:E:282:ALA:O	3:E:283:ILE:C	2.51	0.53
1:A:522:TYR:CE1	2:B:233:PRO:HD3	2.43	0.53
2:B:215:PHE:O	2:B:216:LEU:HB2	2.06	0.53
3:G:117:PRO:O	6:G:419:HOH:O	2.19	0.53
1:C:561:PRO:HA	6:E:447:HOH:O	2.07	0.53
1:C:503:ILE:HD12	1:C:503:ILE:H	1.69	0.53
1:A:462:ALA:HB3	1:A:463:PRO:CD	2.38	0.53
3:G:126:HIS:ND1	6:G:453:HOH:O	2.34	0.53
2:D:258:ASN:ND2	2:D:260:VAL:H	2.00	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:75:ALA:O	3:E:76:ASP:C	2.52	0.53
3:E:235:VAL:HG23	3:E:235:VAL:O	2.08	0.53
1:A:540:ASP:N	3:G:151:GLU:OE1	2.24	0.52
3:G:44:LYS:HD2	6:G:412:HOH:O	2.09	0.52
3:G:118:GLU:CD	3:G:118:GLU:H	2.18	0.52
3:G:198:ALA:HB1	3:G:202:THR:OG1	2.09	0.52
3:G:235:VAL:C	3:G:237:VAL:H	2.16	0.52
3:E:110:ARG:NH1	3:E:117:PRO:CA	2.71	0.52
3:E:254:GLY:HA3	6:E:418:HOH:O	2.08	0.52
1:A:500:ARG:NH1	1:A:514:TYR:CE2	2.78	0.52
1:C:503:ILE:CG1	1:C:506:CYS:HB2	2.40	0.52
2:B:250:ASP:C	2:B:252:SER:N	2.58	0.52
3:G:276:LEU:O	3:G:277:ASP:C	2.51	0.52
1:A:466:LEU:HD12	1:A:497:ILE:HD11	1.92	0.52
3:G:28:LEU:HD13	3:G:32:PHE:CZ	2.45	0.52
3:E:68:PHE:CE1	3:E:70:GLY:C	2.88	0.52
3:E:165:ARG:HH22	5:E:402:FLC:HG1	1.74	0.52
3:G:11:ALA:O	3:G:15:ILE:HG12	2.09	0.52
1:A:541:ILE:HG22	1:A:541:ILE:O	2.09	0.52
3:G:85:TYR:O	3:G:86:GLN:CG	2.57	0.52
3:G:203:LYS:NZ	6:G:501:HOH:O	2.43	0.52
3:E:314:ILE:HG23	3:E:314:ILE:O	2.10	0.52
3:G:139:ARG:C	3:G:141:ARG:N	2.56	0.51
1:C:484:LYS:HB3	1:C:484:LYS:HZ2	1.73	0.51
1:A:489:LYS:CB	6:A:91:HOH:O	2.57	0.51
1:A:533:VAL:HB	2:B:265:LEU:HB3	1.92	0.51
1:A:573:LEU:HD22	3:E:90:PHE:CZ	2.44	0.51
2:B:249:GLU:OE2	3:G:165:ARG:CG	2.49	0.51
3:G:129:MET:HE1	3:G:314:ILE:HG22	1.93	0.51
1:C:500:ARG:CD	1:C:514:TYR:CD2	2.93	0.51
1:A:503:ILE:HB	1:A:506:CYS:HB2	1.93	0.51
3:G:59:PRO:C	3:G:60:LEU:HD23	2.36	0.51
3:E:172:MET:HA	3:E:284:LYS:HE3	1.92	0.51
3:G:215:ASN:HD21	3:G:332:SER:CB	2.14	0.51
3:G:235:VAL:C	3:G:237:VAL:N	2.68	0.51
3:G:252:SER:O	3:G:253:VAL:C	2.53	0.51
3:E:216:ILE:HG22	4:E:401:ATP:H5'2	1.92	0.51
1:A:544:HIS:CG	1:A:545:PRO:CD	2.93	0.51
2:D:226:LEU:CD1	2:D:228:LYS:HE2	2.34	0.51
3:E:47:LEU:HD12	6:E:470:HOH:O	2.11	0.51
3:G:33:ARG:NH1	6:G:448:HOH:O	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:CYS:O	1:A:507:LYS:C	2.53	0.51
3:G:237:VAL:O	3:G:238:MET:C	2.54	0.51
3:E:195:LEU:HA	4:E:401:ATP:C2	2.45	0.51
3:E:309:ILE:O	3:E:313:ILE:HG12	2.10	0.51
3:G:169:PHE:CE1	3:G:173:ASN:ND2	2.79	0.51
3:G:222:VAL:HA	3:G:227:THR:O	2.11	0.51
3:G:258:LEU:HB2	6:G:514:HOH:O	2.11	0.51
3:G:293:VAL:HB	3:G:302:GLY:H	1.75	0.51
3:G:329:ASN:ND2	3:G:330:PHE:H	2.09	0.51
1:A:536:ASN:C	1:A:536:ASN:HD22	2.19	0.51
2:B:240:ILE:C	2:B:242:ASN:N	2.68	0.51
3:G:33:ARG:NH2	6:G:484:HOH:O	2.44	0.51
3:G:96:GLU:C	3:G:98:ASP:N	2.67	0.51
1:A:562:PHE:O	1:A:565:LEU:HD23	2.11	0.50
1:C:561:PRO:O	1:C:562:PHE:C	2.54	0.50
2:D:216:LEU:HA	2:D:221:LEU:HD23	1.93	0.50
1:A:523:GLU:HG3	1:A:529:PHE:CE2	2.46	0.50
2:B:241:LEU:C	2:B:243:SER:H	2.19	0.50
3:G:63:SER:HA	3:G:66:ASN:N	2.24	0.50
1:A:551:HIS:HB3	6:A:353:HOH:O	2.11	0.50
3:G:184:LEU:C	3:G:186:GLN:H	2.19	0.50
3:G:222:VAL:HG12	3:G:228:LEU:HA	1.93	0.50
3:G:281:ASP:OD2	3:G:281:ASP:C	2.55	0.50
3:G:80:VAL:CG2	3:G:97:ILE:CD1	2.83	0.50
3:E:129:MET:HE1	6:E:508:HOH:O	2.11	0.50
1:A:458:CYS:N	1:A:529:PHE:O	2.39	0.50
1:A:500:ARG:NE	6:A:56:HOH:O	2.44	0.50
2:B:222:GLN:OE1	2:B:222:GLN:CA	2.57	0.50
3:G:24:SER:O	3:G:26:ASP:N	2.44	0.50
1:C:506:CYS:C	1:C:508:ARG:H	2.19	0.50
2:B:282:ARG:HB2	2:B:282:ARG:CZ	2.39	0.50
3:E:21:SER:O	6:E:450:HOH:O	2.20	0.50
3:E:237:VAL:O	3:E:238:MET:C	2.54	0.50
3:E:314:ILE:CG2	6:E:508:HOH:O	2.58	0.50
1:A:520:GLN:CG	1:A:522:TYR:CE2	2.94	0.50
2:B:265:LEU:HD12	2:B:266:ALA:N	2.26	0.50
3:G:182:VAL:O	3:G:187:MET:CE	2.46	0.50
3:G:184:LEU:C	3:G:186:GLN:N	2.69	0.50
3:G:257:LEU:HD22	3:G:257:LEU:H	1.75	0.50
1:C:561:PRO:HB2	1:C:565:LEU:HD22	1.92	0.50
3:E:177:THR:CG2	3:E:280:PHE:CD2	2.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ILE:HG22	1:A:519:LEU:CD1	2.41	0.50
3:E:47:LEU:O	3:E:48:SER:C	2.50	0.50
3:G:16:GLN:HG2	3:G:313:ILE:O	2.12	0.49
3:G:167:LEU:O	3:G:170:ILE:HB	2.12	0.49
3:E:181:ARG:NH2	3:E:275:ARG:HH22	2.10	0.49
3:G:5:GLN:O	3:G:9:LYS:HG2	2.12	0.49
3:G:138:SER:O	3:G:139:ARG:C	2.53	0.49
1:C:471:ARG:O	1:C:475:ARG:HG2	2.12	0.49
2:D:213:PRO:O	2:D:217:THR:HG23	2.12	0.49
3:E:149:ASP:O	3:E:153:GLY:N	2.40	0.49
3:E:166:ILE:HD13	3:E:166:ILE:O	2.12	0.49
3:E:248:ASN:O	3:E:251:LEU:HD12	2.12	0.49
3:E:295:ASP:HB3	3:E:301:GLU:OE1	2.12	0.49
1:C:479:GLN:CG	2:D:210:THR:HG22	2.42	0.49
6:C:77:HOH:O	2:D:230:PRO:HD3	2.12	0.49
3:E:253:VAL:O	3:E:254:GLY:C	2.55	0.49
3:E:270:CYS:SG	3:E:293:VAL:HG22	2.52	0.49
1:A:543:SER:H	1:A:544:HIS:HA	1.77	0.49
1:A:560:PHE:HA	1:A:562:PHE:N	2.27	0.49
3:G:135:MET:O	3:G:136:SER:C	2.55	0.49
3:G:139:ARG:CB	3:G:332:SER:CB	2.90	0.49
3:G:162:THR:HG22	3:G:165:ARG:HB2	1.94	0.49
1:C:524:VAL:HG22	2:D:232:LEU:HD23	1.95	0.49
3:E:198:ALA:HB1	3:E:202:THR:CB	2.43	0.49
3:E:207:VAL:O	3:E:211:LEU:HG	2.12	0.49
3:G:76:ASP:O	3:G:80:VAL:HG12	2.12	0.49
3:G:12:LEU:HD21	3:G:180:LEU:HD22	1.95	0.49
3:G:51:THR:CG2	3:G:242:GLN:OE1	2.61	0.49
3:G:149:ASP:OD1	3:G:149:ASP:C	2.53	0.49
1:C:541:ILE:HG23	1:C:541:ILE:O	2.12	0.49
3:E:67:LYS:HA	3:E:155:GLU:HG3	1.93	0.49
3:E:123:HIS:HD2	3:E:125:MET:H	1.61	0.49
1:A:495:TYR:HE1	2:B:227:PRO:O	1.95	0.49
1:C:519:LEU:HD23	1:C:531:LEU:HD21	1.94	0.49
1:A:550:ASP:CG	1:A:551:HIS:H	2.20	0.49
3:G:149:ASP:OD1	3:G:149:ASP:O	2.31	0.49
3:G:294:VAL:HA	3:G:299:LYS:O	2.13	0.49
3:E:231:VAL:C	6:E:486:HOH:O	2.54	0.49
3:E:133:LEU:O	3:E:134:ALA:C	2.55	0.48
3:E:204:VAL:HG11	3:E:240:LEU:HD22	1.95	0.48
3:G:163:GLN:N	6:G:493:HOH:O	1.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:217:SER:N	4:G:401:ATP:O1B	2.44	0.48
1:C:542:TYR:CD1	1:C:542:TYR:C	2.90	0.48
3:E:43:VAL:HG21	3:E:105:LEU:HD13	1.95	0.48
3:G:86:GLN:CB	3:G:209:LYS:NZ	2.77	0.48
3:G:185:ASN:HD22	3:G:185:ASN:C	2.17	0.48
2:D:221:LEU:O	2:D:221:LEU:HD22	2.13	0.48
2:D:225:LYS:CG	2:D:226:LEU:N	2.66	0.48
3:E:274:ASP:O	3:E:275:ARG:HB3	2.13	0.48
2:D:212:ILE:HG13	2:D:217:THR:HG22	1.94	0.48
1:A:535:SER:HB2	1:A:562:PHE:CG	2.47	0.48
1:A:550:ASP:CG	1:A:551:HIS:N	2.71	0.48
2:B:246:ALA:O	2:B:248:LYS:N	2.46	0.48
3:G:85:TYR:O	3:G:86:GLN:HG3	2.12	0.48
3:G:241:ILE:HD12	3:G:246:TYR:CE2	2.49	0.48
3:G:97:ILE:HA	3:G:100:PHE:HD1	1.78	0.48
1:A:503:ILE:CD1	1:A:515:ALA:HB2	2.43	0.48
1:A:503:ILE:HD11	1:A:515:ALA:HB2	1.95	0.48
2:B:250:ASP:HB3	2:B:252:SER:H	1.79	0.48
3:G:96:GLU:O	3:G:97:ILE:C	2.53	0.48
3:E:240:LEU:HD23	3:E:249:LEU:HD23	1.95	0.48
3:G:45:THR:O	3:G:49:LEU:HG	2.13	0.48
2:D:226:LEU:H	2:D:227:PRO:HD3	1.78	0.48
1:A:552:GLY:HA2	1:A:553:MET:HA	1.54	0.48
3:G:86:GLN:HB3	3:G:209:LYS:HZ1	1.79	0.48
2:D:283:TYR:C	2:D:283:TYR:CD2	2.92	0.48
3:E:122:VAL:HG22	3:E:143:ILE:HD11	1.94	0.48
3:E:141:ARG:HH12	3:E:217:SER:N	2.12	0.48
3:E:218:ALA:HB1	3:E:231:VAL:CG2	2.43	0.48
3:E:309:ILE:O	3:E:310:LEU:C	2.57	0.48
1:A:461:ASP:HB2	6:A:234:HOH:O	2.14	0.48
2:B:222:GLN:O	2:B:223:GLU:C	2.57	0.48
1:A:466:LEU:HD22	1:A:495:TYR:CE2	2.49	0.47
2:B:238:LYS:CG	2:B:238:LYS:O	2.62	0.47
3:G:82:LYS:O	3:G:85:TYR:O	2.32	0.47
2:D:225:LYS:NZ	2:D:227:PRO:HD2	2.27	0.47
3:E:142:ARG:HB2	3:E:161:LEU:O	2.14	0.47
3:E:175:LYS:CB	6:E:429:HOH:O	2.61	0.47
2:B:249:GLU:HB3	3:G:168:LYS:NZ	2.27	0.47
3:G:80:VAL:HG23	3:G:84:TYR:CE1	2.50	0.47
3:G:129:MET:HE1	3:G:314:ILE:CG2	2.44	0.47
1:C:561:PRO:HB2	1:C:565:LEU:CD2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:297:ASN:HB3	3:E:299:LYS:NZ	2.28	0.47
1:A:491:ARG:HG2	1:A:492:SER:N	2.29	0.47
2:B:223:GLU:C	2:B:225:LYS:N	2.70	0.47
3:G:189:ILE:HG23	3:G:312:TYR:CD2	2.49	0.47
1:C:521:LEU:HD12	2:D:229:PRO:CB	2.42	0.47
3:E:329:ASN:HB3	3:E:330:PHE:H	1.42	0.47
3:G:75:ALA:HB1	6:G:521:HOH:O	2.13	0.47
3:G:200:MET:O	3:G:252:SER:HB2	2.15	0.47
3:E:312:TYR:C	3:E:314:ILE:N	2.69	0.47
3:E:83:TYR:CE2	3:E:112:ILE:HG21	2.50	0.47
3:G:3:ASP:HB3	3:G:6:GLU:CB	2.45	0.47
1:C:511:LYS:HA	6:C:211:HOH:O	2.13	0.47
3:E:302:GLY:C	3:E:303:ILE:HG13	2.40	0.47
1:A:482:VAL:HG13	2:B:213:PRO:HG3	1.96	0.47
1:C:567:ALA:HB3	6:C:264:HOH:O	2.14	0.47
3:E:191:THR:CG2	3:E:192:TRP:N	2.78	0.47
1:A:449:ARG:HA	1:A:451:LYS:HG2	1.97	0.47
3:G:96:GLU:O	3:G:98:ASP:N	2.48	0.47
3:E:181:ARG:NE	3:E:275:ARG:HH22	2.04	0.47
3:E:265:ASP:OD2	3:E:289:HIS:CE1	2.68	0.47
1:A:561:PRO:HB3	3:G:66:ASN:HD21	1.80	0.46
3:G:43:VAL:CG1	6:G:485:HOH:O	2.39	0.46
1:C:561:PRO:O	1:C:564:ASP:N	2.48	0.46
3:E:255:GLU:C	3:E:257:LEU:N	2.73	0.46
2:B:224:LEU:O	2:B:226:LEU:HD23	2.15	0.46
3:G:2:MET:CB	6:G:464:HOH:O	2.54	0.46
3:G:63:SER:H	3:G:65:ALA:H	1.58	0.46
3:E:216:ILE:HD13	3:E:216:ILE:HG21	1.57	0.46
3:G:39:VAL:HG13	3:G:60:LEU:HB3	1.97	0.46
3:G:271:ARG:NH1	3:G:296:GLU:HA	2.31	0.46
3:E:74:MET:HG2	6:E:497:HOH:O	2.14	0.46
3:E:257:LEU:HA	3:E:257:LEU:HD12	1.51	0.46
1:A:465:ILE:HG12	6:E:454:HOH:O	2.15	0.46
1:C:563:LEU:O	1:C:566:CYS:HB2	2.15	0.46
1:C:556:LEU:HD11	3:E:149:ASP:HA	1.98	0.46
1:A:574:PHE:CG	3:E:93:ALA:HB1	2.51	0.46
3:G:195:LEU:CD2	3:G:303:ILE:HD12	2.36	0.46
1:C:535:SER:HB2	1:C:562:PHE:CD1	2.51	0.46
1:A:465:ILE:O	1:A:468:ALA:N	2.48	0.46
3:G:306:LEU:HD23	3:G:306:LEU:HA	1.61	0.46
2:D:285:ARG:HD2	2:D:285:ARG:HA	1.60	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:185:ASN:HD22	3:G:186:GLN:HG3	1.75	0.46
1:A:507:LYS:HD3	1:A:507:LYS:O	2.16	0.46
3:G:60:LEU:N	3:G:60:LEU:CD2	2.66	0.46
3:G:102:LEU:HD12	3:G:102:LEU:HA	1.79	0.46
3:E:67:LYS:NZ	6:E:459:HOH:O	2.49	0.46
1:A:531:LEU:HD12	1:A:531:LEU:HA	1.75	0.46
3:G:185:ASN:HD22	3:G:186:GLN:H	1.63	0.46
3:E:38:ASP:O	3:E:39:VAL:C	2.57	0.46
3:E:288:VAL:HG12	3:E:290:ARG:H	1.81	0.46
3:G:47:LEU:HA	3:G:50:LEU:HD12	1.97	0.45
1:C:462:ALA:HB1	1:C:495:TYR:CE2	2.51	0.45
3:E:142:ARG:NE	3:E:334:VAL:O	2.35	0.45
1:A:458:CYS:HB3	6:E:454:HOH:O	2.16	0.45
1:A:520:GLN:O	1:A:531:LEU:HD12	2.17	0.45
1:A:573:LEU:HG	6:A:241:HOH:O	2.16	0.45
3:G:23:THR:O	3:G:24:SER:C	2.59	0.45
2:D:247:TYR:CD1	2:D:247:TYR:N	2.83	0.45
3:E:264:PHE:CD2	3:E:265:ASP:O	2.68	0.45
3:G:172:MET:HE2	3:G:172:MET:HB3	1.75	0.45
1:C:505:HIS:O	1:C:508:ARG:HB3	2.17	0.45
3:E:8:GLN:OE1	3:E:180:LEU:HA	2.16	0.45
3:E:68:PHE:CZ	3:E:70:GLY:C	2.95	0.45
3:E:90:PHE:HA	3:E:91:PRO:HD3	1.72	0.45
3:E:190:GLY:HA2	3:E:308:ASP:OD2	2.16	0.45
3:G:18:PHE:O	3:G:19:ILE:C	2.59	0.45
3:G:49:LEU:O	3:G:53:ASN:HB2	2.17	0.45
1:C:535:SER:HB2	1:C:562:PHE:CG	2.51	0.45
3:E:229:LEU:HD23	3:E:229:LEU:HA	1.54	0.45
3:E:317:LYS:HA	3:E:317:LYS:CE	2.44	0.45
3:G:236:ASP:CG	3:G:260:ARG:HH11	2.25	0.45
3:E:225:GLU:H	3:E:225:GLU:HG2	1.49	0.45
1:A:481:THR:HG22	6:A:285:HOH:O	2.16	0.45
2:B:283:TYR:O	2:B:284:HIS:C	2.59	0.45
3:G:38:ASP:C	3:G:40:THR:N	2.71	0.45
3:E:241:ILE:HG21	3:E:246:TYR:CD2	2.52	0.45
3:E:275:ARG:O	3:E:276:LEU:C	2.58	0.45
3:E:288:VAL:CG1	3:E:290:ARG:O	2.64	0.45
1:A:559:SER:O	1:A:562:PHE:HB3	2.16	0.45
3:G:65:ALA:C	3:G:67:LYS:N	2.71	0.45
3:G:80:VAL:HG21	3:G:97:ILE:CD1	2.45	0.45
1:C:494:MET:C	1:C:496:THR:H	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:123:HIS:CD2	3:E:125:MET:H	2.34	0.45
3:E:165:ARG:NH1	5:E:402:FLC:OG2	2.49	0.45
3:E:181:ARG:HE	3:E:181:ARG:HB3	1.71	0.45
3:E:279:ILE:HG23	3:E:291:LEU:CD1	2.47	0.45
1:A:463:PRO:HB2	6:A:234:HOH:O	2.16	0.45
2:B:290:THR:HG23	3:G:36:VAL:HG21	1.99	0.45
3:G:62:ASP:O	3:G:67:LYS:N	2.44	0.45
1:C:529:PHE:N	1:C:529:PHE:CD1	2.85	0.45
3:E:81:ILE:O	3:E:81:ILE:CD1	2.62	0.45
3:E:144:PRO:HA	3:E:160:VAL:HG22	1.99	0.45
2:B:211:GLU:H	2:B:211:GLU:HG3	1.33	0.45
1:C:454:PHE:HB2	1:C:530:MET:HE1	1.98	0.45
1:C:497:ILE:O	1:C:519:LEU:N	2.37	0.45
1:A:533:VAL:CG1	1:A:534:LYS:N	2.80	0.45
3:G:6:GLU:CB	6:G:464:HOH:O	2.65	0.45
3:G:203:LYS:HA	3:G:203:LYS:HD3	1.68	0.45
2:D:232:LEU:HD11	2:D:236:LEU:HB2	1.97	0.44
3:E:20:ARG:HG2	3:E:129:MET:HG3	1.99	0.44
3:E:133:LEU:O	3:E:136:SER:N	2.50	0.44
3:G:126:HIS:HB3	6:G:453:HOH:O	2.15	0.44
3:G:174:CYS:O	3:G:175:LYS:C	2.60	0.44
3:G:184:LEU:O	3:G:186:GLN:N	2.50	0.44
2:D:232:LEU:CD1	2:D:236:LEU:HB2	2.47	0.44
3:E:327:THR:O	3:E:329:ASN:N	2.51	0.44
1:A:533:VAL:CG1	1:A:534:LYS:H	2.26	0.44
3:G:129:MET:CE	3:G:314:ILE:HG22	2.47	0.44
2:D:208:TYR:OH	6:D:323:HOH:O	2.21	0.44
3:E:306:LEU:N	4:E:401:ATP:O1G	2.45	0.44
1:C:519:LEU:N	1:C:519:LEU:HD12	2.32	0.44
2:D:283:TYR:HE2	2:D:284:HIS:HD2	1.58	0.44
3:E:15:ILE:O	3:E:18:PHE:HB3	2.18	0.44
3:E:185:ASN:C	3:E:185:ASN:ND2	2.75	0.44
3:E:314:ILE:HG12	6:E:508:HOH:O	2.17	0.44
1:A:470:TYR:O	1:A:473:LEU:HB2	2.18	0.44
1:C:537:GLY:N	6:C:27:HOH:O	2.44	0.44
3:G:307:ALA:HB3	4:G:401:ATP:O1A	2.18	0.44
3:G:315:TYR:O	3:G:316:ASP:C	2.60	0.44
1:C:469:VAL:O	1:C:473:LEU:HB2	2.17	0.44
3:E:209:LYS:O	3:E:212:ALA:O	2.36	0.44
1:A:574:PHE:CD2	3:E:93:ALA:HB1	2.52	0.44
1:C:572:LYS:HD2	1:C:572:LYS:HA	1.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:78:VAL:CA	3:E:81:ILE:HG22	2.48	0.44
1:C:461:ASP:O	1:C:462:ALA:C	2.60	0.44
3:E:325:GLU:CD	3:E:329:ASN:HD21	2.24	0.44
1:A:459:ARG:HG3	1:A:459:ARG:NH1	2.32	0.44
3:G:310:LEU:HA	3:G:310:LEU:HD23	1.80	0.44
2:D:295:ASN:ND2	3:E:101:ARG:HH12	2.16	0.44
3:E:234:SER:C	3:E:236:ASP:N	2.75	0.44
3:E:305:SER:HB2	4:E:401:ATP:O2B	2.18	0.44
1:A:523:GLU:CA	1:A:529:PHE:CD2	2.96	0.43
1:A:521:LEU:HD23	1:A:531:LEU:HA	2.00	0.43
3:G:165:ARG:HD2	3:G:165:ARG:C	2.43	0.43
1:C:542:TYR:N	1:C:542:TYR:CD1	2.86	0.43
2:D:210:THR:CB	6:D:322:HOH:O	2.11	0.43
2:D:216:LEU:O	2:D:217:THR:O	2.36	0.43
3:E:99:LYS:HG2	3:E:100:PHE:N	2.33	0.43
3:E:210:MET:O	3:E:214:LYS:HB2	2.18	0.43
3:E:215:ASN:ND2	3:E:331:GLU:C	2.75	0.43
3:G:110:ARG:C	6:G:441:HOH:O	2.61	0.43
2:D:220:THR:HG22	2:D:220:THR:O	2.19	0.43
2:D:282:ARG:NH1	2:D:282:ARG:CG	2.74	0.43
3:E:80:VAL:HG12	3:E:109:GLU:HG2	2.01	0.43
2:B:296:PHE:CB	3:E:99:LYS:HD2	2.48	0.43
3:G:132:CYS:HB3	3:G:314:ILE:HD13	1.99	0.43
3:G:207:VAL:O	3:G:208:ILE:C	2.61	0.43
1:C:482:VAL:HG13	1:C:483:PRO:HD2	1.99	0.43
1:C:503:ILE:HD11	1:C:514:TYR:H	1.74	0.43
3:E:166:ILE:HG23	3:E:166:ILE:HD12	1.58	0.43
2:B:280:THR:OG1	2:B:289:THR:HG23	2.18	0.43
3:G:22:ARG:HD3	3:G:22:ARG:HA	1.48	0.43
3:G:73:THR:HG23	3:G:75:ALA:H	1.84	0.43
3:G:170:ILE:C	3:G:172:MET:N	2.74	0.43
2:D:265:LEU:HA	2:D:265:LEU:HD12	1.73	0.43
3:E:231:VAL:HG11	6:E:505:HOH:O	2.17	0.43
1:A:560:PHE:HA	1:A:561:PRO:C	2.42	0.43
1:C:464:GLU:O	1:C:465:ILE:C	2.62	0.43
2:D:237:GLU:O	2:D:237:GLU:CG	2.66	0.43
3:E:255:GLU:HG2	3:E:255:GLU:H	1.60	0.43
1:A:466:LEU:HD11	1:A:497:ILE:HD11	2.00	0.43
1:C:569:LEU:HD22	1:C:573:LEU:HG	2.01	0.43
3:E:51:THR:O	3:E:52:LEU:C	2.60	0.43
3:E:228:LEU:HD23	3:E:228:LEU:HA	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:243:ASP:N	6:E:414:HOH:O	2.42	0.43
3:G:276:LEU:HA	3:G:276:LEU:HD12	1.72	0.43
3:E:83:TYR:C	6:E:452:HOH:O	2.62	0.43
3:E:136:SER:OG	3:E:311:ASN:ND2	2.52	0.43
2:B:220:THR:OG1	2:B:224:LEU:HD13	2.19	0.43
3:G:20:ARG:HG2	3:G:129:MET:HG3	2.00	0.43
1:C:508:ARG:HD2	6:C:376:HOH:O	2.19	0.43
3:E:276:LEU:O	3:E:280:PHE:HB2	2.19	0.43
1:A:491:ARG:C	2:B:227:PRO:HG3	2.44	0.42
3:G:38:ASP:C	3:G:40:THR:H	2.26	0.42
3:G:112:ILE:HD12	3:G:330:PHE:CZ	2.54	0.42
3:G:169:PHE:CA	6:G:507:HOH:O	2.64	0.42
2:D:262:LEU:HD13	2:D:262:LEU:HA	1.68	0.42
3:E:97:ILE:HA	3:E:97:ILE:HD13	1.57	0.42
3:E:288:VAL:HG12	3:E:290:ARG:O	2.18	0.42
3:G:23:THR:O	3:G:26:ASP:HB2	2.19	0.42
3:G:185:ASN:HD21	3:G:186:GLN:HG3	1.82	0.42
3:E:8:GLN:O	3:E:9:LYS:C	2.62	0.42
3:E:128:LEU:HD11	3:E:166:ILE:CG1	2.48	0.42
3:E:141:ARG:HH11	3:E:217:SER:HB3	1.84	0.42
1:A:500:ARG:HG2	1:A:514:TYR:CD2	2.54	0.42
3:G:2:MET:CG	6:G:464:HOH:O	2.66	0.42
3:G:120:ILE:HD13	3:G:120:ILE:H	1.84	0.42
1:C:541:ILE:HD12	1:C:541:ILE:HA	1.81	0.42
2:D:212:ILE:HD12	2:D:213:PRO:HD2	2.02	0.42
3:E:110:ARG:HE	3:E:110:ARG:CA	2.32	0.42
3:E:218:ALA:O	3:E:219:VAL:HG23	2.19	0.42
1:A:461:ASP:O	1:A:464:GLU:N	2.53	0.42
1:A:489:LYS:CA	6:A:91:HOH:O	2.61	0.42
1:A:492:SER:C	1:A:494:MET:N	2.77	0.42
1:A:507:LYS:C	1:A:507:LYS:CD	2.72	0.42
2:B:296:PHE:HB3	3:E:99:LYS:HD2	2.00	0.42
3:G:224:SER:C	3:G:226:GLY:H	2.27	0.42
1:A:491:ARG:O	1:A:492:SER:C	2.61	0.42
3:G:149:ASP:O	3:G:151:GLU:N	2.53	0.42
3:G:305:SER:OG	3:G:306:LEU:N	2.51	0.42
3:E:295:ASP:OD1	3:E:295:ASP:C	2.60	0.42
3:G:306:LEU:HD12	6:G:526:HOH:O	2.18	0.42
1:C:501:TRP:HB2	6:C:213:HOH:O	2.19	0.42
3:G:201:GLU:HA	3:G:252:SER:HB2	2.01	0.42
3:G:295:ASP:HB3	3:G:301:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ARG:O	1:C:494:MET:HG2	2.18	0.42
1:C:515:ALA:HA	1:C:537:GLY:O	2.19	0.42
2:D:272:LEU:HD12	3:E:49:LEU:CD2	2.50	0.42
3:E:307:ALA:O	3:E:308:ASP:C	2.63	0.42
2:B:212:ILE:O	2:B:213:PRO:C	2.63	0.42
3:G:123:HIS:CD2	3:G:125:MET:H	2.37	0.42
2:D:258:ASN:HD22	2:D:258:ASN:C	2.28	0.42
3:E:37:PHE:HB2	3:E:60:LEU:HD23	2.00	0.42
4:E:401:ATP:C8	4:E:401:ATP:C5'	2.85	0.42
3:E:294:VAL:HG12	3:E:300:LEU:HA	2.01	0.42
2:B:236:LEU:HD23	2:B:261:LEU:HD22	2.01	0.42
3:G:24:SER:O	3:G:25:TYR:C	2.63	0.42
1:C:454:PHE:HB2	1:C:530:MET:CE	2.50	0.42
3:E:175:LYS:C	3:E:175:LYS:CD	2.92	0.42
1:A:540:ASP:HB3	3:G:151:GLU:OE1	2.19	0.41
2:B:214:ALA:C	2:B:215:PHE:O	2.54	0.41
2:B:218:SER:O	2:B:219:ASN:HB3	2.20	0.41
2:B:263:ASN:ND2	2:B:279:ALA:HB1	2.34	0.41
3:G:80:VAL:HG22	3:G:97:ILE:CD1	2.37	0.41
3:G:91:PRO:HD2	6:C:17:HOH:O	2.20	0.41
3:G:120:ILE:H	3:G:120:ILE:CD1	2.33	0.41
3:G:294:VAL:HB	3:G:298:LEU:HA	2.01	0.41
1:C:560:PHE:HA	1:C:561:PRO:C	2.45	0.41
2:D:261:LEU:HD21	6:D:307:HOH:O	2.19	0.41
3:E:83:TYR:C	3:E:83:TYR:CD1	2.98	0.41
3:E:115:ILE:HG13	3:E:116:PRO:HD2	2.00	0.41
3:E:162:THR:HG21	6:E:460:HOH:O	2.20	0.41
3:E:240:LEU:HA	3:E:240:LEU:HD12	1.80	0.41
3:E:252:SER:O	3:E:253:VAL:C	2.61	0.41
3:E:323:VAL:HA	3:E:324:PRO:HA	1.85	0.41
3:G:78:VAL:HG13	3:G:208:ILE:HG23	2.02	0.41
1:C:465:ILE:O	1:C:466:LEU:C	2.60	0.41
1:C:479:GLN:NE2	1:C:500:ARG:HH22	2.18	0.41
1:C:484:LYS:NZ	1:C:484:LYS:CB	2.79	0.41
1:C:487:ASN:C	1:C:489:LYS:H	2.27	0.41
3:E:186:GLN:CB	6:E:523:HOH:O	2.47	0.41
1:A:561:PRO:O	1:A:565:LEU:CD2	2.59	0.41
1:A:561:PRO:CA	3:G:66:ASN:HD21	2.34	0.41
3:G:164[B]:TYR:HE1	6:G:493:HOH:O	2.04	0.41
1:C:487:ASN:O	1:C:489:LYS:N	2.43	0.41
3:E:56:VAL:HB	6:E:497:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:206:ASP:O	3:E:209:LYS:HB3	2.19	0.41
3:E:290:ARG:CZ	3:E:290:ARG:HB2	2.50	0.41
1:A:484:LYS:HE3	1:A:484:LYS:HA	2.03	0.41
2:B:250:ASP:CA	2:B:252:SER:H	2.33	0.41
3:G:247:SER:C	3:G:249:LEU:N	2.77	0.41
1:C:472:ALA:CB	1:C:573:LEU:HD23	2.49	0.41
1:C:506:CYS:HB3	1:C:511:LYS:CB	2.50	0.41
2:D:295:ASN:O	2:D:296:PHE:C	2.58	0.41
1:A:464:GLU:O	1:A:467:LEU:HB3	2.20	0.41
2:B:215:PHE:C	2:B:217:THR:H	2.29	0.41
2:B:224:LEU:HB3	2:B:226:LEU:HD21	2.02	0.41
3:G:168:LYS:O	3:G:172:MET:CG	2.66	0.41
6:C:77:HOH:O	2:D:229:PRO:HA	2.20	0.41
1:A:542:TYR:HA	1:A:543:SER:CB	2.50	0.41
1:A:558:SER:HA	3:G:156:MET:HE3	2.02	0.41
3:G:90:PHE:HA	3:G:91:PRO:HD3	1.82	0.41
3:G:130:ASP:OD2	6:G:453:HOH:O	2.22	0.41
1:C:534:LYS:O	1:C:534:LYS:HG2	2.19	0.41
2:D:295:ASN:ND2	3:E:101:ARG:NH1	2.68	0.41
1:A:495:TYR:CE1	2:B:227:PRO:O	2.74	0.41
3:G:96:GLU:C	3:G:98:ASP:H	2.27	0.41
3:G:309:ILE:O	3:G:313:ILE:HG12	2.20	0.41
1:A:561:PRO:O	1:A:562:PHE:C	2.62	0.41
2:B:265:LEU:HD12	2:B:266:ALA:H	1.85	0.41
2:B:270:THR:C	2:B:272:LEU:N	2.77	0.41
3:G:39:VAL:CG2	3:G:61:TRP:O	2.68	0.41
3:G:77:PHE:N	6:G:477:HOH:O	2.53	0.41
3:G:101:ARG:O	3:G:102:LEU:C	2.64	0.41
3:G:248:ASN:O	3:G:251:LEU:HD12	2.20	0.41
3:G:329:ASN:N	3:G:329:ASN:HD22	2.18	0.41
1:C:454:PHE:HE1	2:D:238:LYS:O	2.03	0.41
3:E:15:ILE:O	3:E:16:GLN:C	2.63	0.41
3:E:27:VAL:HG13	3:E:169:PHE:HB2	2.03	0.41
3:E:102:LEU:HD12	3:E:102:LEU:HA	1.87	0.41
3:E:209:LYS:HG2	3:E:213:GLU:OE1	2.20	0.41
3:G:80:VAL:HG23	3:G:84:TYR:CD1	2.56	0.41
3:G:170:ILE:O	3:G:171:SER:C	2.64	0.41
1:C:555:ASP:OD2	1:C:555:ASP:N	2.53	0.41
3:E:327:THR:O	3:E:328:ASP:C	2.64	0.41
1:A:479:GLN:NE2	1:A:500:ARG:NH2	2.69	0.40
1:A:525:MET:HE3	1:A:525:MET:HB3	1.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:LEU:HA	1:A:566:CYS:HB2	2.03	0.40
2:B:238:LYS:O	2:B:238:LYS:HG2	2.21	0.40
3:G:118:GLU:CD	3:G:118:GLU:N	2.78	0.40
3:G:193:SER:O	3:G:194:ASN:CB	2.66	0.40
2:D:209:SER:OG	2:D:210:THR:N	2.54	0.40
3:E:120:ILE:HG23	3:E:143:ILE:HG13	2.03	0.40
3:E:181:ARG:NH2	3:E:275:ARG:NH2	2.68	0.40
3:E:265:ASP:HB2	3:E:289:HIS:CE1	2.56	0.40
1:A:466:LEU:HD21	1:A:494:MET:O	2.21	0.40
3:G:77:PHE:CA	6:G:477:HOH:O	2.69	0.40
3:G:247:SER:C	3:G:249:LEU:H	2.29	0.40
1:C:505:HIS:CE1	1:C:506:CYS:SG	3.14	0.40
3:E:114:ALA:HA	3:E:330:PHE:CD1	2.55	0.40
3:E:309:ILE:H	3:E:309:ILE:HG12	1.45	0.40
3:G:205:TYR:C	3:G:205:TYR:CD2	3.00	0.40
1:C:495:TYR:CZ	2:D:229:PRO:HD3	2.56	0.40
3:E:283:ILE:HD13	3:E:283:ILE:HG21	1.83	0.40
1:C:521:LEU:CD1	2:D:229:PRO:HB3	2.47	0.40
3:G:44:LYS:CD	6:G:412:HOH:O	2.69	0.40
3:G:196:ALA:O	3:G:220:PRO:HD2	2.22	0.40
3:G:307:ALA:CB	4:G:401:ATP:O1A	2.70	0.40
1:C:500:ARG:HG2	1:C:500:ARG:NH1	2.18	0.40
2:D:228:LYS:HA	2:D:228:LYS:HD3	1.82	0.40
3:E:203:LYS:HD3	3:E:203:LYS:HA	1.87	0.40
3:E:234:SER:C	3:E:236:ASP:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	127/137 (93%)	90 (71%)	20 (16%)	17 (13%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	111/137 (81%)	84 (76%)	18 (16%)	9 (8%)	1	1
2	B	91/97 (94%)	60 (66%)	17 (19%)	14 (15%)	0	0
2	D	89/97 (92%)	71 (80%)	11 (12%)	7 (8%)	1	1
3	E	331/333 (99%)	256 (77%)	49 (15%)	26 (8%)	1	1
3	G	321/333 (96%)	265 (83%)	36 (11%)	20 (6%)	1	3
All	All	1070/1134 (94%)	826 (77%)	151 (14%)	93 (9%)	0	1

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	LYS
1	A	542	TYR
1	A	543	SER
1	A	545	PRO
1	A	548	THR
1	A	554	ASP
1	A	555	ASP
2	B	209	SER
2	B	219	ASN
2	B	222	GLN
2	B	243	SER
2	B	247	TYR
2	B	259[A]	HIS
2	B	259[B]	HIS
2	B	262	LEU
3	G	64	GLU
3	G	88	SER
3	G	140	ALA
3	G	141	ARG
3	G	170	ILE
3	G	264	PHE
3	G	316	ASP
1	C	511	LYS
2	D	217	THR
2	D	224	LEU
2	D	225	LYS
2	D	226	LEU
3	E	64	GLU
3	E	93	ALA
1	A	448	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	493	ASP
1	A	534	LYS
1	A	551	HIS
2	B	225	LYS
2	B	245	THR
3	G	89	SER
3	G	110	ARG
3	G	121	TYR
3	G	150	GLY
3	G	200	MET
3	G	215	ASN
3	G	284	LYS
1	C	488	GLY
1	C	502	GLU
1	C	555	ASP
2	D	218	SER
3	E	3	ASP
3	E	26	ASP
3	E	88	SER
3	E	94	ILE
3	E	274	ASP
3	E	309	ILE
3	E	329	ASN
3	E	333	ALA
1	A	511	LYS
2	B	207	GLN
2	B	248	LYS
3	G	138	SER
1	C	483	PRO
1	C	489	LYS
3	E	95	ALA
3	E	97	ILE
3	E	117	PRO
3	E	213	GLU
3	E	254	GLY
3	E	328	ASP
1	A	487	ASN
1	A	556	LEU
3	G	3	ASP
3	G	25	TYR
3	G	248	ASN
1	C	527	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	541	ILE
2	D	262	LEU
3	E	52	LEU
3	E	91	PRO
3	E	211	LEU
3	E	276	LEU
1	A	547	ARG
2	B	241	LEU
2	B	246	ALA
1	C	504	PRO
3	E	139	ARG
3	E	238	MET
3	E	308	ASP
3	E	332	SER
1	A	462	ALA
1	A	544	HIS
3	G	266	GLY
3	G	97	ILE
2	D	230	PRO
3	E	190	GLY
3	E	39	VAL

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	106/120 (88%)	85 (80%)	21 (20%)	1	4
1	C	96/120 (80%)	72 (75%)	24 (25%)	0	2
2	B	80/88 (91%)	58 (72%)	22 (28%)	0	1
2	D	79/88 (90%)	59 (75%)	20 (25%)	0	2
3	E	293/296 (99%)	229 (78%)	64 (22%)	1	2
3	G	283/296 (96%)	221 (78%)	62 (22%)	1	2
All	All	937/1008 (93%)	724 (77%)	213 (23%)	1	2

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	459	ARG
1	A	474	GLN
1	A	481	THR
1	A	484	LYS
1	A	486	VAL
1	A	492	SER
1	A	507	LYS
1	A	511	LYS
1	A	512	ASN
1	A	513	THR
1	A	521	LEU
1	A	525	MET
1	A	534	LYS
1	A	536	ASN
1	A	540	ASP
1	A	543	SER
1	A	546	GLU
1	A	558	SER
1	A	565	LEU
1	A	569	LEU
2	B	207	GLN
2	B	210	THR
2	B	211	GLU
2	B	217	THR
2	B	222	GLN
2	B	224	LEU
2	B	225	LYS
2	B	226	LEU
2	B	231	SER
2	B	232	LEU
2	B	238	LYS
2	B	249	GLU
2	B	253	VAL
2	B	256	ASN
2	B	260	VAL
2	B	262	LEU
2	B	263	ASN
2	B	269	ASN
2	B	271	GLN
2	B	281	THR
2	B	282	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	285	ARG
3	G	13	LYS
3	G	22	ARG
3	G	30	THR
3	G	39	VAL
3	G	46	SER
3	G	52	LEU
3	G	57	SER
3	G	62	ASP
3	G	63	SER
3	G	64	GLU
3	G	80	VAL
3	G	82	LYS
3	G	86	GLN
3	G	87	SER
3	G	92	GLU
3	G	94	ILE
3	G	102	LEU
3	G	118	GLU
3	G	119	THR
3	G	120	ILE
3	G	122	VAL
3	G	129	MET
3	G	137	LYS
3	G	138	SER
3	G	143	ILE
3	G	146	ILE
3	G	154	SER
3	G	155	GLU
3	G	161	LEU
3	G	162	THR
3	G	165	ARG
3	G	172	MET
3	G	175	LYS
3	G	181	ARG
3	G	185	ASN
3	G	189	ILE
3	G	193	SER
3	G	200	MET
3	G	201	GLU
3	G	221	ILE
3	G	225	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	227	THR
3	G	228	LEU
3	G	235	VAL
3	G	236	ASP
3	G	248	ASN
3	G	255	GLU
3	G	258	LEU
3	G	275	ARG
3	G	276	LEU
3	G	279	ILE
3	G	281	ASP
3	G	284	LYS
3	G	286	SER
3	G	289	HIS
3	G	296	GLU
3	G	298	LEU
3	G	305	SER
3	G	309	ILE
3	G	310	LEU
3	G	315	TYR
3	G	329	ASN
1	C	474	GLN
1	C	479	GLN
1	C	483	PRO
1	C	484	LYS
1	C	487	ASN
1	C	492	SER
1	C	500	ARG
1	C	503	ILE
1	C	507	LYS
1	C	512	ASN
1	C	534	LYS
1	C	535	SER
1	C	536	ASN
1	C	539	LYS
1	C	541	ILE
1	C	542	TYR
1	C	555	ASP
1	C	556	LEU
1	C	557	LYS
1	C	559	SER
1	C	564	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	565	LEU
1	C	569	LEU
1	C	572	LYS
2	D	211	GLU
2	D	212	ILE
2	D	221	LEU
2	D	223	GLU
2	D	224	LEU
2	D	225	LYS
2	D	226	LEU
2	D	228	LYS
2	D	232	LEU
2	D	235	HIS
2	D	238	LYS
2	D	247	TYR
2	D	250	ASP
2	D	258	ASN
2	D	261	LEU
2	D	262	LEU
2	D	263	ASN
2	D	282	ARG
2	D	290	THR
2	D	296	PHE
3	E	4	VAL
3	E	8	GLN
3	E	9	LYS
3	E	19	ILE
3	E	30	THR
3	E	31	SER
3	E	35	ILE
3	E	39	VAL
3	E	44	LYS
3	E	64	GLU
3	E	67	LYS
3	E	73	THR
3	E	80	VAL
3	E	81	ILE
3	E	89	SER
3	E	92	GLU
3	E	94	ILE
3	E	97	ILE
3	E	99	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	102	LEU
3	E	110	ARG
3	E	115	ILE
3	E	118	GLU
3	E	119	THR
3	E	120	ILE
3	E	122	VAL
3	E	129	MET
3	E	137	LYS
3	E	143	ILE
3	E	146	ILE
3	E	152	THR
3	E	161	LEU
3	E	162	THR
3	E	166	ILE
3	E	175	LYS
3	E	181	ARG
3	E	185	ASN
3	E	188	THR
3	E	201	GLU
3	E	219	VAL
3	E	223	ASN
3	E	225	GLU
3	E	227	THR
3	E	228	LEU
3	E	230	ASN
3	E	231	VAL
3	E	235	VAL
3	E	255	GLU
3	E	257	LEU
3	E	260	ARG
3	E	265	ASP
3	E	275	ARG
3	E	276	LEU
3	E	277	ASP
3	E	280	PHE
3	E	281	ASP
3	E	305	SER
3	E	309	ILE
3	E	310	LEU
3	E	314	ILE
3	E	316	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	317	LYS
3	E	325	GLU
3	E	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	474	GLN
1	A	505	HIS
1	A	520	GLN
1	A	536	ASN
2	B	207	GLN
2	B	263	ASN
3	G	5	GLN
3	G	8	GLN
3	G	53	ASN
3	G	54	ASN
3	G	66	ASN
3	G	86	GLN
3	G	123	HIS
3	G	163	GLN
3	G	173	ASN
3	G	185	ASN
3	G	230	ASN
3	G	329	ASN
1	C	474	GLN
1	C	505	HIS
1	C	512	ASN
1	C	536	ASN
2	D	235	HIS
2	D	242	ASN
2	D	244	ASN
2	D	258	ASN
2	D	271	GLN
2	D	284	HIS
2	D	295	ASN
3	E	53	ASN
3	E	123	HIS
3	E	185	ASN
3	E	186	GLN
3	E	215	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	242	GLN
3	E	268	HIS
3	E	289	HIS
3	E	311	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 oligosaccharides 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	$\# Z > 2$
4	ATP	E	401	-	32,33,33	2.10	7 (21%)	48,52,52	1.87	11 (22%)
4	ATP	G	401	-	32,33,33	1.63	4 (12%)	48,52,52	1.91	11 (22%)
5	FLC	E	402	-	12,12,12	1.19	0	17,17,17	1.35	1 (5%)

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	E	401	-	-	2/22/38/38	0/3/3/3
4	ATP	G	401	-	-	6/22/38/38	0/3/3/3
5	FLC	E	402	-	-	6/16/16/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	ATP	PB-O3B	7.85	1.68	1.59
4	G	401	ATP	C5-C4	5.87	1.49	1.39
4	E	401	ATP	C5-C4	4.72	1.47	1.39
4	G	401	ATP	C5-C6	3.25	1.50	1.41
4	E	401	ATP	C5-C6	3.18	1.49	1.41
4	E	401	ATP	C5-N7	-2.75	1.34	1.39
4	G	401	ATP	C8-N7	2.69	1.36	1.31
4	E	401	ATP	PB-O3A	2.60	1.62	1.59
4	E	401	ATP	PA-O3A	2.60	1.62	1.59
4	E	401	ATP	C8-N7	2.41	1.36	1.31
4	G	401	ATP	C4-N9	-2.04	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	ATP	C5-C4-N3	-6.03	118.41	126.72
4	E	401	ATP	C5-C4-N3	-5.92	118.56	126.72
4	G	401	ATP	N3-C4-N9	4.20	134.31	127.17
4	G	401	ATP	C4-C5-N7	-4.15	105.84	110.58
4	E	401	ATP	C4-C5-N7	-4.05	105.95	110.58
4	E	401	ATP	N3-C4-N9	4.00	133.96	127.17
4	E	401	ATP	C2-N3-C4	3.87	121.29	111.83
4	G	401	ATP	C2-N3-C4	3.31	119.92	111.83
4	E	401	ATP	N3-C2-N1	-3.13	123.85	128.58
4	G	401	ATP	O5'-C5'-C4'	3.08	119.47	108.99
4	E	401	ATP	C5'-C4'-C3'	-3.07	104.17	115.21
5	E	402	FLC	OB2-CBC-CB	2.93	118.77	113.14
4	G	401	ATP	O3A-PB-O1B	-2.85	102.14	110.70
4	G	401	ATP	O3A-PA-O1A	-2.76	102.39	110.70
4	G	401	ATP	C2'-C3'-C4'	2.74	107.90	102.61
4	E	401	ATP	C5-N7-C8	2.74	107.75	103.45
4	G	401	ATP	C6-C5-N7	2.62	137.14	132.09
4	G	401	ATP	O2B-PB-O3B	2.57	114.23	107.27
4	E	401	ATP	C6-C5-N7	2.47	136.85	132.09
4	E	401	ATP	O3A-PA-O1A	2.42	117.97	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	ATP	C5-N7-C8	2.33	107.12	103.45
4	E	401	ATP	C3'-C2'-C1'	2.09	105.42	101.46
4	E	401	ATP	PA-O5'-C5'	-2.08	109.41	121.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	401	ATP	O4'-C4'-C5'-O5'
4	E	401	ATP	PB-O3A-PA-O5'
5	E	402	FLC	CG-CB-CBC-OB1
5	E	402	FLC	CG-CB-CBC-OB2
5	E	402	FLC	OHB-CB-CBC-OB1
5	E	402	FLC	OHB-CB-CBC-OB2
4	G	401	ATP	C3'-C4'-C5'-O5'
4	G	401	ATP	PB-O3A-PA-O5'
4	G	401	ATP	PB-O3A-PA-O1A
4	G	401	ATP	PB-O3B-PG-O1G
4	E	401	ATP	C4'-C5'-O5'-PA
5	E	402	FLC	CA-CB-CBC-OB1
5	E	402	FLC	CA-CB-CBC-OB2
4	G	401	ATP	PG-O3B-PB-O2B

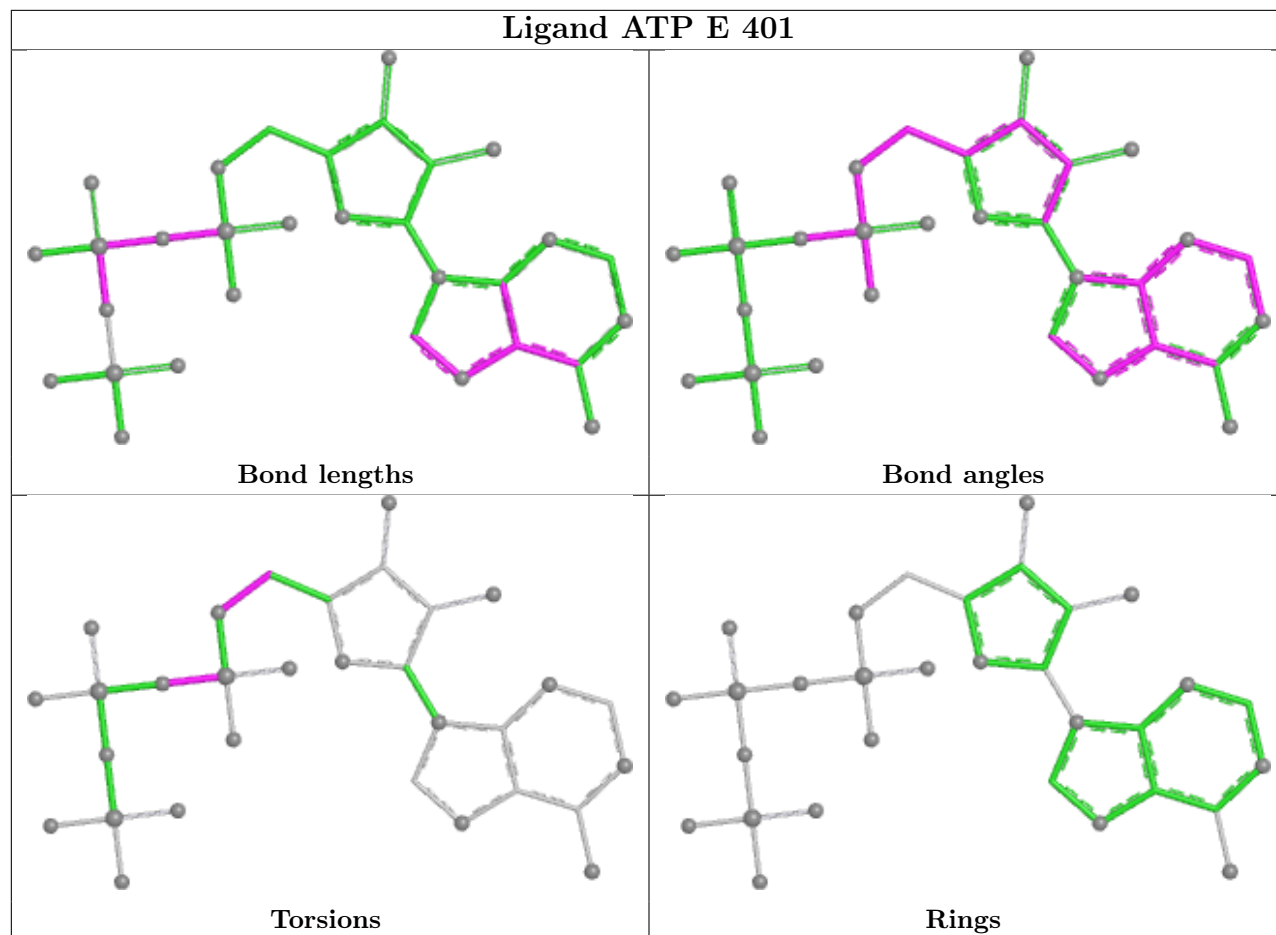
There are no ring outliers.

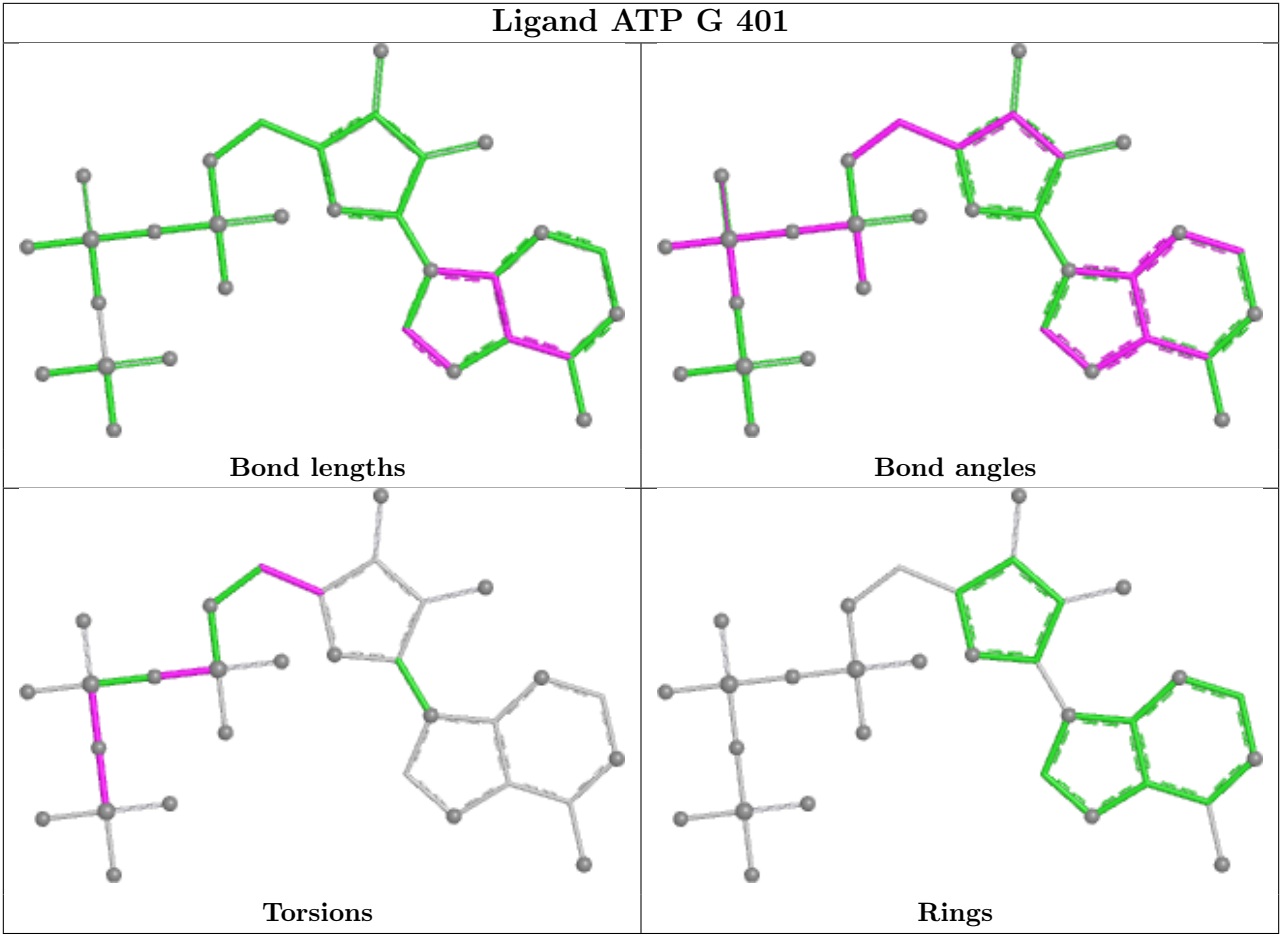
3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	ATP	12	0
4	G	401	ATP	4	0
5	E	402	FLC	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	286:LYS	C	287:TYR	N	1.13

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	129/137 (94%)	-0.62	1 (0%) 82 77	30, 54, 113, 128	0
1	C	115/137 (83%)	-0.74	0 100 100	38, 55, 88, 102	0
2	B	92/97 (94%)	-0.54	0 100 100	23, 64, 94, 100	1 (1%)
2	D	91/97 (93%)	-0.46	1 (1%) 78 72	23, 63, 100, 103	0
3	E	333/333 (100%)	-0.81	1 (0%) 90 87	25, 49, 84, 128	0
3	G	324/333 (97%)	-0.84	1 (0%) 90 87	17, 44, 69, 80	1 (0%)
All	All	1084/1134 (95%)	-0.74	4 (0%) 88 86	17, 50, 91, 128	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	246	ALA	4.7
3	G	63	SER	2.8
3	E	320	THR	2.2
1	A	548	THR	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,

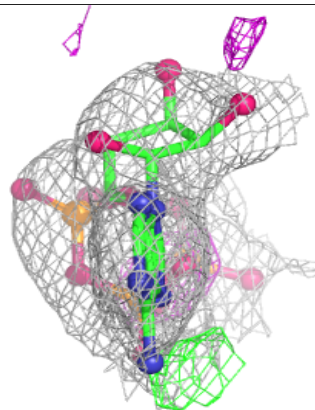
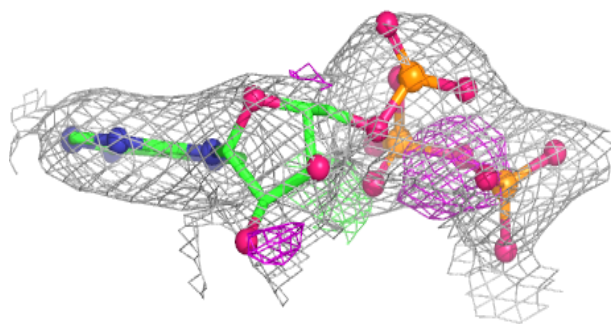
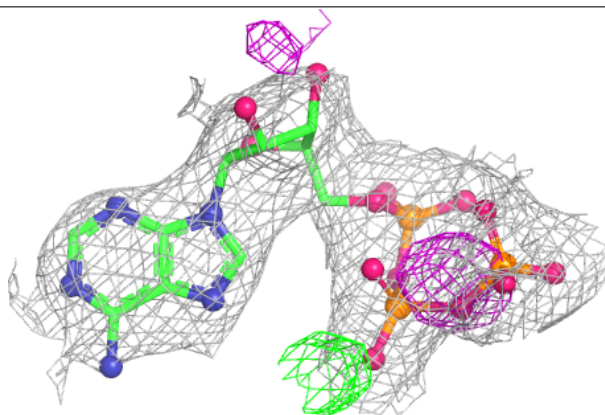
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

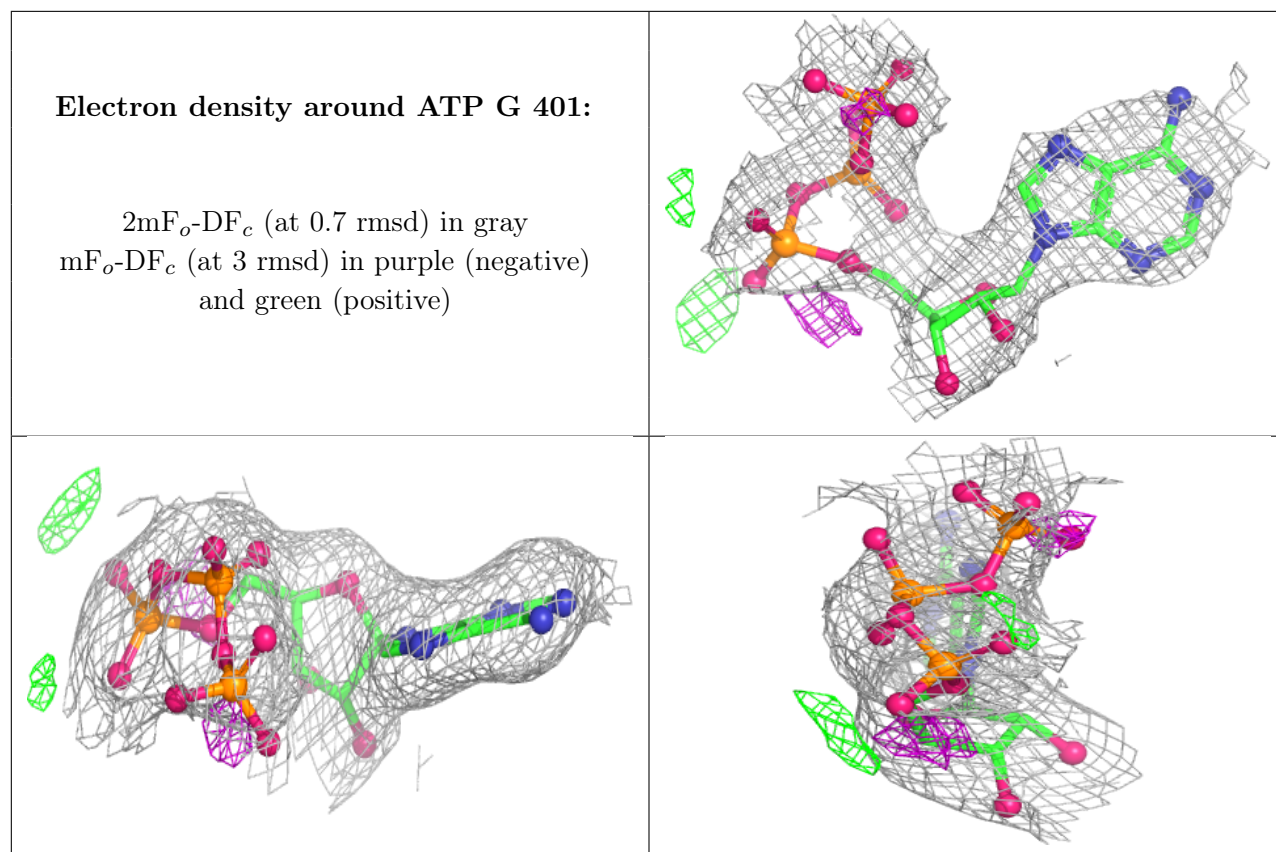
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FLC	E	402	13/13	0.87	0.08	99,101,102,102	0
4	ATP	E	401	31/31	0.90	0.08	55,60,90,92	0
4	ATP	G	401	31/31	0.90	0.09	50,54,98,99	0

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 E 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.