



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:57 AM UTC

PDB ID : 1Y8R / pdb_00001y8r
Title : SUMO E1 ACTIVATING ENZYME SAE1-SAE2-SUMO1-MG-ATP COM-
PLEX
Authors : Lois, L.M.; Lima, C.D.
Deposited on : 2004-12-13
Resolution : 2.75 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:

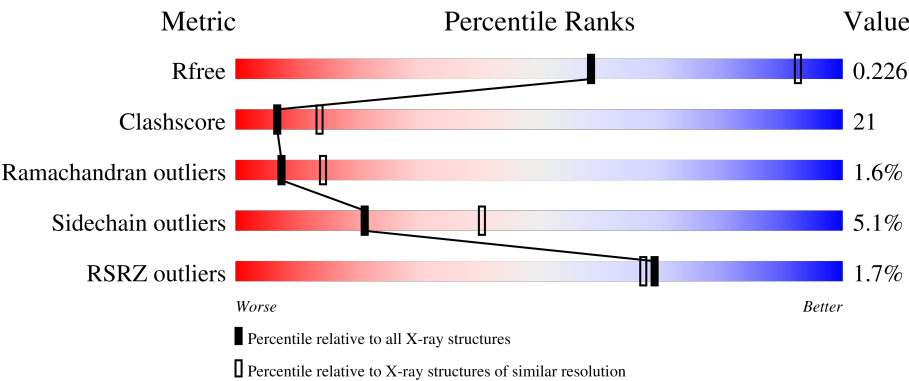
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	346	55%35%•9%
1	D	346	56%30%•10%
2	B	640	2% 48%29%•20%
2	E	640	2% 48%30%••20%
3	C	97	2% 42%41%••13%

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Mol	Chain	Length	Quality of chain
3	F	97	7% 33% 48% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14695 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 Ubiquitin-like 1 activating enzyme E1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2462	1559	418	472	13			
1	D	311	Total	C	N	O	S	0	0	0
			2437	1544	414	466	13			

- Molecule 2 is a protein called Ubiquitin-like 2 activating enzyme E1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	512	Total	C	N	O	S	0	0	0
			4022	2556	695	752	19			
2	E	514	Total	C	N	O	S	0	0	0
			4031	2562	696	754	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	ALA	CYS	engineered mutation	UNP Q9UBT2
E	173	ALA	CYS	engineered mutation	UNP Q9UBT2

- Molecule 3 is a protein called Ubiquitin-like protein SMT3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	84	Total	C	N	O	S	0	0	0
			680	425	117	134	4			
3	F	84	Total	C	N	O	S	0	0	0
			680	425	117	134	4			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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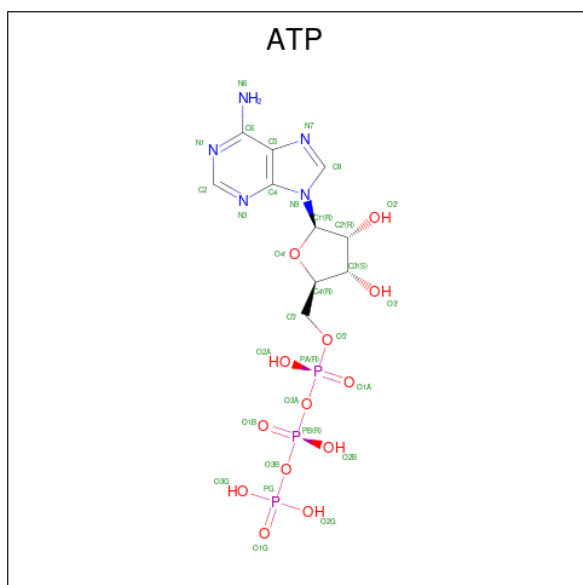
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	61	Total	O	0	0
			61	61		
7	B	89	Total	O	0	0
			89	89		

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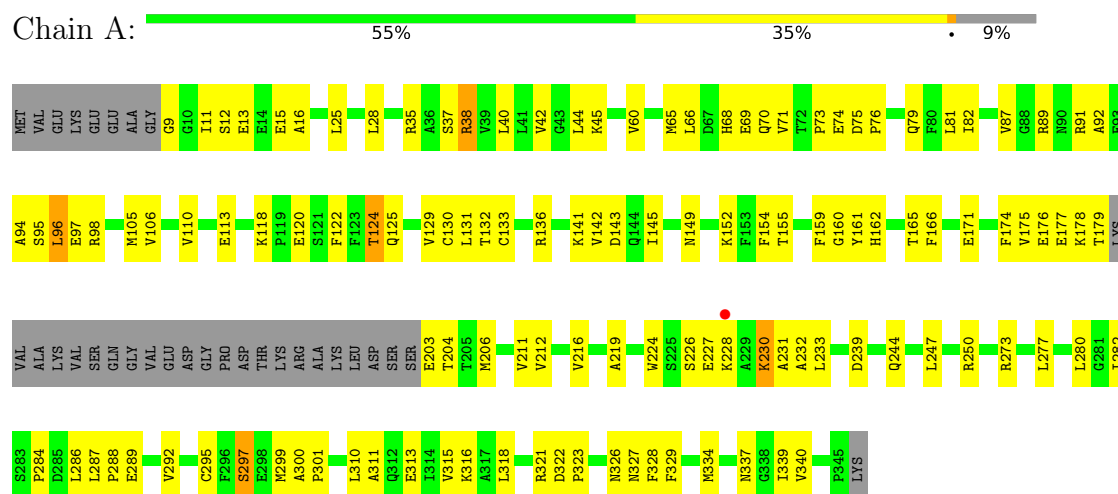
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	13	Total 13	O 13	0	0
7	D	62	Total 62	O 62	0	0
7	E	85	Total 85	O 85	0	0
7	F	7	Total 7	O 7	0	0

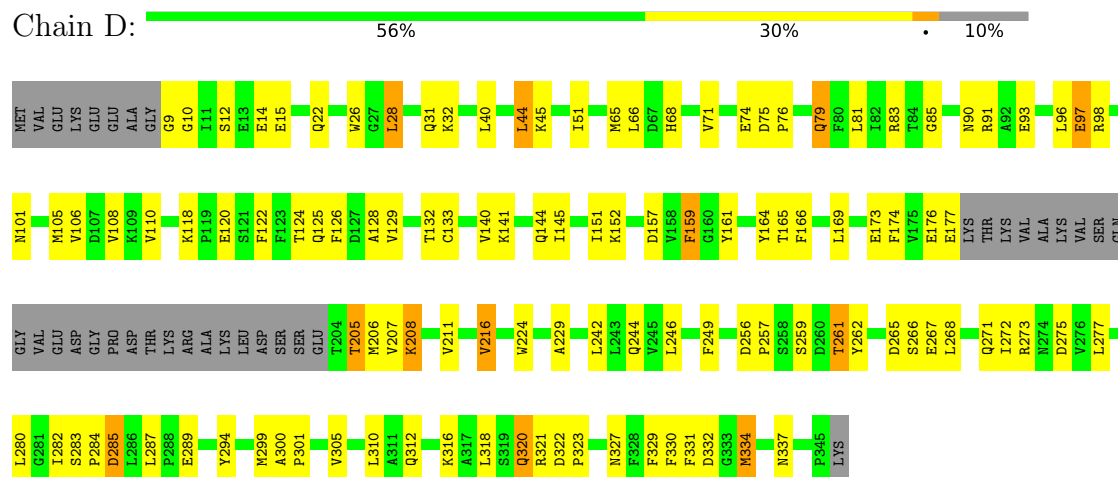
3 Residue-property plots

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: Ubiquitin-like 1 activating enzyme E1A



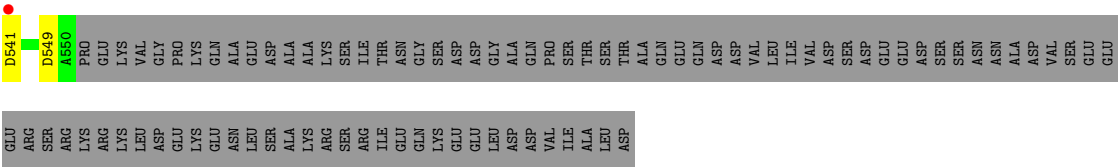
• Molecule 1: Ubiquitin-like 1 activating enzyme E1A



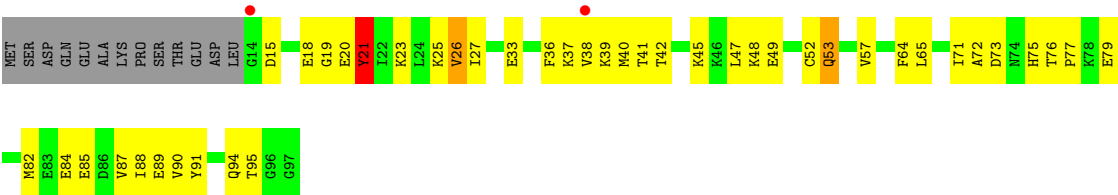
• Molecule 2: Ubiquitin-like 2 activating enzyme E1B



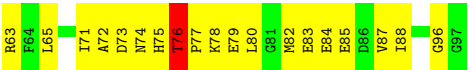




● Molecule 3: Ubiquitin-like protein SMT3C



● Molecule 3: Ubiquitin-like protein SMT3C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.20Å 215.15Å 100.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.75 19.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.99-2.75) 94.7 (19.99-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.276 0.222 , 0.226	Depositor DCC
R_{free} test set	3237 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14695	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.76% 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: MG, ZN, 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	0.56	0/2505	0.89	3/3379 (0.1%)
1	D	0.60	0/2480	0.91	5/3346 (0.1%)
2	B	0.52	1/4099 (0.0%)	0.91	6/5548 (0.1%)
2	E	0.56	1/4108 (0.0%)	0.95	10/5560 (0.2%)
3	C	0.48	0/690	0.83	0/918
3	F	0.42	0/690	0.80	2/918 (0.2%)
All	All	0.55	2/14572 (0.0%)	0.91	26/19669 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	162	HIS	ND1-CE1	5.19	1.37	1.32
2	B	162	HIS	ND1-CE1	5.13	1.37	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	VAL	N-CA-C	6.90	113.84	107.56
2	E	466	ASP	N-CA-C	6.72	118.26	111.07
2	B	162	HIS	CB-CG-CD2	-6.61	122.61	131.20
2	E	162	HIS	CB-CG-CD2	-6.45	122.81	131.20
2	B	109	PHE	N-CA-C	5.82	118.41	110.55
2	E	162	HIS	CB-CG-ND1	5.67	131.20	122.70
2	E	70	ARG	N-CA-C	5.65	117.19	110.19
1	D	44	LEU	N-CA-C	5.62	117.64	109.71
2	E	44	ILE	N-CA-C	5.62	116.20	108.12
1	D	106	VAL	N-CA-C	5.61	116.38	108.36
2	B	162	HIS	CA-C-N	5.61	126.85	119.84
2	B	162	HIS	C-N-CA	5.61	126.85	119.84
2	B	162	HIS	CB-CG-ND1	5.60	131.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	471	GLU	N-CA-C	5.55	118.17	111.40
1	A	118	LYS	CA-C-N	5.52	125.95	119.99
1	A	118	LYS	C-N-CA	5.52	125.95	119.99
1	D	330	PHE	N-CA-C	5.36	117.47	107.99
2	E	277	LYS	CA-C-N	5.32	125.86	120.38
2	E	277	LYS	C-N-CA	5.32	125.86	120.38
1	A	212	VAL	N-CA-C	5.30	115.53	108.11
3	F	76	THR	CA-C-N	5.09	125.12	119.32
3	F	76	THR	C-N-CA	5.09	125.12	119.32
2	E	278	PRO	N-CA-C	5.08	116.90	110.70
2	E	420	LYS	N-CA-C	-5.07	105.41	112.45
1	D	242	LEU	N-CA-C	-5.06	105.76	111.28
1	D	323	PRO	N-CA-C	5.02	116.82	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2462	0	2451	99	0
1	D	2437	0	2425	86	0
2	B	4022	0	4058	166	0
2	E	4031	0	4067	172	0
3	C	680	0	674	43	0
3	F	680	0	674	65	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	31	0	12	0	0
6	E	31	0	12	2	0
7	A	61	0	0	3	0
7	B	89	0	0	6	0
7	C	13	0	0	0	0
7	D	62	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	85	0	0	7	0
7	F	7	0	0	0	0
All	All	14695	0	14373	612	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 21.

All (612) 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)
2:B:465:GLN:HB2	2:B:491:ILE:HD13	1.43	0.99
2:E:97:MET:HE3	2:E:121:ALA:HA	1.45	0.98
1:A:40:LEU:HD12	1:A:129:VAL:HG13	1.51	0.92
2:E:490:LEU:HD11	2:E:511:ILE:HD11	1.52	0.91
3:F:21:TYR:HB3	3:F:22:ILE:HD12	1.54	0.88
1:D:22:GLN:HE21	1:D:31:GLN:HE22	1.23	0.85
1:D:90:ASN:HB3	1:D:93:GLU:HB2	1.58	0.85
2:E:541:ASP:HA	7:E:833:HOH:O	1.75	0.84
1:D:40:LEU:HD12	1:D:129:VAL:HG13	1.59	0.84
3:F:75:HIS:HB3	3:F:80:LEU:HD11	1.57	0.84
1:A:124:THR:HG23	1:A:149:ASN:HD22	1.45	0.82
1:A:282:ILE:HG21	1:A:286:LEU:HD22	1.62	0.81
1:A:334:MET:HE2	1:A:334:MET:HA	1.63	0.80
2:B:455:ASN:HD22	2:B:536:GLU:HA	1.47	0.80
1:A:277:LEU:HD13	1:A:284:PRO:HA	1.64	0.79
2:E:47:ILE:HD13	2:E:96:ILE:HG23	1.65	0.79
2:B:307:LEU:HB2	2:B:310:GLN:HG3	1.63	0.78
2:E:197:PHE:HB3	2:E:333:LEU:HD22	1.63	0.78
3:F:84:GLU:HG3	3:F:85:GLU:HG2	1.63	0.78
2:E:23:VAL:HG12	2:E:116:LEU:HD21	1.66	0.78
1:D:98:ARG:HH12	2:E:83:PHE:HB3	1.46	0.77
2:B:283:ASP:HB3	2:B:286:GLU:HG3	1.65	0.77
2:B:452:VAL:HG12	2:B:454:LEU:HD22	1.66	0.77
2:B:8:PRO:HD2	2:B:9:ARG:H	1.49	0.76
2:B:475:MET:HA	7:B:833:HOH:O	1.85	0.76
1:A:44:LEU:HD21	1:A:65:MET:HB3	1.65	0.76
2:B:18:GLY:HA3	2:B:110:ILE:HD13	1.67	0.76
2:E:491:ILE:HA	2:E:498:THR:HG21	1.66	0.76
2:B:277:LYS:HD2	2:B:278:PRO:HD2	1.66	0.76
1:D:9:GLY:N	1:D:32:LYS:HZ1	1.84	0.75
2:E:177:ASN:HD21	2:E:209:ASP:HB3	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:GLN:HE21	1:D:31:GLN:NE2	1.84	0.75
2:B:465:GLN:HB2	2:B:491:ILE:CD1	2.17	0.74
2:E:305:LEU:HD12	2:E:311:GLN:HE22	1.52	0.74
1:A:299:MET:HE3	2:B:7:LEU:HD11	1.69	0.74
2:B:178:THR:HG21	2:B:276:ARG:HH11	1.53	0.74
2:B:271:LYS:HD2	2:B:271:LYS:H	1.52	0.73
3:C:72:ALA:H	3:C:75:HIS:HD2	1.35	0.73
3:F:43:HIS:HB2	3:F:46:LYS:HE2	1.70	0.73
3:F:25:LYS:HG3	3:F:87:VAL:HG22	1.69	0.73
2:E:171:PRO:HA	2:E:541:ASP:OD2	1.89	0.72
3:F:22:ILE:HG12	3:F:40:MET:HE2	1.69	0.72
2:B:470:LYS:HG2	2:B:475:MET:O	1.89	0.72
2:B:467:LYS:NZ	2:B:467:LYS:HB3	2.06	0.71
1:D:83:ARG:HA	1:D:98:ARG:NH2	2.06	0.71
2:E:183:ILE:O	2:E:187:VAL:HG23	1.90	0.71
2:E:33:LEU:HD23	2:E:80:VAL:HG21	1.73	0.71
2:B:111:LEU:HG	2:B:113:MET:HE2	1.73	0.70
2:B:141:THR:HG22	2:B:394:ILE:HG13	1.74	0.70
1:D:22:GLN:NE2	1:D:31:GLN:HE22	1.89	0.70
1:A:42:VAL:HG12	1:A:66:LEU:HB3	1.74	0.69
1:A:133:CYS:HA	1:A:250:ARG:HH12	1.58	0.69
2:B:482:ILE:HD13	2:B:488:THR:HB	1.74	0.69
1:D:249:PHE:CE1	1:D:268:LEU:HD23	2.28	0.69
1:A:311:ALA:O	1:A:315:VAL:HG23	1.95	0.67
2:B:256:THR:O	2:B:260:LYS:HB3	1.95	0.67
2:E:28:ILE:HD11	2:E:141:THR:HG23	1.76	0.67
3:F:27:ILE:HG12	3:F:33:GLU:HG3	1.74	0.67
1:D:141:LYS:HE2	1:D:145:ILE:HD11	1.76	0.67
3:F:45:LYS:HA	3:F:48:LYS:HD3	1.76	0.67
2:B:423:ASN:HB2	2:B:424:PRO:HD2	1.78	0.66
2:B:454:LEU:HD12	2:B:459:VAL:HG21	1.76	0.66
2:B:316:LYS:HE2	2:B:320:ARG:NH1	2.11	0.66
3:C:76:THR:HG22	3:C:79:GLU:HG3	1.78	0.66
1:D:174:PHE:HE2	1:D:211:VAL:HG23	1.61	0.65
1:A:42:VAL:HG21	1:A:131:LEU:HG	1.78	0.65
3:F:22:ILE:HD13	3:F:40:MET:HB2	1.78	0.65
1:D:273:ARG:HH12	1:D:289:GLU:HG2	1.61	0.65
3:F:25:LYS:HD3	3:F:85:GLU:O	1.97	0.65
2:B:467:LYS:HB3	2:B:467:LYS:HZ3	1.60	0.65
1:A:233:LEU:HD21	1:A:286:LEU:HD21	1.77	0.65
2:E:456:VAL:HG12	2:E:534:HIS:ND1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:LEU:HD11	2:B:353:ASP:HB3	1.78	0.65
2:E:496:GLY:H	2:E:499:GLU:CD	2.05	0.65
2:B:47:ILE:HD12	2:B:92:TYR:HB2	1.78	0.65
2:E:183:ILE:HA	2:E:186:ILE:HD12	1.79	0.65
2:E:25:ALA:HB2	2:E:46:LEU:HD11	1.79	0.64
2:B:145:LEU:HB2	3:C:94:GLN:HE21	1.62	0.64
2:B:465:GLN:O	2:B:465:GLN:HG2	1.96	0.64
2:B:155:VAL:HG12	2:B:156:THR:HG23	1.79	0.64
2:B:263:ILE:HG22	2:B:281:PRO:HG3	1.80	0.64
2:E:194:ASN:HA	2:E:198:GLY:HA3	1.80	0.64
2:E:23:VAL:CG1	2:E:96:ILE:HG12	2.28	0.63
2:E:414:ARG:NE	7:E:802:HOH:O	2.32	0.63
3:F:44:LEU:HD21	3:F:77:PRO:HG3	1.80	0.63
1:A:60:VAL:O	1:A:106:VAL:HG22	1.98	0.63
2:E:499:GLU:HA	2:E:502:ASN:HD21	1.62	0.63
3:F:22:ILE:CD1	3:F:40:MET:HB2	2.29	0.63
1:D:98:ARG:NH1	2:E:83:PHE:HB3	2.11	0.63
1:A:133:CYS:HA	1:A:250:ARG:NH1	2.13	0.63
1:D:83:ARG:HA	1:D:98:ARG:HH21	1.63	0.63
1:A:92:ALA:HB1	1:A:110:VAL:HG13	1.80	0.63
2:B:259:PHE:HB3	2:B:365:ILE:HD11	1.80	0.63
1:A:273:ARG:HG2	1:A:277:LEU:HD12	1.80	0.63
2:B:145:LEU:HB2	3:C:94:GLN:NE2	2.15	0.62
1:D:277:LEU:HD13	1:D:284:PRO:HA	1.80	0.62
1:D:152:LYS:HG2	1:D:169:LEU:HD22	1.81	0.62
2:E:421:GLN:HG3	2:E:422:PRO:HD2	1.80	0.62
2:B:156:THR:O	2:B:437:PRO:HG3	1.98	0.62
2:E:522:PHE:N	7:E:877:HOH:O	2.32	0.62
3:F:55:GLN:HB3	3:F:57:VAL:HG23	1.79	0.62
2:B:215:ALA:HB2	2:B:272:LEU:HB2	1.80	0.62
1:A:42:VAL:HG22	1:A:131:LEU:HA	1.81	0.62
1:A:70:GLN:HE21	1:A:89:ARG:C	2.07	0.62
2:E:134:VAL:HG13	2:E:135:PRO:HD2	1.82	0.62
2:B:71:SER:O	2:B:75:VAL:HG23	2.00	0.61
2:E:156:THR:O	2:E:437:PRO:HG3	2.00	0.61
2:B:423:ASN:HD21	2:B:425:ARG:HE	1.49	0.61
3:F:17:LYS:HG3	3:F:18:GLU:H	1.65	0.61
3:C:45:LYS:HD2	3:C:73:ASP:HB3	1.81	0.61
3:F:43:HIS:HA	3:F:76:THR:HG23	1.81	0.61
1:A:71:VAL:HG22	1:A:91:ARG:HA	1.81	0.61
2:E:456:VAL:HG21	2:E:511:ILE:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:CYS:HB2	3:C:57:VAL:O	2.00	0.61
1:A:337:ASN:HB3	1:A:339:ILE:HD11	1.81	0.61
1:D:10:GLY:H	1:D:32:LYS:HE2	1.67	0.60
1:A:42:VAL:CG2	1:A:131:LEU:HG	2.30	0.60
2:B:142:ALA:HB3	3:C:94:GLN:NE2	2.16	0.60
1:A:120:GLU:HG3	1:A:145:ILE:HG23	1.81	0.60
2:B:23:VAL:HG12	2:B:116:LEU:HD21	1.83	0.60
2:E:360:ASN:HA	2:E:363:MET:HE3	1.83	0.60
1:A:273:ARG:HG3	1:A:287:LEU:HD23	1.83	0.60
1:A:299:MET:HE3	2:B:7:LEU:HD21	1.84	0.59
2:E:84:TYR:N	2:E:85:PRO:HD3	2.17	0.59
3:F:23:LYS:HE2	3:F:37:LYS:HE2	1.83	0.59
1:D:205:THR:HG22	1:D:207:VAL:HG23	1.83	0.59
2:B:371:LYS:HD3	2:B:379:MET:HE1	1.85	0.59
1:D:334:MET:HE2	1:D:334:MET:HA	1.83	0.59
1:A:132:THR:HG22	1:A:133:CYS:SG	2.42	0.59
1:A:339:ILE:HD12	1:A:339:ILE:N	2.18	0.59
2:E:455:ASN:C	2:E:455:ASN:HD22	2.11	0.59
1:A:38:ARG:HH11	1:A:38:ARG:HB2	1.68	0.59
1:A:165:THR:OG1	1:A:329:PHE:HB3	2.03	0.59
2:E:499:GLU:HA	2:E:502:ASN:ND2	2.18	0.59
1:A:161:TYR:CD2	1:A:334:MET:HE3	2.37	0.58
1:D:118:LYS:HG2	1:D:122:PHE:CD2	2.38	0.58
3:C:76:THR:CG2	3:C:79:GLU:HG3	2.34	0.58
1:A:82:ILE:HG23	1:A:94:ALA:HB1	1.84	0.58
2:B:538:LEU:HD11	2:B:545:GLU:HG2	1.86	0.58
3:C:82:MET:HE1	3:C:88:ILE:HD11	1.85	0.58
2:E:89:ILE:N	2:E:89:ILE:HD12	2.19	0.58
1:A:131:LEU:HD12	1:A:131:LEU:N	2.19	0.57
2:B:73:ALA:HB1	2:B:91:ALA:HB1	1.87	0.57
1:A:131:LEU:HD21	1:A:142:VAL:HG21	1.85	0.57
2:B:215:ALA:HB1	2:B:271:LYS:HD3	1.86	0.57
3:C:39:LYS:HE2	3:C:41:THR:O	2.05	0.57
1:D:165:THR:HG23	1:D:310:LEU:HD13	1.86	0.57
2:E:371:LYS:HD3	2:E:379:MET:HE1	1.86	0.57
1:A:11:ILE:HG22	1:A:35:ARG:CZ	2.35	0.57
1:D:312:GLN:O	1:D:316:LYS:HG3	2.05	0.57
3:F:63:ARG:HG2	3:F:65:LEU:CD1	2.34	0.57
2:E:97:MET:HE3	2:E:121:ALA:CA	2.28	0.57
3:F:45:LYS:HD2	3:F:73:ASP:HB3	1.87	0.57
2:B:8:PRO:HD2	2:B:9:ARG:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:TYR:HA	7:B:855:HOH:O	2.04	0.56
3:C:64:PHE:HB3	3:C:71:ILE:HD12	1.87	0.56
2:B:141:THR:CG2	2:B:394:ILE:HG13	2.34	0.56
1:D:45:LYS:HE3	1:D:91:ARG:HH12	1.70	0.56
2:B:215:ALA:HA	2:B:271:LYS:HB2	1.87	0.56
2:E:418:LEU:HD13	2:E:429:LEU:HD21	1.87	0.56
1:A:224:TRP:HE1	1:A:280:LEU:HD23	1.70	0.56
2:E:498:THR:C	2:E:500:ALA:H	2.13	0.56
1:D:176:GLU:O	1:D:206:MET:HA	2.05	0.56
1:D:273:ARG:NH1	1:D:289:GLU:HG2	2.19	0.56
3:F:21:TYR:HB2	3:F:39:LYS:HA	1.87	0.56
3:F:72:ALA:H	3:F:75:HIS:CG	2.23	0.55
1:A:71:VAL:HG23	1:A:89:ARG:O	2.06	0.55
1:A:179:THR:HG21	1:A:203:GLU:HG3	1.88	0.55
1:A:226:SER:O	1:A:230:LYS:HG2	2.07	0.55
2:B:425:ARG:O	2:B:426:LYS:HB2	2.06	0.55
2:B:461:VAL:HG12	7:B:887:HOH:O	2.06	0.55
3:F:44:LEU:HG	3:F:77:PRO:HD3	1.88	0.55
3:C:72:ALA:H	3:C:75:HIS:CD2	2.21	0.55
1:A:300:ALA:HB3	1:A:301:PRO:HD3	1.89	0.55
2:E:49:LEU:HD12	2:E:49:LEU:C	2.32	0.55
2:E:188:TRP:NE1	2:E:362:ARG:NH2	2.55	0.55
2:B:450:VAL:HG22	2:B:451:THR:N	2.20	0.55
1:D:157:ASP:HB2	1:D:164:TYR:HE2	1.71	0.55
2:E:243:TRP:CH2	2:E:257:LYS:HG3	2.41	0.55
2:B:65:LYS:O	2:B:68:VAL:HG23	2.07	0.55
3:C:19:GLY:H	3:C:39:LYS:HB2	1.71	0.55
1:D:273:ARG:HG3	1:D:287:LEU:HD23	1.89	0.55
1:D:165:THR:HB	1:D:329:PHE:HB3	1.90	0.54
2:E:77:LYS:HG3	2:E:89:ILE:HB	1.88	0.54
1:A:299:MET:CE	2:B:7:LEU:HD11	2.35	0.54
2:B:316:LYS:HG2	2:B:320:ARG:CZ	2.37	0.54
2:B:484:ASP:OD1	2:B:486:LYS:HD2	2.06	0.54
1:D:45:LYS:HE3	1:D:91:ARG:NH1	2.23	0.54
3:F:72:ALA:O	3:F:75:HIS:HB2	2.07	0.54
1:A:141:LYS:HE2	1:A:145:ILE:HD11	1.90	0.54
2:E:23:VAL:HG13	2:E:96:ILE:HG12	1.90	0.54
1:A:124:THR:HG23	1:A:149:ASN:ND2	2.18	0.54
2:B:20:VAL:HG13	2:B:113:MET:HE3	1.90	0.54
2:B:244:ALA:HB1	2:B:249:TYR:CE1	2.43	0.54
1:D:9:GLY:HA3	2:E:306:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:HA	1:D:206:MET:H	1.72	0.54
2:E:273:TRP:HA	2:E:276:ARG:CG	2.37	0.54
1:A:42:VAL:CG2	1:A:131:LEU:HA	2.38	0.54
2:B:240:THR:HA	2:B:242:GLU:OE2	2.07	0.54
3:C:20:GLU:OE1	3:C:37:LYS:HB3	2.07	0.54
2:E:283:ASP:O	2:E:287:VAL:HG23	2.07	0.54
1:A:66:LEU:HD21	1:A:113:GLU:O	2.08	0.54
1:D:68:HIS:HB3	7:D:381:HOH:O	2.07	0.54
2:E:19:ARG:HH21	2:E:90:VAL:HG21	1.73	0.54
2:E:65:LYS:O	2:E:68:VAL:HG23	2.08	0.54
1:A:44:LEU:CD2	1:A:65:MET:HB3	2.38	0.53
1:A:68:HIS:HB2	7:A:376:HOH:O	2.08	0.53
1:D:173:GLU:HG2	1:D:208:LYS:HE2	1.91	0.53
2:E:181:GLU:HB2	2:E:184:HIS:CE1	2.42	0.53
2:B:47:ILE:CD1	2:B:92:TYR:HB2	2.39	0.53
3:C:84:GLU:HG3	3:C:85:GLU:HG2	1.90	0.53
2:E:257:LYS:O	2:E:257:LYS:HD3	2.08	0.53
2:B:181:GLU:HB2	2:B:183:ILE:HG22	1.90	0.53
3:F:49:GLU:O	3:F:53:GLN:HB2	2.09	0.53
2:B:456:VAL:HG11	2:B:511:ILE:O	2.08	0.53
2:E:188:TRP:NE1	2:E:362:ARG:HH21	2.07	0.53
2:E:188:TRP:HE1	2:E:362:ARG:HH21	1.56	0.53
3:F:40:MET:HA	3:F:77:PRO:HB2	1.91	0.53
2:B:412:GLN:O	2:B:414:ARG:HD2	2.08	0.53
2:B:500:ALA:HA	2:B:503:HIS:HE1	1.74	0.53
2:E:37:VAL:HG23	2:E:38:LEU:N	2.23	0.53
2:E:141:THR:O	3:F:96:GLY:HA3	2.09	0.53
2:B:459:VAL:O	2:B:506:LEU:HG	2.08	0.53
3:C:49:GLU:O	3:C:53:GLN:HB2	2.09	0.53
1:D:165:THR:HG22	7:D:373:HOH:O	2.08	0.53
2:E:243:TRP:CZ3	2:E:257:LYS:HG3	2.43	0.53
3:F:24:LEU:HD13	3:F:88:ILE:HD11	1.91	0.53
2:B:81:LEU:HD23	2:B:87:ALA:HB3	1.89	0.53
1:D:280:LEU:O	1:D:282:ILE:HG13	2.08	0.53
2:E:118:ASN:C	2:E:118:ASN:ND2	2.65	0.53
2:E:454:LEU:HD21	2:E:532:ILE:HG23	1.91	0.53
1:D:176:GLU:HG2	1:D:177:GLU:H	1.73	0.52
2:B:28:ILE:HD11	2:B:141:THR:HG23	1.92	0.52
2:E:257:LYS:HD3	2:E:257:LYS:C	2.34	0.52
3:F:25:LYS:HB3	3:F:35:HIS:CD2	2.44	0.52
2:B:201:ASP:HB3	2:B:204:GLN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:102:ASN:O	2:E:105:PHE:HB3	2.09	0.52
2:E:210:ARG:HA	2:E:210:ARG:CZ	2.39	0.52
2:E:158:CYS:O	2:E:161:CYS:HB2	2.09	0.52
2:E:457:HIS:O	2:E:505:LYS:HG2	2.10	0.52
2:B:199:GLU:HA	2:B:341:GLU:OE2	2.09	0.52
2:B:420:LYS:NZ	2:B:420:LYS:HB3	2.25	0.52
3:F:23:LYS:HG2	3:F:24:LEU:N	2.25	0.52
2:B:540:LYS:HA	7:B:807:HOH:O	2.09	0.52
2:E:365:ILE:HG22	2:E:365:ILE:O	2.08	0.52
3:F:75:HIS:CB	3:F:80:LEU:HD11	2.34	0.52
1:A:313:GLU:OE2	1:A:316:LYS:HE2	2.10	0.51
1:D:321:ARG:O	1:D:322:ASP:HB2	2.09	0.51
2:B:33:LEU:HD11	2:B:46:LEU:CD1	2.41	0.51
1:A:136:ARG:HG3	1:A:247:LEU:HD13	1.92	0.51
1:D:75:ASP:N	1:D:76:PRO:HD2	2.25	0.51
1:A:179:THR:HG21	1:A:203:GLU:O	2.10	0.51
2:B:423:ASN:OD1	2:B:427:LYS:HB2	2.09	0.51
2:B:470:LYS:HA	2:B:475:MET:O	2.09	0.51
3:C:26:VAL:HG12	3:C:90:VAL:HG23	1.91	0.51
2:E:273:TRP:HB3	2:E:278:PRO:HG3	1.93	0.51
1:A:176:GLU:HG3	1:A:323:PRO:HD3	1.91	0.51
2:E:348:ASP:HB3	2:E:351:ALA:HB3	1.93	0.51
2:E:482:ILE:HD12	2:E:488:THR:HB	1.92	0.51
1:D:268:LEU:O	1:D:271:GLN:HB3	2.11	0.51
3:F:43:HIS:CD2	3:F:74:ASN:HA	2.46	0.51
2:E:71:SER:HB3	2:E:74:GLN:HB2	1.93	0.51
3:F:48:LYS:HB2	3:F:59:MET:HE1	1.93	0.51
1:D:71:VAL:HG22	1:D:91:ARG:HA	1.93	0.51
3:C:19:GLY:O	3:C:20:GLU:HG2	2.10	0.50
1:D:14:GLU:OE1	1:D:105:MET:HE3	2.11	0.50
1:D:74:GLU:OE2	1:D:74:GLU:N	2.43	0.50
2:E:102:ASN:HD22	2:E:102:ASN:H	1.59	0.50
3:F:76:THR:OG1	3:F:79:GLU:HB2	2.11	0.50
2:B:8:PRO:CD	2:B:9:ARG:H	2.21	0.50
1:D:265:ASP:O	1:D:266:SER:C	2.52	0.50
2:E:288:GLN:N	2:E:288:GLN:HE21	2.09	0.50
1:A:340:VAL:HG21	2:B:422:PRO:HG3	1.93	0.50
2:B:257:LYS:HA	2:B:261:ASP:HB2	1.92	0.50
2:E:37:VAL:HG23	2:E:38:LEU:H	1.76	0.50
1:A:143:ASP:OD1	1:A:216:VAL:HG12	2.12	0.50
1:D:97:GLU:O	1:D:98:ARG:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:260:LYS:HB2	2:E:282:LEU:O	2.12	0.50
3:F:52:CYS:HB2	3:F:57:VAL:O	2.11	0.50
2:B:496:GLY:H	2:B:499:GLU:CD	2.20	0.50
3:C:27:ILE:HG12	3:C:33:GLU:HG2	1.93	0.50
1:A:179:THR:OG1	1:A:204:THR:HA	2.10	0.50
2:B:240:THR:HG23	2:B:242:GLU:OE1	2.11	0.50
1:D:310:LEU:O	1:D:310:LEU:HD12	2.12	0.50
2:E:352:MET:SD	2:E:377:LYS:HG3	2.52	0.50
3:F:63:ARG:HG2	3:F:65:LEU:HD11	1.93	0.50
2:E:164:LYS:HB3	2:E:165:PRO:HD2	1.94	0.50
2:E:268:THR:HB	2:E:269:MET:HE3	1.93	0.50
1:A:162:HIS:HD2	1:A:239:ASP:OD2	1.95	0.49
2:B:30:CYS:SG	2:B:62:LEU:HD12	2.51	0.49
2:E:212:ASP:O	2:E:214:GLU:N	2.45	0.49
2:B:111:LEU:CG	2:B:113:MET:HE2	2.42	0.49
2:B:482:ILE:HD12	2:B:482:ILE:N	2.28	0.49
1:D:332:ASP:OD1	1:D:334:MET:HB2	2.12	0.49
2:B:482:ILE:O	2:B:487:GLY:HA2	2.12	0.49
3:C:45:LYS:HA	3:C:48:LYS:HD3	1.94	0.49
1:A:175:VAL:CG2	1:A:206:MET:HB2	2.43	0.49
2:B:344:TRP:NE1	2:B:355:VAL:HG21	2.28	0.49
1:D:166:PHE:CE2	1:D:216:VAL:HG22	2.48	0.49
2:E:492:SER:N	2:E:498:THR:HG21	2.27	0.49
2:E:497:GLU:O	2:E:498:THR:HG23	2.13	0.49
7:D:402:HOH:O	2:E:389:THR:HG23	2.12	0.49
3:F:72:ALA:HB3	3:F:75:HIS:ND1	2.27	0.49
2:B:26:GLY:O	2:B:60:GLN:HG2	2.13	0.49
2:B:283:ASP:O	2:B:287:VAL:HG23	2.12	0.49
3:C:20:GLU:OE1	3:C:37:LYS:HD3	2.13	0.49
1:A:130:CYS:HA	1:A:154:PHE:O	2.13	0.49
2:E:122:ARG:HD3	2:E:159:TYR:CZ	2.47	0.49
2:B:210:ARG:HG3	2:B:211:ALA:N	2.27	0.49
3:F:43:HIS:HA	3:F:76:THR:CG2	2.43	0.49
2:B:34:LYS:HD2	2:B:35:ASN:OD1	2.13	0.49
2:B:450:VAL:CG2	2:B:451:THR:N	2.76	0.49
2:E:241:LYS:O	2:E:245:LYS:HG2	2.13	0.49
1:A:224:TRP:NE1	1:A:280:LEU:HD23	2.28	0.48
2:B:98:ASN:HB3	2:B:101:TYR:CE1	2.47	0.48
2:B:208:PRO:HB3	2:B:266:LEU:HD13	1.94	0.48
2:E:271:LYS:O	2:E:274:ARG:HB2	2.13	0.48
1:A:161:TYR:CE2	1:A:334:MET:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:THR:HG22	1:D:133:CYS:SG	2.53	0.48
1:A:230:LYS:HB3	1:A:230:LYS:HZ3	1.78	0.48
2:B:18:GLY:CA	2:B:110:ILE:HD13	2.41	0.48
2:E:256:THR:O	2:E:260:LYS:HB3	2.12	0.48
2:B:263:ILE:N	2:B:263:ILE:HD12	2.28	0.48
2:E:193:PHE:CD2	2:E:344:TRP:HB2	2.48	0.48
1:A:321:ARG:O	1:A:322:ASP:HB2	2.13	0.48
2:B:179:PRO:HD2	2:B:366:PHE:CE2	2.48	0.48
2:B:217:TRP:HB2	2:B:269:MET:HE3	1.96	0.48
2:B:418:LEU:HA	2:B:429:LEU:HD23	1.95	0.48
1:D:305:VAL:HG23	2:E:396:GLY:HA3	1.94	0.48
2:B:98:ASN:HB3	2:B:101:TYR:CD1	2.49	0.48
2:B:364:HIS:ND1	2:B:370:MET:HE2	2.29	0.48
2:B:429:LEU:O	2:B:431:PRO:HD3	2.13	0.48
2:B:455:ASN:ND2	2:B:536:GLU:HA	2.21	0.48
2:E:167:GLN:H	2:E:167:GLN:CD	2.22	0.48
1:A:81:LEU:O	1:A:95:SER:HA	2.13	0.48
1:A:96:LEU:HD13	1:A:110:VAL:HG23	1.96	0.48
2:E:492:SER:H	2:E:498:THR:HG21	1.79	0.48
3:F:22:ILE:HD12	3:F:22:ILE:N	2.29	0.48
2:B:76:ALA:O	2:B:80:VAL:HG23	2.13	0.47
2:B:420:LYS:HZ3	2:B:421:GLN:HG3	1.79	0.47
2:B:7:LEU:H	2:B:8:PRO:HA	1.79	0.47
2:B:469:VAL:O	2:B:475:MET:HB2	2.14	0.47
1:D:161:TYR:CE2	1:D:334:MET:HE3	2.49	0.47
3:F:36:PHE:HZ	3:F:51:TYR:HA	1.79	0.47
2:B:33:LEU:HD11	2:B:46:LEU:HD11	1.96	0.47
2:E:77:LYS:O	2:E:81:LEU:HB2	2.15	0.47
1:A:178:LYS:O	1:A:178:LYS:HG3	2.14	0.47
2:B:71:SER:HB3	2:B:74:GLN:HB2	1.96	0.47
1:D:10:GLY:H	1:D:32:LYS:CE	2.26	0.47
2:E:418:LEU:HD13	2:E:429:LEU:CD2	2.45	0.47
2:E:188:TRP:HE1	2:E:362:ARG:NH2	2.12	0.47
3:F:75:HIS:CD2	3:F:80:LEU:HD21	2.50	0.47
1:A:334:MET:HA	1:A:334:MET:CE	2.39	0.47
2:B:33:LEU:HD13	2:B:80:VAL:HG21	1.96	0.47
2:B:327:GLU:O	2:B:331:VAL:HG23	2.13	0.47
2:B:454:LEU:N	2:B:454:LEU:HD23	2.29	0.47
2:E:197:PHE:CD1	2:E:197:PHE:N	2.83	0.47
2:E:415:THR:HB	7:E:834:HOH:O	2.15	0.47
2:E:423:ASN:OD1	2:E:423:ASN:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HD11	2:B:340:ALA:O	2.15	0.47
2:E:242:GLU:HA	2:E:245:LYS:HB2	1.97	0.47
2:E:134:VAL:CG1	2:E:135:PRO:HD2	2.45	0.47
1:A:174:PHE:HE2	1:A:211:VAL:HG23	1.80	0.46
3:C:64:PHE:CD2	3:C:90:VAL:HG22	2.50	0.46
2:E:334:ALA:C	2:E:336:LYS:H	2.24	0.46
2:B:49:LEU:CD1	2:B:49:LEU:C	2.88	0.46
1:D:65:MET:HE2	1:D:108:VAL:CG1	2.45	0.46
3:F:22:ILE:HG22	3:F:23:LYS:N	2.30	0.46
2:B:250:ASP:HB3	2:B:253:LYS:HB2	1.96	0.46
2:B:105:PHE:O	2:B:108:GLN:HG3	2.15	0.46
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.80	0.46
3:C:26:VAL:HG13	3:C:88:ILE:HB	1.97	0.46
1:D:128:ALA:HB2	1:D:318:LEU:HD21	1.96	0.46
2:E:150:THR:CG2	2:E:405:ILE:HD11	2.46	0.46
2:E:208:PRO:HG3	2:E:266:LEU:HD13	1.97	0.46
2:E:322:PHE:CE1	2:E:326:ILE:HD11	2.51	0.46
3:F:71:ILE:HA	3:F:75:HIS:CD2	2.51	0.46
2:B:52:ILE:HD12	2:B:52:ILE:H	1.80	0.46
2:B:414:ARG:HB2	2:B:432:CYS:O	2.14	0.46
1:D:259:SER:C	1:D:261:THR:N	2.74	0.46
3:F:47:LEU:HA	3:F:50:SER:HB3	1.98	0.46
2:B:124:HIS:O	2:B:128:MET:HG2	2.16	0.46
2:B:214:GLU:HB3	2:B:272:LEU:HG	1.97	0.46
2:B:263:ILE:CG2	2:B:281:PRO:HG3	2.44	0.46
2:B:455:ASN:OD1	2:B:457:HIS:HB2	2.16	0.46
3:C:26:VAL:HG12	3:C:90:VAL:CG2	2.46	0.46
2:E:381:GLY:O	2:E:382:ASN:C	2.58	0.46
3:F:45:LYS:HB2	3:F:73:ASP:CA	2.46	0.46
2:B:49:LEU:HD23	2:B:95:SER:HB2	1.97	0.46
2:E:425:ARG:O	2:E:426:LYS:HB2	2.16	0.46
2:B:170:PHE:CB	2:B:175:ILE:HD11	2.46	0.45
1:D:244:GLN:HA	1:D:244:GLN:HE21	1.81	0.45
2:E:161:CYS:SG	2:E:438:ASN:HB3	2.57	0.45
1:A:299:MET:HE3	2:B:7:LEU:CD1	2.43	0.45
2:B:308:LYS:HB3	2:B:308:LYS:NZ	2.31	0.45
3:C:25:LYS:HG3	3:C:87:VAL:HG22	1.97	0.45
2:E:34:LYS:HD3	2:E:61:PHE:CZ	2.51	0.45
2:E:510:GLY:O	2:E:512:ARG:HD3	2.16	0.45
3:F:39:LYS:HB3	3:F:42:THR:OG1	2.17	0.45
1:A:11:ILE:HA	1:A:35:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PRO:HG3	1:A:87:VAL:HG11	1.98	0.45
3:C:38:VAL:HG21	3:C:47:LEU:HD12	1.99	0.45
1:D:44:LEU:HD21	1:D:65:MET:HB3	1.96	0.45
1:A:230:LYS:HB3	1:A:230:LYS:NZ	2.32	0.45
2:B:446:SER:O	2:B:447:LYS:HD2	2.16	0.45
1:D:66:LEU:C	1:D:66:LEU:HD23	2.42	0.45
2:E:376:ILE:HA	2:E:379:MET:HE3	1.97	0.45
2:E:407:SER:HB3	2:E:409:LYS:HE3	1.99	0.45
2:B:482:ILE:HD12	2:B:482:ILE:H	1.82	0.45
3:C:89:GLU:OE1	3:C:91:TYR:OH	2.31	0.45
2:E:23:VAL:CG1	2:E:116:LEU:HD21	2.42	0.45
2:B:94:ASP:OD2	2:B:98:ASN:ND2	2.50	0.45
1:A:230:LYS:NZ	1:A:230:LYS:CB	2.80	0.45
3:C:82:MET:HE1	3:C:88:ILE:CG1	2.47	0.45
2:E:19:ARG:NH2	2:E:90:VAL:HG21	2.32	0.45
2:E:188:TRP:O	2:E:191:TYR:HB2	2.17	0.45
3:F:75:HIS:CD2	3:F:80:LEU:HD11	2.51	0.45
1:A:154:PHE:HB3	1:A:310:LEU:HD11	1.98	0.45
2:B:34:LYS:O	2:B:38:LEU:HG	2.16	0.45
2:B:116:LEU:HD13	2:B:121:ALA:CB	2.47	0.45
1:D:224:TRP:HA	1:D:229:ALA:HB1	1.98	0.45
2:E:34:LYS:HE2	2:E:34:LYS:HB3	1.77	0.45
3:F:21:TYR:HB3	3:F:22:ILE:CD1	2.37	0.45
2:B:195:GLN:NE2	2:B:201:ASP:H	2.15	0.45
2:E:535:SER:HB3	2:E:538:LEU:HD21	1.98	0.45
1:A:73:PRO:O	1:A:74:GLU:HB2	2.17	0.45
1:A:228:LYS:N	1:A:228:LYS:HD2	2.32	0.45
2:B:418:LEU:HD13	2:B:429:LEU:HD21	1.99	0.45
2:E:76:ALA:O	2:E:80:VAL:HG23	2.17	0.45
2:E:276:ARG:O	2:E:278:PRO:HD3	2.17	0.45
1:A:244:GLN:NE2	7:A:354:HOH:O	2.49	0.44
3:C:64:PHE:O	3:C:65:LEU:HD12	2.16	0.44
2:E:178:THR:HG21	2:E:276:ARG:CZ	2.47	0.44
2:E:447:LYS:HD3	2:E:447:LYS:HA	1.75	0.44
2:E:496:GLY:C	2:E:499:GLU:OE2	2.61	0.44
3:F:44:LEU:CD2	3:F:77:PRO:HG3	2.46	0.44
1:A:9:GLY:HA2	2:B:306:GLY:O	2.17	0.44
1:A:28:LEU:HD23	2:B:306:GLY:HA2	2.00	0.44
2:B:67:HIS:CD2	2:B:75:VAL:HG13	2.53	0.44
2:B:207:SER:HB3	2:B:208:PRO:HD2	2.00	0.44
2:B:451:THR:HA	2:B:531:ASN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:LYS:HA	3:C:36:PHE:O	2.17	0.44
2:E:415:THR:O	2:E:432:CYS:N	2.50	0.44
1:A:122:PHE:O	1:A:125:GLN:HG2	2.17	0.44
3:C:77:PRO:HA	3:C:82:MET:HG3	1.98	0.44
1:D:79:GLN:OE1	1:D:81:LEU:HB2	2.17	0.44
2:E:119:ARG:O	2:E:123:ASN:ND2	2.51	0.44
2:E:421:GLN:CG	2:E:422:PRO:HD2	2.47	0.44
2:E:491:ILE:CA	2:E:498:THR:HG21	2.43	0.44
3:C:19:GLY:N	3:C:39:LYS:HB2	2.32	0.44
2:E:199:GLU:HA	2:E:341:GLU:OE2	2.18	0.44
2:E:238:ILE:HG23	7:E:870:HOH:O	2.17	0.44
2:E:263:ILE:CG2	2:E:281:PRO:HG3	2.48	0.44
2:E:438:ASN:OD1	2:E:440:ASN:N	2.47	0.44
2:E:454:LEU:O	2:E:534:HIS:HA	2.18	0.44
3:F:23:LYS:HD2	3:F:85:GLU:OE1	2.17	0.44
3:F:27:ILE:HD12	3:F:87:VAL:HG11	1.99	0.44
2:B:49:LEU:C	2:B:49:LEU:HD12	2.42	0.44
2:E:102:ASN:O	2:E:105:PHE:N	2.47	0.44
2:E:139:SER:OG	2:E:398:ILE:HD11	2.17	0.44
3:F:27:ILE:HG23	3:F:32:SER:O	2.17	0.44
1:A:175:VAL:HG21	1:A:206:MET:HB2	2.00	0.44
2:B:48:ASP:HB3	7:B:856:HOH:O	2.16	0.44
1:D:283:SER:HB2	1:D:285:ASP:OD1	2.17	0.44
2:B:117:ASP:OD1	2:B:117:ASP:C	2.61	0.44
2:B:315:VAL:HG22	2:B:370:MET:HE1	2.00	0.44
2:E:14:ALA:O	2:E:18:GLY:N	2.51	0.44
2:E:423:ASN:HB2	2:E:424:PRO:CD	2.48	0.44
3:F:25:LYS:O	3:F:87:VAL:HA	2.17	0.44
1:A:337:ASN:HB3	1:A:339:ILE:CD1	2.47	0.44
2:B:171:PRO:HG2	2:B:174:THR:OG1	2.18	0.44
2:B:8:PRO:CD	2:B:9:ARG:N	2.79	0.43
2:E:77:LYS:HG3	2:E:89:ILE:CG2	2.48	0.43
3:F:55:GLN:C	3:F:57:VAL:H	2.26	0.43
1:A:155:THR:HG22	1:A:166:PHE:HB3	1.98	0.43
1:A:233:LEU:CD2	1:A:286:LEU:HD21	2.46	0.43
2:B:461:VAL:CG1	2:B:490:LEU:HD22	2.48	0.43
1:D:120:GLU:HG3	1:D:145:ILE:HG23	2.00	0.43
2:E:185:CYS:O	2:E:188:TRP:HB3	2.18	0.43
2:E:377:LYS:HG2	2:E:383:ILE:HD11	2.00	0.43
3:F:22:ILE:HG23	3:F:84:GLU:CD	2.43	0.43
1:A:12:SER:HB3	1:A:15:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LEU:HB2	1:D:110:VAL:HG11	2.00	0.43
2:E:150:THR:HG23	2:E:405:ILE:HD11	2.00	0.43
1:A:326:ASN:HA	1:A:327:ASN:HA	1.79	0.43
1:D:98:ARG:O	1:D:101:ASN:HB2	2.18	0.43
1:D:272:ILE:HA	1:D:275:ASP:OD1	2.19	0.43
2:E:152:LYS:HB3	2:E:155:VAL:HB	2.00	0.43
3:F:30:ASP:OD1	3:F:32:SER:HB2	2.18	0.43
3:F:42:THR:O	3:F:77:PRO:HD2	2.19	0.43
1:D:273:ARG:HG2	1:D:277:LEU:HD12	2.01	0.43
2:E:23:VAL:HG11	2:E:96:ILE:HG12	2.00	0.43
3:F:44:LEU:HD11	3:F:82:MET:SD	2.57	0.43
3:F:75:HIS:HB3	3:F:80:LEU:CD1	2.40	0.43
3:C:84:GLU:O	3:C:85:GLU:HB2	2.18	0.43
1:D:12:SER:OG	1:D:15:GLU:HG3	2.19	0.43
1:D:300:ALA:HB3	1:D:301:PRO:HD3	2.00	0.43
3:C:64:PHE:CB	3:C:71:ILE:HD12	2.48	0.43
1:A:28:LEU:HD22	2:B:307:LEU:HG	2.00	0.43
2:E:6:GLY:HA3	7:E:844:HOH:O	2.18	0.43
2:E:421:GLN:HB3	3:F:31:SER:HB2	2.00	0.43
1:A:131:LEU:N	1:A:131:LEU:CD1	2.82	0.43
1:A:224:TRP:CD1	1:A:282:ILE:HD11	2.54	0.43
1:A:289:GLU:O	1:A:292:VAL:HG22	2.19	0.43
2:B:7:LEU:N	2:B:8:PRO:HA	2.34	0.43
2:B:32:LEU:HD22	2:B:36:LEU:HG	2.01	0.43
1:D:256:ASP:HB3	1:D:257:PRO:HD2	2.01	0.43
2:E:114:ASN:OD1	2:E:136:LEU:HD11	2.19	0.43
2:E:214:GLU:HB3	2:E:272:LEU:HD23	2.00	0.43
2:B:378:SER:HA	2:B:383:ILE:HD12	2.01	0.42
2:B:456:VAL:O	2:B:507:SER:HB3	2.19	0.42
1:D:177:GLU:HA	1:D:205:THR:HB	2.01	0.42
2:E:19:ARG:HG3	2:E:43:HIS:HB3	2.01	0.42
1:A:75:ASP:N	1:A:76:PRO:CD	2.81	0.42
2:B:81:LEU:CD2	2:B:87:ALA:HB3	2.50	0.42
3:C:76:THR:HG1	3:C:77:PRO:HD2	1.84	0.42
1:D:51:ILE:HD11	1:D:310:LEU:HD23	2.01	0.42
1:D:85:GLY:HA2	7:D:386:HOH:O	2.20	0.42
2:E:360:ASN:HB3	2:E:370:MET:SD	2.59	0.42
1:A:287:LEU:HA	1:A:288:PRO:HD2	1.87	0.42
3:C:38:VAL:HG12	3:C:39:LYS:N	2.34	0.42
2:E:34:LYS:HE3	2:E:35:ASN:OD1	2.19	0.42
2:E:48:ASP:CG	6:E:801:ATP:HO2'	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:ASN:ND2	2:E:120:ALA:H	2.17	0.42
1:A:227:GLU:O	1:A:231:ALA:HB3	2.20	0.42
2:B:461:VAL:HG13	2:B:490:LEU:HD22	2.01	0.42
2:E:540:LYS:HE2	2:E:540:LYS:HB3	1.92	0.42
3:F:42:THR:O	3:F:76:THR:HG22	2.20	0.42
1:A:162:HIS:CE1	7:A:396:HOH:O	2.72	0.42
3:C:76:THR:OG1	3:C:77:PRO:HD2	2.20	0.42
1:A:160:GLY:HA3	1:A:295:CYS:HA	2.01	0.42
3:F:45:LYS:HB2	3:F:73:ASP:HB3	2.02	0.42
2:B:32:LEU:CD2	2:B:36:LEU:HG	2.50	0.42
1:D:140:VAL:O	1:D:144:GLN:HG3	2.20	0.42
1:D:207:VAL:HG12	1:D:208:LYS:N	2.35	0.42
2:E:171:PRO:HA	2:E:541:ASP:CG	2.43	0.42
2:E:496:GLY:N	2:E:499:GLU:CD	2.75	0.42
1:D:122:PHE:O	1:D:125:GLN:HG2	2.20	0.42
1:D:157:ASP:HB2	1:D:164:TYR:CE2	2.52	0.42
2:E:499:GLU:CD	2:E:499:GLU:H	2.28	0.42
1:A:129:VAL:HG12	1:A:131:LEU:CD1	2.49	0.42
2:B:89:ILE:HG22	2:B:90:VAL:N	2.35	0.42
1:D:28:LEU:O	1:D:31:GLN:HB3	2.20	0.42
1:D:166:PHE:HE1	1:D:327:ASN:ND2	2.18	0.42
2:E:23:VAL:HA	2:E:47:ILE:CG2	2.50	0.42
2:E:48:ASP:OD2	6:E:801:ATP:O2'	2.36	0.42
2:E:81:LEU:HD12	2:E:81:LEU:HA	1.81	0.42
2:E:513:ASN:HB2	2:E:534:HIS:HB3	2.01	0.42
3:F:22:ILE:HD11	3:F:40:MET:HB2	2.02	0.42
1:A:37:SER:HB3	1:A:318:LEU:HD22	2.02	0.41
1:A:96:LEU:O	1:A:97:GLU:C	2.63	0.41
1:A:233:LEU:HD11	1:A:282:ILE:HD13	2.01	0.41
2:E:33:LEU:CD2	2:E:80:VAL:HG21	2.45	0.41
2:E:454:LEU:HD12	2:E:459:VAL:HG21	2.01	0.41
2:B:40:GLY:O	2:B:41:PHE:C	2.63	0.41
2:B:92:TYR:CD1	2:B:92:TYR:N	2.88	0.41
2:B:96:ILE:O	2:B:96:ILE:HG13	2.19	0.41
2:B:178:THR:HG21	2:B:276:ARG:NH1	2.27	0.41
2:B:496:GLY:N	2:B:499:GLU:CD	2.78	0.41
2:E:46:LEU:HD13	2:E:47:ILE:N	2.35	0.41
2:E:360:ASN:O	2:E:361:LEU:C	2.62	0.41
2:E:491:ILE:HA	2:E:498:THR:CG2	2.42	0.41
2:E:498:THR:C	2:E:500:ALA:N	2.78	0.41
3:F:22:ILE:HG12	3:F:40:MET:CE	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ASP:OD1	2:B:485:GLY:N	2.54	0.41
2:E:528:LEU:HD12	2:E:529:LEU:H	1.85	0.41
3:F:76:THR:HA	3:F:77:PRO:HD3	1.94	0.41
1:A:219:ALA:HB1	1:A:328:PHE:HE1	1.86	0.41
2:B:402:GLY:O	2:B:406:LEU:HG	2.21	0.41
1:D:244:GLN:HA	1:D:244:GLN:NE2	2.35	0.41
1:A:13:GLU:O	1:A:16:ALA:HB3	2.20	0.41
1:A:98:ARG:HH12	2:B:83:PHE:HB3	1.85	0.41
2:B:47:ILE:HD12	2:B:92:TYR:O	2.20	0.41
1:D:40:LEU:HB2	1:D:126:PHE:CG	2.55	0.41
2:E:81:LEU:HD13	2:E:89:ILE:HD13	2.01	0.41
2:E:97:MET:HE2	2:E:124:HIS:HB2	2.03	0.41
2:E:360:ASN:CA	2:E:363:MET:HE3	2.49	0.41
2:B:165:PRO:HA	7:B:849:HOH:O	2.21	0.41
3:C:76:THR:HG23	3:C:79:GLU:H	1.85	0.41
2:E:273:TRP:HA	2:E:276:ARG:HG3	2.02	0.41
2:E:359:ALA:O	2:E:363:MET:HG3	2.20	0.41
2:B:117:ASP:HA	3:C:95:THR:O	2.21	0.41
1:D:26:TRP:HE1	1:D:31:GLN:HE21	1.68	0.41
2:E:322:PHE:HE1	2:E:354:PHE:CE1	2.38	0.41
1:A:152:LYS:H	1:A:152:LYS:HG2	1.64	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.90	0.41
2:B:161:CYS:HA	2:B:441:CYS:SG	2.60	0.41
2:B:185:CYS:SG	2:B:363:MET:HG2	2.60	0.41
2:B:465:GLN:OE1	2:B:491:ILE:HG23	2.20	0.41
3:C:18:GLU:OE2	3:C:18:GLU:HA	2.19	0.41
3:C:71:ILE:HD11	3:C:88:ILE:HG23	2.02	0.41
1:D:259:SER:C	1:D:261:THR:H	2.28	0.41
2:E:110:ILE:HG22	7:E:861:HOH:O	2.21	0.41
2:E:118:ASN:ND2	2:E:119:ARG:N	2.69	0.41
1:D:124:THR:HA	1:D:151:ILE:HD11	2.03	0.41
1:D:159:PHE:CG	1:D:246:LEU:HD13	2.56	0.41
2:E:20:VAL:HG12	2:E:111:LEU:HB3	2.03	0.41
2:E:405:ILE:HG12	2:E:410:ILE:HD13	2.03	0.41
3:F:78:LYS:C	3:F:80:LEU:H	2.29	0.41
3:C:82:MET:HE1	3:C:88:ILE:CD1	2.49	0.40
2:E:8:PRO:O	2:E:9:ARG:C	2.64	0.40
2:E:119:ARG:HG3	2:E:120:ALA:N	2.36	0.40
2:B:414:ARG:HA	2:B:434:LEU:HG	2.04	0.40
2:E:331:VAL:O	2:E:331:VAL:HG12	2.21	0.40
3:C:21:TYR:HD2	3:C:21:TYR:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLN:HE21	1:D:320:GLN:HB2	1.59	0.40
2:E:501:ASN:HB3	2:E:509:PHE:CZ	2.56	0.40
2:E:518:GLN:HG3	2:E:529:LEU:CD2	2.52	0.40
3:F:22:ILE:O	3:F:37:LYS:HA	2.20	0.40
2:B:170:PHE:HB3	2:B:175:ILE:HD11	2.02	0.40
1:D:299:MET:O	1:D:300:ALA:C	2.64	0.40
1:D:331:PHE:HA	1:D:337:ASN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/346 (90%)	264 (85%)	43 (14%)	3 (1%)	12	24
1	D	307/346 (89%)	264 (86%)	40 (13%)	3 (1%)	12	24
2	B	506/640 (79%)	433 (86%)	67 (13%)	6 (1%)	10	20
2	E	508/640 (79%)	452 (89%)	46 (9%)	10 (2%)	6	11
3	C	82/97 (84%)	70 (85%)	9 (11%)	3 (4%)	2	4
3	F	82/97 (84%)	68 (83%)	10 (12%)	4 (5%)	1	2
All	All	1795/2166 (83%)	1551 (86%)	215 (12%)	29 (2%)	7	14

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	PRO
1	D	205	THR
2	B	7	LEU
2	B	205	GLU
2	B	206	VAL

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Mol	Chain	Res	Type
3	C	15	ASP
3	C	21	TYR
1	D	97	GLU
2	E	214	GLU
2	E	217	TRP
2	E	498	THR
2	E	549	ASP
3	F	21	TYR
3	F	61	SER
3	F	83	GLU
1	A	96	LEU
2	E	278	PRO
3	F	43	HIS
1	A	297	SER
2	E	540	LYS
1	A	232	ALA
1	D	262	TYR
2	E	367	SER
2	B	472	LYS
3	C	40	MET
2	E	84	TYR
2	E	213	PRO
2	E	499	GLU
2	B	337	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	270/296 (91%)	258 (96%)	12 (4%)	25	47
1	D	267/296 (90%)	256 (96%)	11 (4%)	27	49
2	B	442/551 (80%)	414 (94%)	28 (6%)	16	30
2	E	443/551 (80%)	422 (95%)	21 (5%)	23	45
3	C	75/87 (86%)	71 (95%)	4 (5%)	20	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	75/87 (86%)	71 (95%)	4 (5%)	20	39
All	All	1572/1868 (84%)	1492 (95%)	80 (5%)	21	40

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	38	ARG
1	A	45	LYS
1	A	69	GLU
1	A	79	GLN
1	A	105	MET
1	A	124	THR
1	A	159	PHE
1	A	171	GLU
1	A	177	GLU
1	A	230	LYS
1	A	297	SER
2	B	11	LEU
2	B	32	LEU
2	B	46	LEU
2	B	47	ILE
2	B	49	LEU
2	B	65	LYS
2	B	66	LYS
2	B	138	GLU
2	B	205	GLU
2	B	242	GLU
2	B	256	THR
2	B	270	ASP
2	B	272	LEU
2	B	275	LYS
2	B	290	GLN
2	B	308	LYS
2	B	342	LEU
2	B	362	ARG
2	B	414	ARG
2	B	420	LYS
2	B	458	LYS
2	B	467	LYS
2	B	479	ASP
2	B	483	GLU

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Mol	Chain	Res	Type
2	B	484	ASP
2	B	486	LYS
2	B	490	LEU
2	B	499	GLU
3	C	21	TYR
3	C	26	VAL
3	C	42	THR
3	C	53	GLN
1	D	28	LEU
1	D	79	GLN
1	D	159	PHE
1	D	208	LYS
1	D	216	VAL
1	D	261	THR
1	D	267	GLU
1	D	285	ASP
1	D	294	TYR
1	D	320	GLN
1	D	334	MET
2	E	32	LEU
2	E	49	LEU
2	E	96	ILE
2	E	97	MET
2	E	102	ASN
2	E	161	CYS
2	E	197	PHE
2	E	200	GLU
2	E	206	VAL
2	E	214	GLU
2	E	256	THR
2	E	269	MET
2	E	288	GLN
2	E	305	LEU
2	E	371	LYS
2	E	454	LEU
2	E	481	GLN
2	E	492	SER
2	E	498	THR
2	E	499	GLU
2	E	520	ASP
3	F	18	GLU
3	F	21	TYR

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Mol	Chain	Res	Type
3	F	55	GLN
3	F	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	125	GLN
1	A	149	ASN
1	A	162	HIS
1	A	168	ASN
1	A	244	GLN
2	B	56	ASN
2	B	64	GLN
2	B	67	HIS
2	B	88	ASN
2	B	123	ASN
2	B	167	GLN
2	B	195	GLN
2	B	204	GLN
2	B	288	GLN
2	B	311	GLN
2	B	412	GLN
2	B	440	ASN
3	C	55	GLN
3	C	74	ASN
3	C	75	HIS
3	C	94	GLN
1	D	31	GLN
1	D	162	HIS
1	D	168	ASN
1	D	244	GLN
1	D	320	GLN
2	E	43	HIS
2	E	102	ASN
2	E	108	GLN
2	E	204	GLN
2	E	288	GLN
2	E	311	GLN
2	E	421	GLN
2	E	455	ASN
2	E	502	ASN

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Mol	Chain	Res	Type
3	F	35	HIS
3	F	43	HIS
3	F	55	GLN
3	F	60	ASN
3	F	69	GLN
3	F	92	GLN
3	F	94	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 6 ligands modelled in this entry, 4 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
6	ATP	B	802	4	32,33,33	1.23	4 (12%)	48,52,52	2.00	10 (20%)
6	ATP	E	801	4	32,33,33	1.24	3 (9%)	48,52,52	2.05	12 (25%)

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
6	ATP	B	802	4	-	5/22/38/38	0/3/3/3
6	ATP	E	801	4	-	5/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	801	ATP	PB-O3B	-3.89	1.55	1.59
6	B	802	ATP	C2-N3	2.77	1.38	1.33
6	B	802	ATP	C2-N1	2.75	1.38	1.33
6	E	801	ATP	C2-N3	2.60	1.38	1.33
6	B	802	ATP	C4-N3	2.51	1.39	1.34
6	B	802	ATP	PB-O3B	-2.31	1.57	1.59
6	E	801	ATP	C2-N1	2.15	1.37	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	802	ATP	N3-C2-N1	-5.71	119.94	128.58
6	E	801	ATP	N3-C2-N1	-5.67	120.00	128.58
6	B	802	ATP	C5-N7-C8	5.25	111.71	103.45
6	E	801	ATP	C5-N7-C8	5.24	111.69	103.45
6	B	802	ATP	N9-C8-N7	-5.06	106.76	113.94
6	E	801	ATP	N9-C8-N7	-4.84	107.08	113.94
6	B	802	ATP	C4-C5-N7	-4.74	105.16	110.58
6	E	801	ATP	C4-C5-N7	-4.59	105.33	110.58
6	E	801	ATP	C5-C4-N3	-3.12	122.42	126.72
6	E	801	ATP	C2'-C1'-N9	3.10	121.02	113.30
6	E	801	ATP	C2-N3-C4	3.08	119.36	111.83
6	B	802	ATP	C5-C4-N3	-2.87	122.76	126.72
6	B	802	ATP	C4-N9-C8	2.84	108.72	105.74
6	E	801	ATP	O4'-C1'-N9	-2.82	102.66	108.09
6	E	801	ATP	C6-C5-N7	2.79	137.46	132.09
6	B	802	ATP	C2-N3-C4	2.58	118.13	111.83
6	E	801	ATP	C4-N9-C8	2.56	108.43	105.74
6	B	802	ATP	C6-C5-N7	2.51	136.94	132.09
6	B	802	ATP	O4'-C1'-N9	-2.40	103.49	108.09
6	B	802	ATP	O2'-C2'-C3'	2.38	119.43	111.82
6	E	801	ATP	O2G-PG-O3B	2.10	111.68	104.64
6	E	801	ATP	O2B-PB-O3B	2.04	112.78	107.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

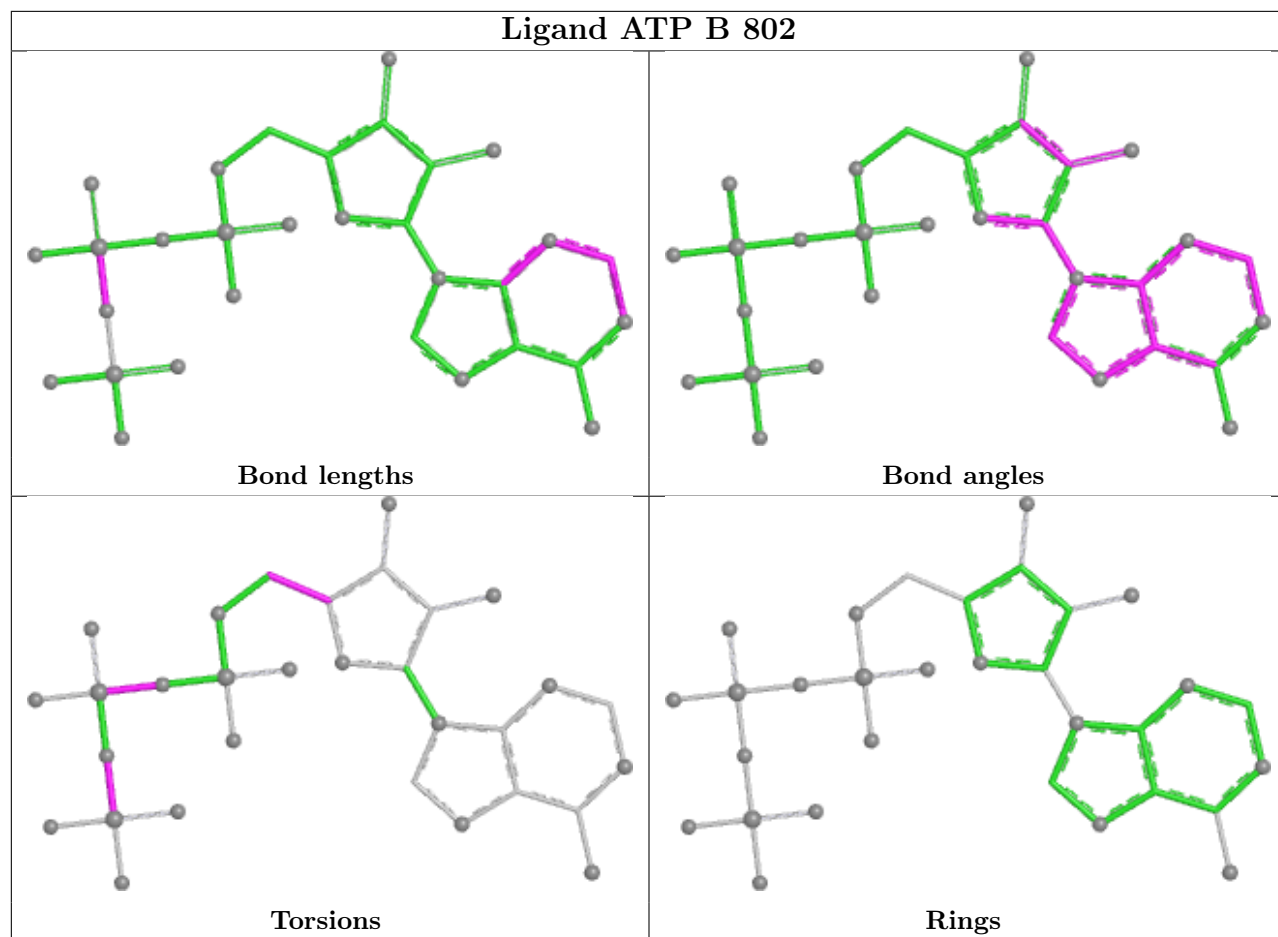
Mol	Chain	Res	Type	Atoms
6	B	802	ATP	PB-O3B-PG-O3G
6	B	802	ATP	PA-O3A-PB-O3B
6	E	801	ATP	C5'-O5'-PA-O1A
6	E	801	ATP	C5'-O5'-PA-O2A
6	E	801	ATP	C5'-O5'-PA-O3A
6	E	801	ATP	PB-O3A-PA-O2A
6	B	802	ATP	O4'-C4'-C5'-O5'
6	B	802	ATP	PA-O3A-PB-O1B
6	B	802	ATP	PA-O3A-PB-O2B
6	E	801	ATP	PB-O3A-PA-O1A

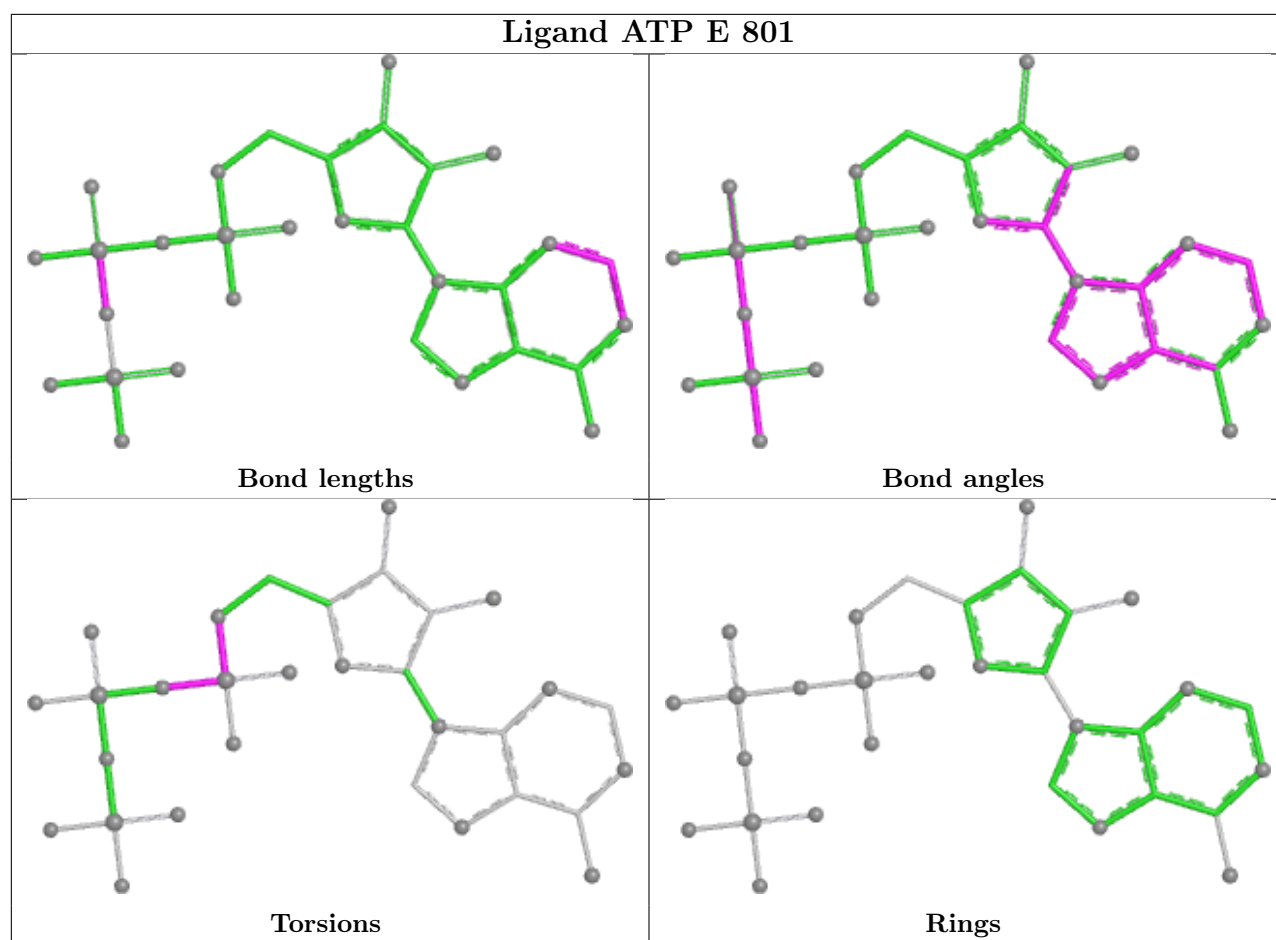
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	801	ATP	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/346 (90%)	-0.28	1 (0%) 90 91	13, 41, 82, 112	0
1	D	311/346 (89%)	-0.40	0 100 100	11, 39, 73, 94	0
2	B	512/640 (80%)	-0.10	7 (1%) 73 73	17, 53, 101, 131	0
2	E	514/640 (80%)	-0.14	14 (2%) 56 54	15, 44, 102, 133	0
3	C	84/97 (86%)	-0.00	2 (2%) 59 57	26, 63, 91, 101	0
3	F	84/97 (86%)	0.73	7 (8%) 17 18	29, 86, 107, 115	0
All	All	1819/2166 (83%)	-0.15	31 (1%) 69 67	11, 46, 97, 133	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	7	LEU	3.8
3	C	14	GLY	3.7
2	E	217	TRP	3.6
2	E	272	LEU	3.3
2	E	169	THR	3.1
3	F	14	GLY	3.0
2	E	267	LEU	3.0
3	F	38	VAL	3.0
2	E	166	THR	2.9
2	B	216	ALA	2.8
2	E	4	SER	2.8
2	E	211	ALA	2.5
3	F	19	GLY	2.4
1	A	228	LYS	2.4
2	E	165	PRO	2.4
2	B	217	TRP	2.3
2	E	175	ILE	2.3
3	C	38	VAL	2.3
2	E	206	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	197	PHE	2.2
2	B	8	PRO	2.2
3	F	20	GLU	2.2
2	E	266	LEU	2.2
2	E	271	LYS	2.2
2	E	215	ALA	2.2
3	F	22	ILE	2.1
2	B	4	SER	2.1
2	B	266	LEU	2.1
2	E	541	ASP	2.1
3	F	58	PRO	2.0
3	F	60	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

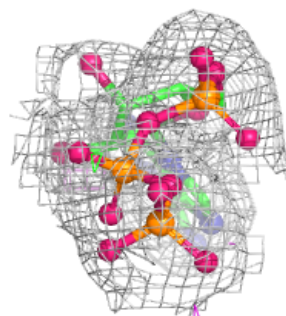
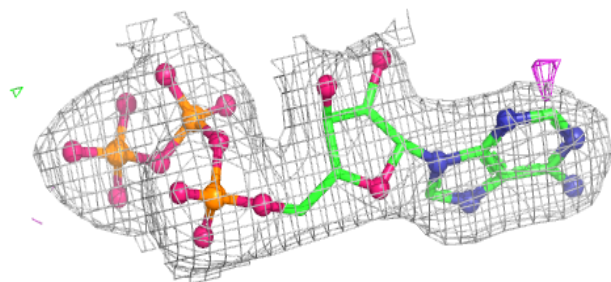
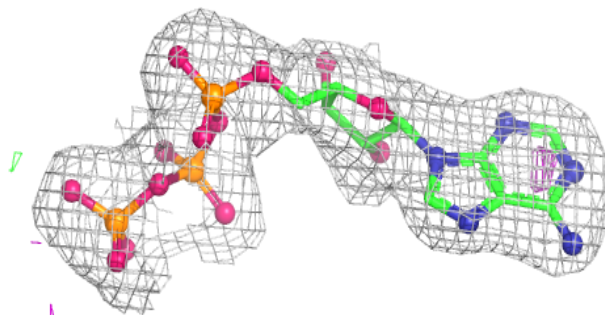
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	E	641	1/1	0.95	0.07	31,31,31,31	0
4	MG	B	641	1/1	0.96	0.04	16,16,16,16	0
6	ATP	B	802	31/31	0.98	0.06	19,28,34,35	0
6	ATP	E	801	31/31	0.98	0.04	20,26,29,32	0
5	ZN	E	642	1/1	0.99	0.03	31,31,31,31	0
5	ZN	B	642	1/1	1.00	0.01	37,37,37,37	0

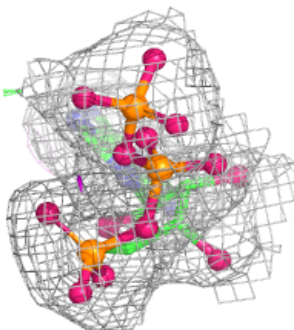
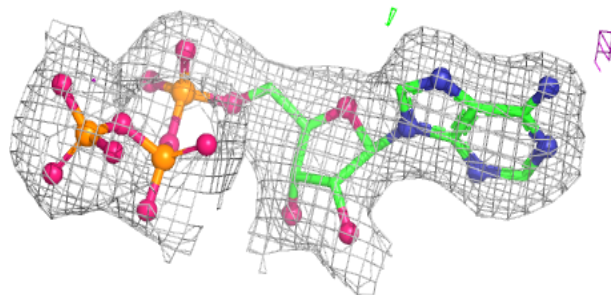
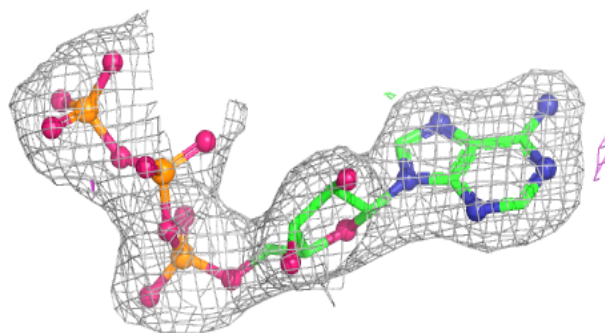
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 802:

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

**Electron density around ATP E 801:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.