



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:56 PM UTC

PDB ID : 3B2E / pdb_00003b2e
Title : Crystal structure of *S. cerevisiae* Get3 in the open conformation in complex with Get1 cytosolic domain
Authors : Kubota, K.; Yamagata, A.; Fukai, S.
Deposited on : 2011-07-30
Resolution : 3.00 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:

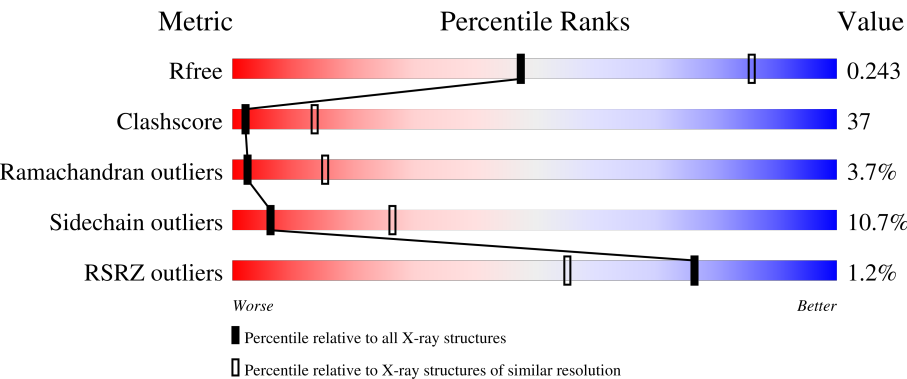
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	% 40%36%9%15%
1	B	362	% 37%43%9%10%
1	C	362	% 37%43%11%7%
1	D	362	% 35%42%8%15%
2	E	84	2% 33%36%11%20%

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Mol	Chain	Length	Quality of chain
2	F	84	2% 31% 35% 8% 26%
2	G	84	% 35% 36% 10% 20%
2	H	84	% 36% 32% 8% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12146 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2416	1525	401	474	16			
1	B	325	Total	C	N	O	S	0	0	0
			2495	1575	414	487	19			
1	C	335	Total	C	N	O	S	0	0	0
			2592	1632	436	505	19			
1	D	307	Total	C	N	O	S	0	0	0
			2385	1507	395	466	17			

- Molecule 2 is a protein called Golgi to ER traffic protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	67	Total	C	N	O	0	0	0
			555	345	101	109			
2	F	62	Total	C	N	O	0	0	0
			512	316	93	103			
2	G	67	Total	C	N	O	0	0	0
			551	343	99	109			
2	H	64	Total	C	N	O	0	0	0
			532	330	96	106			

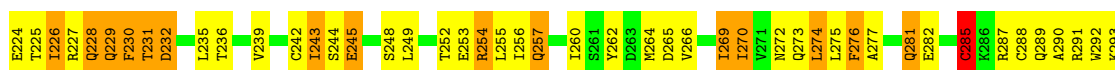
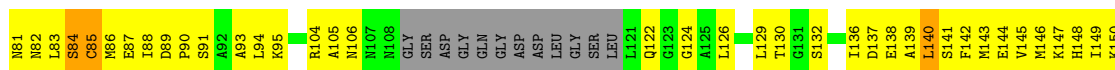
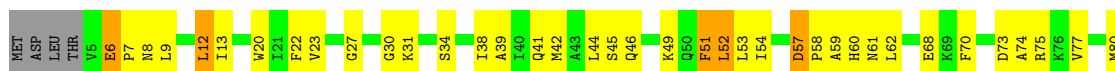
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



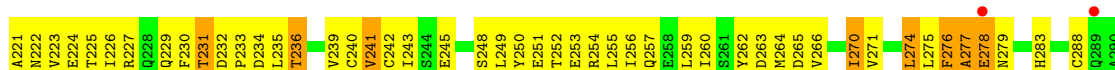
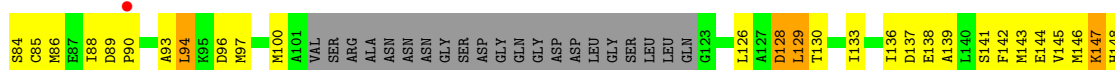
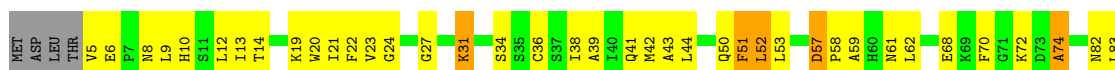
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



• Molecule 1: ATPase GET3



• Molecule 1: ATPase GET3



• Molecule 2: Golgi to ER traffic protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.34Å 167.66Å 244.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 94.5 (50.00-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.306 0.252 , 0.243	Depositor DCC
R_{free} test set	2243 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12146	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: ADP

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	0.71	1/2455 (0.0%)	1.11	22/3313 (0.7%)
1	B	0.68	1/2536 (0.0%)	1.17	29/3426 (0.8%)
1	C	0.55	2/2634 (0.1%)	1.13	24/3556 (0.7%)
1	D	0.50	0/2423	1.07	18/3270 (0.6%)
2	E	0.43	0/563	1.05	8/751 (1.1%)
2	F	0.43	0/518	1.05	5/690 (0.7%)
2	G	0.40	0/558	0.98	4/744 (0.5%)
2	H	0.38	0/539	1.02	5/718 (0.7%)
All	All	0.59	4/12226 (0.0%)	1.10	115/16468 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	PHE	CE2-CZ	6.01	1.56	1.38
1	B	204	PHE	CG-CD2	5.70	1.50	1.38
1	C	204	PHE	CG-CD1	5.39	1.50	1.38
1	A	294	MET	SD-CE	5.05	1.92	1.79

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	82	ILE	N-CA-C	-11.33	102.43	113.53
2	G	82	ILE	N-CA-C	-11.24	102.51	113.53
2	E	82	ILE	N-CA-C	-11.18	102.57	113.53
2	H	82	ILE	N-CA-C	-11.02	102.73	113.53
1	B	201	LEU	N-CA-C	-9.00	102.44	113.97
1	A	334	LEU	N-CA-C	-8.30	103.28	113.50
1	B	334	LEU	N-CA-C	-8.04	103.61	113.50
1	C	188	GLU	N-CA-C	-7.90	103.77	113.41
1	B	217	ASN	N-CA-C	-7.89	104.25	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	LEU	N-CA-C	-7.89	102.63	111.07
1	A	276	PHE	N-CA-C	-7.82	101.44	111.92
2	E	94	LYS	N-CA-C	-7.76	103.54	113.16
1	D	278	GLU	N-CA-C	-7.74	102.78	111.07
1	C	334	LEU	N-CA-C	-7.59	104.16	113.50
1	C	289	GLN	N-CA-C	-7.56	103.61	114.12
1	B	224	GLU	N-CA-C	-7.50	105.31	114.75
1	B	229	GLN	N-CA-C	-7.44	101.46	111.96
1	B	216	LEU	N-CA-C	-7.44	104.16	112.57
1	D	334	LEU	N-CA-C	-7.39	104.41	113.50
1	C	225	THR	N-CA-C	-7.27	103.88	112.89
1	B	225	THR	N-CA-C	-7.20	101.68	112.04
1	B	193	ILE	N-CA-C	-7.14	106.53	113.53
1	A	269	ILE	CB-CA-C	-7.12	100.09	110.63
1	A	225	THR	N-CA-C	-7.07	103.62	111.82
1	C	218	GLU	N-CA-C	-6.79	104.97	113.18
1	B	203	SER	N-CA-C	-6.79	104.10	112.38
1	B	95	LYS	N-CA-C	-6.66	105.48	112.93
1	D	219	LEU	N-CA-C	-6.55	104.14	111.28
1	D	341	ILE	CB-CA-C	-6.48	100.66	111.29
1	B	312	VAL	N-CA-C	6.39	117.03	107.51
1	D	94	LEU	N-CA-C	-6.36	106.06	113.88
1	C	51	PHE	N-CA-C	6.31	119.82	109.72
1	A	277	ALA	N-CA-C	6.29	118.94	111.33
1	B	269	ILE	CB-CA-C	-6.24	101.39	110.63
1	B	51	PHE	N-CA-C	6.21	119.67	109.72
1	A	57	ASP	CA-C-N	6.20	125.76	119.19
1	A	57	ASP	C-N-CA	6.20	125.76	119.19
1	A	27	GLY	N-CA-C	-6.17	104.90	112.68
1	D	51	PHE	N-CA-C	6.17	119.59	109.72
1	A	51	PHE	N-CA-C	6.13	119.53	109.72
1	C	57	ASP	N-CA-C	6.03	116.99	109.57
1	C	57	ASP	CA-C-N	6.00	125.55	119.19
1	C	57	ASP	C-N-CA	6.00	125.55	119.19
1	A	217	ASN	N-CA-C	-5.94	105.11	112.90
1	A	312	VAL	N-CA-C	5.93	116.65	107.99
1	B	349	GLU	N-CA-C	-5.93	105.81	113.16
1	C	27	GLY	N-CA-C	-5.93	105.21	112.68
1	A	232	ASP	CA-C-N	5.91	127.22	119.84
1	A	232	ASP	C-N-CA	5.91	127.22	119.84
1	B	57	ASP	CA-C-N	5.88	125.43	119.19
1	B	57	ASP	C-N-CA	5.88	125.43	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	GLY	N-CA-C	-5.84	105.32	112.68
1	D	339	ASN	CA-C-N	5.84	126.25	119.47
1	D	339	ASN	C-N-CA	5.84	126.25	119.47
1	C	6	GLU	CA-C-N	5.82	129.77	121.91
1	C	6	GLU	C-N-CA	5.82	129.77	121.91
2	E	98	ALA	N-CA-C	-5.82	106.18	113.28
1	D	27	GLY	N-CA-C	-5.81	105.36	112.68
1	C	312	VAL	N-CA-C	5.78	116.12	107.51
2	F	93	ASN	N-CA-C	-5.77	106.14	112.72
1	A	339	ASN	CA-C-N	5.75	126.14	119.47
1	A	339	ASN	C-N-CA	5.75	126.14	119.47
1	D	312	VAL	N-CA-C	5.75	116.38	107.99
1	D	57	ASP	CA-C-N	5.73	125.27	119.19
1	D	57	ASP	C-N-CA	5.73	125.27	119.19
2	G	61	ALA	N-CA-C	-5.71	106.02	112.87
1	D	253	GLU	N-CA-C	-5.67	105.10	111.28
2	F	61	ALA	N-CA-C	-5.65	106.09	112.87
1	D	57	ASP	N-CA-C	5.61	116.47	109.57
2	E	61	ALA	N-CA-C	-5.61	106.14	112.87
1	B	253	GLU	N-CA-C	-5.59	105.18	111.28
2	E	83	ASN	N-CA-C	-5.59	106.12	113.17
1	B	46	GLN	CA-C-N	5.54	125.64	119.32
1	B	46	GLN	C-N-CA	5.54	125.64	119.32
2	H	61	ALA	N-CA-C	-5.54	106.22	112.87
1	B	57	ASP	N-CA-C	5.53	116.37	109.57
1	A	253	GLU	N-CA-C	-5.52	105.26	111.28
1	D	168	ALA	CA-C-N	5.52	124.98	119.24
1	D	168	ALA	C-N-CA	5.52	124.98	119.24
1	D	349	GLU	N-CA-C	-5.51	106.33	113.16
1	C	226	ILE	N-CA-C	-5.50	105.49	110.82
2	H	83	ASN	N-CA-C	-5.50	106.25	113.17
2	H	96	PHE	N-CA-C	-5.48	105.80	113.37
2	F	83	ASN	N-CA-C	-5.47	106.27	113.17
1	A	211	ASP	N-CA-C	-5.46	106.46	113.01
1	C	228	GLN	N-CA-C	-5.45	105.26	112.94
1	C	253	GLU	N-CA-C	-5.43	105.36	111.28
1	A	349	GLU	N-CA-C	-5.43	106.65	113.28
2	G	83	ASN	N-CA-C	-5.41	106.35	113.17
1	C	243	ILE	N-CA-C	-5.35	100.93	109.17
1	C	168	ALA	CA-C-N	5.33	124.51	118.97
1	C	168	ALA	C-N-CA	5.33	124.51	118.97
1	C	221	ALA	N-CA-C	-5.29	105.64	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	91	SER	N-CA-C	-5.27	106.85	113.28
1	A	243	ILE	N-CA-C	-5.26	101.06	109.17
1	B	168	ALA	CA-C-N	5.26	124.71	119.24
1	B	168	ALA	C-N-CA	5.26	124.71	119.24
1	B	339	ASN	CA-C-N	5.24	125.55	119.47
1	B	339	ASN	C-N-CA	5.24	125.55	119.47
1	B	93	ALA	N-CA-C	-5.17	108.24	114.75
1	B	202	ASN	N-CA-C	-5.16	104.60	112.04
1	A	57	ASP	N-CA-C	5.12	115.87	109.57
1	B	286	LYS	N-CA-C	5.11	116.66	111.14
1	D	243	ILE	N-CA-C	-5.11	101.31	109.17
1	C	232	ASP	CA-C-N	5.10	126.22	119.84
1	C	232	ASP	C-N-CA	5.10	126.22	119.84
2	F	84	ASN	N-CA-C	-5.08	106.77	113.12
1	A	168	ALA	CA-C-N	5.07	124.24	118.97
1	A	168	ALA	C-N-CA	5.07	124.24	118.97
2	G	84	ASN	N-CA-C	-5.06	106.79	113.12
2	E	70	LYS	N-CA-C	-5.06	105.46	110.97
1	C	104	ARG	N-CA-C	-5.06	107.77	114.04
2	H	84	ASN	N-CA-C	-5.04	106.82	113.12
2	E	84	ASN	N-CA-C	-5.03	106.83	113.12
1	B	144	GLU	N-CA-C	-5.02	106.00	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2416	0	2392	159	0
1	B	2495	0	2433	190	1
1	C	2592	0	2549	205	1
1	D	2385	0	2349	198	0
2	E	555	0	551	37	0
2	F	512	0	511	43	0
2	G	551	0	553	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	532	0	528	33	1
3	A	27	0	12	2	0
3	B	27	0	12	5	0
3	C	27	0	12	3	0
3	D	27	0	12	3	0
All	All	12146	0	11914	891	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (891) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:HD22	1:B:48:ASN:N	1.46	1.11
1:A:257:GLN:HE21	1:A:257:GLN:HA	1.15	1.10
1:B:48:ASN:H	1:B:48:ASN:ND2	1.42	1.09
1:B:200:MET:O	1:B:204:PHE:HB2	1.59	1.00
2:E:38:LEU:HD13	2:E:89:ILE:HG13	1.41	1.00
1:A:143:MET:HE1	1:A:219:LEU:HD11	1.42	1.00
2:H:38:LEU:HD13	2:H:89:ILE:HG13	1.41	1.00
2:G:38:LEU:HD13	2:G:89:ILE:HG13	1.41	0.99
1:B:20:TRP:HB2	1:B:236:THR:HG22	1.44	0.98
1:B:320:GLU:HA	3:B:401:ADP:O2'	1.63	0.98
2:F:38:LEU:HD13	2:F:89:ILE:HG13	1.42	0.98
2:H:67:LYS:H	2:H:67:LYS:HD2	1.30	0.96
1:C:198:GLY:HA2	1:C:202:ASN:HB2	1.47	0.95
2:F:67:LYS:HD2	2:F:67:LYS:H	1.31	0.95
2:E:67:LYS:H	2:E:67:LYS:HD2	1.30	0.94
1:C:256:ILE:O	1:C:260:ILE:HG13	1.68	0.93
1:B:209:ASN:H	1:B:209:ASN:HD22	1.12	0.92
2:G:67:LYS:H	2:G:67:LYS:HD2	1.31	0.92
1:A:133:ILE:HB	1:A:136:ILE:HD11	1.50	0.91
1:A:88:ILE:HD11	1:A:145:VAL:HG13	1.52	0.90
1:D:39:ALA:HB2	1:D:53:LEU:HD13	1.54	0.89
1:A:320:GLU:HA	3:A:401:ADP:O2'	1.72	0.89
1:B:209:ASN:HD22	1:B:209:ASN:N	1.68	0.88
1:D:320:GLU:HA	3:D:401:ADP:O2'	1.74	0.88
1:B:22:PHE:CE1	1:B:165:PHE:HD1	1.91	0.88
1:A:257:GLN:HA	1:A:257:GLN:NE2	1.81	0.87
1:A:12:LEU:O	1:A:12:LEU:HD23	1.75	0.87
1:C:291:ARG:HH12	1:D:291:ARG:HH12	1.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLN:HG2	2:E:65:TYR:HB3	1.54	0.86
1:B:88:ILE:HD11	1:B:145:VAL:HG13	1.57	0.86
1:C:257:GLN:NE2	1:C:260:ILE:HD12	1.90	0.85
1:A:179:LEU:HB3	1:A:180:PRO:HD3	1.59	0.84
1:C:248:SER:O	1:C:252:THR:HG23	1.77	0.84
1:B:86:MET:HE1	1:B:152:GLN:HG3	1.61	0.83
1:C:54:ILE:HD12	1:C:86:MET:HE3	1.58	0.83
1:D:314:MET:HE3	1:D:330:PHE:CZ	2.14	0.83
1:C:51:PHE:CE2	1:C:162:THR:HB	2.14	0.82
2:F:91:SER:HA	2:F:94:LYS:HD2	1.62	0.82
1:C:291:ARG:NH1	1:D:291:ARG:HH12	1.79	0.81
1:A:148:HIS:CE1	1:A:151:ARG:HH22	1.98	0.81
1:D:242:CYS:HB3	1:D:252:THR:HG21	1.62	0.80
1:D:178:GLN:HA	1:D:178:GLN:HE21	1.47	0.80
1:B:76:LYS:HG2	1:B:84:SER:OG	1.80	0.80
1:B:20:TRP:HB2	1:B:236:THR:CG2	2.11	0.80
1:A:341:ILE:HG22	1:A:342:THR:N	1.96	0.79
1:D:34:SER:O	1:D:38:ILE:HG13	1.83	0.79
1:A:12:LEU:HD23	1:A:12:LEU:C	2.08	0.78
1:A:219:LEU:C	1:A:221:ALA:H	1.92	0.78
1:A:136:ILE:HG22	1:A:140:LEU:HD11	1.66	0.78
1:C:94:LEU:HD11	1:C:140:LEU:HD22	1.66	0.78
1:B:270:ILE:HD12	1:B:270:ILE:C	2.09	0.77
1:C:184:SER:O	1:C:188:GLU:HG2	1.84	0.77
1:C:174:LEU:HD11	1:C:264:MET:HE2	1.66	0.77
1:B:97:MET:HE1	1:B:147:LYS:NZ	1.99	0.77
2:F:52:LEU:HB3	2:F:75:LEU:HD21	1.66	0.77
1:A:64:ASP:HB3	1:A:322:ARG:HH21	1.49	0.76
2:G:52:LEU:HB3	2:G:75:LEU:HD21	1.67	0.76
2:H:52:LEU:HB3	2:H:75:LEU:HD21	1.66	0.76
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.51	0.76
1:D:126:LEU:HD12	1:D:129:LEU:HD21	1.68	0.76
1:A:130:THR:HA	1:A:136:ILE:HD12	1.65	0.76
2:G:30:SER:HA	2:G:34:PRO:HD2	1.66	0.75
1:D:23:VAL:O	1:D:167:THR:HG22	1.86	0.75
1:D:42:MET:HE1	1:D:164:ILE:CG1	2.16	0.75
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.51	0.75
2:E:52:LEU:HB3	2:E:75:LEU:HD21	1.66	0.74
1:A:50:GLN:HG2	1:A:158:GLU:OE2	1.87	0.74
1:D:275:LEU:C	1:D:277:ALA:H	1.94	0.74
1:D:174:LEU:HD23	1:D:174:LEU:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HD22	1:C:201:LEU:HB2	1.69	0.74
1:C:51:PHE:HE2	1:C:162:THR:HB	1.52	0.73
2:G:34:PRO:HA	2:G:38:LEU:HD12	1.67	0.73
1:C:287:ARG:HB3	1:D:318:ALA:HA	1.69	0.73
1:C:320:GLU:HA	3:C:401:ADP:O2'	1.88	0.73
1:A:337:GLU:OE2	1:A:337:GLU:N	2.14	0.73
2:H:95:ALA:C	2:H:97:GLN:H	1.97	0.73
1:B:22:PHE:CE1	1:B:165:PHE:CD1	2.76	0.73
1:C:254:ARG:HH11	1:C:254:ARG:HB3	1.52	0.72
1:C:257:GLN:HE22	1:C:260:ILE:HD12	1.50	0.72
1:D:70:PHE:CD2	1:D:85:CYS:HB2	2.24	0.72
1:A:242:CYS:HB3	1:A:252:THR:HG21	1.70	0.72
1:C:62:LEU:HD13	1:C:85:CYS:SG	2.29	0.72
1:B:209:ASN:H	1:B:209:ASN:ND2	1.86	0.71
1:D:227:ARG:O	1:D:231:THR:HG22	1.90	0.71
1:D:128:ASP:C	1:D:130:THR:H	1.95	0.71
2:H:67:LYS:HD2	2:H:67:LYS:N	2.06	0.71
1:D:94:LEU:HG	1:D:144:GLU:OE2	1.90	0.71
1:B:26:LYS:HE2	1:B:251:GLU:OE1	1.90	0.71
1:A:219:LEU:O	1:A:221:ALA:N	2.24	0.71
1:A:8:ASN:HA	1:A:312:VAL:HG22	1.73	0.71
1:C:34:SER:OG	1:C:270:ILE:HD11	1.90	0.70
1:C:8:ASN:HA	1:C:312:VAL:HG22	1.73	0.70
1:D:50:GLN:HE21	1:D:158:GLU:CD	1.98	0.70
1:A:227:ARG:O	1:A:231:THR:HG22	1.92	0.70
1:C:139:ALA:HB1	1:C:223:VAL:HG21	1.74	0.70
1:B:200:MET:HA	1:B:203:SER:OG	1.92	0.70
2:F:38:LEU:HD22	2:F:89:ILE:HB	1.73	0.69
2:F:67:LYS:HD2	2:F:67:LYS:N	2.07	0.69
2:G:38:LEU:HD22	2:G:89:ILE:HB	1.74	0.69
1:B:74:ALA:HB2	1:B:86:MET:HE3	1.73	0.69
1:A:52:LEU:HD12	1:A:163:VAL:HG22	1.73	0.69
1:C:23:VAL:HG22	1:C:239:VAL:CG2	2.23	0.69
2:G:67:LYS:HD2	2:G:67:LYS:N	2.07	0.69
1:D:337:GLU:H	1:D:337:GLU:CD	2.00	0.69
1:D:13:ILE:HD13	1:D:41:GLN:HG2	1.74	0.69
2:G:33:ALA:HB3	2:G:34:PRO:CD	2.23	0.69
1:A:133:ILE:HB	1:A:136:ILE:CD1	2.20	0.69
2:E:38:LEU:HD22	2:E:89:ILE:HB	1.75	0.69
1:D:90:PRO:O	1:D:94:LEU:HB2	1.92	0.69
1:B:97:MET:HE1	1:B:147:LYS:HZ1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:GLU:O	2:F:41:LYS:HB2	1.92	0.69
1:C:126:LEU:HD11	1:C:216:LEU:HD21	1.75	0.69
1:A:20:TRP:HB2	1:A:236:THR:HB	1.74	0.69
2:G:30:SER:O	2:G:34:PRO:HG2	1.92	0.69
1:D:42:MET:HE1	1:D:164:ILE:HG12	1.75	0.68
1:D:53:LEU:HD12	1:D:164:ILE:HB	1.74	0.68
1:D:23:VAL:HG21	1:D:38:ILE:HD12	1.73	0.68
1:B:228:GLN:HA	1:B:231:THR:HG22	1.76	0.68
1:C:20:TRP:HB2	1:C:236:THR:OG1	1.93	0.68
1:B:13:ILE:HD13	1:B:41:GLN:CG	2.24	0.68
1:C:152:GLN:O	1:C:156:GLU:HB2	1.94	0.68
2:H:38:LEU:HD22	2:H:89:ILE:HB	1.73	0.68
1:C:242:CYS:HB3	1:C:252:THR:HG21	1.74	0.68
2:G:37:GLU:C	2:G:39:SER:H	2.01	0.68
1:A:86:MET:HE2	1:A:152:GLN:HG3	1.75	0.67
1:D:52:LEU:HD23	1:D:84:SER:O	1.93	0.67
1:C:249:LEU:HD21	1:C:302:ILE:HD11	1.75	0.67
1:B:142:PHE:CE2	1:B:226:ILE:HD11	2.30	0.67
1:D:13:ILE:HD13	1:D:41:GLN:CG	2.25	0.67
1:A:282:GLU:CD	1:A:283:HIS:H	2.02	0.67
1:B:219:LEU:C	1:B:221:ALA:H	2.03	0.67
1:B:205:MET:HE3	1:B:205:MET:O	1.94	0.67
1:B:175:ARG:HA	1:B:262:TYR:CE1	2.30	0.66
1:A:17:THR:OG1	1:A:234:ASP:O	2.12	0.66
1:B:97:MET:HE2	1:B:144:GLU:HG2	1.78	0.66
1:D:12:LEU:HD23	1:D:12:LEU:O	1.95	0.66
1:D:230:PHE:HA	1:D:236:THR:HG21	1.77	0.66
1:D:96:ASP:O	1:D:100:MET:HG2	1.96	0.66
1:D:226:ILE:O	1:D:229:GLN:HB3	1.94	0.66
1:A:257:GLN:HE21	1:A:257:GLN:CA	1.92	0.66
1:A:72:LYS:HG3	1:A:88:ILE:HG22	1.78	0.66
1:C:298:TYR:OH	2:G:62:GLN:HG3	1.95	0.66
1:D:12:LEU:HD21	1:D:21:ILE:HD13	1.77	0.65
1:D:264:MET:HG3	1:D:265:ASP:N	2.10	0.65
1:A:137:ASP:HA	1:A:140:LEU:HD12	1.79	0.65
1:C:291:ARG:NH1	1:D:291:ARG:NH1	2.45	0.65
1:B:321:ILE:O	1:B:321:ILE:HG22	1.97	0.64
1:D:20:TRP:HB2	1:D:236:THR:HB	1.78	0.64
1:A:128:ASP:OD2	1:A:129:LEU:HD12	1.96	0.64
1:A:226:ILE:HG22	1:A:227:ARG:N	2.12	0.64
1:B:20:TRP:CB	1:B:236:THR:HG22	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:SER:HB3	1:B:310:HIS:HB2	1.79	0.64
1:C:254:ARG:HH11	1:C:254:ARG:CB	2.11	0.64
1:A:22:PHE:CD1	1:A:165:PHE:HB2	2.32	0.64
1:D:88:ILE:HG22	1:D:89:ASP:N	2.12	0.64
1:B:179:LEU:HB3	1:B:180:PRO:HD3	1.80	0.64
1:D:240:CYS:SG	1:D:255:LEU:HD23	2.37	0.64
2:E:37:GLU:O	2:E:41:LYS:HB2	1.98	0.64
1:D:241:VAL:HG13	1:D:270:ILE:HG13	1.79	0.64
1:C:73:ASP:HB2	1:C:75:ARG:HH12	1.64	0.63
1:C:12:LEU:C	1:C:12:LEU:HD23	2.23	0.63
1:D:24:GLY:HA3	1:D:167:THR:HG21	1.81	0.63
2:E:67:LYS:HD2	2:E:67:LYS:N	2.06	0.63
1:B:254:ARG:HG2	1:B:254:ARG:NH1	2.08	0.63
1:C:52:LEU:HD23	1:C:84:SER:O	1.99	0.63
1:D:51:PHE:CE2	1:D:162:THR:HB	2.33	0.63
1:D:68:GLU:HB2	1:D:70:PHE:CE1	2.34	0.63
1:A:253:GLU:HG3	2:E:69:THR:HG21	1.79	0.63
1:C:206:GLY:O	1:C:210:VAL:HG23	1.98	0.63
1:B:255:LEU:C	1:B:255:LEU:HD23	2.24	0.63
1:C:272:ASN:ND2	1:C:273:GLN:HG3	2.14	0.63
1:C:275:LEU:CD2	1:C:295:GLN:HE22	2.11	0.62
1:A:94:LEU:HD23	1:A:94:LEU:O	1.99	0.62
1:A:219:LEU:C	1:A:221:ALA:N	2.58	0.62
1:B:13:ILE:HD13	1:B:41:GLN:HG2	1.81	0.62
1:B:142:PHE:HE2	1:B:226:ILE:HD11	1.63	0.62
1:B:158:GLU:HA	1:B:158:GLU:OE2	1.97	0.62
2:E:34:PRO:HA	2:E:38:LEU:HD12	1.81	0.62
1:C:229:GLN:C	1:C:231:THR:H	2.07	0.62
2:H:90:GLN:O	2:H:94:LYS:HG3	2.00	0.62
2:E:47:LYS:O	2:E:51:GLU:HG3	2.00	0.62
2:G:47:LYS:O	2:G:51:GLU:HG3	2.00	0.62
1:A:13:ILE:HD13	1:A:41:GLN:HG2	1.81	0.62
1:A:31:LYS:NZ	1:A:31:LYS:HB3	2.15	0.62
1:A:52:LEU:HD12	1:A:163:VAL:CG2	2.29	0.62
1:A:238:PHE:CD2	1:A:259:LEU:HD11	2.35	0.62
2:G:57:ASN:N	2:G:57:ASN:HD22	1.98	0.62
1:B:270:ILE:HD13	1:B:314:MET:HG3	1.81	0.61
1:C:275:LEU:HD22	1:C:295:GLN:HE22	1.65	0.61
1:C:291:ARG:HH12	1:D:291:ARG:NH1	1.96	0.61
1:D:270:ILE:HG22	1:D:312:VAL:HB	1.81	0.61
1:D:278:GLU:HB2	1:D:292:TRP:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:O	1:A:229:GLN:N	2.34	0.61
1:D:9:LEU:O	1:D:13:ILE:HG13	2.01	0.61
1:C:287:ARG:HG3	1:C:288:CYS:SG	2.40	0.61
1:B:249:LEU:CD2	1:B:302:ILE:HD11	2.29	0.61
2:G:33:ALA:HB3	2:G:34:PRO:HD2	1.83	0.61
1:D:12:LEU:HD21	1:D:21:ILE:CD1	2.30	0.61
1:A:271:VAL:HG12	1:A:274:LEU:HD11	1.83	0.61
2:E:57:ASN:N	2:E:57:ASN:HD22	1.98	0.61
1:B:188:GLU:O	1:B:188:GLU:HG2	2.01	0.61
1:D:31:LYS:HA	1:D:241:VAL:HG21	1.83	0.61
2:H:47:LYS:O	2:H:51:GLU:HG3	2.00	0.61
1:A:38:ILE:O	1:A:42:MET:HG3	2.01	0.61
1:C:46:GLN:OE1	1:C:49:LYS:HE2	2.01	0.61
1:C:68:GLU:HB2	1:C:70:PHE:CE1	2.35	0.61
1:C:139:ALA:O	1:C:143:MET:HE2	2.01	0.61
1:C:264:MET:HG3	1:C:265:ASP:N	2.16	0.61
1:D:337:GLU:CD	1:D:337:GLU:N	2.59	0.60
2:H:57:ASN:N	2:H:57:ASN:HD22	1.97	0.60
2:F:57:ASN:HD22	2:F:57:ASN:N	1.97	0.60
1:C:60:HIS:HA	1:C:87:GLU:OE1	2.01	0.60
1:A:238:PHE:CE2	1:A:255:LEU:HD21	2.36	0.60
1:D:12:LEU:HD23	1:D:12:LEU:C	2.25	0.60
1:A:52:LEU:CD1	1:A:163:VAL:HG22	2.30	0.60
1:A:282:GLU:CD	1:A:283:HIS:N	2.59	0.60
1:B:93:ALA:O	1:B:97:MET:HG2	2.02	0.60
1:B:345:LYS:HA	1:B:345:LYS:HE2	1.82	0.60
1:C:198:GLY:CA	1:C:202:ASN:HB2	2.28	0.60
1:D:74:ALA:HB2	1:D:86:MET:HE2	1.82	0.60
2:F:47:LYS:O	2:F:51:GLU:HG3	2.00	0.60
1:A:177:LEU:HD12	1:A:262:TYR:HB3	1.84	0.60
1:D:39:ALA:CB	1:D:53:LEU:HD13	2.31	0.60
1:D:147:LYS:HE3	1:D:147:LYS:HA	1.82	0.60
1:C:52:LEU:HB3	1:C:163:VAL:HG22	1.84	0.60
1:C:223:VAL:HG12	1:C:223:VAL:O	2.01	0.60
1:D:324:LEU:HD23	1:D:324:LEU:C	2.27	0.60
1:C:122:GLN:CD	1:C:126:LEU:HB3	2.26	0.60
1:A:247:LEU:CD2	1:B:27:GLY:HA3	2.31	0.59
1:A:344:GLY:O	1:A:347:ILE:HG12	2.01	0.59
1:A:249:LEU:HD21	1:A:302:ILE:HD11	1.85	0.59
1:D:19:LYS:HG3	1:D:161:ASP:O	2.02	0.59
1:B:57:ASP:OD2	1:B:59:ALA:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TRP:O	1:C:236:THR:HA	2.03	0.59
2:H:37:GLU:O	2:H:41:LYS:HB2	2.02	0.59
1:B:31:LYS:N	3:B:401:ADP:O1B	2.36	0.59
1:B:223:VAL:HG12	1:B:223:VAL:O	2.02	0.59
1:A:246:PHE:C	1:A:246:PHE:CD2	2.79	0.59
1:B:139:ALA:HB2	1:B:176:PHE:HB2	1.85	0.59
1:D:276:PHE:HE1	1:D:315:PRO:HB3	1.67	0.59
1:C:174:LEU:HD11	1:C:264:MET:CE	2.33	0.59
1:D:178:GLN:HA	1:D:178:GLN:NE2	2.14	0.59
1:A:52:LEU:HB3	1:A:163:VAL:HG22	1.83	0.59
1:C:242:CYS:CB	1:C:252:THR:HG21	2.33	0.59
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.83	0.59
2:G:38:LEU:HB3	2:G:89:ILE:HD12	1.85	0.59
1:A:313:LYS:HD3	1:A:313:LYS:N	2.18	0.58
1:B:304:GLU:OE2	2:F:67:LYS:HE3	2.03	0.58
1:D:128:ASP:C	1:D:130:THR:N	2.61	0.58
2:H:38:LEU:HB3	2:H:89:ILE:HD12	1.85	0.58
1:A:247:LEU:HD21	1:B:27:GLY:HA3	1.84	0.58
1:B:275:LEU:C	1:B:277:ALA:H	2.12	0.58
1:C:347:ILE:HD12	1:C:347:ILE:O	2.03	0.58
1:D:174:LEU:HG	1:D:174:LEU:O	2.04	0.58
1:A:12:LEU:C	1:A:12:LEU:CD2	2.77	0.58
1:A:152:GLN:O	1:A:156:GLU:HB2	2.04	0.58
1:C:75:ARG:HG3	1:C:75:ARG:HH11	1.68	0.58
1:C:222:ASN:C	1:C:224:GLU:H	2.11	0.58
1:D:275:LEU:C	1:D:277:ALA:N	2.61	0.58
1:A:285:CYS:SG	1:A:287:ARG:HG3	2.43	0.58
1:C:189:LYS:C	1:C:191:GLY:H	2.10	0.58
1:D:176:PHE:HD2	1:D:177:LEU:N	2.02	0.58
1:B:314:MET:HE3	1:B:330:PHE:CZ	2.39	0.58
1:D:8:ASN:HA	1:D:312:VAL:HG22	1.86	0.58
1:A:90:PRO:HB2	1:A:141:SER:OG	2.04	0.58
2:E:38:LEU:HB3	2:E:89:ILE:HD12	1.86	0.58
2:G:39:SER:O	2:G:43:LEU:HG	2.04	0.58
1:A:136:ILE:HG22	1:A:140:LEU:CD1	2.32	0.58
1:C:305:LEU:HD11	2:G:73:ARG:NH2	2.19	0.58
1:D:242:CYS:CB	1:D:252:THR:HG21	2.34	0.58
2:H:39:SER:O	2:H:43:LEU:HG	2.04	0.58
1:D:20:TRP:O	1:D:236:THR:HA	2.04	0.58
1:B:177:LEU:HD12	1:B:262:TYR:HB3	1.85	0.57
1:B:278:GLU:HB2	1:B:292:TRP:HE1	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:LEU:HB3	2:F:89:ILE:HD12	1.85	0.57
1:D:275:LEU:HD23	1:D:295:GLN:OE1	2.04	0.57
1:D:324:LEU:HD23	1:D:324:LEU:O	2.04	0.57
1:B:227:ARG:O	1:B:231:THR:HG22	2.04	0.57
1:C:139:ALA:HB2	1:C:176:PHE:HB2	1.87	0.57
1:D:139:ALA:HA	1:D:176:PHE:CD1	2.40	0.57
1:D:179:LEU:HB3	1:D:180:PRO:HD3	1.86	0.57
1:A:96:ASP:C	1:A:98:ASN:H	2.13	0.57
1:C:38:ILE:O	1:C:42:MET:HG3	2.04	0.57
1:C:51:PHE:CD2	1:C:162:THR:HB	2.39	0.57
2:F:39:SER:O	2:F:43:LEU:HG	2.04	0.57
1:D:152:GLN:O	1:D:156:GLU:HB3	2.03	0.57
1:B:20:TRP:O	1:B:236:THR:HA	2.04	0.57
1:B:285:CYS:SG	1:B:287:ARG:HG2	2.44	0.57
1:C:142:PHE:CZ	1:C:230:PHE:HE2	2.23	0.57
2:H:90:GLN:HG3	2:H:94:LYS:HE3	1.85	0.57
1:A:129:LEU:HD22	1:A:212:ILE:HG21	1.85	0.57
1:C:215:LYS:C	1:C:217:ASN:H	2.13	0.57
1:C:257:GLN:NE2	1:C:257:GLN:HA	2.19	0.57
1:D:89:ASP:O	1:D:93:ALA:HB3	2.05	0.57
1:D:249:LEU:HD12	1:D:298:TYR:HD2	1.69	0.57
1:C:23:VAL:CG2	1:C:38:ILE:HD12	2.35	0.57
1:B:86:MET:HE1	1:B:152:GLN:CG	2.33	0.57
1:C:315:PRO:HB3	1:C:338:TYR:CE2	2.39	0.56
1:D:138:GLU:OE2	1:D:175:ARG:HD2	2.04	0.56
2:F:46:VAL:HG22	2:F:82:ILE:HD13	1.87	0.56
1:C:200:MET:O	1:C:203:SER:HB2	2.05	0.56
1:C:275:LEU:HD23	1:C:275:LEU:H	1.69	0.56
2:G:37:GLU:C	2:G:39:SER:N	2.62	0.56
1:D:179:LEU:HD23	1:D:223:VAL:HG21	1.85	0.56
1:B:136:ILE:HD13	1:B:179:LEU:HD11	1.85	0.56
2:F:60:SER:C	2:F:62:GLN:H	2.12	0.56
1:A:253:GLU:HG2	1:A:306:TYR:OH	2.04	0.56
2:E:39:SER:O	2:E:43:LEU:HG	2.05	0.56
1:C:105:ALA:HB2	1:C:124:GLY:HA2	1.88	0.56
1:C:227:ARG:O	1:C:227:ARG:HG2	2.05	0.56
1:B:249:LEU:HD22	1:B:302:ILE:HD11	1.88	0.56
1:D:44:LEU:HD23	1:D:44:LEU:O	2.06	0.56
1:B:228:GLN:HA	1:B:231:THR:CG2	2.35	0.56
1:C:86:MET:HE1	1:C:149:ILE:HG12	1.88	0.56
1:C:242:CYS:SG	1:C:269:ILE:HD11	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:PHE:O	1:D:279:ASN:N	2.38	0.56
1:A:254:ARG:NH1	1:A:254:ARG:HG2	2.19	0.56
1:C:219:LEU:C	1:C:221:ALA:H	2.14	0.56
2:G:35:GLY:O	2:G:39:SER:HB2	2.06	0.56
1:B:129:LEU:HD12	1:B:129:LEU:C	2.31	0.56
1:C:148:HIS:O	1:C:152:GLN:HG2	2.06	0.56
2:G:46:VAL:HG22	2:G:82:ILE:HD13	1.87	0.56
1:A:179:LEU:HD23	1:A:223:VAL:HG21	1.88	0.55
2:E:60:SER:C	2:E:62:GLN:H	2.13	0.55
1:B:32:THR:HG23	1:B:61:ASN:HD22	1.71	0.55
2:F:45:LYS:HB3	2:F:82:ILE:HD11	1.88	0.55
1:D:227:ARG:HG2	1:D:227:ARG:NH1	2.21	0.55
1:A:20:TRP:O	1:A:236:THR:HA	2.06	0.55
1:A:271:VAL:HG12	1:A:274:LEU:CD1	2.36	0.55
2:H:60:SER:C	2:H:62:GLN:N	2.63	0.55
2:F:60:SER:C	2:F:62:GLN:N	2.62	0.55
1:D:222:ASN:O	1:D:226:ILE:HG13	2.06	0.55
1:A:20:TRP:HB2	1:A:236:THR:CB	2.36	0.55
1:A:70:PHE:CD1	1:A:85:CYS:HB2	2.41	0.55
1:C:243:ILE:HG23	1:C:245:GLU:HG3	1.88	0.55
2:H:95:ALA:C	2:H:97:GLN:N	2.62	0.55
1:B:129:LEU:HD22	1:B:216:LEU:HD11	1.88	0.55
1:B:297:LYS:HE2	2:F:63:ASP:HA	1.89	0.55
1:D:164:ILE:HD12	1:D:164:ILE:N	2.21	0.55
2:E:46:VAL:HG22	2:E:82:ILE:HD13	1.88	0.55
1:C:183:LEU:HD12	1:C:220:LYS:HB2	1.88	0.55
1:C:294:MET:O	1:C:297:LYS:HB3	2.06	0.55
2:G:60:SER:C	2:G:62:GLN:N	2.63	0.55
1:B:249:LEU:HD11	1:B:298:TYR:HB3	1.89	0.55
1:C:23:VAL:HG21	1:C:38:ILE:HD12	1.88	0.55
1:C:31:LYS:N	3:C:401:ADP:O1B	2.39	0.55
2:G:60:SER:C	2:G:62:GLN:H	2.14	0.55
2:H:92:GLU:O	2:H:92:GLU:HG2	2.06	0.55
1:C:297:LYS:NZ	2:G:62:GLN:HG2	2.21	0.55
1:D:5:VAL:HG12	1:D:6:GLU:N	2.22	0.55
1:D:168:ALA:HB3	1:D:173:THR:CG2	2.37	0.55
1:C:52:LEU:HD11	1:C:86:MET:CE	2.36	0.54
1:C:208:GLY:O	1:C:211:ASP:HB3	2.06	0.54
2:G:45:LYS:HB3	2:G:82:ILE:HD11	1.89	0.54
1:D:348:TYR:HD1	1:D:351:GLU:OE1	1.88	0.54
2:E:50:HIS:HD2	1:B:131:GLY:CA	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD11	1:C:86:MET:HE2	1.89	0.54
1:D:312:VAL:HG11	1:D:334:LEU:HD23	1.88	0.54
1:B:22:PHE:HE1	1:B:165:PHE:CD1	2.24	0.54
1:B:98:ASN:C	1:B:100:MET:H	2.15	0.54
2:E:45:LYS:HB3	2:E:82:ILE:HD11	1.89	0.54
1:B:320:GLU:CA	3:B:401:ADP:O2'	2.49	0.54
1:C:93:ALA:C	1:C:95:LYS:H	2.16	0.54
1:C:142:PHE:CZ	1:C:230:PHE:CE2	2.95	0.54
1:B:221:ALA:C	1:B:223:VAL:H	2.16	0.54
1:B:276:PHE:O	1:B:278:GLU:N	2.41	0.54
1:C:222:ASN:O	1:C:224:GLU:N	2.34	0.54
1:C:276:PHE:CD1	1:C:276:PHE:N	2.75	0.54
1:D:51:PHE:HE2	1:D:162:THR:HB	1.72	0.54
1:D:139:ALA:HB2	1:D:176:PHE:HB2	1.90	0.54
2:H:60:SER:C	2:H:62:GLN:H	2.13	0.54
2:H:46:VAL:HG22	2:H:82:ILE:HD13	1.88	0.54
2:H:45:LYS:HB3	2:H:82:ILE:HD11	1.88	0.54
1:B:341:ILE:HG22	1:B:342:THR:N	2.23	0.54
2:G:90:GLN:C	2:G:92:GLU:H	2.15	0.54
1:B:7:PRO:HG2	1:B:337:GLU:OE1	2.08	0.54
1:B:72:LYS:O	1:B:86:MET:HE2	2.07	0.54
1:D:329:LYS:O	1:D:332:GLN:HG2	2.07	0.54
1:A:256:ILE:HG12	1:A:266:VAL:HG11	1.90	0.53
1:B:176:PHE:C	1:B:176:PHE:CD2	2.85	0.53
1:D:22:PHE:CD1	1:D:165:PHE:HB2	2.43	0.53
1:B:174:LEU:O	1:B:262:TYR:CE1	2.61	0.53
1:C:230:PHE:N	1:C:230:PHE:CD1	2.76	0.53
1:B:52:LEU:HD22	1:B:84:SER:O	2.09	0.53
2:F:86:LYS:O	2:F:90:GLN:HB2	2.08	0.53
1:C:197:LEU:HD13	1:C:201:LEU:HD12	1.90	0.53
1:C:321:ILE:HG12	1:C:350:LEU:CD1	2.38	0.53
1:D:168:ALA:HB3	1:D:173:THR:HG21	1.91	0.53
1:D:294:MET:HE2	1:D:295:GLN:N	2.23	0.53
1:B:245:GLU:O	1:B:249:LEU:HG	2.08	0.53
1:C:266:VAL:HG12	1:C:309:PHE:CZ	2.44	0.53
1:B:12:LEU:HD23	1:B:12:LEU:O	2.09	0.53
1:B:20:TRP:CD1	1:B:236:THR:HG22	2.44	0.53
1:D:128:ASP:O	1:D:130:THR:N	2.42	0.53
1:D:146:MET:HA	1:D:149:ILE:HD12	1.90	0.53
2:F:37:GLU:OE2	2:F:38:LEU:HD23	2.09	0.53
1:D:176:PHE:HD2	1:D:176:PHE:C	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HE2	1:A:151:ARG:HH21	1.73	0.53
1:A:174:LEU:O	1:A:174:LEU:HG	2.09	0.53
1:B:141:SER:O	1:B:145:VAL:HG23	2.08	0.53
1:D:176:PHE:C	1:D:176:PHE:CD2	2.87	0.53
1:A:306:TYR:HB3	1:A:309:PHE:CD2	2.44	0.53
1:B:22:PHE:CD1	1:B:165:PHE:HD1	2.27	0.53
1:C:292:TRP:O	1:C:296:LYS:HG3	2.07	0.53
1:A:212:ILE:O	1:A:216:LEU:HB2	2.08	0.53
1:A:19:LYS:HA	1:A:162:THR:OG1	2.09	0.52
1:C:297:LYS:HZ3	2:G:62:GLN:HG2	1.74	0.52
1:C:22:PHE:CD1	1:C:165:PHE:HB2	2.43	0.52
1:A:180:PRO:HA	1:A:220:LYS:HG3	1.91	0.52
1:C:220:LYS:HG2	1:C:220:LYS:O	2.10	0.52
1:D:177:LEU:HD12	1:D:262:TYR:HB3	1.91	0.52
1:B:149:ILE:HG22	1:B:150:LYS:N	2.23	0.52
1:D:141:SER:O	1:D:145:VAL:HG23	2.09	0.52
1:D:338:TYR:CZ	1:D:340:PRO:HA	2.44	0.52
1:B:287:ARG:HG3	1:B:288:CYS:N	2.24	0.52
1:A:299:LEU:HD22	1:A:313:LYS:NZ	2.25	0.52
1:B:254:ARG:HH11	1:B:254:ARG:CG	2.22	0.52
1:D:274:LEU:HD21	1:D:299:LEU:HD11	1.92	0.52
1:C:254:ARG:HH11	1:C:254:ARG:CG	2.23	0.51
1:D:74:ALA:HB2	1:D:86:MET:CE	2.39	0.51
1:C:146:MET:HB3	1:C:150:LYS:NZ	2.25	0.51
1:D:257:GLN:HA	1:D:257:GLN:NE2	2.24	0.51
2:G:35:GLY:O	2:G:39:SER:CB	2.59	0.51
1:B:32:THR:HG21	1:B:61:ASN:HB2	1.92	0.51
1:B:219:LEU:C	1:B:221:ALA:N	2.68	0.51
1:C:219:LEU:C	1:C:221:ALA:N	2.69	0.51
1:D:130:THR:HA	1:D:136:ILE:HD12	1.93	0.51
1:D:183:LEU:C	1:D:185:LYS:H	2.18	0.51
1:D:212:ILE:C	1:D:214:GLY:H	2.17	0.51
1:D:341:ILE:HG22	1:D:342:THR:N	2.24	0.51
2:E:60:SER:C	2:E:62:GLN:N	2.63	0.51
1:D:212:ILE:C	1:D:214:GLY:N	2.67	0.51
1:A:341:ILE:HG22	1:A:342:THR:HG23	1.92	0.51
1:C:90:PRO:HB2	1:C:141:SER:OG	2.11	0.51
1:C:337:GLU:CD	1:C:337:GLU:H	2.19	0.51
1:A:179:LEU:HB3	1:A:180:PRO:CD	2.37	0.51
1:B:229:GLN:OE1	1:B:229:GLN:HA	2.11	0.51
2:G:33:ALA:CB	2:G:34:PRO:CD	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:LEU:O	1:D:277:ALA:N	2.42	0.51
1:A:130:THR:HG23	1:A:136:ILE:HB	1.92	0.51
1:B:224:GLU:OE2	1:B:224:GLU:O	2.28	0.51
1:D:254:ARG:HH12	1:D:255:LEU:CD1	2.22	0.51
1:A:20:TRP:HB2	1:A:236:THR:CG2	2.41	0.51
1:C:180:PRO:C	1:C:182:THR:H	2.19	0.51
1:C:287:ARG:O	1:C:290:ALA:HB3	2.11	0.51
1:D:339:ASN:OD1	1:D:341:ILE:HB	2.11	0.51
1:A:31:LYS:HB3	1:A:31:LYS:HZ2	1.76	0.50
1:B:91:SER:C	1:B:93:ALA:H	2.18	0.50
1:C:229:GLN:C	1:C:231:THR:N	2.70	0.50
1:C:244:SER:C	1:C:245:GLU:HG2	2.36	0.50
1:A:72:LYS:HE2	1:A:148:HIS:CE1	2.46	0.50
1:B:256:ILE:HG12	1:B:266:VAL:HG11	1.92	0.50
1:B:326:ASN:HB3	1:B:350:LEU:HD22	1.93	0.50
1:C:8:ASN:C	1:C:8:ASN:OD1	2.54	0.50
2:F:38:LEU:HD22	2:F:89:ILE:CB	2.42	0.50
1:C:57:ASP:OD2	1:C:59:ALA:HB3	2.11	0.50
1:C:77:VAL:HG23	1:C:83:LEU:O	2.11	0.50
1:C:230:PHE:N	1:C:230:PHE:HD1	2.10	0.50
1:D:275:LEU:O	1:D:292:TRP:CE3	2.64	0.50
1:A:158:GLU:O	1:A:158:GLU:HG3	2.10	0.50
1:C:52:LEU:HD22	1:C:53:LEU:N	2.27	0.50
1:D:175:ARG:O	1:D:175:ARG:HG2	2.12	0.50
1:B:249:LEU:HD21	1:B:302:ILE:HD11	1.94	0.50
1:D:19:LYS:HE2	1:D:235:LEU:CD2	2.40	0.50
1:A:12:LEU:HD21	1:A:21:ILE:HD13	1.94	0.50
1:B:209:ASN:N	1:B:209:ASN:ND2	2.41	0.50
1:C:77:VAL:HB	1:C:80:MET:HB2	1.93	0.50
1:B:23:VAL:HA	1:B:239:VAL:HG23	1.93	0.50
1:B:146:MET:O	1:B:150:LYS:HE2	2.11	0.50
1:B:174:LEU:O	1:B:262:TYR:HE1	1.95	0.50
1:C:126:LEU:HD21	1:C:216:LEU:CD2	2.41	0.50
1:C:174:LEU:O	1:C:262:TYR:CE1	2.64	0.50
1:A:96:ASP:HA	1:A:99:ASP:OD2	2.10	0.50
1:B:281:GLN:CB	1:B:345:LYS:HZ2	2.24	0.50
1:C:209:ASN:C	1:C:211:ASP:N	2.68	0.50
2:F:64:ASN:O	2:F:65:TYR:C	2.55	0.49
1:C:90:PRO:O	1:C:94:LEU:HB2	2.12	0.49
1:D:83:LEU:HD12	1:D:84:SER:N	2.26	0.49
2:F:90:GLN:HA	2:F:90:GLN:OE1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:SER:O	1:C:38:ILE:HG13	2.11	0.49
2:H:57:ASN:N	2:H:57:ASN:ND2	2.60	0.49
1:A:139:ALA:HB2	1:A:176:PHE:HB2	1.95	0.49
1:C:287:ARG:HG3	1:C:288:CYS:N	2.27	0.49
1:D:275:LEU:HD23	1:D:275:LEU:H	1.77	0.49
1:D:321:ILE:O	1:D:321:ILE:HG22	2.11	0.49
2:F:57:ASN:N	2:F:57:ASN:ND2	2.60	0.49
1:C:275:LEU:CD2	1:C:295:GLN:NE2	2.76	0.49
2:H:64:ASN:O	2:H:65:TYR:C	2.55	0.49
1:B:262:TYR:O	1:B:263:ASP:HB2	2.13	0.49
1:B:287:ARG:HG3	1:B:288:CYS:H	1.78	0.49
1:C:222:ASN:C	1:C:224:GLU:N	2.71	0.49
2:G:34:PRO:HB3	2:G:92:GLU:OE1	2.12	0.49
1:B:271:VAL:HG12	1:B:274:LEU:HD13	1.95	0.49
1:D:256:ILE:HG12	1:D:266:VAL:HG11	1.95	0.49
1:D:257:GLN:HA	1:D:257:GLN:HE21	1.78	0.49
1:A:285:CYS:SG	1:A:287:ARG:CG	3.01	0.49
1:B:175:ARG:O	1:B:175:ARG:HG2	2.12	0.49
1:B:320:GLU:HA	3:B:401:ADP:HO2'	1.74	0.49
2:G:57:ASN:N	2:G:57:ASN:ND2	2.61	0.49
1:D:52:LEU:HB3	1:D:163:VAL:HG22	1.95	0.49
1:A:5:VAL:HG12	1:A:310:HIS:CE1	2.47	0.49
1:B:211:ASP:OD1	1:B:212:ILE:HD12	2.13	0.49
1:C:229:GLN:O	1:C:231:THR:N	2.38	0.49
1:A:94:LEU:HD23	1:A:94:LEU:C	2.38	0.49
1:A:298:TYR:O	1:A:302:ILE:HG13	2.13	0.49
1:C:226:ILE:C	1:C:228:GLN:H	2.20	0.49
1:C:249:LEU:HD21	1:C:302:ILE:CD1	2.43	0.49
2:G:64:ASN:O	2:G:65:TYR:C	2.55	0.49
1:D:274:LEU:HG	1:D:292:TRP:CZ3	2.48	0.49
1:A:13:ILE:HD13	1:A:41:GLN:CG	2.43	0.48
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.25	0.48
2:E:35:GLY:O	2:E:39:SER:HB2	2.13	0.48
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.76	0.48
1:B:176:PHE:C	1:B:176:PHE:HD2	2.21	0.48
2:E:64:ASN:O	2:E:65:TYR:C	2.55	0.48
1:C:269:ILE:HG22	1:C:309:PHE:HD1	1.77	0.48
1:A:39:ALA:HB1	1:A:83:LEU:HD11	1.95	0.48
1:B:231:THR:O	1:B:233:PRO:HD3	2.13	0.48
1:B:271:VAL:HG12	1:B:274:LEU:CD1	2.43	0.48
1:D:339:ASN:CG	1:D:342:THR:HG23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HG23	1:A:42:MET:HA	1.93	0.48
1:D:230:PHE:C	1:D:232:ASP:H	2.22	0.48
2:E:50:HIS:HD2	1:B:131:GLY:HA3	1.77	0.48
1:B:26:LYS:HE2	1:B:251:GLU:CD	2.37	0.48
1:B:219:LEU:O	1:B:221:ALA:N	2.47	0.48
1:B:275:LEU:O	1:B:277:ALA:N	2.39	0.48
1:B:221:ALA:C	1:B:223:VAL:N	2.71	0.48
1:D:23:VAL:HA	1:D:239:VAL:HG23	1.96	0.48
1:A:126:LEU:C	1:A:128:ASP:H	2.22	0.48
2:E:38:LEU:HD22	2:E:89:ILE:CB	2.43	0.48
1:A:31:LYS:N	3:A:401:ADP:O1B	2.47	0.48
1:A:50:GLN:HA	1:A:50:GLN:NE2	2.28	0.48
1:A:274:LEU:HD21	1:A:299:LEU:HD11	1.95	0.48
1:B:136:ILE:CD1	1:B:179:LEU:HD11	2.44	0.48
1:B:209:ASN:C	1:B:211:ASP:H	2.21	0.48
1:C:23:VAL:HG22	1:C:239:VAL:HG23	1.96	0.48
2:G:38:LEU:HD22	2:G:89:ILE:CB	2.43	0.48
1:D:43:ALA:HA	1:D:51:PHE:CE1	2.49	0.48
1:A:249:LEU:HD11	1:A:298:TYR:HB3	1.95	0.48
1:B:74:ALA:HB2	1:B:86:MET:CE	2.41	0.48
1:D:88:ILE:CG2	1:D:89:ASP:N	2.77	0.48
1:D:271:VAL:HG12	1:D:274:LEU:HD13	1.96	0.48
2:F:90:GLN:HG3	2:F:94:LYS:HE3	1.96	0.47
1:D:241:VAL:HG13	1:D:270:ILE:CG1	2.43	0.47
1:B:174:LEU:O	1:B:174:LEU:HG	2.14	0.47
1:B:278:GLU:HB2	1:B:292:TRP:NE1	2.29	0.47
2:F:91:SER:HA	2:F:94:LYS:CD	2.40	0.47
1:D:249:LEU:HD12	1:D:298:TYR:CD2	2.49	0.47
1:A:266:VAL:HG12	1:A:309:PHE:HE1	1.79	0.47
1:C:139:ALA:O	1:C:143:MET:HG3	2.14	0.47
1:C:176:PHE:C	1:C:176:PHE:CD2	2.92	0.47
1:C:187:LEU:HD13	1:C:217:ASN:HD22	1.80	0.47
1:B:261:SER:HG	1:B:262:TYR:HD2	1.62	0.47
2:F:37:GLU:HG3	2:F:38:LEU:N	2.29	0.47
1:D:23:VAL:HG22	1:D:239:VAL:CG2	2.44	0.47
1:D:344:GLY:O	1:D:347:ILE:HG12	2.14	0.47
1:C:285:CYS:HB2	1:C:288:CYS:SG	2.54	0.47
1:C:301:GLN:OE1	2:G:66:ALA:HB2	2.13	0.47
2:G:37:GLU:O	2:G:39:SER:N	2.47	0.47
1:B:30:GLY:HA2	3:B:401:ADP:O1A	2.14	0.47
1:C:276:PHE:HD1	1:C:276:PHE:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:LEU:HD23	1:C:328:THR:OG1	2.14	0.47
1:D:44:LEU:HD23	1:D:44:LEU:C	2.39	0.47
2:H:38:LEU:HD22	2:H:89:ILE:CB	2.42	0.47
1:B:249:LEU:HD12	1:B:298:TYR:CD2	2.49	0.47
2:G:90:GLN:O	2:G:90:GLN:OE1	2.33	0.47
1:D:34:SER:HB3	1:D:270:ILE:CD1	2.45	0.47
1:D:274:LEU:HG	1:D:292:TRP:HZ3	1.80	0.47
1:D:311:VAL:HG23	1:D:311:VAL:O	2.14	0.47
1:B:39:ALA:HA	1:B:164:ILE:CD1	2.45	0.47
1:B:298:TYR:OH	2:F:62:GLN:HG3	2.15	0.47
1:C:38:ILE:CD1	1:C:239:VAL:HG21	2.44	0.47
1:C:215:LYS:C	1:C:217:ASN:N	2.73	0.47
1:B:189:LYS:C	1:B:191:GLY:N	2.73	0.47
1:C:129:LEU:HA	1:C:132:SER:OG	2.14	0.47
1:A:249:LEU:HD21	1:A:302:ILE:CD1	2.44	0.46
1:C:198:GLY:O	1:C:199:PRO:C	2.58	0.46
1:A:299:LEU:HD22	1:A:313:LYS:HZ2	1.80	0.46
1:D:212:ILE:O	1:D:212:ILE:HG13	2.15	0.46
1:A:257:GLN:NE2	1:A:257:GLN:CA	2.55	0.46
1:B:97:MET:HE1	1:B:147:LYS:HZ2	1.77	0.46
1:B:166:ASP:O	1:B:167:THR:C	2.59	0.46
1:C:243:ILE:HG22	1:C:248:SER:CB	2.44	0.46
1:D:292:TRP:CE2	1:D:296:LYS:HG3	2.50	0.46
1:C:166:ASP:O	1:C:167:THR:C	2.59	0.46
1:D:31:LYS:NZ	1:D:31:LYS:HB3	2.31	0.46
1:D:126:LEU:HD13	1:D:212:ILE:HD11	1.98	0.46
1:D:136:ILE:O	1:D:137:ASP:C	2.58	0.46
1:B:13:ILE:HG23	1:B:42:MET:HA	1.97	0.46
1:B:32:THR:CG2	1:B:61:ASN:HD22	2.29	0.46
1:C:73:ASP:O	1:C:75:ARG:HG3	2.16	0.46
1:C:281:GLN:O	1:C:282:GLU:C	2.58	0.46
1:D:166:ASP:O	1:D:167:THR:C	2.58	0.46
1:A:39:ALA:HA	1:A:164:ILE:HD13	1.97	0.46
1:A:317:CYS:SG	1:A:350:LEU:HD12	2.56	0.46
1:D:342:THR:OG1	1:D:343:ASP:N	2.47	0.46
1:A:22:PHE:HB2	1:A:238:PHE:CD1	2.50	0.46
1:A:166:ASP:O	1:A:167:THR:C	2.58	0.46
2:F:66:ALA:HB3	2:F:67:LYS:HD2	1.98	0.46
1:C:57:ASP:HA	1:C:58:PRO:HD3	1.74	0.46
1:C:306:TYR:HB3	1:C:309:PHE:HB2	1.98	0.46
2:E:90:GLN:HG3	2:E:94:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:O	1:C:305:LEU:HD12	2.15	0.46
2:G:49:ARG:HG2	2:G:49:ARG:HH11	1.81	0.46
1:D:339:ASN:OD1	1:D:342:THR:HG23	2.16	0.46
1:B:82:ASN:OD1	1:B:82:ASN:N	2.49	0.46
1:B:305:LEU:HD12	1:B:305:LEU:O	2.16	0.46
1:C:139:ALA:C	1:C:143:MET:HE2	2.40	0.46
1:C:175:ARG:HA	1:C:262:TYR:CE1	2.50	0.46
1:C:256:ILE:HG12	1:C:266:VAL:HG11	1.98	0.46
2:G:66:ALA:HB3	2:G:67:LYS:HD2	1.98	0.46
1:D:97:MET:O	1:D:97:MET:SD	2.74	0.46
1:A:127:ALA:O	1:A:130:THR:N	2.34	0.46
1:B:223:VAL:HA	1:B:226:ILE:HG22	1.97	0.46
2:F:41:LYS:C	2:F:43:LEU:H	2.24	0.46
1:A:136:ILE:O	1:A:137:ASP:C	2.58	0.45
1:A:288:CYS:O	1:A:291:ARG:N	2.45	0.45
1:B:48:ASN:N	1:B:48:ASN:ND2	2.18	0.45
1:B:347:ILE:HD11	1:B:348:TYR:CE2	2.51	0.45
1:B:262:TYR:CD2	1:B:262:TYR:N	2.83	0.45
1:C:53:LEU:HD23	1:C:85:CYS:SG	2.56	0.45
1:C:272:ASN:HD22	1:C:273:GLN:HG3	1.78	0.45
1:D:338:TYR:OH	1:D:340:PRO:HA	2.17	0.45
1:A:136:ILE:O	1:A:140:LEU:HG	2.17	0.45
1:C:6:GLU:HG2	1:C:7:PRO:HD2	1.98	0.45
1:C:183:LEU:O	1:C:184:SER:C	2.58	0.45
1:D:178:GLN:HE21	1:D:178:GLN:CA	2.18	0.45
1:A:289:GLN:O	1:A:289:GLN:HG2	2.14	0.45
1:A:297:LYS:NZ	2:E:62:GLN:HG2	2.31	0.45
2:F:49:ARG:HG2	2:F:49:ARG:HH11	1.81	0.45
1:C:9:LEU:O	1:C:13:ILE:HG13	2.16	0.45
1:C:243:ILE:CG2	1:C:245:GLU:HG3	2.46	0.45
1:C:336:LYS:HE3	1:C:336:LYS:HB3	1.87	0.45
2:H:66:ALA:HB3	2:H:67:LYS:HD2	1.99	0.45
1:A:262:TYR:CD2	1:A:262:TYR:N	2.83	0.45
1:B:210:VAL:HG12	1:B:210:VAL:O	2.17	0.45
1:B:347:ILE:HD11	1:B:348:TYR:CZ	2.51	0.45
1:C:13:ILE:HG22	1:C:45:SER:OG	2.16	0.45
1:D:20:TRP:HB2	1:D:236:THR:CB	2.45	0.45
1:D:317:CYS:SG	1:D:321:ILE:HD11	2.56	0.45
2:H:90:GLN:OE1	2:H:90:GLN:HA	2.16	0.45
1:A:20:TRP:CD1	1:A:236:THR:HG22	2.52	0.45
1:A:271:VAL:CG1	1:A:274:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:GLU:CD	2:F:38:LEU:HG	2.41	0.45
1:C:219:LEU:O	1:C:221:ALA:N	2.50	0.45
2:E:41:LYS:C	2:E:43:LEU:N	2.75	0.45
2:E:66:ALA:HB3	2:E:67:LYS:HD2	1.98	0.45
1:B:48:ASN:HD22	1:B:48:ASN:H	0.64	0.45
1:B:264:MET:HG2	1:B:265:ASP:N	2.32	0.45
1:C:136:ILE:O	1:C:137:ASP:C	2.58	0.45
2:G:41:LYS:C	2:G:43:LEU:N	2.75	0.45
1:D:31:LYS:N	3:D:401:ADP:O1B	2.50	0.45
2:E:49:ARG:HG2	2:E:49:ARG:HH11	1.82	0.45
1:B:204:PHE:O	1:B:206:GLY:N	2.49	0.45
2:F:49:ARG:NE	2:F:79:ASP:OD2	2.50	0.45
1:C:189:LYS:C	1:C:191:GLY:N	2.75	0.45
1:A:20:TRP:HD1	1:A:236:THR:HG22	1.82	0.45
1:A:23:VAL:O	1:A:167:THR:HG23	2.16	0.45
1:B:209:ASN:C	1:B:211:ASP:N	2.74	0.45
1:B:281:GLN:CB	1:B:345:LYS:NZ	2.80	0.45
1:C:232:ASP:OD2	1:C:235:LEU:HG	2.17	0.45
2:E:49:ARG:NE	2:E:79:ASP:OD2	2.50	0.44
1:B:51:PHE:CE2	1:B:162:THR:HB	2.52	0.44
1:B:90:PRO:HB2	1:B:141:SER:OG	2.17	0.44
1:B:172:HIS:ND1	1:B:172:HIS:N	2.65	0.44
1:C:126:LEU:HD21	1:C:216:LEU:HD23	1.99	0.44
1:D:126:LEU:CD1	1:D:129:LEU:HD21	2.45	0.44
1:A:139:ALA:O	1:A:143:MET:HG3	2.17	0.44
1:B:94:LEU:HD23	1:B:94:LEU:O	2.16	0.44
2:F:41:LYS:C	2:F:43:LEU:N	2.75	0.44
1:C:82:ASN:OD1	1:C:82:ASN:N	2.51	0.44
1:C:209:ASN:C	1:C:211:ASP:H	2.23	0.44
1:C:275:LEU:CD2	1:C:275:LEU:H	2.31	0.44
1:D:133:ILE:HB	1:D:136:ILE:CD1	2.47	0.44
1:D:254:ARG:NH1	1:D:255:LEU:HA	2.32	0.44
2:H:49:ARG:NE	2:H:79:ASP:OD2	2.50	0.44
1:C:20:TRP:HE3	1:C:165:PHE:HE1	1.65	0.44
2:G:49:ARG:NE	2:G:79:ASP:OD2	2.50	0.44
1:D:36:CYS:CB	1:D:327:LEU:HD23	2.47	0.44
1:D:147:LYS:HA	1:D:147:LYS:CE	2.48	0.44
1:D:248:SER:O	1:D:252:THR:HG23	2.17	0.44
1:C:39:ALA:HA	1:C:164:ILE:CD1	2.47	0.44
1:C:274:LEU:HD21	1:C:313:LYS:HG3	1.99	0.44
2:G:78:LEU:HA	2:G:81:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:GLN:OE1	2:H:65:TYR:N	2.50	0.44
2:E:41:LYS:C	2:E:43:LEU:H	2.25	0.44
1:B:136:ILE:O	1:B:137:ASP:C	2.59	0.44
1:C:89:ASP:O	1:C:93:ALA:HB2	2.18	0.44
1:D:51:PHE:CD2	1:D:162:THR:HB	2.53	0.44
1:D:130:THR:HG23	1:D:136:ILE:HB	2.00	0.44
1:D:259:LEU:HB2	1:D:266:VAL:HG21	1.99	0.44
1:A:276:PHE:HE1	1:A:315:PRO:HA	1.83	0.44
1:C:8:ASN:HA	1:C:312:VAL:CG2	2.46	0.44
1:C:139:ALA:HB1	1:C:223:VAL:CG2	2.46	0.44
1:C:168:ALA:HB3	1:C:173:THR:CG2	2.48	0.44
1:B:242:CYS:HB3	1:B:252:THR:HG21	1.99	0.44
1:B:346:VAL:HA	1:B:349:GLU:CG	2.48	0.44
2:F:36:ASN:O	2:F:40:LYS:N	2.48	0.44
1:C:314:MET:CE	1:C:330:PHE:CZ	3.01	0.44
1:D:227:ARG:C	1:D:229:GLN:N	2.72	0.44
2:H:41:LYS:C	2:H:43:LEU:H	2.25	0.44
1:A:291:ARG:NH1	1:B:291:ARG:NH1	2.66	0.44
2:E:57:ASN:N	2:E:57:ASN:ND2	2.60	0.44
1:B:54:ILE:HG13	1:B:86:MET:O	2.18	0.44
1:C:73:ASP:HB2	1:C:75:ARG:NH1	2.31	0.44
1:D:241:VAL:HG13	1:D:270:ILE:CD1	2.47	0.44
1:B:232:ASP:O	1:B:234:ASP:N	2.51	0.44
1:B:270:ILE:HD11	1:B:272:ASN:HB2	1.99	0.44
1:D:224:GLU:HA	1:D:224:GLU:OE1	2.17	0.44
1:D:278:GLU:HB2	1:D:292:TRP:HD1	1.78	0.44
2:H:41:LYS:C	2:H:43:LEU:N	2.75	0.44
1:A:12:LEU:HD21	1:A:21:ILE:CD1	2.48	0.43
1:B:129:LEU:HD12	1:B:130:THR:N	2.33	0.43
2:F:38:LEU:HB3	2:F:89:ILE:CD1	2.48	0.43
1:C:350:LEU:O	1:C:351:GLU:HB3	2.18	0.43
1:D:24:GLY:O	1:D:241:VAL:HG23	2.18	0.43
1:A:22:PHE:HD1	1:A:165:PHE:CB	2.31	0.43
1:A:70:PHE:CD1	1:A:85:CYS:CB	3.01	0.43
1:A:232:ASP:OD2	1:A:235:LEU:HG	2.17	0.43
2:E:92:GLU:HG2	2:E:92:GLU:O	2.18	0.43
1:B:321:ILE:HG22	1:B:327:LEU:HD23	1.99	0.43
2:F:52:LEU:O	2:F:55:PHE:N	2.52	0.43
1:C:168:ALA:HB3	1:C:173:THR:HG21	1.99	0.43
1:D:211:ASP:O	1:D:212:ILE:C	2.60	0.43
1:A:126:LEU:C	1:A:128:ASP:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:LEU:HB3	2:E:89:ILE:CD1	2.49	0.43
1:B:204:PHE:O	1:B:204:PHE:CD2	2.71	0.43
1:D:276:PHE:CE1	1:D:338:TYR:CE2	3.06	0.43
2:H:49:ARG:HG2	2:H:49:ARG:HH11	1.82	0.43
1:A:261:SER:OG	1:A:262:TYR:CD2	2.71	0.43
1:C:80:MET:HG2	1:C:324:LEU:HD11	1.99	0.43
1:A:22:PHE:CD1	1:A:165:PHE:CB	3.00	0.43
1:A:95:LYS:O	1:A:95:LYS:HG2	2.17	0.43
1:A:238:PHE:HE2	1:A:255:LEU:HD21	1.78	0.43
1:B:52:LEU:HB3	1:B:163:VAL:HG22	1.99	0.43
1:B:230:PHE:N	1:B:230:PHE:CD1	2.86	0.43
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.88	0.43
2:E:78:LEU:HA	2:E:81:GLU:HG2	1.99	0.43
1:B:220:LYS:O	1:B:220:LYS:HG2	2.18	0.43
1:C:31:LYS:HB3	1:C:31:LYS:HE3	1.67	0.43
1:C:270:ILE:O	1:C:270:ILE:CG1	2.67	0.43
1:D:327:LEU:O	1:D:331:SER:HB3	2.19	0.43
1:D:348:TYR:HA	1:D:351:GLU:OE1	2.18	0.43
1:A:253:GLU:O	1:A:257:GLN:HG2	2.18	0.43
1:B:19:LYS:HG3	1:B:235:LEU:HD23	2.01	0.43
2:F:78:LEU:HA	2:F:81:GLU:HG2	2.00	0.43
1:C:350:LEU:O	1:C:351:GLU:CB	2.67	0.43
1:D:13:ILE:HD13	1:D:41:GLN:HG3	1.99	0.43
1:D:20:TRP:HD1	1:D:236:THR:HG22	1.83	0.43
1:D:42:MET:CE	1:D:164:ILE:HG12	2.47	0.43
1:D:214:GLY:O	1:D:218:GLU:N	2.51	0.43
1:B:54:ILE:CG2	1:B:165:PHE:CD2	3.01	0.43
2:G:41:LYS:C	2:G:43:LEU:H	2.25	0.43
1:B:191:GLY:C	1:B:193:ILE:H	2.26	0.43
1:B:270:ILE:HD12	1:B:270:ILE:O	2.19	0.43
1:C:197:LEU:CD1	1:C:201:LEU:HD12	2.49	0.43
1:D:218:GLU:O	1:D:221:ALA:HB3	2.17	0.43
1:B:51:PHE:N	1:B:82:ASN:O	2.44	0.43
1:C:44:LEU:HD23	1:C:80:MET:HE1	2.00	0.43
1:D:23:VAL:CG2	1:D:38:ILE:HD12	2.46	0.43
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.78	0.42
2:H:38:LEU:HB3	2:H:89:ILE:CD1	2.48	0.42
1:A:130:THR:HA	1:A:136:ILE:CD1	2.44	0.42
1:A:218:GLU:O	1:A:218:GLU:HG2	2.19	0.42
1:B:201:LEU:HA	1:B:204:PHE:HB3	2.01	0.42
1:B:292:TRP:CZ2	1:B:296:LYS:HG2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ALA:O	1:C:293:LYS:HB3	2.19	0.42
1:D:24:GLY:CA	1:D:167:THR:CG2	2.97	0.42
1:A:50:GLN:CA	1:A:50:GLN:HE21	2.30	0.42
1:A:184:SER:C	1:A:186:LEU:H	2.26	0.42
1:B:139:ALA:HA	1:B:176:PHE:CD1	2.54	0.42
1:B:301:GLN:OE1	2:F:66:ALA:HB2	2.20	0.42
1:C:39:ALA:HA	1:C:164:ILE:HD13	2.00	0.42
1:C:61:ASN:OD1	1:C:61:ASN:N	2.52	0.42
1:C:88:ILE:HD11	1:C:145:VAL:HG13	2.01	0.42
1:A:22:PHE:HD1	1:A:165:PHE:HB2	1.78	0.42
1:C:30:GLY:HA2	3:C:401:ADP:O1A	2.20	0.42
1:C:176:PHE:C	1:C:176:PHE:HD2	2.28	0.42
1:D:147:LYS:HE3	1:D:147:LYS:CA	2.48	0.42
1:D:176:PHE:CD2	1:D:177:LEU:N	2.85	0.42
1:A:270:ILE:HG12	1:A:270:ILE:O	2.19	0.42
1:A:281:GLN:O	1:A:282:GLU:HB2	2.19	0.42
2:E:67:LYS:O	2:E:68:TRP:C	2.63	0.42
1:B:74:ALA:CB	1:B:86:MET:HE3	2.45	0.42
1:C:89:ASP:OD1	1:C:91:SER:HB3	2.19	0.42
1:C:198:GLY:O	1:C:202:ASN:HB3	2.19	0.42
1:C:198:GLY:O	1:C:202:ASN:CB	2.68	0.42
1:C:314:MET:HE3	1:C:330:PHE:CE1	2.55	0.42
1:A:226:ILE:C	1:A:228:GLN:N	2.77	0.42
1:B:38:ILE:O	1:B:42:MET:HG3	2.20	0.42
1:B:189:LYS:C	1:B:191:GLY:H	2.26	0.42
1:B:270:ILE:O	1:B:270:ILE:HG13	2.19	0.42
1:C:130:THR:HG21	1:C:137:ASP:OD1	2.19	0.42
1:C:215:LYS:HE3	1:C:215:LYS:HB2	1.87	0.42
1:C:243:ILE:HG23	1:C:245:GLU:CG	2.49	0.42
2:H:78:LEU:HA	2:H:81:GLU:HG2	2.00	0.42
1:A:57:ASP:OD2	1:A:59:ALA:HB3	2.19	0.42
1:A:227:ARG:O	1:A:231:THR:CG2	2.64	0.42
1:C:38:ILE:HD13	1:C:239:VAL:HG21	2.02	0.42
2:G:38:LEU:HB3	2:G:89:ILE:CD1	2.49	0.42
2:G:87:ASP:HA	2:G:90:GLN:HB3	2.01	0.42
1:B:74:ALA:N	1:B:86:MET:HE3	2.35	0.42
1:B:255:LEU:HD23	1:B:255:LEU:O	2.19	0.42
1:C:122:GLN:NE2	1:C:126:LEU:HB3	2.35	0.42
1:D:142:PHE:CB	1:D:176:PHE:HE1	2.32	0.42
1:D:229:GLN:NE2	1:D:235:LEU:HD13	2.34	0.42
1:A:82:ASN:OD1	1:A:82:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:CYS:O	1:A:290:ALA:N	2.53	0.42
1:B:187:LEU:HD11	1:B:217:ASN:HA	2.01	0.42
1:D:61:ASN:OD1	1:D:62:LEU:N	2.53	0.42
1:D:174:LEU:HD23	1:D:174:LEU:N	2.27	0.42
1:A:22:PHE:HB2	1:A:238:PHE:HD1	1.84	0.41
1:A:39:ALA:HA	1:A:164:ILE:CD1	2.50	0.41
1:B:38:ILE:CD1	1:B:239:VAL:HG21	2.50	0.41
1:C:158:GLU:O	1:C:158:GLU:HG2	2.20	0.41
1:D:10:HIS:ND1	1:D:10:HIS:C	2.77	0.41
1:D:225:THR:O	1:D:229:GLN:HB2	2.20	0.41
1:D:227:ARG:NH1	1:D:227:ARG:CG	2.81	0.41
1:D:317:CYS:N	3:D:401:ADP:N1	2.59	0.41
1:A:175:ARG:HA	1:A:262:TYR:CE1	2.55	0.41
1:B:94:LEU:C	1:B:96:ASP:H	2.27	0.41
1:B:227:ARG:C	1:B:229:GLN:H	2.28	0.41
1:B:327:LEU:O	1:B:331:SER:HB3	2.21	0.41
2:G:33:ALA:O	2:G:35:GLY:N	2.53	0.41
1:D:34:SER:HB3	1:D:270:ILE:HD12	2.01	0.41
1:A:70:PHE:CE1	1:A:85:CYS:HB2	2.55	0.41
1:A:226:ILE:O	1:A:227:ARG:C	2.62	0.41
1:B:306:TYR:HB3	1:B:309:PHE:HB2	2.02	0.41
1:C:13:ILE:HD13	1:C:41:GLN:HG2	2.02	0.41
1:C:126:LEU:HD11	1:C:216:LEU:CD2	2.47	0.41
1:C:174:LEU:O	1:C:174:LEU:HG	2.20	0.41
1:C:176:PHE:HE2	1:C:177:LEU:HD21	1.85	0.41
1:D:57:ASP:OD2	1:D:59:ALA:HB3	2.20	0.41
1:D:57:ASP:HA	1:D:58:PRO:HD3	1.81	0.41
1:D:139:ALA:HA	1:D:176:PHE:HD1	1.83	0.41
1:B:32:THR:HG23	1:B:61:ASN:ND2	2.33	0.41
1:B:250:TYR:O	1:B:251:GLU:C	2.63	0.41
1:C:147:LYS:HE3	1:C:147:LYS:HB2	1.83	0.41
1:D:318:ALA:HB3	1:D:351:GLU:OE2	2.21	0.41
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.77	0.41
1:C:254:ARG:CG	1:C:254:ARG:NH1	2.83	0.41
1:D:227:ARG:C	1:D:229:GLN:H	2.27	0.41
1:B:174:LEU:HD12	1:B:264:MET:HE1	2.02	0.41
2:F:43:LEU:O	2:F:47:LYS:HB2	2.21	0.41
1:A:51:PHE:CE2	1:A:162:THR:HB	2.55	0.41
1:A:180:PRO:HD3	1:A:223:VAL:HG11	2.03	0.41
1:D:138:GLU:OE2	1:D:175:ARG:NH1	2.54	0.41
1:B:55:SER:HB2	1:B:62:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:VAL:CG2	2:F:82:ILE:HD13	2.50	0.41
2:G:46:VAL:CG2	2:G:82:ILE:HD13	2.50	0.41
1:D:276:PHE:C	1:D:278:GLU:N	2.76	0.41
2:H:46:VAL:CG2	2:H:82:ILE:HD13	2.51	0.41
1:A:20:TRP:HB2	1:A:236:THR:HG22	2.01	0.41
1:A:347:ILE:HG13	1:A:348:TYR:CD2	2.56	0.41
1:B:13:ILE:O	1:B:13:ILE:HG22	2.20	0.41
1:B:138:GLU:N	1:B:138:GLU:OE1	2.54	0.41
1:B:201:LEU:CA	1:B:204:PHE:HB3	2.50	0.41
2:F:90:GLN:O	2:F:94:LYS:HG3	2.21	0.41
1:C:308:ASP:OD1	1:C:308:ASP:N	2.53	0.41
2:G:52:LEU:O	2:G:55:PHE:N	2.52	0.41
1:D:24:GLY:HA3	1:D:167:THR:CG2	2.49	0.41
1:D:183:LEU:C	1:D:185:LYS:N	2.79	0.41
1:D:226:ILE:HG22	1:D:230:PHE:CE2	2.55	0.41
1:A:283:HIS:NE2	1:A:289:GLN:OE1	2.53	0.41
1:B:197:LEU:O	1:B:201:LEU:CB	2.69	0.41
2:F:52:LEU:HD23	2:F:52:LEU:HA	1.85	0.41
1:C:180:PRO:O	1:C:182:THR:N	2.54	0.41
1:B:46:GLN:OE1	1:B:49:LYS:HD2	2.20	0.40
1:C:179:LEU:HA	1:C:179:LEU:HD12	1.89	0.40
2:G:35:GLY:O	2:G:39:SER:OG	2.39	0.40
2:G:67:LYS:O	2:G:70:LYS:HB2	2.22	0.40
1:D:13:ILE:HG21	1:D:41:GLN:HG3	2.03	0.40
1:D:43:ALA:HA	1:D:51:PHE:CD1	2.56	0.40
1:A:327:LEU:O	1:A:331:SER:HB3	2.20	0.40
1:B:70:PHE:CD1	1:B:85:CYS:HB2	2.56	0.40
1:B:346:VAL:O	1:B:346:VAL:HG12	2.21	0.40
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.85	0.40
1:A:145:VAL:O	1:A:146:MET:C	2.64	0.40
2:E:43:LEU:O	2:E:47:LYS:HB2	2.21	0.40
2:E:52:LEU:O	2:E:55:PHE:N	2.52	0.40
2:F:45:LYS:C	2:F:47:LYS:N	2.79	0.40
1:D:5:VAL:CG1	1:D:310:HIS:CE1	3.04	0.40
1:D:249:LEU:HD23	1:D:249:LEU:HA	1.81	0.40
1:D:250:TYR:O	1:D:251:GLU:C	2.65	0.40
1:C:139:ALA:HA	1:C:176:PHE:CD1	2.56	0.40
2:G:43:LEU:O	2:G:47:LYS:HB2	2.21	0.40
1:D:346:VAL:O	1:D:346:VAL:HG12	2.21	0.40
2:H:52:LEU:O	2:H:55:PHE:N	2.52	0.40
2:E:45:LYS:C	2:E:47:LYS:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PHE:CE2	1:B:177:LEU:HD23	2.57	0.40
1:D:148:HIS:O	1:D:152:GLN:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:ALA:CB	2:H:95:ALA:CB[3_554]	1.74	0.46
1:B:125:ALA:CB	1:C:204:PHE:CE2[3_654]	1.96	0.24

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	301/362 (83%)	248 (82%)	43 (14%)	10 (3%)	3	17
1	B	321/362 (89%)	258 (80%)	50 (16%)	13 (4%)	2	14
1	C	331/362 (91%)	259 (78%)	59 (18%)	13 (4%)	2	14
1	D	301/362 (83%)	246 (82%)	42 (14%)	13 (4%)	2	12
2	E	65/84 (77%)	52 (80%)	12 (18%)	1 (2%)	8	35
2	F	60/84 (71%)	48 (80%)	11 (18%)	1 (2%)	7	32
2	G	65/84 (77%)	49 (75%)	13 (20%)	3 (5%)	2	11
2	H	62/84 (74%)	50 (81%)	11 (18%)	1 (2%)	7	34
All	All	1506/1784 (84%)	1210 (80%)	241 (16%)	55 (4%)	2	15

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	LYS
1	A	320	GLU

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Mol	Chain	Res	Type
1	B	277	ALA
1	D	129	LEU
1	A	74	ALA
1	A	173	THR
2	E	66	ALA
1	B	74	ALA
1	B	173	THR
1	B	205	MET
1	B	220	LYS
1	B	276	PHE
1	B	320	GLU
2	F	66	ALA
1	C	74	ALA
1	C	173	THR
1	C	206	GLY
1	C	223	VAL
1	C	277	ALA
1	C	320	GLU
2	G	38	LEU
2	G	66	ALA
1	D	74	ALA
1	D	173	THR
1	D	234	ASP
1	D	277	ALA
1	D	320	GLU
2	H	66	ALA
1	A	289	GLN
1	B	99	ASP
1	C	181	ASN
1	C	230	PHE
1	C	281	GLN
1	C	346	VAL
2	G	33	ALA
1	D	231	THR
1	D	283	HIS
1	A	185	LYS
1	A	346	VAL
1	B	209	ASN
1	C	220	LYS
1	D	180	PRO
1	D	233	PRO
1	D	341	ILE

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Mol	Chain	Res	Type
1	D	346	VAL
1	A	233	PRO
1	B	233	PRO
1	B	346	VAL
1	C	285	CYS
1	D	276	PHE
1	C	180	PRO
1	A	341	ILE
1	A	180	PRO
1	B	206	GLY
1	B	341	ILE

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	273/318 (86%)	239 (88%)	34 (12%)	4	20
1	B	272/318 (86%)	240 (88%)	32 (12%)	5	22
1	C	286/318 (90%)	252 (88%)	34 (12%)	5	22
1	D	264/318 (83%)	243 (92%)	21 (8%)	11	38
2	E	61/77 (79%)	55 (90%)	6 (10%)	7	30
2	F	57/77 (74%)	52 (91%)	5 (9%)	9	35
2	G	61/77 (79%)	56 (92%)	5 (8%)	10	37
2	H	59/77 (77%)	54 (92%)	5 (8%)	10	36
All	All	1333/1580 (84%)	1191 (89%)	142 (11%)	6	26

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	THR
1	A	5	VAL
1	A	14	THR

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Mol	Chain	Res	Type
1	A	17	THR
1	A	31	LYS
1	A	48	ASN
1	A	52	LEU
1	A	56	THR
1	A	126	LEU
1	A	128	ASP
1	A	137	ASP
1	A	155	ASP
1	A	156	GLU
1	A	158	GLU
1	A	162	THR
1	A	163	VAL
1	A	173	THR
1	A	180	PRO
1	A	211	ASP
1	A	216	LEU
1	A	218	GLU
1	A	228	GLN
1	A	236	THR
1	A	239	VAL
1	A	247	LEU
1	A	254	ARG
1	A	263	ASP
1	A	270	ILE
1	A	288	CYS
1	A	301	GLN
1	A	305	LEU
1	A	308	ASP
1	A	313	LYS
2	E	37	GLU
2	E	41	LYS
2	E	43	LEU
2	E	52	LEU
2	E	67	LYS
2	E	92	GLU
1	B	4	THR
1	B	11	SER
1	B	12	LEU
1	B	14	THR
1	B	17	THR
1	B	32	THR

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Mol	Chain	Res	Type
1	B	48	ASN
1	B	50	GLN
1	B	52	LEU
1	B	64	ASP
1	B	75	ARG
1	B	144	GLU
1	B	149	ILE
1	B	159	THR
1	B	161	ASP
1	B	173	THR
1	B	205	MET
1	B	209	ASN
1	B	218	GLU
1	B	224	GLU
1	B	239	VAL
1	B	260	ILE
1	B	261	SER
1	B	269	ILE
1	B	270	ILE
1	B	275	LEU
1	B	296	LYS
1	B	315	PRO
1	B	316	LEU
1	B	320	GLU
1	B	328	THR
1	B	349	GLU
2	F	37	GLU
2	F	41	LYS
2	F	43	LEU
2	F	52	LEU
2	F	67	LYS
1	C	12	LEU
1	C	52	LEU
1	C	81	ASN
1	C	84	SER
1	C	85	CYS
1	C	106	ASN
1	C	138	GLU
1	C	140	LEU
1	C	144	GLU
1	C	158	GLU
1	C	159	THR

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Mol	Chain	Res	Type
1	C	173	THR
1	C	176	PHE
1	C	180	PRO
1	C	197	LEU
1	C	204	PHE
1	C	205	MET
1	C	229	GLN
1	C	231	THR
1	C	245	GLU
1	C	254	ARG
1	C	255	LEU
1	C	257	GLN
1	C	269	ILE
1	C	270	ILE
1	C	274	LEU
1	C	276	PHE
1	C	285	CYS
1	C	308	ASP
1	C	324	LEU
1	C	332	GLN
1	C	337	GLU
1	C	347	ILE
1	C	350	LEU
2	G	41	LYS
2	G	43	LEU
2	G	52	LEU
2	G	67	LYS
2	G	94	LYS
1	D	14	THR
1	D	31	LYS
1	D	52	LEU
1	D	72	LYS
1	D	82	ASN
1	D	128	ASP
1	D	143	MET
1	D	147	LYS
1	D	170	THR
1	D	176	PHE
1	D	236	THR
1	D	241	VAL
1	D	245	GLU
1	D	260	ILE

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Mol	Chain	Res	Type
1	D	263	ASP
1	D	270	ILE
1	D	274	LEU
1	D	288	CYS
1	D	308	ASP
1	D	337	GLU
1	D	342	THR
2	H	41	LYS
2	H	43	LEU
2	H	52	LEU
2	H	57	ASN
2	H	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	178	GLN
1	A	217	ASN
1	A	222	ASN
1	A	257	GLN
1	A	267	ASN
2	E	57	ASN
1	B	41	GLN
1	B	48	ASN
1	B	50	GLN
1	B	60	HIS
1	B	178	GLN
1	B	209	ASN
1	B	222	ASN
1	B	257	GLN
2	F	57	ASN
2	F	62	GLN
1	C	98	ASN
1	C	122	GLN
1	C	152	GLN
1	C	178	GLN
1	C	181	ASN
1	C	217	ASN
1	C	222	ASN
1	C	228	GLN
1	C	257	GLN

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Mol	Chain	Res	Type
1	C	267	ASN
1	C	273	GLN
1	C	295	GLN
1	C	310	HIS
2	G	57	ASN
2	G	62	GLN
2	G	90	GLN
1	D	178	GLN
1	D	222	ASN
1	D	229	GLN
1	D	257	GLN
1	D	267	ASN
1	D	335	ASN
2	H	36	ASN
2	H	57	ASN
2	H	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	401	-	28,29,29	2.19	4 (14%)	43,45,45	1.98	11 (25%)
3	ADP	D	401	-	28,29,29	2.21	2 (7%)	43,45,45	1.89	8 (18%)
3	ADP	A	401	-	28,29,29	2.19	4 (14%)	43,45,45	1.97	11 (25%)
3	ADP	C	401	-	28,29,29	2.08	2 (7%)	43,45,45	1.88	8 (18%)

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
3	ADP	B	401	-	-	0/16/32/32	0/3/3/3
3	ADP	D	401	-	-	0/16/32/32	0/3/3/3
3	ADP	A	401	-	-	0/16/32/32	0/3/3/3
3	ADP	C	401	-	-	0/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	O4'-C4'	-10.26	1.22	1.45
3	A	401	ADP	O4'-C4'	-9.63	1.23	1.45
3	C	401	ADP	O4'-C4'	-9.41	1.24	1.45
3	B	401	ADP	O4'-C4'	-8.79	1.25	1.45
3	B	401	ADP	PA-O3A	4.84	1.64	1.59
3	A	401	ADP	PA-O3A	2.87	1.62	1.59
3	C	401	ADP	PA-O3A	2.68	1.62	1.59
3	D	401	ADP	PA-O3A	2.56	1.62	1.59
3	B	401	ADP	O4'-C1'	2.47	1.47	1.42
3	A	401	ADP	O5'-C5'	-2.27	1.36	1.44
3	A	401	ADP	C5-N7	-2.18	1.35	1.39
3	B	401	ADP	O5'-C5'	-2.10	1.36	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C5-C4-N3	-5.21	119.54	126.72
3	B	401	ADP	C5-C4-N3	-5.15	119.63	126.72
3	A	401	ADP	C5-C4-N3	-5.12	119.66	126.72
3	C	401	ADP	C5-C4-N3	-5.06	119.75	126.72
3	A	401	ADP	N3-C2-N1	-5.00	121.02	128.58
3	C	401	ADP	N3-C2-N1	-4.84	121.26	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	N3-C2-N1	-4.78	121.34	128.58
3	B	401	ADP	N3-C2-N1	-4.53	121.72	128.58
3	D	401	ADP	N3-C4-N9	4.39	134.63	127.17
3	A	401	ADP	N3-C4-N9	4.09	134.12	127.17
3	C	401	ADP	N3-C4-N9	4.04	134.03	127.17
3	B	401	ADP	N3-C4-N9	4.00	133.96	127.17
3	B	401	ADP	O4'-C4'-C3'	3.98	113.06	105.15
3	D	401	ADP	C2-N3-C4	3.92	121.41	111.83
3	B	401	ADP	C2-N3-C4	3.89	121.33	111.83
3	C	401	ADP	C2-N3-C4	3.85	121.24	111.83
3	A	401	ADP	C2-N3-C4	3.84	121.20	111.83
3	A	401	ADP	C5-N7-C8	3.77	109.38	103.45
3	A	401	ADP	O4'-C4'-C3'	3.75	112.60	105.15
3	D	401	ADP	C5-N7-C8	3.71	109.29	103.45
3	C	401	ADP	C5-N7-C8	3.64	109.17	103.45
3	B	401	ADP	C5-N7-C8	3.56	109.04	103.45
3	C	401	ADP	O4'-C4'-C3'	3.43	111.95	105.15
3	B	401	ADP	C4-C5-N7	-3.13	107.00	110.58
3	D	401	ADP	O4'-C4'-C3'	3.08	111.27	105.15
3	A	401	ADP	C4-C5-N7	-2.94	107.22	110.58
3	D	401	ADP	C4-C5-N7	-2.92	107.24	110.58
3	C	401	ADP	C4-C5-N7	-2.91	107.26	110.58
3	A	401	ADP	N9-C8-N7	-2.85	109.89	113.94
3	B	401	ADP	C5'-C4'-C3'	-2.78	105.20	115.21
3	D	401	ADP	N9-C8-N7	-2.70	110.11	113.94
3	B	401	ADP	N9-C8-N7	-2.64	110.19	113.94
3	B	401	ADP	PA-O5'-C5'	-2.63	106.28	121.35
3	C	401	ADP	N9-C8-N7	-2.58	110.27	113.94
3	A	401	ADP	C5'-C4'-C3'	-2.35	106.77	115.21
3	A	401	ADP	O4'-C1'-N9	2.31	112.53	108.09
3	A	401	ADP	PA-O5'-C5'	-2.28	108.27	121.35
3	B	401	ADP	O4'-C1'-N9	2.19	112.30	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

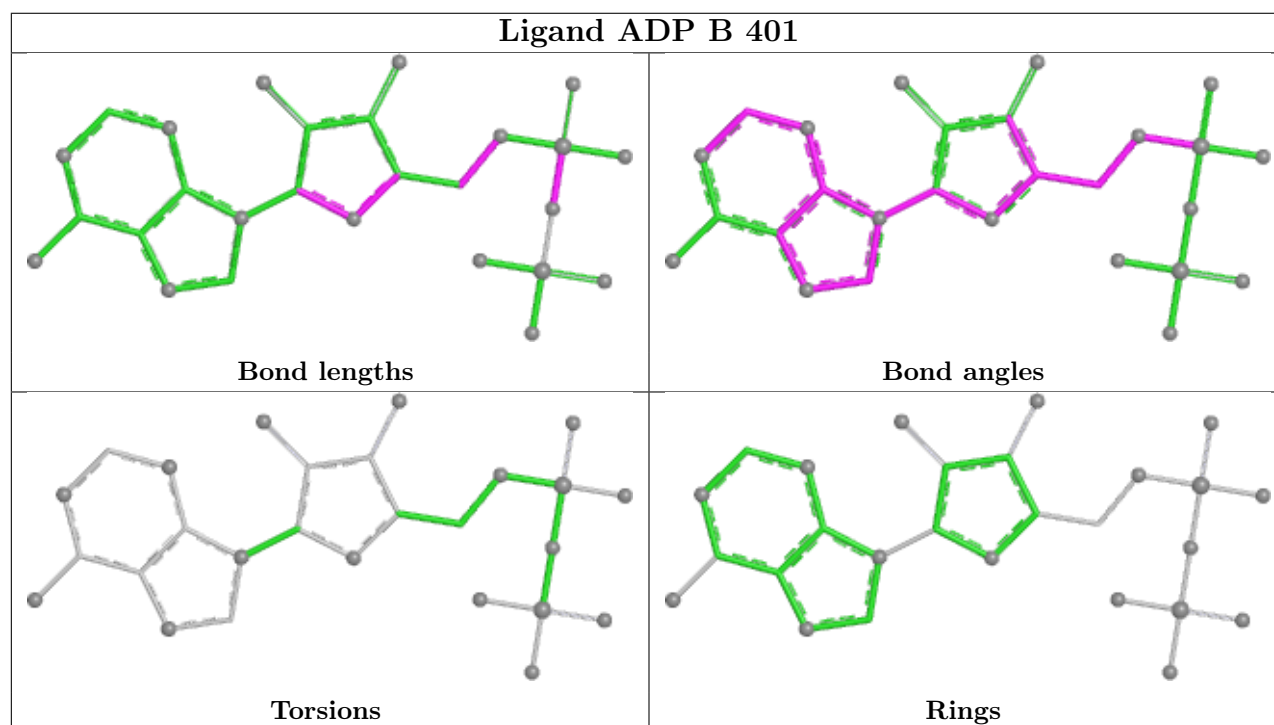
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ADP	5	0
3	D	401	ADP	3	0

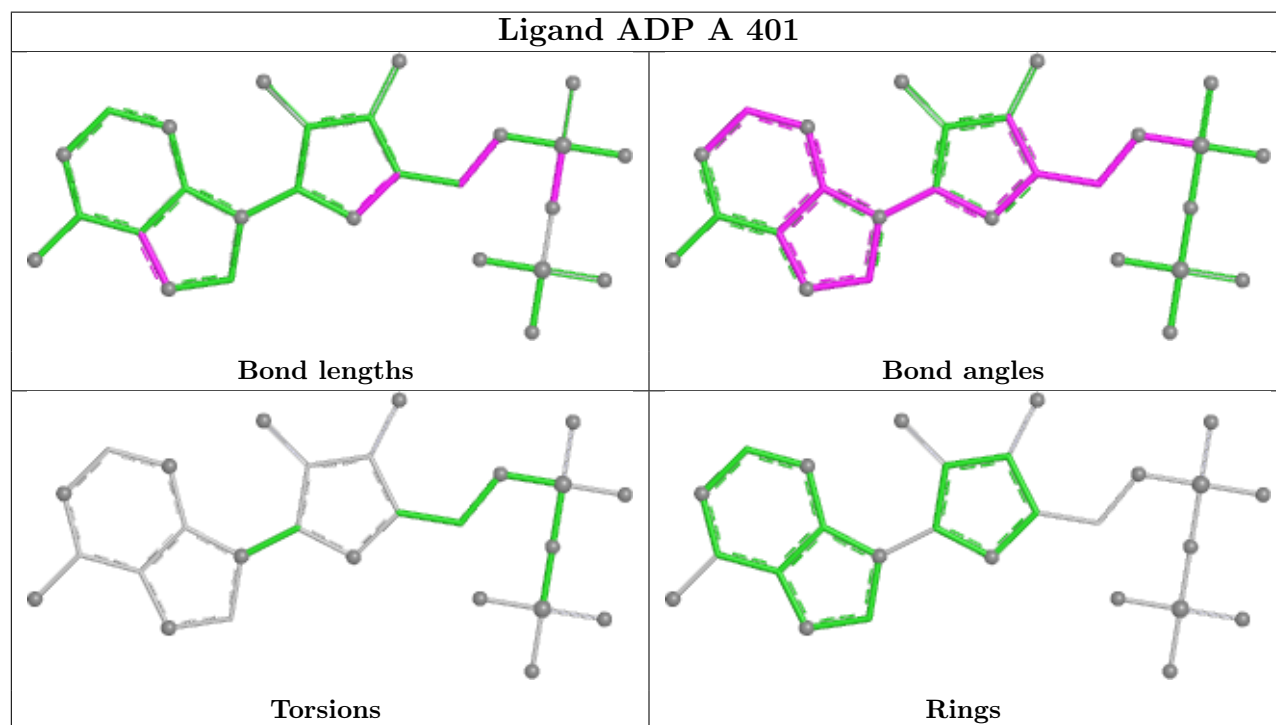
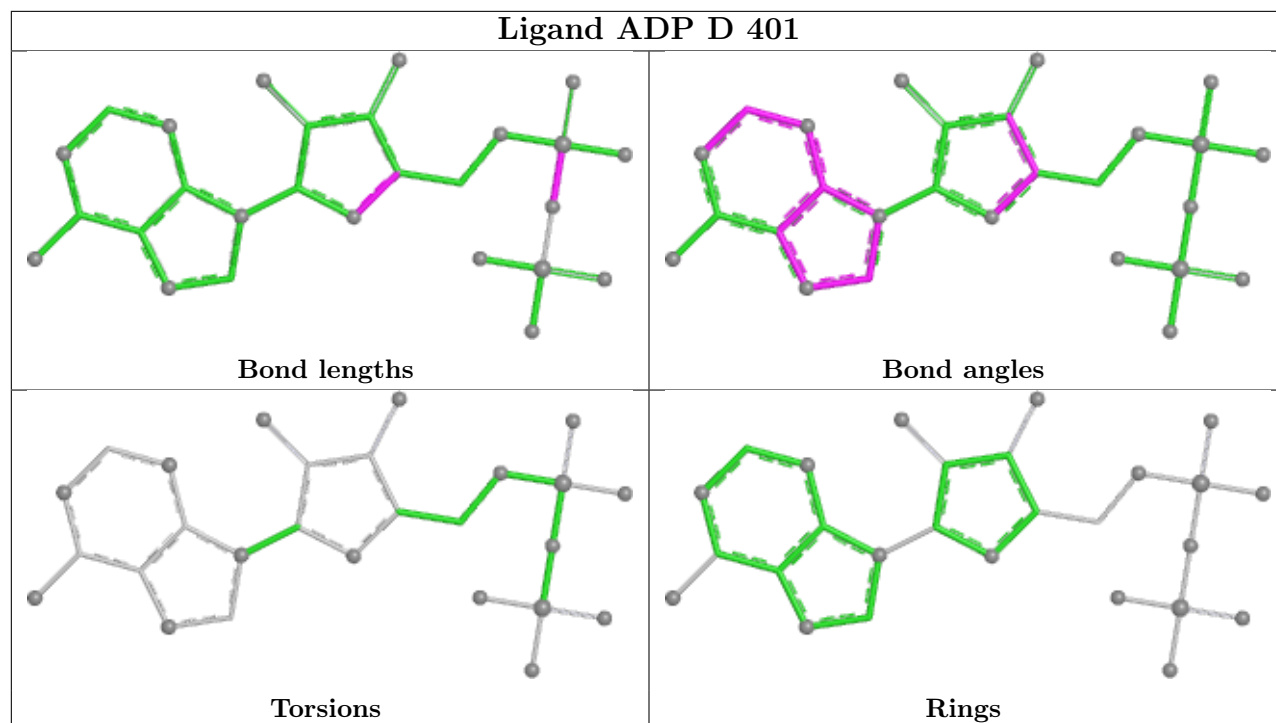
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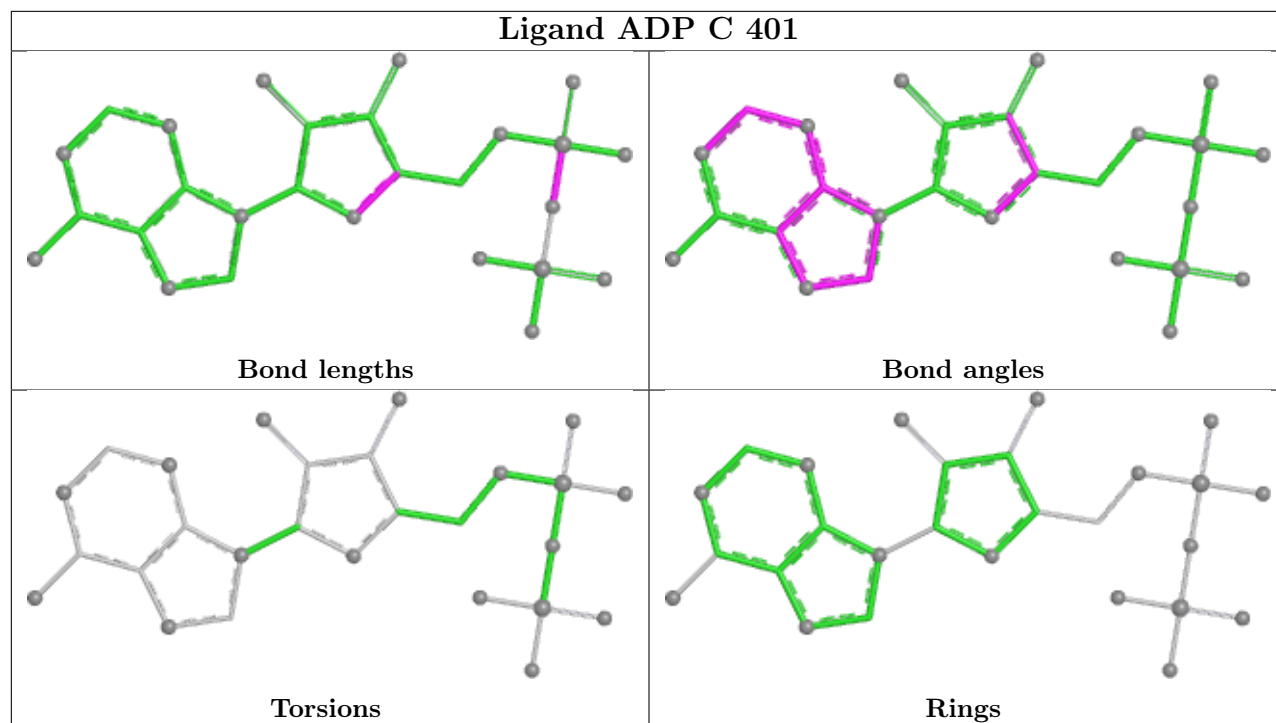
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	2	0
3	C	401	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	307/362 (84%)	-0.21	2 (0%) 84 66	43, 86, 147, 169	0
1	B	325/362 (89%)	-0.06	5 (1%) 72 49	43, 89, 169, 192	0
1	C	335/362 (92%)	0.02	2 (0%) 85 69	66, 113, 185, 193	0
1	D	307/362 (84%)	0.16	4 (1%) 75 53	80, 133, 181, 188	0
2	E	67/84 (79%)	0.12	2 (2%) 52 30	61, 111, 159, 167	0
2	F	62/84 (73%)	0.19	2 (3%) 50 29	66, 121, 164, 167	0
2	G	67/84 (79%)	0.41	1 (1%) 72 49	112, 165, 195, 197	0
2	H	64/84 (76%)	0.01	1 (1%) 70 47	105, 145, 174, 179	0
All	All	1534/1784 (85%)	0.01	19 (1%) 76 55	43, 114, 178, 197	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	79	ASP	5.1
1	B	200	MET	4.2
2	G	85	LEU	4.2
2	H	95	ALA	3.9
1	B	137	ASP	3.5
2	E	100	LEU	3.1
1	A	128	ASP	3.1
1	B	126	LEU	3.0
2	E	36	ASN	2.9
1	D	278	GLU	2.7
1	B	212	ILE	2.7
1	D	289	GLN	2.5
1	C	173	THR	2.4
1	C	346	VAL	2.2
1	D	90	PRO	2.2
1	A	73	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	209	ASN	2.1
2	F	42	TYR	2.1
1	D	162	THR	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](#)

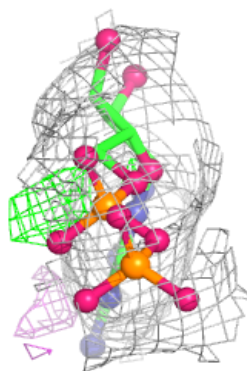
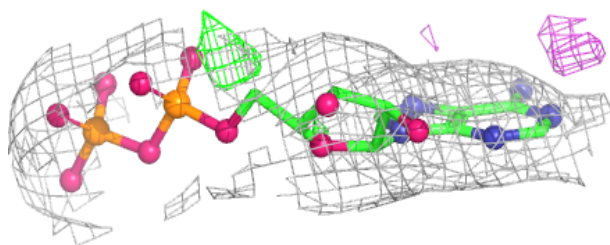
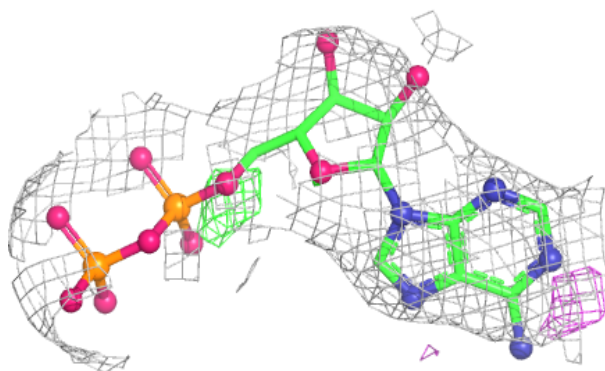
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	D	401	27/27	0.90	0.10	104,107,110,113	0
3	ADP	C	401	27/27	0.93	0.10	91,99,102,106	0
3	ADP	A	401	27/27	0.94	0.09	65,72,77,85	0
3	ADP	B	401	27/27	0.96	0.07	64,73,78,85	0

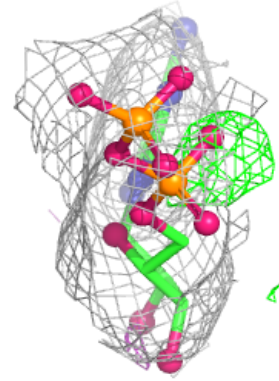
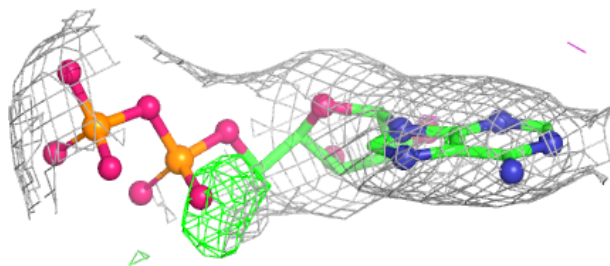
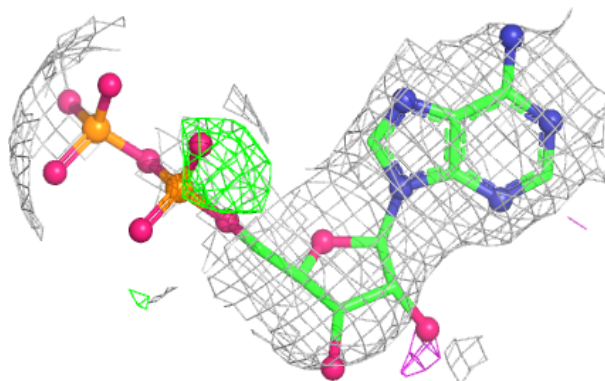
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 401:

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

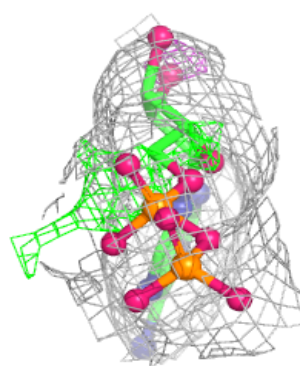
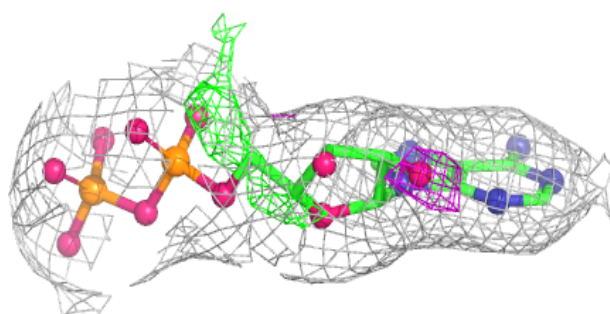
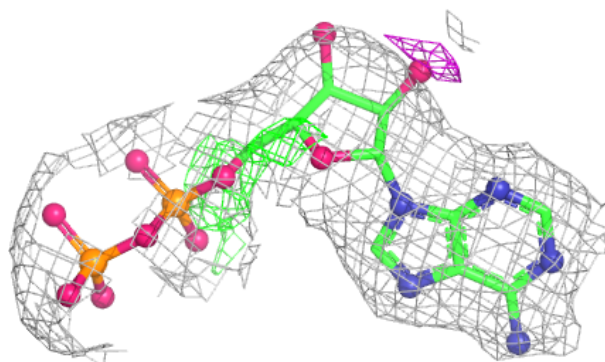
**Electron density around ADP C 401:**

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

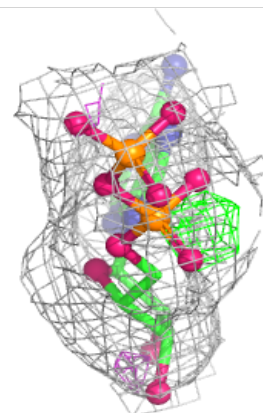
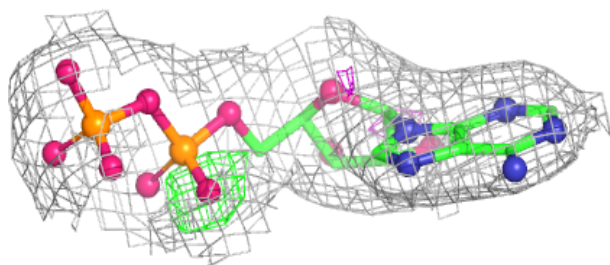
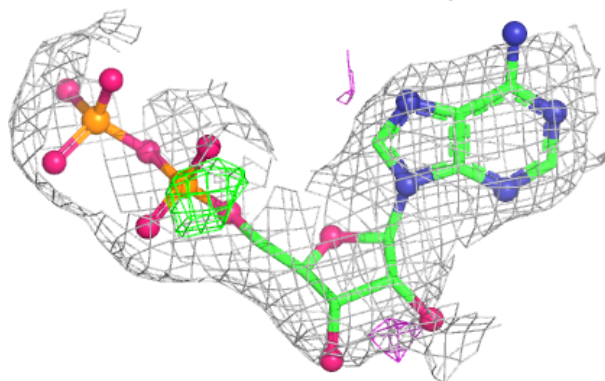


Electron density around ADP A 401:

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

**Electron density around ADP B 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.