



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:11 am BST

PDB ID : 3B2E
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

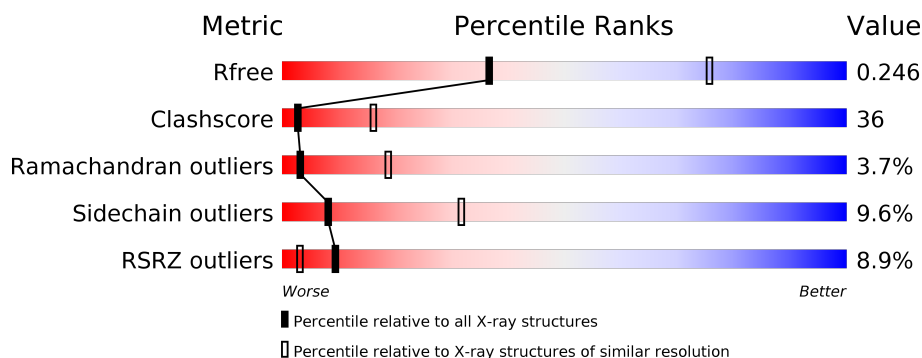
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	<div> <div>3%</div> <div> <div>44%</div> <div>34%</div> <div>6%</div> <div>15%</div> </div> </div>
1	B	362	<div> <div>5%</div> <div> <div>42%</div> <div>41%</div> <div>7%</div> <div>10%</div> </div> </div>
1	C	362	<div> <div>7%</div> <div> <div>39%</div> <div>45%</div> <div>8%</div> <div>7%</div> </div> </div>
1	D	362	<div> <div>8%</div> <div> <div>38%</div> <div>41%</div> <div>6%</div> <div>15%</div> </div> </div>
2	E	84	<div> <div>7%</div> <div> <div>42%</div> <div>30%</div> <div>8%</div> <div>20%</div> </div> </div>
2	F	84	<div> <div>10%</div> <div> <div>36%</div> <div>31%</div> <div>7%</div> <div>26%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	84	<div><div></div><div>32%</div><div>38%</div><div>35%</div><div>7%</div><div>20%</div></div>
2	H	84	<div><div></div><div>17%</div><div>40%</div><div>30%</div><div>6%</div><div>24%</div></div>

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.

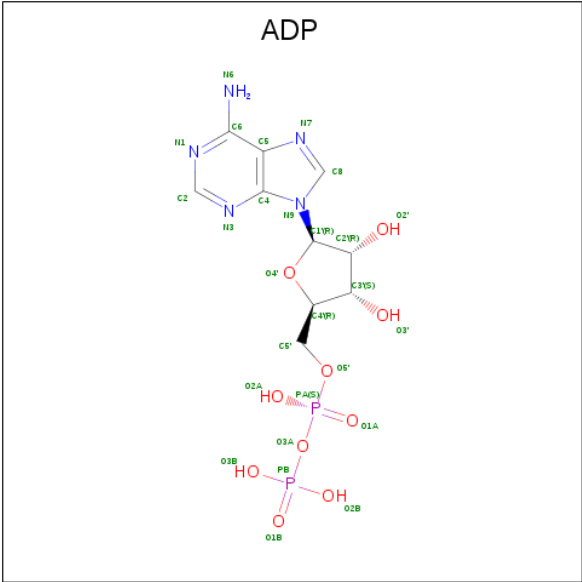
- Molecule 1 is a protein called ATPase GET3.

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 (three-letter code: 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		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

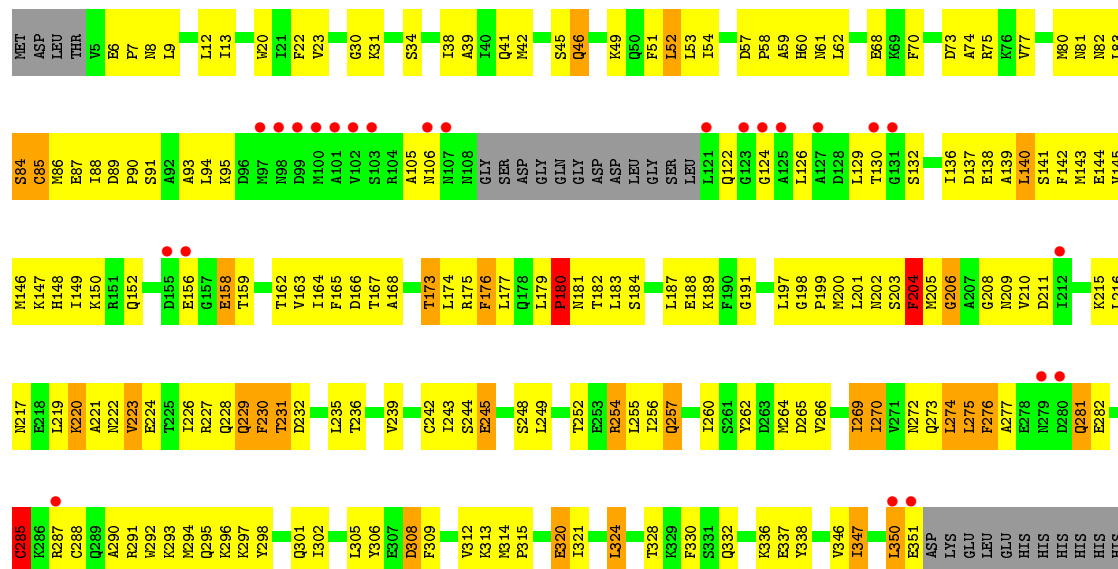
Chain B:

42% 41% 5% 10%

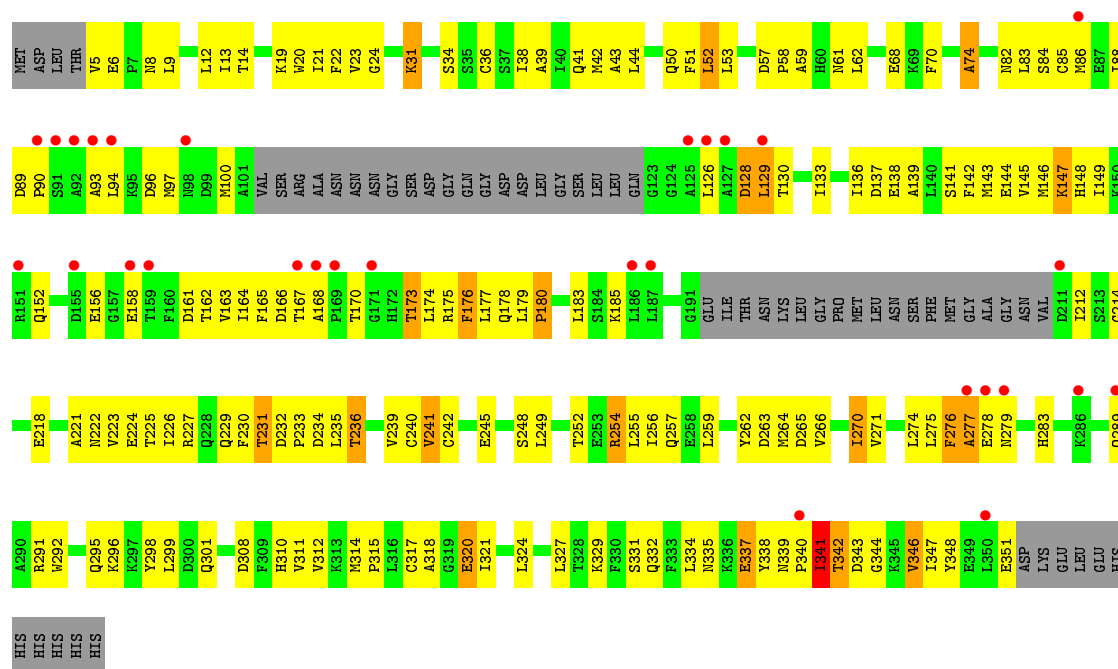
MET	ASP	LEU	T4	P7	S11	I12	I13	T14	T17	H18	K19	H20	T21	F22	V23	K26	G27	G30	K31	T32	I38	A39	I40	Q41	N42	Q46	P47	N48	K49	F50	F51	L52	L53	L54	S55	T56	D57	P58	A59	H60	I61	L62	S63	D64	F70	A74	R75	K76	N82
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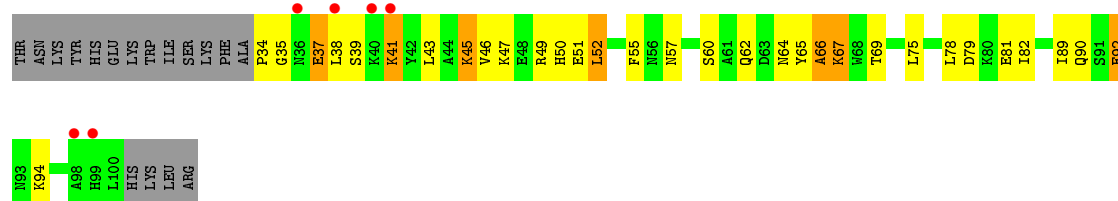
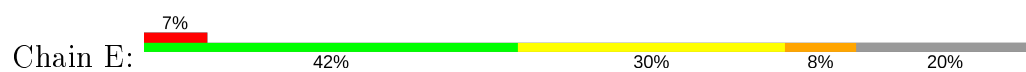
• Molecule 1: ATPase GET3



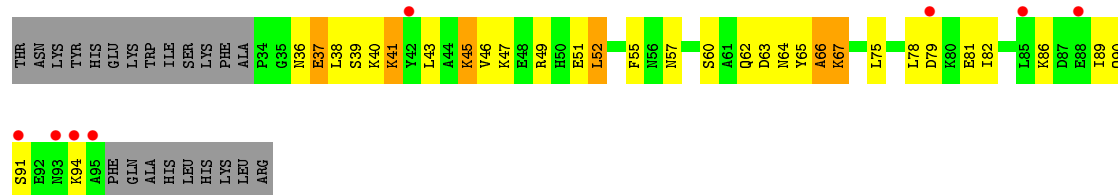
• Molecule 1: ATPase GET3



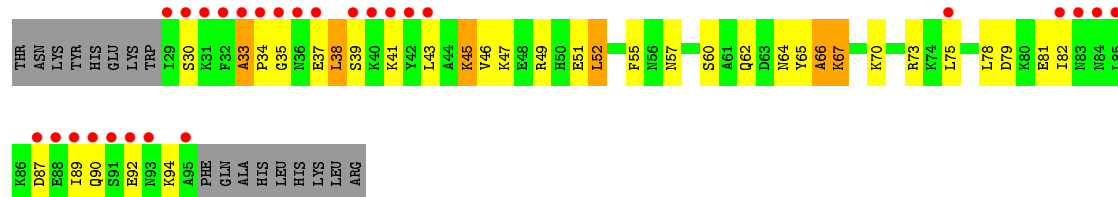
• Molecule 2: Golgi to ER traffic protein 1



- Molecule 2: Golgi to ER traffic protein 1



- Molecule 2: Golgi to ER traffic protein 1



- 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 42.25 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 94.5 (42.25-3.01)	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 0.256 , 0.246	Depositor DCC
R_{free} test set	2243 reflections (5.05%)	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)	0.25 , 40.0	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	0.90	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 [i](#)

5.1 Standard geometry [i](#)

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	0.59	1/2455 (0.0%)	0.74	2/3313 (0.1%)
1	B	0.61	2/2536 (0.1%)	0.74	2/3426 (0.1%)
1	C	0.53	3/2634 (0.1%)	0.72	1/3556 (0.0%)
1	D	0.42	0/2423	0.69	1/3270 (0.0%)
2	E	0.37	0/563	0.54	0/751
2	F	0.37	0/518	0.55	0/690
2	G	0.35	0/558	0.54	0/744
2	H	0.34	0/539	0.54	0/718
All	All	0.51	6/12226 (0.0%)	0.70	6/16468 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	PHE	CE2-CZ	10.18	1.56	1.37
1	B	204	PHE	CG-CD2	8.05	1.50	1.38
1	C	204	PHE	CG-CD1	7.62	1.50	1.38
1	B	204	PHE	CE2-CZ	6.40	1.49	1.37
1	C	204	PHE	CD2-CE2	-5.98	1.27	1.39
1	A	240	CYS	CB-SG	-5.36	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	269	ILE	CB-CA-C	-5.75	100.09	111.60
1	D	341	ILE	CB-CA-C	-5.47	100.66	111.60
1	C	204	PHE	CG-CD2-CE2	-5.42	114.84	120.80
1	B	269	ILE	CB-CA-C	-5.10	101.39	111.60
1	A	52	LEU	CA-CB-CG	5.01	126.83	115.30

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	160	0
1	B	2495	0	2433	174	1
1	C	2592	0	2549	200	1
1	D	2385	0	2349	191	0
2	E	555	0	551	35	0
2	F	512	0	511	42	0
2	G	551	0	553	45	0
2	H	532	0	528	31	1
3	A	27	0	12	3	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	855	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 36.

All (855) 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:N	1:B:48:ASN:HD22	1.46	1.11
1:A:257:GLN:HA	1:A:257:GLN:HE21	1.15	1.10
1:B:48:ASN:ND2	1:B:48:ASN:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLN:HA	1:A:257:GLN:NE2	1.81	0.96
1:C:198:GLY:HA2	1:C:202:ASN:HB2	1.47	0.95
2:F:67:LYS:H	2:F:67:LYS:HD2	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:HD22	1:B:209:ASN:H	1.12	0.92
2:G:67:LYS:HD2	2:G:67:LYS:H	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:12:LEU:HD23	1:A:12:LEU:O	1.75	0.87
1:C:291:ARG:HH12	1:D:291:ARG:HH12	1.21	0.87
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: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:74:ALA:HB2	1:B:86:MET:HE3	1.62	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: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:C:184:SER:O	1:C:188:GLU:HG2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:HA	1:A:136:ILE:HD12	1.65	0.76
1:D:23:VAL:O	1:D:167:THR:HG22	1.86	0.75
2:G:30:SER:HA	2:G:34:PRO:HD2	1.66	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:174:LEU:H	1:D:174:LEU:HD23	1.52	0.74
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:A:12:LEU:HD23	1:A:12:LEU:C	2.08	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
1:B:22:PHE:CE1	1:B:165:PHE:CD1	2.76	0.73
1:B:270:ILE:C	1:B:270:ILE:HD12	2.09	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:B:209:ASN:H	1:B:209:ASN:ND2	1.86	0.72
1:C:62:LEU:HD13	1:C:85:CYS:SG	2.29	0.72
1:D:227:ARG:O	1:D:231:THR:HG22	1.90	0.71
2:H:67:LYS:N	2:H:67:LYS:HD2	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:A:219:LEU:C	1:A:221:ALA:H	1.92	0.70
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: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
1:D:275:LEU:C	1:D:277:ALA:H	1.94	0.70
2:F:67:LYS:N	2:F:67:LYS:HD2	2.07	0.69
2:F:38:LEU:HD22	2:F:89:ILE:HB	1.73	0.69
2:G:38:LEU:HD22	2:G:89:ILE:HB	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:90:PRO:O	1:D:94:LEU:HB2	1.92	0.69
2:E:38:LEU:HD22	2:E:89:ILE:HB	1.75	0.69
1:C:126:LEU:HD11	1:C:216:LEU:HD21	1.75	0.69
2:F:37:GLU:O	2:F:41:LYS:HB2	1.92	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: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
2:H:95:ALA:C	2:H:97:GLN:H	1.97	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
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:B:175:ARG:HA	1:B:262:TYR:CE1	2.30	0.66
1:D:128:ASP:C	1:D:130:THR:H	1.95	0.66
1:A:17:THR:OG1	1:A:234:ASP:O	2.12	0.66
1:D:12:LEU:O	1:D:12:LEU:HD23	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:D:314:MET:HE1	1:D:334:LEU:HG	1.77	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:50:GLN:HE21	1:D:158:GLU:CD	1.98	0.65
1:D:12:LEU:HD21	1:D:21:ILE:HD13	1.77	0.65
1:D:74:ALA:HB2	1:D:86:MET:HE2	1.78	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:HG22	1:B:321:ILE:O	1.97	0.64
1:D:337:GLU:CD	1:D:337:GLU:H	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:TRP:HB2	1:D:236:THR:HB	1.78	0.64
1:D:42:MET:HE1	1:D:164:ILE:CG1	2.28	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
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:D:42:MET:HE1	1:D:164:ILE:HG12	1.80	0.64
1:B:158:GLU:OE2	1:B:158:GLU:HA	1.97	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
1:D:241:VAL:HG13	1:D:270:ILE:HG13	1.79	0.64
2:E:37:GLU:O	2:E:41:LYS:HB2	1.98	0.64
1:C:73:ASP:HB2	1:C:75:ARG:HH12	1.64	0.63
1:D:24:GLY:HA3	1:D:167:THR:HG21	1.81	0.63
2:E:67:LYS:N	2:E:67:LYS:HD2	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:C:206:GLY:O	1:C:210:VAL:HG23	1.98	0.63
1:A:253:GLU:HG3	2:E:69:THR:HG21	1.79	0.63
1:C:272:ASN:ND2	1:C:273:GLN:HG3	2.14	0.63
2:G:37:GLU:C	2:G:39:SER:H	2.01	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:282:GLU:CD	1:A:283:HIS:H	2.02	0.62
1:C:52:LEU:HD11	1:C:86:MET:HE1	1.81	0.62
1:B:142:PHE:HE2	1:B:226:ILE:HD11	1.63	0.62
1:B:13:ILE:HD13	1:B:41:GLN:HG2	1.81	0.62
1:B:219:LEU:C	1:B:221:ALA:H	2.03	0.62
2:E:34:PRO:HA	2:E:38:LEU:HD12	1.81	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: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
1:A:31:LYS:NZ	1:A:31:LYS:HB3	2.15	0.62
1:A:13:ILE:HD13	1:A:41:GLN:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:188:GLU:O	1:B:188:GLU:HG2	2.01	0.61
1:C:264:MET:HG3	1:C:265:ASP:N	2.16	0.61
1:D:31:LYS:HA	1:D:241:VAL:HG21	1.83	0.61
2:E:57:ASN:HD22	2:E:57:ASN:N	1.98	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
2:H:57:ASN:HD22	2:H:57:ASN:N	1.97	0.60
1:C:174:LEU:HD11	1:C:264:MET:HE2	1.83	0.60
1:C:60:HIS:HA	1:C:87:GLU:OE1	2.01	0.60
2:F:57:ASN:HD22	2:F:57:ASN:N	1.97	0.60
1:A:238:PHE:CE2	1:A:255:LEU:HD21	2.36	0.60
1:A:52:LEU:CD1	1:A:163:VAL:HG22	2.30	0.60
1:B:345:LYS:HE2	1:B:345:LYS:HA	1.82	0.60
1:B:93:ALA:O	1:B:97:MET:HG2	2.02	0.60
1:C:198:GLY:CA	1:C:202:ASN:HB2	2.28	0.60
1:C:86:MET:HE3	1:C:149:ILE:HG12	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:147:LYS:HE3	1:D:147:LYS:HA	1.82	0.60
1:D:39:ALA:CB	1:D:53:LEU:HD13	2.31	0.60
1:C:223:VAL:HG12	1:C:223:VAL:O	2.01	0.60
1:C:52:LEU:HB3	1:C:163:VAL:HG22	1.84	0.60
1:A:344:GLY:O	1:A:347:ILE:HG12	2.01	0.59
1:A:247:LEU:CD2	1:B:27:GLY:HA3	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:OD2	1:B:59:ALA:HB3	2.01	0.59
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:223:VAL:HG12	1:B:223:VAL:O	2.02	0.59
1:B:31:LYS:N	3:B:401:ADP:O1B	2.36	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:12:LEU:HD23	1:C:12:LEU:C	2.23	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
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:C:347:ILE:O	1:C:347:ILE:HD12	2.03	0.58
1:D:174:LEU:HG	1:D:174:LEU:O	2.04	0.58
1:A:152:GLN:O	1:A:156:GLU:HB2	2.04	0.58
1:C:75:ARG:HH11	1:C:75:ARG:HG3	1.68	0.58
1:A:285:CYS:SG	1:A:287:ARG:HG3	2.43	0.58
1:D:176:PHE:HD2	1:D:177:LEU:N	2.02	0.58
1:D:8:ASN:HA	1:D:312:VAL:HG22	1.86	0.58
1:B:255:LEU:C	1:B:255:LEU:HD23	2.24	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:D:242:CYS:CB	1:D:252:THR:HG21	2.34	0.58
1:C:305:LEU:HD11	2:G:73:ARG:NH2	2.19	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
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
2:F:38:LEU:HB3	2:F:89:ILE:HD12	1.85	0.57
1:A:219:LEU:C	1:A:221:ALA:N	2.58	0.57
1:B:227:ARG:O	1:B:231:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:51:PHE:CD2	1:C:162:THR:HB	2.39	0.57
1:C:38:ILE:O	1:C:42:MET:HG3	2.04	0.57
1:C:229:GLN:C	1:C:231:THR:H	2.07	0.57
1:D:152:GLN:O	1:D:156:GLU:HB3	2.03	0.57
2:F:39:SER:O	2:F:43:LEU:HG	2.04	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:257:GLN:HA	1:C:257:GLN:NE2	2.19	0.57
1:D:249:LEU:HD12	1:D:298:TYR:HD2	1.69	0.57
1:D:89:ASP:O	1:D:93:ALA:HB3	2.05	0.57
1:C:23:VAL:CG2	1:C:38:ILE:HD12	2.35	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
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
1:D:179:LEU:HD23	1:D:223:VAL:HG21	1.85	0.56
2:F:46:VAL:HG22	2:F:82:ILE:HD13	1.87	0.56
1:B:136:ILE:HD13	1:B:179:LEU:HD11	1.85	0.56
1:D:12:LEU:HD23	1:D:12:LEU:C	2.25	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:HG2	1:C:227:ARG:O	2.05	0.56
1:A:143:MET:CE	1:A:219:LEU:HD11	2.35	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:A:282:GLU:CD	1:A:283:HIS:N	2.59	0.56
1:B:228:GLN:HA	1:B:231:THR:CG2	2.35	0.56
1:C:242:CYS:SG	1:C:269:ILE:HD11	2.46	0.56
1:D:276:PHE:O	1:D:279:ASN:N	2.38	0.56
1:D:337:GLU:N	1:D:337:GLU:CD	2.59	0.56
1:A:254:ARG:NH1	1:A:254:ARG:HG2	2.19	0.56
2:G:35:GLY:O	2:G:39:SER:HB2	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD23	1:A:223:VAL:HG21	1.88	0.55
1:B:32:THR:HG23	1:B:61:ASN:HD22	1.71	0.55
1:D:227:ARG:HG2	1:D:227:ARG:NH1	2.21	0.55
2:F:45:LYS:HB3	2:F:82:ILE:HD11	1.88	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
1:D:222:ASN:O	1:D:226:ILE:HG13	2.06	0.55
1:D:324:LEU:HD23	1:D:324:LEU:C	2.27	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
1:A:246:PHE:C	1:A:246:PHE:CD2	2.79	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:C:122:GLN:CD	1:C:126:LEU:HB3	2.26	0.55
1:D:164:ILE:HD12	1:D:164:ILE:N	2.21	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:E:46:VAL:HG22	2:E:82:ILE:HD13	1.88	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:H:92:GLU:HG2	2:H:92:GLU:O	2.06	0.55
1:D:5:VAL:HG12	1:D:6:GLU:N	2.22	0.55
1:C:297:LYS:NZ	2:G:62:GLN:HG2	2.21	0.55
1:D:168:ALA:HB3	1:D:173:THR:CG2	2.37	0.55
1:C:208:GLY:O	1:C:211:ASP:HB3	2.06	0.54
1:C:52:LEU:HD11	1:C:86:MET:CE	2.36	0.54
1:D:348:TYR:HD1	1:D:351:GLU:OE1	1.88	0.54
2:G:45:LYS:HB3	2:G:82:ILE:HD11	1.89	0.54
2:E:50:HIS:HD2	1:B:131:GLY:CA	2.21	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:320:GLU:CA	3:B:401:ADP:O2'	2.49	0.54
1:C:142:PHE:CZ	1:C:230:PHE:CE2	2.95	0.54
2:E:45:LYS:HB3	2:E:82:ILE:HD11	1.89	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:N	1:C:276:PHE:CD1	2.75	0.54
1:D:139:ALA:HB2	1:D:176:PHE:HB2	1.90	0.54
1:D:51:PHE:HE2	1:D:162:THR:HB	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASP:C	1:D:130:THR:N	2.61	0.54
2:H:46:VAL:HG22	2:H:82:ILE:HD13	1.88	0.54
1:B:275:LEU:C	1:B:277:ALA:H	2.12	0.54
1:C:189:LYS:C	1:C:191:GLY:H	2.10	0.54
2:H:45:LYS:HB3	2:H:82:ILE:HD11	1.88	0.54
1:A:12:LEU:C	1:A:12:LEU:CD2	2.77	0.54
1:B:341:ILE:HG22	1:B:342:THR:N	2.23	0.54
1:D:275:LEU:C	1:D:277:ALA:N	2.61	0.54
1:B:7:PRO:HG2	1:B:337:GLU:OE1	2.08	0.54
1:C:222:ASN:C	1:C:224:GLU:H	2.11	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: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:CD1	1:C:230:PHE:N	2.76	0.53
1:C:314:MET:HE2	1:C:330:PHE:CZ	2.43	0.53
1:B:52:LEU:HD22	1:B:84:SER:O	2.09	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
2:F:60:SER:C	2:F:62:GLN:H	2.12	0.53
2:F:86:LYS:O	2:F:90:GLN:HB2	2.08	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:O	1:B:12:LEU:HD23	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:A:147:LYS:HE2	1:A:151:ARG:HH21	1.73	0.53
1:A:174:LEU:HG	1:A:174:LEU:O	2.09	0.53
1:B:141:SER:O	1:B:145:VAL:HG23	2.08	0.53
1:A:306:TYR:HB3	1:A:309:PHE:CD2	2.44	0.53
1:A:96:ASP:C	1:A:98:ASN:H	2.13	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:215:LYS:C	1:C:217:ASN:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:37:GLU:C	2:G:39:SER:N	2.62	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:CG	1:B:254:ARG:HH11	2.22	0.52
1:D:274:LEU:HD21	1:D:299:LEU:HD11	1.92	0.52
2:E:60:SER:C	2:E:62:GLN:N	2.63	0.52
1:C:254:ARG:CG	1:C:254:ARG:HH11	2.23	0.51
1:D:74:ALA:HB2	1:D:86:MET:CE	2.39	0.51
2:H:60:SER:C	2:H:62:GLN:N	2.63	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:D:130:THR:HA	1:D:136:ILE:HD12	1.93	0.51
1:D:341:ILE:HG22	1:D:342:THR:N	2.24	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:219:LEU:C	1:C:221:ALA:H	2.14	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
1:D:275:LEU:O	1:D:277:ALA:N	2.42	0.51
2:E:60:SER:C	2:E:62:GLN:H	2.13	0.51
2:F:60:SER:C	2:F:62:GLN:N	2.62	0.51
2:G:33:ALA:CB	2:G:34:PRO:CD	2.88	0.51
2:G:60:SER:C	2:G:62:GLN:N	2.63	0.51
1:A:130:THR:HG23	1:A:136:ILE:HB	1.92	0.51
1:A:320:GLU:HA	3:A:401:ADP:HO2'	1.73	0.51
1:B:129:LEU:HD12	1:B:129:LEU:C	2.31	0.51
1:B:224:GLU:O	1:B:224:GLU:OE2	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:SER:C	2:G:62:GLN:H	2.14	0.50
2:H:60:SER:C	2:H:62:GLN:H	2.13	0.50
1:C:230:PHE:HD1	1:C:230:PHE:N	2.10	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:D:275:LEU:O	1:D:292:TRP:CE3	2.64	0.50
2:F:38:LEU:HD22	2:F:89:ILE:CB	2.42	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:ND2	1:B:209:ASN:N	2.41	0.50
1:C:77:VAL:HB	1:C:80:MET:HB2	1.93	0.50
1:B:146:MET:O	1:B:150:LYS:HE2	2.11	0.50
1:B:23:VAL:HA	1:B:239:VAL:HG23	1.93	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: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
1:C:34:SER:O	1:C:38:ILE:HG13	2.11	0.49
2:F:90:GLN:OE1	2:F:90:GLN:HA	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:C:93:ALA:C	1:C:95:LYS:H	2.16	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
1:A:31:LYS:HB3	1:A:31:LYS:HZ3	1.76	0.49
1:B:262:TYR:O	1:B:263:ASP:HB2	2.13	0.49
1:C:275:LEU:CD2	1:C:295:GLN:NE2	2.76	0.49
2:F:57:ASN:N	2:F:57:ASN:ND2	2.60	0.49
1:B:287:ARG:HG3	1:B:288:CYS:H	1.78	0.49
1:B:98:ASN:C	1:B:100:MET:H	2.15	0.49
2:G:34:PRO:HB3	2:G:92:GLU:OE1	2.12	0.49
2:G:90:GLN:C	2:G:92:GLU:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:52:LEU:HB3	1:D:163:VAL:HG22	1.95	0.49
2:G:57:ASN:N	2:G:57:ASN:ND2	2.61	0.49
2:H:95:ALA:C	2:H:97:GLN:N	2.62	0.49
1:A:5:VAL:HG12	1:A:310:HIS:CE1	2.47	0.49
1:B:176:PHE:CD2	1:B:176:PHE:C	2.85	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:298:TYR:O	1:A:302:ILE:HG13	2.13	0.49
1:C:249:LEU:HD21	1:C:302:ILE:CD1	2.43	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:HH11	1:A:254:ARG:HG2	1.76	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:A:13:ILE:HG23	1:A:42:MET:HA	1.93	0.48
1:D:176:PHE:C	1:D:176:PHE:HD2	2.17	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:D:176:PHE:CD2	1:D:176:PHE:C	2.87	0.48
2:E:50:HIS:HD2	1:B:131:GLY:HA3	1.77	0.48
1:A:50:GLN:HA	1:A:50:GLN:NE2	2.28	0.48
1:D:23:VAL:HA	1:D:239:VAL:HG23	1.96	0.48
2:E:38:LEU:HD22	2:E:89:ILE:CB	2.43	0.48
2:E:57:ASN:ND2	2:E:57:ASN:N	2.60	0.48
1:A:274:LEU:HD21	1:A:299:LEU:HD11	1.95	0.48
1:A:31:LYS:N	3:A:401:ADP:O1B	2.47	0.48
1:B:136:ILE:CD1	1:B:179:LEU:HD11	2.44	0.48
1:B:221:ALA:C	1:B:223:VAL:H	2.16	0.48
1:C:23:VAL:HG22	1:C:239:VAL:HG23	1.96	0.48
1:D:43:ALA:HA	1:D:51:PHE:CE1	2.49	0.48
2:G:38:LEU:HD22	2:G:89:ILE:CB	2.43	0.48
1:A:249:LEU:HD11	1:A:298:TYR:HB3	1.95	0.48
1:D:271:VAL:HG12	1:D:274:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ILE:CG2	1:D:89:ASP:N	2.77	0.48
1:D:212:ILE:C	1:D:214:GLY:N	2.67	0.47
1:D:241:VAL:HG13	1:D:270:ILE:CG1	2.43	0.47
2:F:90:GLN:HG3	2:F:94:LYS:HE3	1.96	0.47
1:B:174:LEU:HG	1:B:174:LEU:O	2.14	0.47
1:B:278:GLU:HB2	1:B:292:TRP:NE1	2.29	0.47
1:D:249:LEU:HD12	1:D:298:TYR:CD2	2.49	0.47
2:F:91:SER:HA	2:F:94:LYS:CD	2.40	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:187:LEU:HD13	1:C:217:ASN:HD22	1.80	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:B:97:MET:HE1	1:B:144:GLU:HG2	1.96	0.47
1:C:285:CYS:HB2	1:C:288:CYS:SG	2.54	0.47
2:G:37:GLU:O	2:G:39:SER:N	2.47	0.47
1:C:301:GLN:OE1	2:G:66:ALA:HB2	2.13	0.47
1:B:30:GLY:HA2	3:B:401:ADP:O1A	2.14	0.47
1:D:183:LEU:C	1:D:185:LYS:H	2.18	0.47
1:C:276:PHE:HD1	1:C:276:PHE:H	1.63	0.47
1:C:324:LEU:HD23	1:C:328:THR:OG1	2.14	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
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
2:G:90:GLN:OE1	2:G:90:GLN:O	2.33	0.47
1:B:219:LEU:C	1:B:221:ALA:N	2.68	0.47
1:B:298:TYR:OH	2:F:62:GLN:HG3	2.15	0.47
1:B:39:ALA:HA	1:B:164:ILE:CD1	2.45	0.47
1:C:38:ILE:CD1	1:C:239:VAL:HG21	2.44	0.47
1:D:212:ILE:C	1:D:214:GLY:H	2.17	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:219:LEU:C	1:C:221:ALA:N	2.69	0.46
1:C:54:ILE:HD12	1:C:86:MET:HE2	1.96	0.46
1:D:212:ILE:HG13	1:D:212:ILE:O	2.15	0.46
1:A:257:GLN:NE2	1:A:257:GLN:CA	2.55	0.46
1:C:243:ILE:HG22	1:C:248:SER:CB	2.44	0.46
1:C:337:GLU:CD	1:C:337:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TRP:CE2	1:D:296:LYS:HG3	2.50	0.46
1:D:126:LEU:HD13	1:D:212:ILE:HD11	1.98	0.46
1:D:31:LYS:NZ	1:D:31:LYS:HB3	2.31	0.46
1:B:32:THR:CG2	1:B:61:ASN:HD22	2.29	0.46
1:B:13:ILE:HG23	1:B:42:MET:HA	1.97	0.46
1:C:73:ASP:O	1:C:75:ARG:HG3	2.16	0.46
1:A:317:CYS:SG	1:A:350:LEU:HD12	2.56	0.46
1:A:39:ALA:HA	1:A:164:ILE:HD13	1.97	0.46
1:D:342:THR:OG1	1:D:343:ASP:N	2.47	0.46
1:A:143:MET:HE2	1:A:219:LEU:HD11	1.97	0.46
1:A:22:PHE:HB2	1:A:238:PHE:CD1	2.50	0.46
1:C:180:PRO:C	1:C:182:THR:H	2.19	0.46
1:C:306:TYR:HB3	1:C:309:PHE:HB2	1.98	0.46
1:C:57:ASP:HA	1:C:58:PRO:HD3	1.74	0.46
2:F:66:ALA:HB3	2:F:67:LYS:HD2	1.98	0.46
1:C:305:LEU:O	1:C:305:LEU:HD12	2.15	0.46
1:D:339:ASN:OD1	1:D:342:THR:HG23	2.16	0.46
2:E:90:GLN:HG3	2:E:94:LYS:HE3	1.98	0.46
2:G:49:ARG:HG2	2:G:49:ARG:HH11	1.81	0.46
1:B:305:LEU:HD12	1:B:305:LEU:O	2.16	0.46
1:B:82:ASN:OD1	1:B:82:ASN:N	2.49	0.46
1:C:256:ILE:HG12	1:C:266:VAL:HG11	1.98	0.46
1:C:175:ARG:HA	1:C:262:TYR:CE1	2.50	0.46
1:D:97:MET:SD	1:D:97:MET:O	2.74	0.46
2:G:66:ALA:HB3	2:G:67:LYS:HD2	1.98	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
1:B:91:SER:C	1:B:93:ALA:H	2.18	0.46
1:C:8:ASN:C	1:C:8:ASN:OD1	2.54	0.46
1:A:288:CYS:O	1:A:291:ARG:N	2.45	0.45
1:B:347:ILE:HD11	1:B:348:TYR:CE2	2.51	0.45
1:B:48:ASN:N	1:B:48:ASN:ND2	2.18	0.45
1:B:262:TYR:CD2	1:B:262:TYR:N	2.83	0.45
1:C:272:ASN:HD22	1:C:273:GLN:HG3	1.78	0.45
1:C:53:LEU:HD23	1:C:85:CYS:SG	2.56	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:D:178:GLN:CA	1:D:178:GLN:HE21	2.18	0.45
1:A:289:GLN:O	1:A:289:GLN:HG2	2.14	0.45
1:C:243:ILE:CG2	1:C:245:GLU:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:HE3	1:C:336:LYS:HB3	1.87	0.45
1:C:9:LEU:O	1:C:13:ILE:HG13	2.16	0.45
1:A:297:LYS:NZ	2:E:62:GLN:HG2	2.31	0.45
2:F:49:ARG:HH11	2:F:49:ARG:HG2	1.81	0.45
2:H:66:ALA:HB3	2:H:67:LYS:HD2	1.99	0.45
1:A:143:MET:HE1	1:A:219:LEU:HD11	1.97	0.45
1:A:262:TYR:N	1:A:262:TYR:CD2	2.83	0.45
1:B:210:VAL:O	1:B:210:VAL:HG12	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:C:229:GLN:C	1:C:231:THR:N	2.70	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:HA	2:H:90:GLN:OE1	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
1:C:209:ASN:C	1:C:211:ASP:N	2.68	0.45
1:C:219:LEU:O	1:C:221:ALA:N	2.50	0.45
1:C:244:SER:C	1:C:245:GLU:HG2	2.36	0.45
1:B:48:ASN:HD22	1:B:48:ASN:H	0.64	0.45
2:E:66:ALA:HB3	2:E:67:LYS:HD2	1.98	0.45
2:F:64:ASN:O	2:F:65:TYR:C	2.55	0.45
1:B:264:MET:HG2	1:B:265:ASP:N	2.32	0.45
1:D:31:LYS:N	3:D:401:ADP:O1B	2.50	0.45
1:B:204:PHE:O	1:B:206:GLY:N	2.49	0.45
2:E:49:ARG:HG2	2:E:49:ARG:HH11	1.82	0.45
2:F:49:ARG:NE	2:F:79:ASP:OD2	2.50	0.45
1:A:23:VAL:O	1:A:167:THR:HG23	2.16	0.45
1:A:20:TRP:HD1	1:A:236:THR:HG22	1.82	0.45
1:A:74:ALA:HB2	1:A:86:MET:HE2	1.99	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
1:B:90:PRO:HB2	1:B:141:SER:OG	2.17	0.44
1:B:172:HIS:N	1:B:172:HIS:ND1	2.65	0.44
1:B:51:PHE:CE2	1:B:162:THR:HB	2.52	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
2:E:49:ARG:NE	2:E:79:ASP:OD2	2.50	0.44
2:H:64:ASN:O	2:H:65:TYR:C	2.55	0.44
1:A:139:ALA:O	1:A:143:MET:HG3	2.17	0.44
1:B:94:LEU:O	1:B:94:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LEU:CD2	1:C:275:LEU:H	2.31	0.44
1:C:82:ASN:OD1	1:C:82:ASN:N	2.51	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
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:D:36:CYS:CB	1:D:327:LEU:HD23	2.47	0.44
2:G:49:ARG:NE	2:G:79:ASP:OD2	2.50	0.44
1:B:221:ALA:C	1:B:223:VAL:N	2.71	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
1:D:301:GLN:OE1	2:H:65:TYR:N	2.50	0.44
2:G:78:LEU:HA	2:G:81:GLU:HG2	1.99	0.44
1:C:222:ASN:C	1:C:224:GLU:N	2.71	0.44
1:C:89:ASP:O	1:C:93:ALA:HB2	2.18	0.44
1:D:130:THR:HG23	1:D:136:ILE:HB	2.00	0.44
1:D:51:PHE:CD2	1:D:162:THR:HB	2.53	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:A:94:LEU:HD23	1:A:94:LEU:C	2.38	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:C:226:ILE:C	1:C:228:GLN:H	2.20	0.44
1:C:8:ASN:HA	1:C:312:VAL:CG2	2.46	0.44
1:A:270:ILE:CG1	1:A:270:ILE:O	2.66	0.44
1:B:176:PHE:C	1:B:176:PHE:HD2	2.21	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
1:C:314:MET:CE	1:C:330:PHE:CZ	3.01	0.44
2:F:36:ASN:O	2:F:40:LYS:N	2.48	0.44
2:G:64:ASN:O	2:G:65:TYR:C	2.55	0.44
1:A:291:ARG:NH1	1:B:291:ARG:NH1	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:64:ASN:O	2:E:65:TYR:C	2.55	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
1:B:261:SER:HG	1:B:262:TYR:HD2	1.66	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:D:339:ASN:CG	1:D:342:THR:HG23	2.39	0.43
2:F:38:LEU:HB3	2:F:89:ILE:CD1	2.48	0.43
1:A:22:PHE:HD1	1:A:165:PHE:CB	2.31	0.43
1:A:232:ASP:OD2	1:A:235:LEU:HG	2.17	0.43
1:A:70:PHE:CD1	1:A:85:CYS:CB	3.01	0.43
1:B:321:ILE:HG22	1:B:327:LEU:HD23	1.99	0.43
1:C:168:ALA:HB3	1:C:173:THR:HG21	1.99	0.43
1:D:227:ARG:C	1:D:229:GLN:N	2.72	0.43
2:E:92:GLU:O	2:E:92:GLU:HG2	2.18	0.43
2:F:52:LEU:O	2:F:55:PHE:N	2.52	0.43
1:A:126:LEU:C	1:A:128:ASP:H	2.22	0.43
1:B:204:PHE:CD2	1:B:204:PHE:O	2.71	0.43
1:B:26:LYS:HE2	1:B:251:GLU:CD	2.37	0.43
1:D:276:PHE:CE1	1:D:338:TYR:CE2	3.06	0.43
2:E:38:LEU:HB3	2:E:89:ILE:CD1	2.49	0.43
2:H:49:ARG:HH11	2:H:49:ARG:HG2	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:238:PHE:HE2	1:A:255:LEU:HD21	1.78	0.43
1:A:95:LYS:HG2	1:A:95:LYS:O	2.17	0.43
1:B:230:PHE:N	1:B:230:PHE:CD1	2.86	0.43
1:B:52:LEU:HB3	1:B:163:VAL:HG22	1.99	0.43
1:C:83:LEU:HA	1:C:83:LEU:HD12	1.88	0.43
1:B:209:ASN:C	1:B:211:ASP:H	2.21	0.43
1:B:220:LYS:O	1:B:220:LYS:HG2	2.18	0.43
1:C:270:ILE:CG1	1:C:270:ILE:O	2.67	0.43
1:C:31:LYS:HE3	1:C:31:LYS:HB3	1.67	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
2:E:78:LEU:HA	2:E:81:GLU:HG2	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:20:TRP:HD1	1:D:236:THR:HG22	1.83	0.43
2:F:78:LEU:HA	2:F:81:GLU:HG2	2.00	0.43
1:B:54:ILE:CG2	1:B:165:PHE:CD2	3.01	0.43
1:B:270:ILE:O	1:B:270:ILE:HD12	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:A:299:LEU:HD22	1:A:313:LYS:HZ3	1.84	0.43
1:B:51:PHE:N	1:B:82:ASN:O	2.44	0.43
1:C:176:PHE:CD2	1:C:176:PHE:C	2.92	0.43
1:D:23:VAL:CG2	1:D:38:ILE:HD12	2.46	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD23	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:HG2	1:A:218:GLU:O	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
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:B:139:ALA:HA	1:B:176:PHE:CD1	2.54	0.42
1:C:88:ILE:HD11	1:C:145:VAL:HG13	2.01	0.42
1:C:39:ALA:HA	1:C:164:ILE:HD13	2.00	0.42
1:C:61:ASN:N	1:C:61:ASN:OD1	2.52	0.42
1:B:301:GLN:OE1	2:F:66:ALA:HB2	2.20	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: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:D:44:LEU:C	1:D:44:LEU:HD23	2.39	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
1:B:22:PHE:CE2	1:B:264:MET:HE1	2.55	0.42
1:C:198:GLY:O	1:C:202:ASN:HB3	2.19	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:CB	2.68	0.42
1:D:230:PHE:C	1:D:232:ASP:H	2.22	0.42
1:B:270:ILE:HG13	1:B:270:ILE:O	2.19	0.42
1:B:38:ILE:O	1:B:42:MET:HG3	2.20	0.42
1:B:74:ALA:HB2	1:B:86:MET:CE	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:227:ARG:O	1:A:231:THR:CG2	2.64	0.42
1:A:57:ASP:OD2	1:A:59:ALA:HB3	2.19	0.42
1:B:189:LYS:C	1:B:191:GLY:N	2.73	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:255:LEU:O	1:B:255:LEU:HD23	2.19	0.42
1:C:122:GLN:NE2	1:C:126:LEU:HB3	2.35	0.42
1:C:198:GLY:O	1:C:199:PRO:C	2.58	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:288:CYS:O	1:A:290:ALA:N	2.53	0.42
1:A:82:ASN:OD1	1:A:82:ASN:N	2.52	0.42
1:B:187:LEU:HD11	1:B:217:ASN:HA	2.01	0.42
1:C:281:GLN:O	1:C:282:GLU:C	2.58	0.42
1:D:174:LEU:N	1:D:174:LEU:HD23	2.27	0.42
1:D:61:ASN:OD1	1:D:62:LEU:N	2.53	0.42
1:A:297:LYS:HZ1	2:E:62:GLN:HG2	1.85	0.42
1:A:39:ALA:HA	1:A:164:ILE:CD1	2.50	0.41
1:A:22:PHE:HB2	1:A:238:PHE:HD1	1.84	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:C:54:ILE:HD12	1:C:86:MET:CE	2.50	0.41
1:D:227:ARG:CG	1:D:227:ARG:NH1	2.81	0.41
1:D:225:THR:O	1:D:229:GLN:HB2	2.20	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:166:ASP:O	1:B:167:THR:C	2.59	0.41
1:B:327:LEU:O	1:B:331:SER:HB3	2.21	0.41
1:C:166:ASP:O	1:C:167:THR:C	2.59	0.41
1:C:215:LYS:C	1:C:217:ASN:N	2.73	0.41
1:D:136:ILE:O	1:D:137:ASP:C	2.58	0.41
1:D:34:SER:HB3	1:D:270:ILE:HD12	2.01	0.41
2:G:33:ALA:O	2:G:35:GLY:N	2.53	0.41
1:A:70:PHE:CE1	1:A:85:CYS:HB2	2.55	0.41
1:B:306:TYR:HB3	1:B:309:PHE:HB2	2.02	0.41
1:C:126:LEU:HD11	1:C:216:LEU:CD2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ILE:HD13	1:C:41:GLN:HG2	2.02	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:139:ALA:HA	1:D:176:PHE:HD1	1.83	0.41
1:D:166:ASP:O	1:D:167:THR:C	2.58	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:B:209:ASN:C	1:B:211:ASP:N	2.74	0.41
1:B:32:THR:HG23	1:B:61:ASN:ND2	2.33	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:A:166:ASP:O	1:A:167:THR:C	2.58	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
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
2:H:46:VAL:CG2	2:H:82:ILE:HD13	2.51	0.41
1:A:136:ILE:O	1:A:137:ASP:C	2.58	0.41
1:B:13:ILE:HG22	1:B:13:ILE:O	2.20	0.41
1:B:201:LEU:CA	1:B:204:PHE:HB3	2.50	0.41
1:D:226:ILE:HG22	1:D:230:PHE:CE2	2.55	0.41
1:D:24:GLY:HA3	1:D:167:THR:CG2	2.49	0.41
2:F:41:LYS:C	2:F:43:LEU:H	2.24	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:138:GLU:OE1	1:B:138:GLU:N	2.54	0.41
1:C:308:ASP:N	1:C:308:ASP:OD1	2.53	0.41
2:F:41:LYS:C	2:F:43:LEU:N	2.75	0.41
2:F:90:GLN:O	2:F:94:LYS:HG3	2.21	0.41
2:G:52:LEU:O	2:G:55:PHE:N	2.52	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
1:C:180:PRO:O	1:C:182:THR:N	2.54	0.41
1:C:183:LEU:O	1:C:184:SER:C	2.58	0.41
2:F:52:LEU:HD23	2:F:52:LEU:HA	1.85	0.41
1:A:86:MET:HE2	1:A:152:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:O	1:B:137:ASP:C	2.59	0.40
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
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
2:G:67:LYS:O	2:G:70:LYS:HB2	2.22	0.40
1:A:327:LEU:O	1:A:331:SER:HB3	2.20	0.40
1:B:346:VAL:HG12	1:B:346:VAL:O	2.21	0.40
1:B:70:PHE:CD1	1:B:85:CYS:HB2	2.56	0.40
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.85	0.40
1:D:249:LEU:HD23	1:D:249:LEU:HA	1.81	0.40
1:D:5:VAL:CG1	1:D:310:HIS:CE1	3.04	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:37:GLU:CD	2:F:38:LEU:HG	2.41	0.40
1:C:139:ALA:HA	1:C:176:PHE:CD1	2.56	0.40
1:D:346:VAL:O	1:D:346:VAL:HG12	2.21	0.40
2:G:43:LEU:O	2:G:47:LYS:HB2	2.21	0.40
2:H:52:LEU:O	2:H:55:PHE:N	2.52	0.40
1:B:176:PHE:CE2	1:B:177:LEU:HD23	2.57	0.40
1:C:136:ILE:O	1:C:137:ASP:C	2.58	0.40
1:C:209:ASN:C	1:C:211:ASP:H	2.23	0.40
1:D:148:HIS:O	1:D:152:GLN:HG2	2.21	0.40
2:E:41:LYS:C	2:E:43:LEU:N	2.75	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	301/362 (83%)	248 (82%)	43 (14%)	10 (3%)	4	21
1	B	321/362 (89%)	258 (80%)	50 (16%)	13 (4%)	3	17
1	C	331/362 (91%)	259 (78%)	59 (18%)	13 (4%)	3	17
1	D	301/362 (83%)	246 (82%)	42 (14%)	13 (4%)	2	15
2	E	65/84 (77%)	52 (80%)	12 (18%)	1 (2%)	10	42
2	F	60/84 (71%)	48 (80%)	11 (18%)	1 (2%)	9	39
2	G	65/84 (77%)	49 (75%)	13 (20%)	3 (5%)	2	14
2	H	62/84 (74%)	50 (81%)	11 (18%)	1 (2%)	9	40
All	All	1506/1784 (84%)	1210 (80%)	241 (16%)	55 (4%)	3	19

All (55) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	273/318 (86%)	247 (90%)	26 (10%)	8 32
1	B	272/318 (86%)	242 (89%)	30 (11%)	6 25
1	C	286/318 (90%)	254 (89%)	32 (11%)	6 24
1	D	264/318 (83%)	244 (92%)	20 (8%)	13 43
2	E	61/77 (79%)	55 (90%)	6 (10%)	8 30
2	F	57/77 (74%)	52 (91%)	5 (9%)	10 36
2	G	61/77 (79%)	56 (92%)	5 (8%)	11 39
2	H	59/77 (77%)	55 (93%)	4 (7%)	16 48
All	All	1333/1580 (84%)	1205 (90%)	128 (10%)	8 32

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	17	THR
1	A	31	LYS
1	A	48	ASN
1	A	52	LEU
1	A	126	LEU
1	A	128	ASP
1	A	137	ASP
1	A	138	GLU
1	A	156	GLU
1	A	158	GLU
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	254	ARG
1	A	261	SER
1	A	263	ASP
1	A	270	ILE
1	A	288	CYS
1	A	301	GLN

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Mol	Chain	Res	Type
1	A	308	ASP
1	A	313	LYS
2	E	37	GLU
2	E	41	LYS
2	E	45	LYS
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
1	B	48	ASN
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	176	PHE
1	B	205	MET
1	B	209	ASN
1	B	218	GLU
1	B	222	ASN
1	B	224	GLU
1	B	239	VAL
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	349	GLU
2	F	37	GLU
2	F	41	LYS
2	F	45	LYS
2	F	52	LEU

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Mol	Chain	Res	Type
2	F	67	LYS
1	C	46	GLN
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
1	C	176	PHE
1	C	180	PRO
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	275	LEU
1	C	276	PHE
1	C	285	CYS
1	C	308	ASP
1	C	324	LEU
1	C	332	GLN
1	C	347	ILE
1	C	350	LEU
2	G	41	LYS
2	G	45	LYS
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	82	ASN

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Mol	Chain	Res	Type
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	254	ARG
1	D	263	ASP
1	D	270	ILE
1	D	289	GLN
1	D	308	ASP
1	D	335	ASN
1	D	337	GLU
1	D	342	THR
2	H	41	LYS
2	H	45	LYS
2	H	52	LEU
2	H	67	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	178	GLN
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	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	178	GLN
1	C	181	ASN

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Mol	Chain	Res	Type
1	C	217	ASN
1	C	222	ASN
1	C	228	GLN
1	C	257	GLN
1	C	273	GLN
1	C	295	GLN
1	C	335	ASN
2	G	57	ASN
2	G	90	GLN
1	D	50	GLN
1	D	98	ASN
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	57	ASN
2	H	62	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	24,29,29	2.29	4 (16%)	29,45,45	1.83	6 (20%)
3	ADP	D	401	-	24,29,29	2.38	3 (12%)	29,45,45	1.82	4 (13%)
3	ADP	A	401	-	24,29,29	2.40	5 (20%)	29,45,45	1.91	6 (20%)
3	ADP	C	401	-	24,29,29	2.23	3 (12%)	29,45,45	1.83	4 (13%)

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	-	-	0/12/32/32	0/3/3/3
3	ADP	D	401	-	-	0/12/32/32	0/3/3/3
3	ADP	A	401	-	-	0/12/32/32	0/3/3/3
3	ADP	C	401	-	-	0/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	O4'-C4'	-10.21	1.22	1.45
3	A	401	ADP	O4'-C4'	-9.58	1.23	1.45
3	C	401	ADP	O4'-C4'	-9.36	1.24	1.45
3	B	401	ADP	O4'-C4'	-8.75	1.25	1.45
3	B	401	ADP	O4'-C1'	4.75	1.47	1.41
3	A	401	ADP	O4'-C1'	3.35	1.45	1.41
3	C	401	ADP	O4'-C1'	3.04	1.45	1.41
3	D	401	ADP	C8-N7	-2.80	1.29	1.34
3	A	401	ADP	C8-N7	-2.78	1.29	1.34
3	A	401	ADP	C2'-C1'	-2.50	1.50	1.53
3	B	401	ADP	C8-N7	-2.35	1.30	1.34
3	A	401	ADP	O5'-C5'	-2.28	1.36	1.44
3	C	401	ADP	C8-N7	-2.28	1.30	1.34
3	B	401	ADP	O5'-C5'	-2.11	1.36	1.44
3	D	401	ADP	O4'-C1'	2.09	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	PA-O3A-PB	-6.40	110.88	132.83
3	C	401	ADP	PA-O3A-PB	-6.28	111.29	132.83
3	A	401	ADP	PA-O3A-PB	-6.23	111.44	132.83
3	B	401	ADP	PA-O3A-PB	-5.14	115.20	132.83
3	A	401	ADP	N3-C2-N1	-4.90	121.02	128.68
3	C	401	ADP	N3-C2-N1	-4.75	121.26	128.68
3	D	401	ADP	N3-C2-N1	-4.69	121.34	128.68
3	B	401	ADP	N3-C2-N1	-4.45	121.72	128.68
3	B	401	ADP	O4'-C4'-C3'	4.01	113.06	105.11
3	A	401	ADP	O4'-C4'-C3'	3.78	112.60	105.11
3	C	401	ADP	O4'-C4'-C3'	3.46	111.95	105.11
3	D	401	ADP	O4'-C4'-C3'	3.11	111.27	105.11
3	B	401	ADP	C5'-C4'-C3'	-2.66	105.20	115.18
3	B	401	ADP	PA-O5'-C5'	-2.63	106.28	121.68
3	B	401	ADP	C4-C5-N7	-2.30	107.00	109.40
3	A	401	ADP	PA-O5'-C5'	-2.29	108.27	121.68
3	A	401	ADP	C5'-C4'-C3'	-2.25	106.77	115.18
3	A	401	ADP	C4-C5-N7	-2.10	107.22	109.40
3	D	401	ADP	C4-C5-N7	-2.07	107.24	109.40
3	C	401	ADP	C4-C5-N7	-2.06	107.26	109.40

There are no chirality outliers.

There are no torsion outliers.

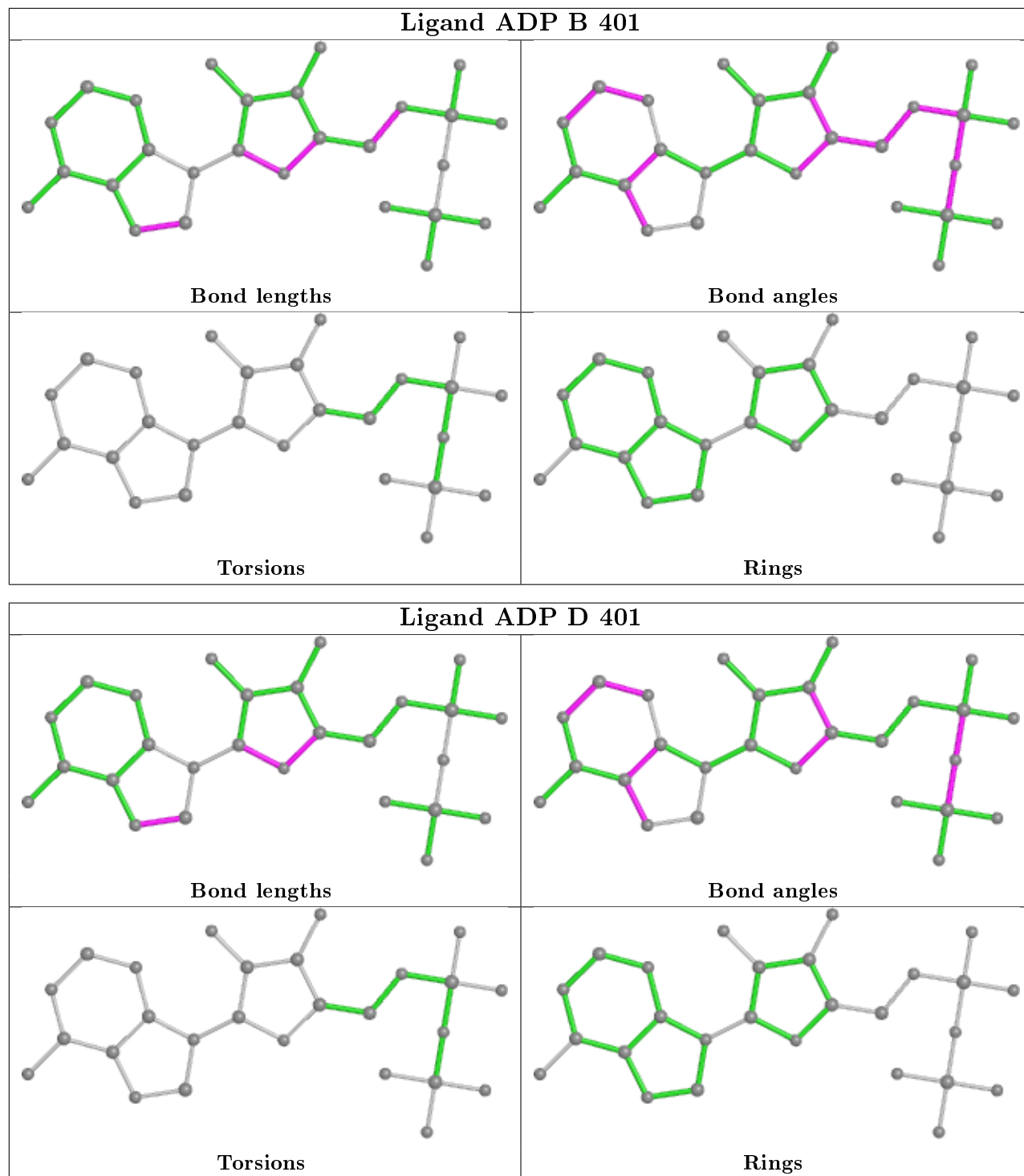
There are no ring outliers.

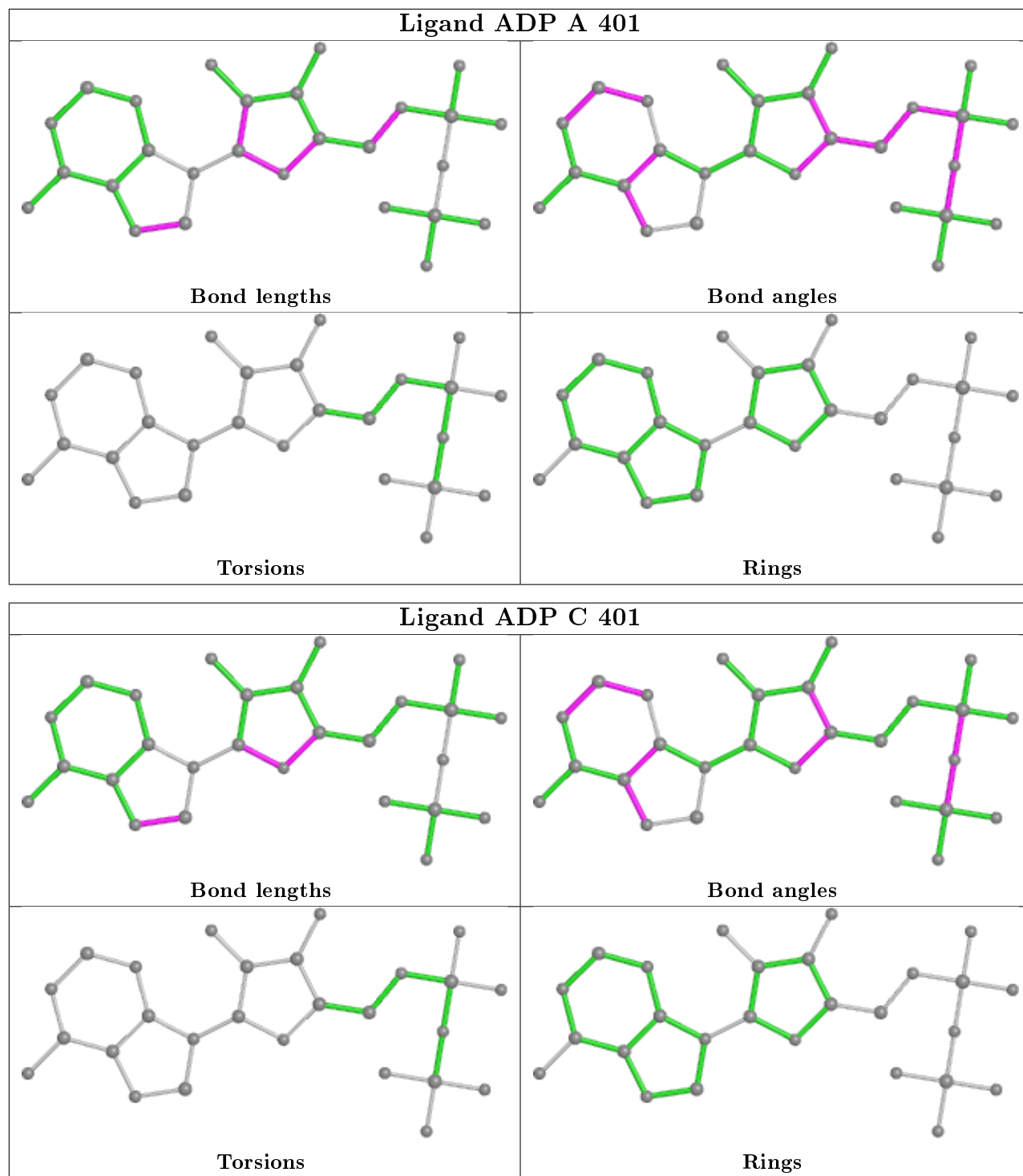
4 monomers are involved in 14 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	307/362 (84%)	0.08	11 (3%)	42	17	43, 86, 147, 169	0
1	B	325/362 (89%)	0.09	18 (5%)	25	9	43, 89, 169, 192	0
1	C	335/362 (92%)	0.30	24 (7%)	15	4	66, 113, 185, 193	0
1	D	307/362 (84%)	0.39	29 (9%)	8	3	80, 133, 181, 188	0
2	E	67/84 (79%)	0.20	6 (8%)	9	3	61, 111, 159, 167	0
2	F	62/84 (73%)	0.55	8 (12%)	3	1	66, 121, 164, 167	0
2	G	67/84 (79%)	1.57	27 (40%)	0	0	112, 165, 195, 197	0
2	H	64/84 (76%)	0.90	14 (21%)	0	0	105, 145, 174, 179	0
All	All	1534/1784 (85%)	0.32	137 (8%)	9	3	43, 115, 178, 197	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	95	ALA	9.8
1	C	99	ASP	6.9
2	F	95	ALA	6.7
2	G	88	GLU	6.4
1	C	121	LEU	5.8
2	G	93	ASN	5.8
1	D	126	LEU	5.5
1	B	281	GLN	5.4
1	C	102	VAL	5.3
2	G	91	SER	5.3
2	H	91	SER	5.2
2	G	95	ALA	5.1
1	C	106	ASN	4.9
1	C	280	ASP	4.9
1	B	200	MET	4.8
1	C	98	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	36	ASN	4.6
2	G	39	SER	4.6
1	B	209	ASN	4.5
2	G	92	GLU	4.5
1	D	289	GLN	4.5
1	D	186	LEU	4.4
1	C	103	SER	4.3
1	C	279	ASN	4.3
2	G	82	ILE	4.2
1	C	351	GLU	4.2
2	H	41	LYS	4.1
1	A	128	ASP	4.1
2	G	30	SER	4.1
1	D	278	GLU	4.1
2	G	29	ILE	4.0
1	C	212	ILE	4.0
1	C	107	ASN	3.8
1	D	86	MET	3.8
1	C	123	GLY	3.7
1	D	91	SER	3.7
1	A	279	ASN	3.7
1	C	127	ALA	3.6
1	B	278	GLU	3.6
1	C	125	ALA	3.6
1	A	286	LYS	3.5
1	C	97	MET	3.5
2	G	43	LEU	3.5
2	E	40	LYS	3.5
2	H	36	ASN	3.5
1	D	90	PRO	3.4
2	H	37	GLU	3.4
2	G	41	LYS	3.3
2	H	96	PHE	3.3
2	H	39	SER	3.3
1	D	350	LEU	3.2
1	C	124	GLY	3.2
1	C	350	LEU	3.2
1	D	127	ALA	3.2
2	H	40	LYS	3.2
1	A	284	ASN	3.2
1	A	212	ILE	3.2
2	G	33	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	34	PRO	3.1
1	A	97	MET	3.1
1	B	280	ASP	3.1
1	D	277	ALA	3.1
1	A	209	ASN	3.1
2	G	83	ASN	3.1
2	G	35	GLY	3.0
1	B	351	GLU	3.0
1	C	101	ALA	3.0
2	G	37	GLU	2.9
1	D	167	THR	2.9
1	B	288	CYS	2.9
2	G	85	LEU	2.9
1	B	99	ASP	2.8
2	G	36	ASN	2.8
1	D	98	ASN	2.8
1	D	125	ALA	2.8
2	H	92	GLU	2.7
1	C	100	MET	2.7
2	H	88	GLU	2.7
2	G	32	PHE	2.7
1	B	204	PHE	2.7
2	G	87	ASP	2.7
1	D	168	ALA	2.6
1	D	211	ASP	2.6
2	G	90	GLN	2.6
1	D	159	THR	2.6
1	D	158	GLU	2.6
2	H	45	LYS	2.6
1	B	94	LEU	2.5
2	F	79	ASP	2.5
1	B	199	PRO	2.5
1	D	340	PRO	2.5
2	G	31	LYS	2.5
1	B	287	ARG	2.5
1	C	287	ARG	2.5
2	F	91	SER	2.5
2	E	99	HIS	2.5
1	D	129	LEU	2.5
1	A	283	HIS	2.5
1	C	155	ASP	2.5
2	G	84	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	40	LYS	2.5
1	D	94	LEU	2.4
2	F	94	LYS	2.4
1	D	286	LYS	2.4
1	B	198	GLY	2.4
1	D	279	ASN	2.3
1	D	155	ASP	2.3
2	G	34	PRO	2.3
1	A	3	LEU	2.3
2	G	42	TYR	2.3
1	A	133	ILE	2.3
1	B	137	ASP	2.3
1	A	98	ASN	2.2
1	C	156	GLU	2.2
2	F	93	ASN	2.2
2	H	93	ASN	2.2
1	D	93	ALA	2.2
2	F	85	LEU	2.2
1	D	151	ARG	2.2
1	C	130	THR	2.2
1	B	212	ILE	2.1
1	D	92	ALA	2.1
2	E	38	LEU	2.1
1	B	279	ASN	2.1
2	G	89	ILE	2.1
1	D	171	GLY	2.1
2	E	98	ALA	2.1
2	F	88	GLU	2.1
1	B	283	HIS	2.1
2	H	42	TYR	2.1
2	G	75	LEU	2.1
2	F	42	TYR	2.0
1	C	131	GLY	2.0
1	D	187	LEU	2.0
1	D	169	PRO	2.0
1	B	216	LEU	2.0
2	E	41	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

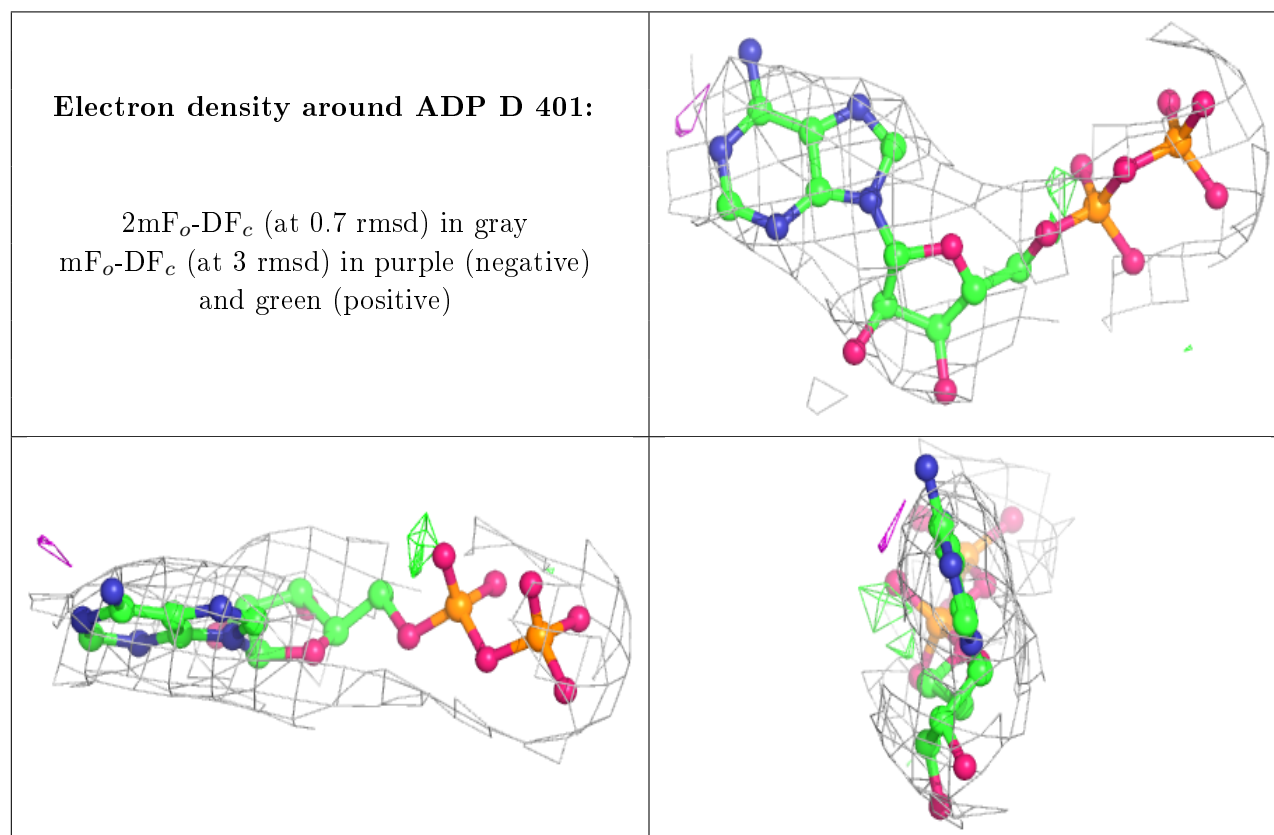
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

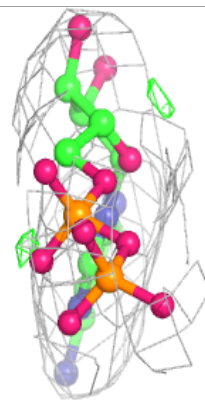
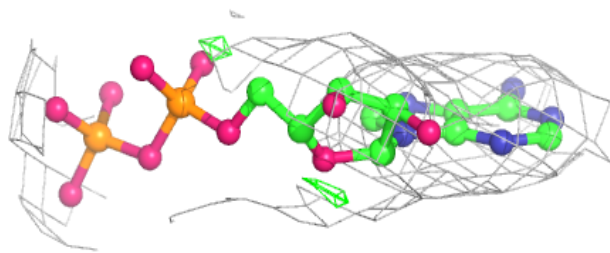
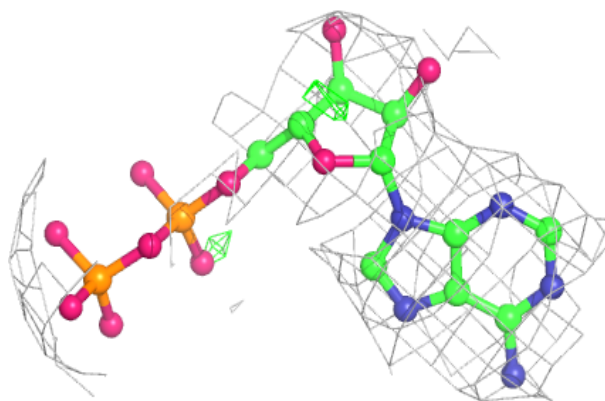
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	D	401	27/27	0.84	0.33	104,107,110,113	0
3	ADP	C	401	27/27	0.88	0.30	91,99,102,106	0
3	ADP	A	401	27/27	0.92	0.27	65,72,77,85	0
3	ADP	B	401	27/27	0.93	0.25	64,73,78,85	0

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.

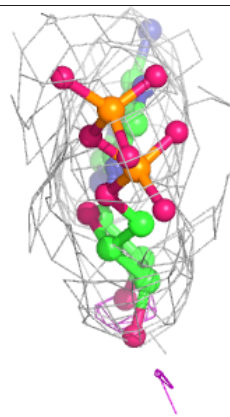
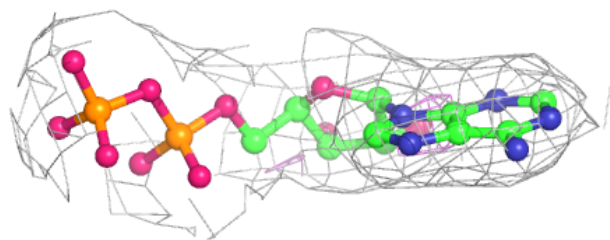
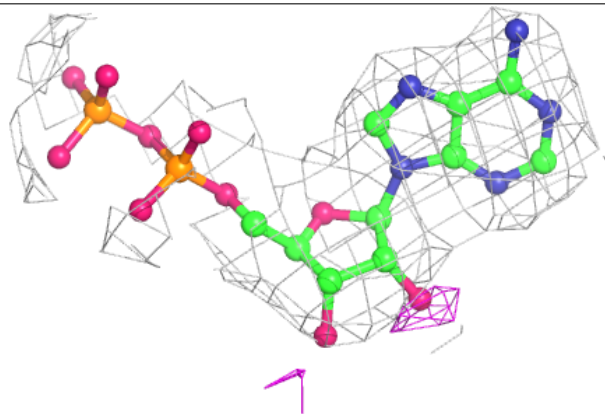


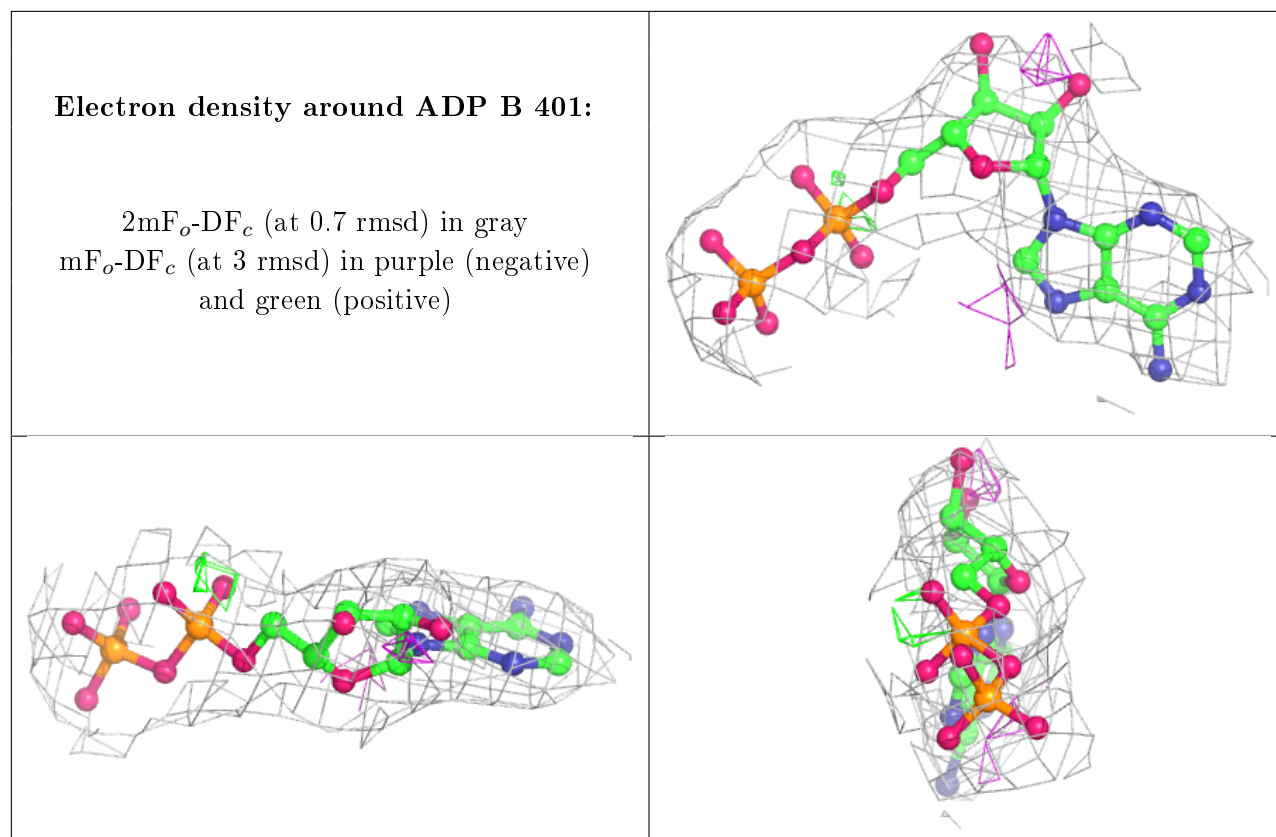
Electron density around ADP C 401:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.