



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:23 pm BST

PDB ID : 1Q95
Title : Aspartate Transcarbamylase (ATCase) of Escherichia coli: A New Crystalline R State Bound to PALA, or to Product Analogues Phosphate and Citrate
Authors : Huang, J.; Lipscomb, W.N.
Deposited on : 2003-08-22
Resolution : 2.46 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

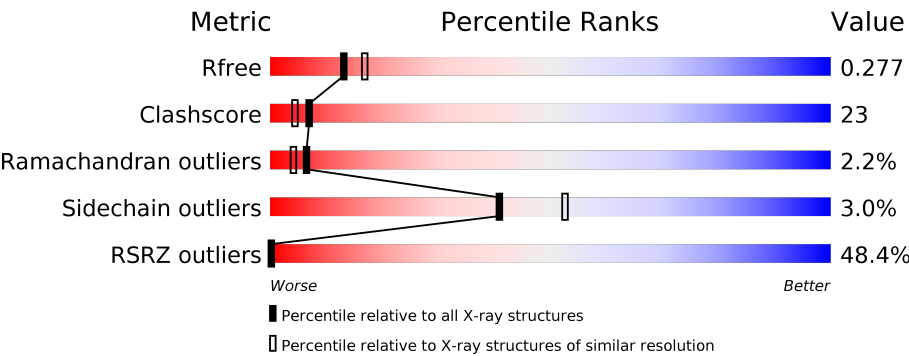
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	310	<div><div>39%</div><div><div></div><div></div><div></div><div></div></div><div>70%</div><div>27%</div><div>..</div></div>
1	B	310	<div><div>33%</div><div><div></div><div></div><div></div><div></div></div><div>71%</div><div>26%</div><div>.</div></div>
1	C	310	<div><div>44%</div><div><div></div><div></div><div></div><div></div></div><div>70%</div><div>27%</div><div>.</div></div>
1	D	310	<div><div>51%</div><div><div></div><div></div><div></div><div></div></div><div>66%</div><div>31%</div><div>.</div></div>
1	E	310	<div><div>56%</div><div><div></div><div></div><div></div><div></div></div><div>67%</div><div>30%</div><div>.</div></div>
1	F	310	<div><div>41%</div><div><div></div><div></div><div></div><div></div></div><div>69%</div><div>29%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	G	153	<div><div><div>47%</div><div>52%</div><div>45%</div><div></div></div></div>
2	H	153	<div><div><div>41%</div><div>54%</div><div>43%</div><div></div></div></div>
2	I	153	<div><div><div>80%</div><div>48%</div><div>48%</div><div></div></div></div>
2	J	153	<div><div><div>31%</div><div>55%</div><div>41%</div><div>5%</div></div></div>
2	K	153	<div><div><div>57%</div><div>52%</div><div>45%</div><div></div></div></div>
2	L	153	<div><div><div>88%</div><div>27%</div><div>63%</div><div>10%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22620 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.

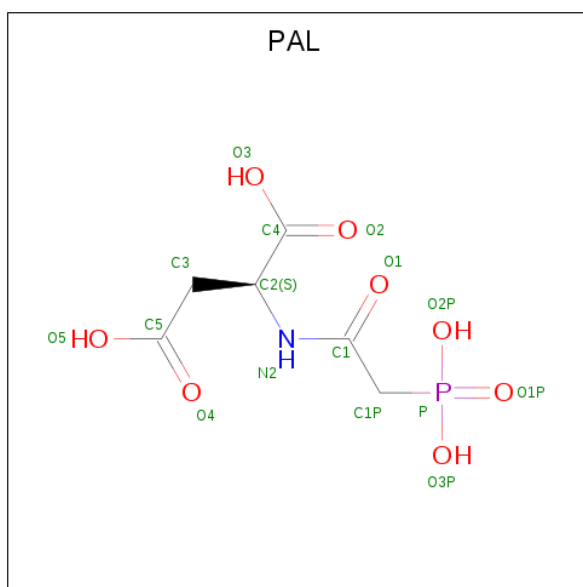
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	B	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	D	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	E	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	F	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	H	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	I	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	J	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	K	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	L	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (three-letter code: PAL) (formula: C₆H₁₀NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	D	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	E	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	F	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

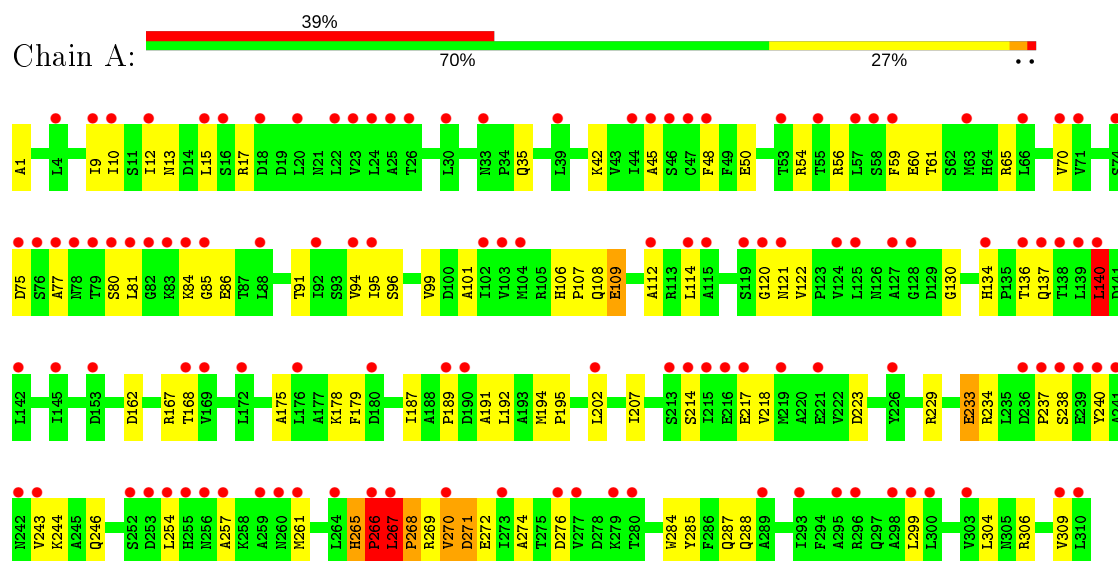
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total 122	O 122	0	0
5	B	120	Total 120	O 120	0	0
5	C	99	Total 99	O 99	0	0
5	D	70	Total 70	O 70	0	0
5	E	72	Total 72	O 72	0	0
5	F	128	Total 128	O 128	0	0
5	G	49	Total 49	O 49	0	0
5	H	45	Total 45	O 45	0	0
5	I	25	Total 25	O 25	0	0
5	J	41	Total 41	O 41	0	0
5	K	26	Total 26	O 26	0	0
5	L	25	Total 25	O 25	0	0

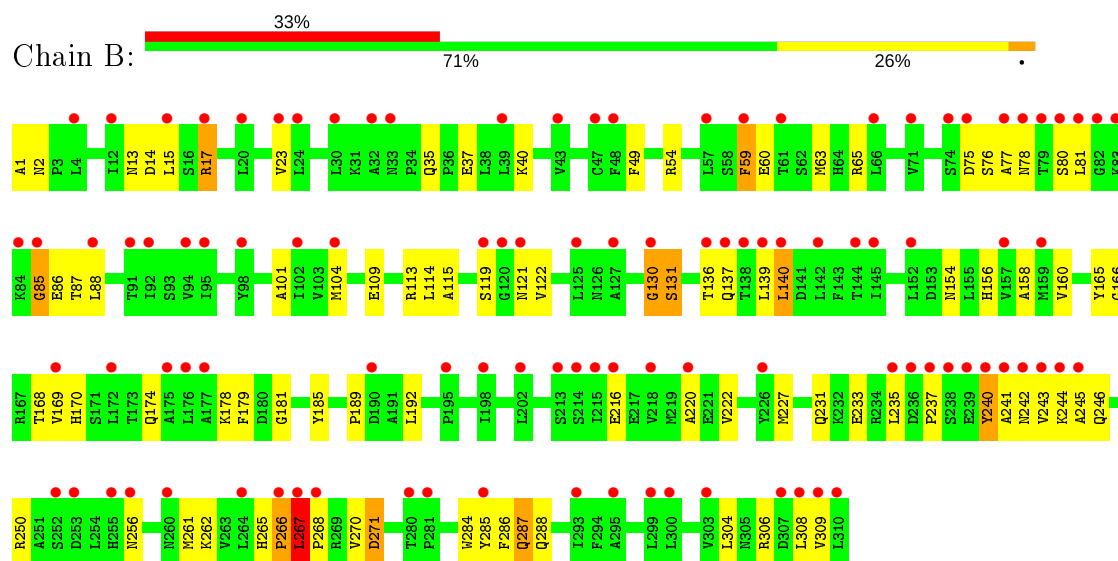
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

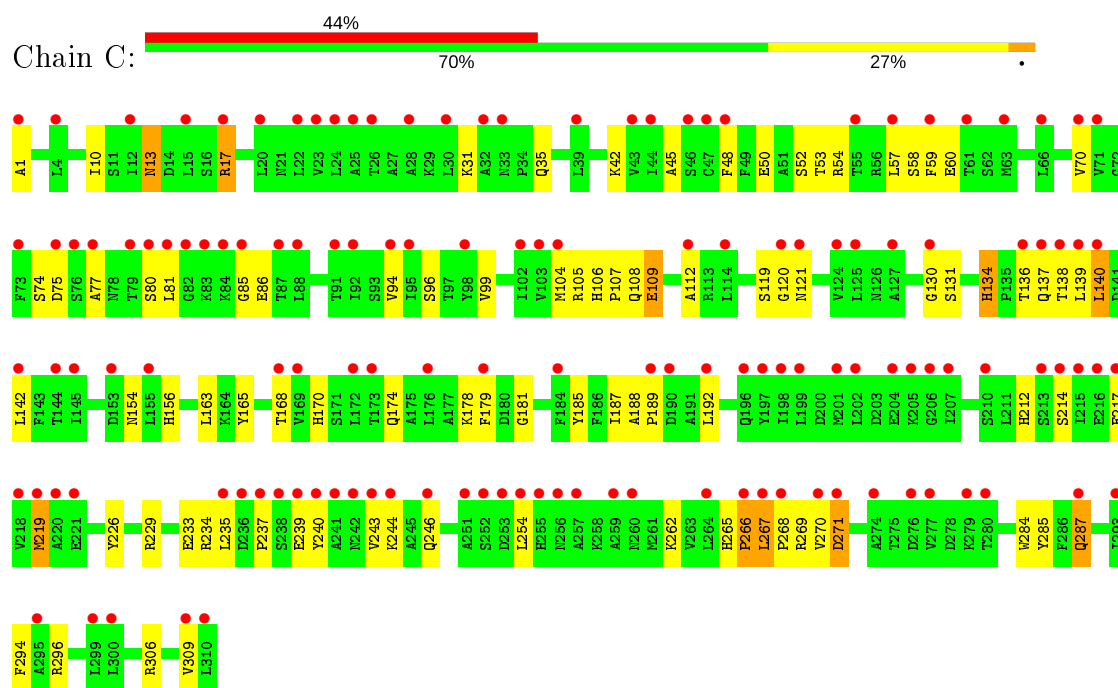
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



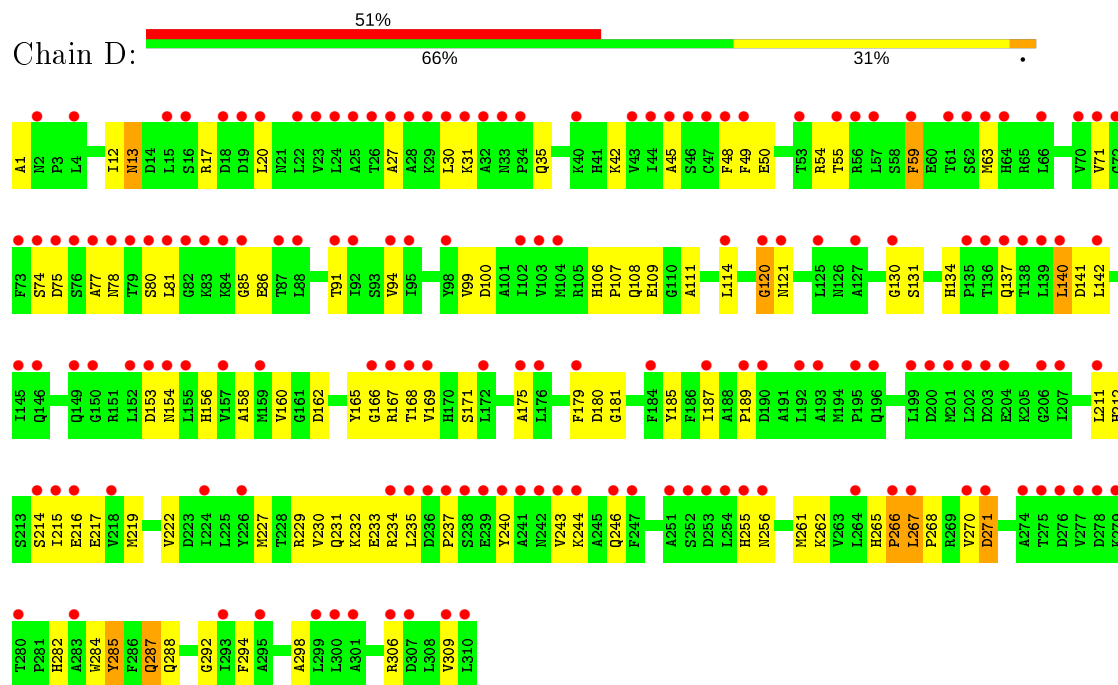
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



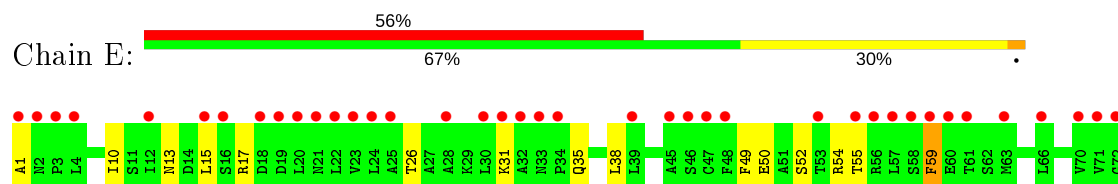
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

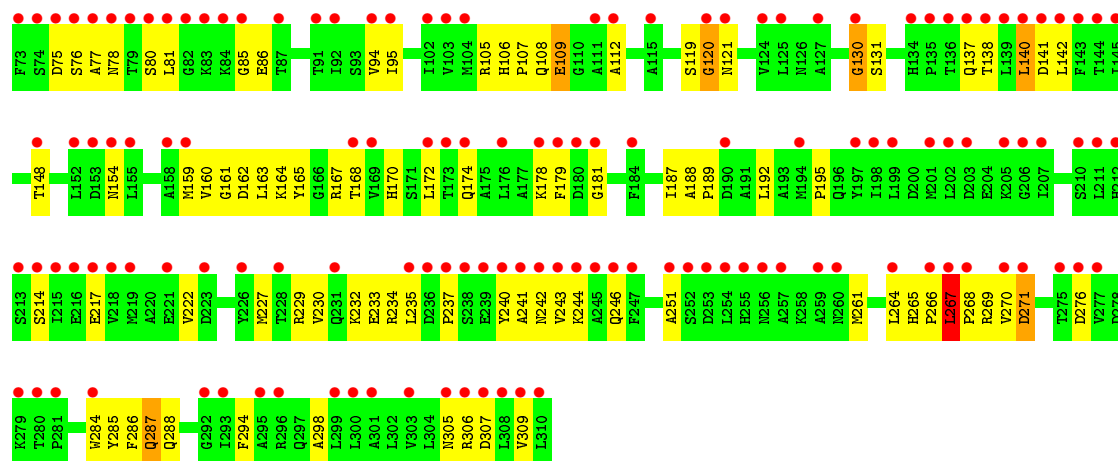


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

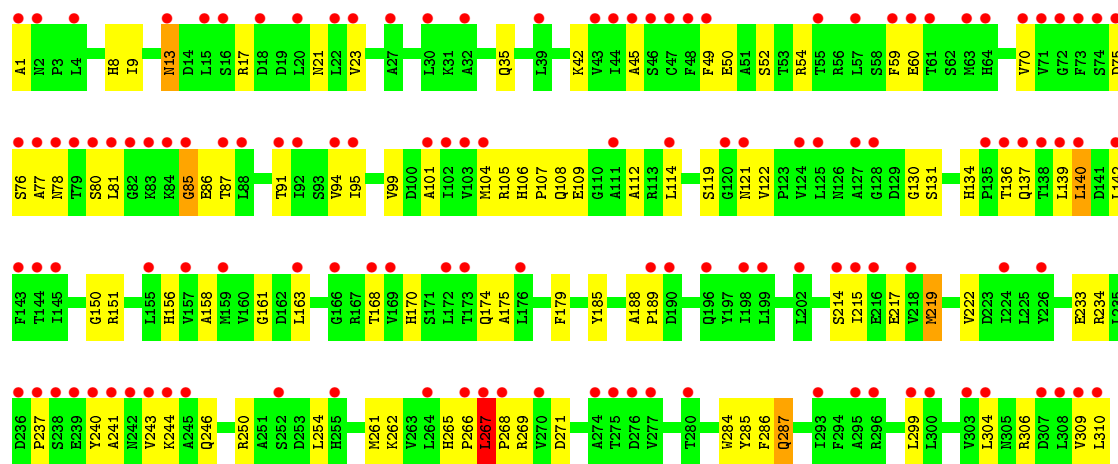
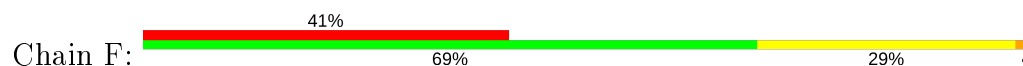


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

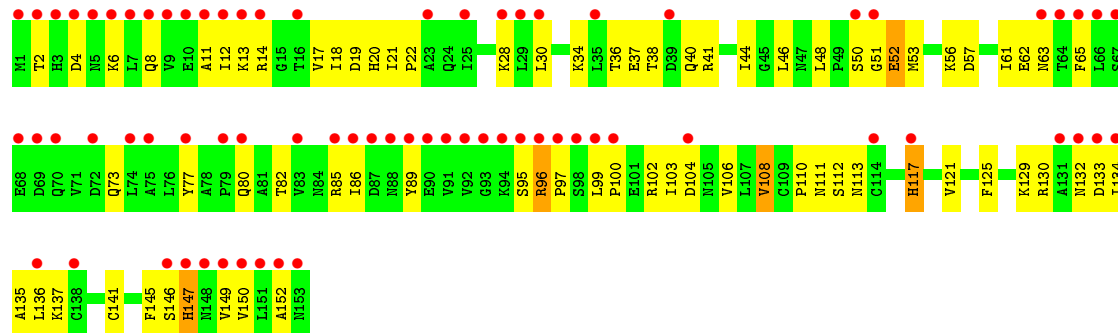




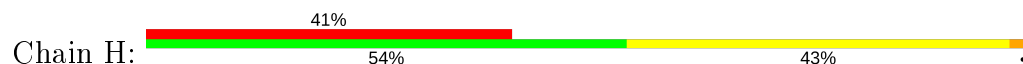
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

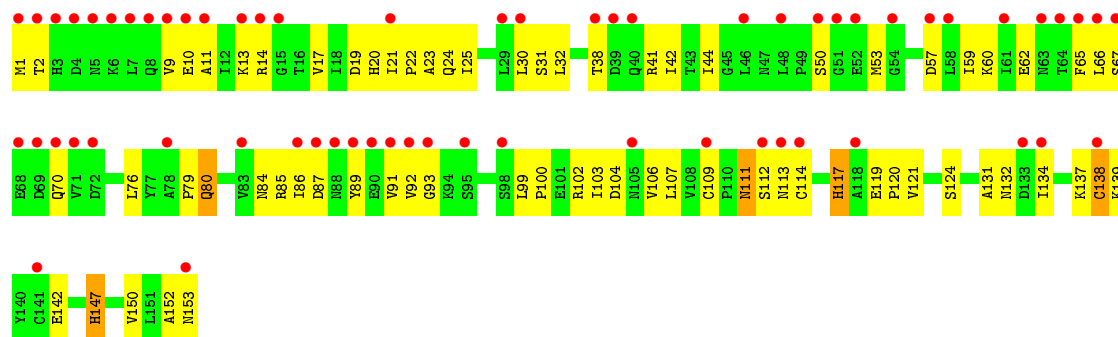


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

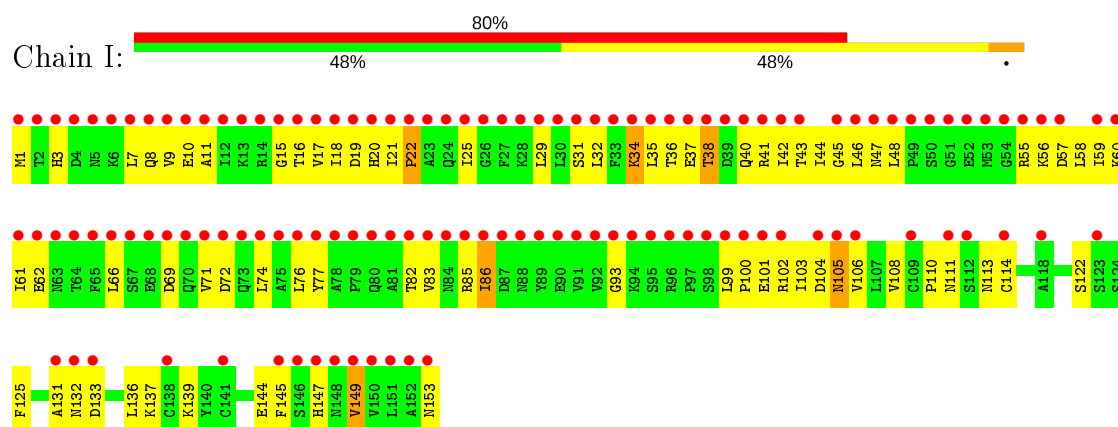


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

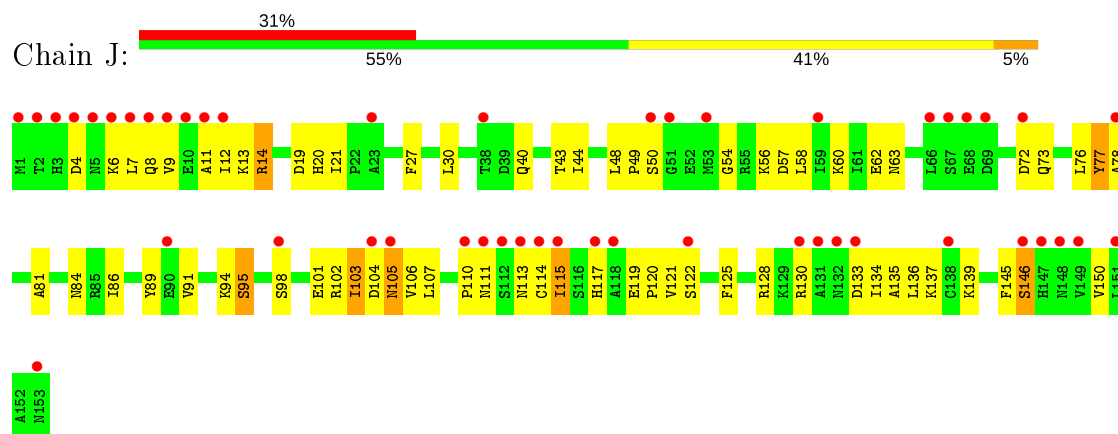




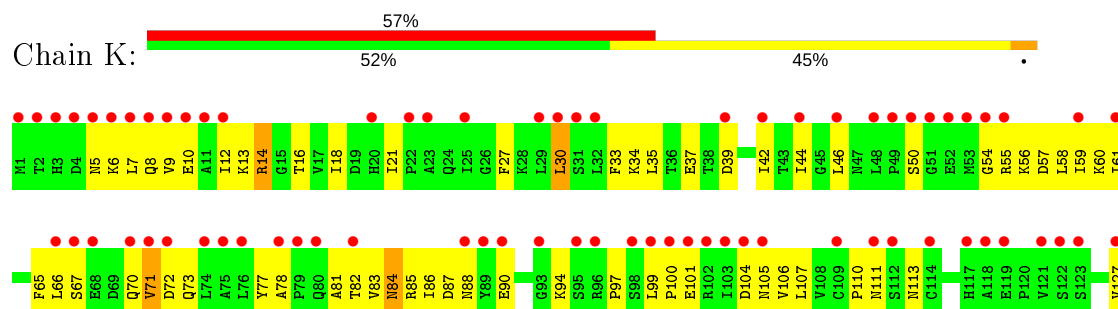
- Molecule 2: Aspartate carbamoyltransferase regulatory chain



- Molecule 2: Aspartate carbamoyltransferase regulatory chain

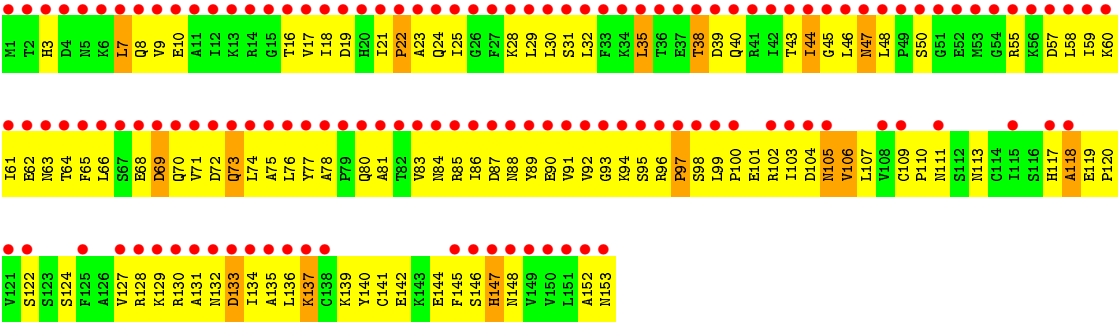
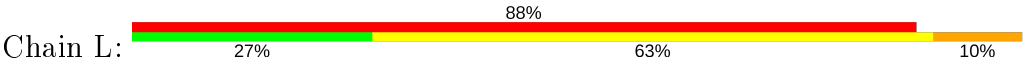


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





● Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.51Å 153.49Å 185.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.46 41.89 – 2.46	Depositor EDS
% Data completeness (in resolution range)	84.7 (8.00-2.46) 83.5 (41.89-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.270 0.239 , 0.277	Depositor DCC
R_{free} test set	5883 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22620	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: ZN, PAL

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	0.44	0/2461	0.76	8/3339 (0.2%)
1	B	0.40	0/2461	0.70	3/3339 (0.1%)
1	C	0.38	0/2461	0.68	3/3339 (0.1%)
1	D	0.37	0/2461	0.65	2/3339 (0.1%)
1	E	0.35	0/2461	0.66	4/3339 (0.1%)
1	F	0.38	0/2461	0.69	3/3339 (0.1%)
2	G	0.36	0/1219	0.65	0/1647
2	H	0.36	0/1219	0.62	0/1647
2	I	0.31	0/1219	0.57	0/1647
2	J	0.36	0/1219	0.63	1/1647 (0.1%)
2	K	0.35	0/1219	0.66	1/1647 (0.1%)
2	L	0.31	0/1219	0.64	0/1647
All	All	0.37	0/22080	0.67	25/29916 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	N-CA-C	9.15	135.71	111.00
1	F	267	LEU	N-CA-C	8.21	133.16	111.00
1	B	267	LEU	N-CA-C	8.15	133.00	111.00
1	D	267	LEU	N-CA-C	8.12	132.93	111.00
1	A	267	LEU	C-N-CA	-7.68	89.75	122.00
1	E	267	LEU	N-CA-C	7.62	131.58	111.00
1	D	266	PRO	N-CA-C	-7.35	92.99	112.10
1	C	266	PRO	N-CA-C	-7.30	93.12	112.10
1	A	267	LEU	C-N-CD	7.14	143.40	128.40
1	A	267	LEU	N-CA-C	6.57	128.74	111.00
1	B	266	PRO	N-CA-C	-6.42	95.42	112.10
1	A	266	PRO	N-CA-C	-6.29	95.75	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	CA-CB-CG	-6.20	101.05	115.30
1	A	267	LEU	CA-CB-CG	-6.13	101.19	115.30
2	J	105	ASN	N-CA-C	5.71	126.42	111.00
1	F	266	PRO	N-CA-C	-5.68	97.33	112.10
1	A	140	LEU	CA-CB-CG	5.64	128.28	115.30
1	F	140	LEU	CA-CB-CG	5.49	127.92	115.30
1	E	267	LEU	C-N-CD	5.38	139.70	128.40
1	A	268	PRO	N-CA-C	-5.34	98.22	112.10
1	B	267	LEU	CA-CB-CG	-5.33	103.03	115.30
1	E	266	PRO	N-CA-C	-5.17	98.64	112.10
1	A	140	LEU	CB-CG-CD1	-5.11	102.32	111.00
2	K	71	VAL	N-CA-C	-5.10	97.22	111.00
1	E	267	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	86	0
1	B	2415	0	2422	99	0
1	C	2415	0	2422	70	0
1	D	2415	0	2422	114	0
1	E	2415	0	2422	97	0
1	F	2415	0	2422	101	0
2	G	1201	0	1219	64	0
2	H	1201	0	1219	79	0
2	I	1201	0	1219	91	0
2	J	1201	0	1219	72	0
2	K	1201	0	1219	75	0
2	L	1201	0	1219	136	0
3	A	16	0	6	1	0
3	B	16	0	6	2	0
3	C	16	0	6	0	0
3	D	16	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	16	0	6	1	0
3	F	16	0	6	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	122	0	0	4	0
5	B	120	0	0	15	0
5	C	99	0	0	9	0
5	D	70	0	0	4	0
5	E	72	0	0	8	0
5	F	128	0	0	15	0
5	G	49	0	0	1	0
5	H	45	0	0	2	0
5	I	25	0	0	2	0
5	J	41	0	0	3	0
5	K	26	0	0	2	0
5	L	25	0	0	6	0
All	All	22620	0	21882	1005	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1005) 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:241:ALA:HB2	1:F:241:ALA:HB2	1.25	1.18
2:L:10:GLU:HB3	2:L:16:THR:HG21	1.22	1.18
2:J:84:ASN:HD21	2:J:94:LYS:HD3	1.18	1.09
1:B:114:LEU:HD21	2:H:119:GLU:HG2	1.36	1.07
2:K:30:LEU:HD21	2:K:44:ILE:HD13	1.31	1.06
1:B:81:LEU:HA	1:B:86:GLU:HB3	1.35	1.06
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.38	1.05
2:L:72:ASP:HB3	2:L:100:PRO:HG3	1.38	1.04
1:B:60:GLU:HA	1:B:63:MET:HE3	1.40	1.03
2:L:50:SER:HB2	2:L:55:ARG:HG2	1.39	1.02
1:B:60:GLU:HA	1:B:63:MET:CE	1.91	0.99
2:H:102:ARG:HH11	2:H:139:LYS:HE3	1.28	0.98
2:H:30:LEU:HD21	2:H:44:ILE:HD13	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG11	1:E:54:ARG:HG2	1.46	0.95
2:I:10:GLU:HG2	2:I:11:ALA:H	1.30	0.95
1:F:81:LEU:HA	1:F:86:GLU:HB3	1.48	0.94
2:I:21:ILE:HB	2:I:57:ASP:HB2	1.50	0.94
1:D:81:LEU:HA	1:D:86:GLU:HB3	1.51	0.93
2:L:32:LEU:HD22	2:L:152:ALA:HB3	1.48	0.92
2:L:101:GLU:HA	2:L:127:VAL:HG22	1.53	0.91
2:L:105:ASN:OD1	2:L:122:SER:HB3	1.71	0.91
1:C:267:LEU:HD21	1:C:285:TYR:HB2	1.51	0.91
1:B:54:ARG:HD3	1:B:267:LEU:HB2	1.51	0.90
2:I:15:GLY:HA3	2:I:62:GLU:HA	1.52	0.90
2:K:128:ARG:HH11	2:K:128:ARG:HB3	1.37	0.89
2:L:87:ASP:HB2	2:L:92:VAL:HG21	1.54	0.89
2:J:7:LEU:HD22	2:J:48:LEU:HB3	1.55	0.89
2:L:44:ILE:HG22	2:L:45:GLY:H	1.37	0.88
2:H:67:SER:H	2:H:70:GLN:HE21	1.20	0.88
1:C:81:LEU:HA	1:C:86:GLU:HB3	1.55	0.87
1:E:243:VAL:HG13	1:E:244:LYS:HD2	1.57	0.87
2:I:46:LEU:HD21	2:I:58:LEU:H	1.39	0.87
2:K:67:SER:HB3	2:K:85:ARG:NH2	1.88	0.87
1:E:81:LEU:HA	1:E:86:GLU:HB3	1.55	0.87
2:I:76:LEU:HD22	2:I:103:ILE:HD13	1.57	0.86
1:B:109:GLU:HG3	1:B:130:GLY:O	1.75	0.85
2:L:71:VAL:HG22	2:L:97:PRO:HG2	1.58	0.85
1:C:54:ARG:HD3	1:C:267:LEU:HB2	1.60	0.84
1:D:94:VAL:HG11	1:E:54:ARG:CG	2.06	0.84
2:L:21:ILE:HB	2:L:57:ASP:HB2	1.60	0.83
1:B:85:GLY:HA2	5:B:1119:HOH:O	1.79	0.83
1:E:237:PRO:HA	1:E:240:TYR:CE2	2.13	0.82
1:D:267:LEU:HD21	1:D:285:TYR:HB2	1.59	0.82
1:E:159:MET:HE2	1:E:172:LEU:HD23	1.59	0.82
1:C:42:LYS:HE3	5:C:1015:HOH:O	1.80	0.82
1:E:284:TRP:CD2	1:E:287:GLN:HG3	2.15	0.82
1:F:243:VAL:HG13	1:F:244:LYS:HD2	1.61	0.82
2:J:14:ARG:HA	2:J:86:ILE:O	1.79	0.82
1:B:241:ALA:CB	1:F:241:ALA:HB2	2.09	0.81
2:G:12:ILE:HG22	2:G:13:LYS:H	1.46	0.81
1:A:265:HIS:ND1	1:A:266:PRO:O	2.13	0.81
2:L:81:ALA:N	2:L:96:ARG:HH12	1.79	0.81
2:I:48:LEU:HD11	2:I:58:LEU:HG	1.63	0.80
1:F:310:LEU:HG	5:F:1046:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:HG22	2:H:60:LYS:HG2	1.65	0.79
1:D:237:PRO:HA	1:D:240:TYR:CE2	2.17	0.79
2:J:12:ILE:HD11	2:J:62:GLU:HA	1.63	0.79
1:B:284:TRP:CE2	1:B:287:GLN:HG3	2.19	0.78
2:H:13:LYS:HD3	2:H:89:TYR:CE1	2.18	0.78
2:J:12:ILE:HD11	2:J:62:GLU:CA	2.12	0.78
1:D:108:GLN:HG3	2:J:113:ASN:ND2	2.00	0.77
1:D:284:TRP:CE2	1:D:287:GLN:HG3	2.20	0.77
2:K:130:ARG:NE	2:K:135:ALA:HB2	1.99	0.77
2:L:72:ASP:CB	2:L:100:PRO:HG3	2.15	0.77
1:A:35:GLN:NE2	1:A:309:VAL:HG13	1.99	0.76
2:I:108:VAL:HG21	2:I:153:ASN:HD22	1.50	0.76
1:C:119:SER:C	5:C:1042:HOH:O	2.23	0.76
1:E:35:GLN:NE2	1:E:309:VAL:HG13	2.00	0.76
2:L:61:ILE:HB	2:L:63:ASN:HD21	1.48	0.76
2:H:102:ARG:NH1	2:H:139:LYS:HE3	2.02	0.75
2:I:20:HIS:HA	2:I:56:LYS:HG3	1.66	0.75
1:A:121:ASN:HB3	5:A:1070:HOH:O	1.86	0.75
1:A:54:ARG:HD3	1:A:267:LEU:HB2	1.68	0.75
2:H:99:LEU:HD12	2:H:100:PRO:HD2	1.69	0.75
2:J:84:ASN:ND2	2:J:94:LYS:HD3	1.97	0.75
1:C:189:PRO:HB3	1:C:246:GLN:NE2	2.01	0.75
1:C:284:TRP:CE2	1:C:287:GLN:HG3	2.22	0.75
1:A:243:VAL:HG13	1:A:244:LYS:HD2	1.69	0.74
2:I:19:ASP:HB2	2:I:82:THR:HG23	1.70	0.74
2:L:31:SER:O	2:L:32:LEU:HD23	1.87	0.74
2:I:99:LEU:HD12	2:I:100:PRO:HD2	1.68	0.74
1:B:243:VAL:HG13	1:B:244:LYS:HD2	1.67	0.74
1:A:257:ALA:HB1	1:A:261:MET:CE	2.17	0.74
2:I:111:ASN:HD22	2:I:114:CYS:HB2	1.52	0.74
5:B:1055:HOH:O	2:H:137:LYS:HE2	1.88	0.74
2:L:10:GLU:CB	2:L:16:THR:HG21	2.13	0.73
2:I:10:GLU:HA	2:I:44:ILE:HD12	1.70	0.73
1:A:265:HIS:C	1:A:266:PRO:O	2.23	0.73
1:D:31:LYS:HE2	1:D:294:PHE:CE2	2.24	0.73
2:K:34:LYS:HE2	2:K:37:GLU:OE1	1.88	0.73
1:B:267:LEU:HD12	1:C:94:VAL:CG1	2.19	0.73
1:F:35:GLN:NE2	1:F:309:VAL:HG13	2.04	0.73
1:D:54:ARG:HD3	1:D:267:LEU:HB2	1.70	0.73
1:D:42:LYS:HE3	5:D:1018:HOH:O	1.89	0.72
2:I:61:ILE:HG22	2:I:62:GLU:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:105:ASN:OD1	2:J:122:SER:HB3	1.88	0.72
1:F:287:GLN:HE21	1:F:287:GLN:H	1.37	0.72
2:L:25:ILE:HG23	2:L:28:LYS:HB2	1.70	0.72
1:B:75:ASP:HB3	5:B:1069:HOH:O	1.89	0.72
1:D:114:LEU:HG	2:J:115:ILE:HG21	1.72	0.72
1:C:121:ASN:HA	5:C:1033:HOH:O	1.88	0.71
1:F:170:HIS:O	1:F:174:GLN:HG3	1.89	0.71
2:I:35:LEU:HD22	2:I:40:GLN:HG3	1.72	0.71
2:J:58:LEU:HD21	2:J:60:LYS:HE3	1.71	0.71
2:J:7:LEU:HD23	2:J:49:PRO:HD2	1.71	0.71
2:L:69:ASP:HA	5:L:2023:HOH:O	1.90	0.71
2:L:8:GLN:HG3	5:L:2024:HOH:O	1.89	0.71
2:J:84:ASN:HD21	2:J:94:LYS:CD	2.01	0.71
2:J:13:LYS:HB2	2:J:89:TYR:CZ	2.25	0.71
1:B:119:SER:C	5:B:1051:HOH:O	2.27	0.71
1:B:265:HIS:CD2	1:B:266:PRO:O	2.44	0.71
1:D:35:GLN:NE2	1:D:309:VAL:HG13	2.06	0.71
2:K:70:GLN:HG3	2:K:73:GLN:HE21	1.55	0.71
2:J:9:VAL:HG13	2:J:43:THR:HG21	1.71	0.70
2:G:28:LYS:HD3	2:G:77:TYR:OH	1.92	0.70
2:H:109:CYS:HB2	2:H:138:CYS:SG	2.30	0.70
1:B:54:ARG:HD3	1:B:267:LEU:CB	2.20	0.70
2:H:111:ASN:ND2	2:H:113:ASN:H	1.89	0.70
2:I:46:LEU:CD2	2:I:58:LEU:H	2.05	0.70
1:B:54:ARG:CD	1:B:267:LEU:HB2	2.19	0.70
1:D:243:VAL:HG13	1:D:244:LYS:HD2	1.73	0.70
1:F:287:GLN:NE2	1:F:287:GLN:H	1.90	0.70
2:L:43:THR:HB	2:L:60:LYS:O	1.92	0.70
2:G:41:ARG:HD3	5:J:2024:HOH:O	1.90	0.70
2:K:99:LEU:HD22	2:K:127:VAL:HG11	1.74	0.70
1:C:237:PRO:HA	1:C:240:TYR:CE2	2.26	0.70
1:F:78:ASN:HB2	5:F:1047:HOH:O	1.92	0.70
1:C:214:SER:OG	1:C:217:GLU:HG3	1.92	0.69
1:A:130:GLY:O	1:A:167:ARG:HD3	1.91	0.69
1:C:284:TRP:CD2	1:C:287:GLN:HG3	2.27	0.69
1:C:189:PRO:HB3	1:C:246:GLN:HE22	1.55	0.69
2:I:56:LYS:HE2	2:I:58:LEU:HD21	1.73	0.69
2:L:50:SER:HA	2:L:55:ARG:HA	1.73	0.69
1:B:60:GLU:HA	1:B:63:MET:HE2	1.75	0.69
1:C:108:GLN:HG3	5:I:2007:HOH:O	1.91	0.69
2:J:30:LEU:HD11	2:J:44:ILE:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:CD2	2:H:119:GLU:HG2	2.19	0.68
2:I:10:GLU:HG2	2:I:11:ALA:N	2.07	0.68
1:F:76:SER:HB2	5:F:1029:HOH:O	1.92	0.68
2:L:73:GLN:NE2	2:L:106:VAL:HG21	2.08	0.68
2:L:19:ASP:O	2:L:21:ILE:HG13	1.93	0.68
2:K:50:SER:HB2	2:K:56:LYS:HG2	1.75	0.68
1:A:214:SER:OG	1:A:217:GLU:HG3	1.94	0.68
1:F:243:VAL:HG13	1:F:244:LYS:CD	2.24	0.68
1:F:23:VAL:HG11	1:F:139:LEU:HD13	1.76	0.67
1:E:159:MET:CE	1:E:172:LEU:HD23	2.22	0.67
2:L:61:ILE:HB	2:L:63:ASN:ND2	2.08	0.67
1:A:189:PRO:HB3	1:A:246:GLN:NE2	2.10	0.67
1:B:220:ALA:HB2	1:B:256:ASN:ND2	2.09	0.67
1:E:243:VAL:HG13	1:E:244:LYS:CD	2.23	0.67
2:H:41:ARG:HD3	2:H:62:GLU:OE2	1.95	0.67
1:D:111:ALA:HB2	2:J:115:ILE:HD11	1.77	0.67
1:F:189:PRO:HB3	1:F:246:GLN:NE2	2.10	0.67
1:F:49:PHE:HE2	1:F:81:LEU:HD13	1.59	0.67
2:L:128:ARG:HB3	2:L:128:ARG:NH1	2.10	0.67
1:B:192:LEU:HD11	1:B:242:ASN:HB3	1.77	0.66
1:F:284:TRP:CE2	1:F:287:GLN:HG3	2.31	0.66
2:I:85:ARG:HG2	5:I:2020:HOH:O	1.95	0.66
2:K:84:ASN:N	2:K:84:ASN:HD22	1.93	0.66
1:E:140:LEU:HD21	1:E:288:GLN:HG2	1.76	0.66
1:F:119:SER:C	5:F:1054:HOH:O	2.33	0.66
2:L:44:ILE:HG22	2:L:45:GLY:N	2.09	0.66
2:L:75:ALA:HB1	2:L:99:LEU:HD23	1.77	0.66
1:C:287:GLN:H	1:C:287:GLN:NE2	1.94	0.66
1:B:23:VAL:HG11	1:B:139:LEU:HD13	1.77	0.66
1:B:241:ALA:HB2	1:F:241:ALA:CB	2.15	0.66
2:J:9:VAL:HG13	2:J:43:THR:CG2	2.25	0.66
2:L:85:ARG:HH21	2:L:93:GLY:HA3	1.60	0.66
1:D:81:LEU:HD12	1:D:91:THR:OG1	1.96	0.66
2:K:70:GLN:CG	2:K:73:GLN:HE21	2.08	0.66
2:G:36:THR:HG21	2:J:27:PHE:CD2	2.31	0.65
2:L:72:ASP:OD1	2:L:97:PRO:HB3	1.95	0.65
1:E:15:LEU:O	1:E:178:LYS:HE3	1.96	0.65
1:D:49:PHE:HE2	1:D:81:LEU:HD13	1.61	0.65
1:B:114:LEU:CD1	2:H:121:VAL:HG11	2.25	0.65
2:I:10:GLU:CG	2:I:11:ALA:H	2.06	0.65
2:I:9:VAL:HG13	2:I:47:ASN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:GLN:HE22	1:F:309:VAL:HG13	1.60	0.65
2:H:79:PRO:HD2	2:H:80:GLN:NE2	2.12	0.65
2:L:17:VAL:HG21	5:L:2007:HOH:O	1.96	0.65
1:A:81:LEU:HD11	5:A:1017:HOH:O	1.96	0.65
1:B:75:ASP:OD2	1:B:77:ALA:HB3	1.96	0.65
2:L:32:LEU:HD22	2:L:152:ALA:CB	2.26	0.65
1:B:166:GLY:O	1:B:169:VAL:HG22	1.96	0.64
2:K:33:PHE:HB2	2:K:35:LEU:HG	1.77	0.64
2:H:30:LEU:HD13	2:H:59:ILE:HD13	1.78	0.64
2:L:72:ASP:HB3	2:L:100:PRO:CG	2.23	0.64
1:D:108:GLN:HB3	2:J:115:ILE:HD12	1.79	0.64
1:F:237:PRO:HA	1:F:240:TYR:CE2	2.32	0.64
2:H:152:ALA:O	2:H:153:ASN:HB2	1.96	0.64
2:H:30:LEU:HD21	2:H:44:ILE:CD1	2.25	0.64
1:D:45:ALA:HB2	1:D:99:VAL:HG11	1.79	0.64
1:B:216:GLU:HG3	5:B:1046:HOH:O	1.97	0.64
1:D:284:TRP:CD2	1:D:287:GLN:HG3	2.32	0.64
1:E:154:ASN:HA	1:E:181:GLY:O	1.98	0.64
2:I:131:ALA:O	2:I:132:ASN:HB2	1.97	0.64
1:B:109:GLU:CG	1:B:130:GLY:O	2.44	0.64
2:K:16:THR:OG1	2:K:65:PHE:HA	1.96	0.64
1:C:265:HIS:CD2	1:C:266:PRO:O	2.50	0.64
2:L:104:ASP:OD1	2:L:124:SER:HB2	1.97	0.64
1:C:240:TYR:O	1:C:243:VAL:HG12	1.97	0.64
1:C:229:ARG:HD3	1:C:268:PRO:O	1.98	0.64
1:E:94:VAL:CG1	1:F:267:LEU:HD12	2.27	0.64
1:F:189:PRO:HB3	1:F:246:GLN:HE22	1.62	0.64
2:J:133:ASP:OD1	2:J:146:SER:HB2	1.98	0.64
2:K:70:GLN:OE1	2:K:72:ASP:HB2	1.98	0.63
2:K:67:SER:HB3	2:K:85:ARG:HH22	1.63	0.63
2:I:58:LEU:O	2:I:60:LYS:HG3	1.98	0.63
1:A:35:GLN:HE22	1:A:309:VAL:HG13	1.62	0.63
1:A:1:ALA:HA	1:A:306:ARG:HG2	1.80	0.63
1:B:237:PRO:HA	1:B:240:TYR:CE2	2.33	0.63
1:E:284:TRP:CE2	1:E:287:GLN:HG3	2.33	0.63
2:K:83:VAL:C	2:K:84:ASN:HD22	2.02	0.63
1:D:229:ARG:HD3	1:D:268:PRO:O	1.99	0.62
2:I:56:LYS:HE2	2:I:58:LEU:CD2	2.28	0.62
2:K:110:PRO:HB2	2:K:145:PHE:CE2	2.33	0.62
1:A:237:PRO:HA	1:A:240:TYR:CE2	2.34	0.62
1:F:81:LEU:HD22	5:F:1029:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:76:LEU:HD23	2:J:134:ILE:HD12	1.81	0.62
1:D:261:MET:HG2	1:D:262:LYS:N	2.14	0.62
1:E:137:GLN:HG2	1:E:168:THR:HG22	1.81	0.62
1:F:284:TRP:CD2	1:F:287:GLN:HG3	2.34	0.62
1:F:42:LYS:HE3	5:F:1086:HOH:O	1.99	0.62
2:G:30:LEU:HD11	2:G:44:ILE:HD13	1.82	0.62
1:E:49:PHE:HE2	1:E:81:LEU:HD13	1.63	0.62
1:F:85:GLY:HA2	5:F:1062:HOH:O	2.00	0.62
2:L:71:VAL:HG23	2:L:83:VAL:HG21	1.82	0.62
1:F:158:ALA:HB2	1:F:222:VAL:HG11	1.81	0.62
2:I:61:ILE:HG22	2:I:62:GLU:N	2.14	0.62
1:D:140:LEU:HD23	1:D:141:ASP:N	2.14	0.62
1:F:137:GLN:HG2	1:F:168:THR:HG22	1.81	0.61
1:A:114:LEU:HD22	2:G:121:VAL:HG11	1.81	0.61
2:H:10:GLU:HG2	2:H:11:ALA:N	2.14	0.61
2:H:76:LEU:HD23	2:H:99:LEU:HD11	1.82	0.61
2:I:56:LYS:HG2	2:I:57:ASP:N	2.15	0.61
1:F:267:LEU:HD11	1:F:286:PHE:CD1	2.34	0.61
1:F:75:ASP:OD2	1:F:77:ALA:HB3	2.00	0.61
2:H:14:ARG:HA	2:H:86:ILE:O	2.01	0.61
2:J:130:ARG:HD2	2:J:135:ALA:HB2	1.80	0.61
1:E:189:PRO:HB3	1:E:246:GLN:NE2	2.16	0.61
1:F:17:ARG:HD2	1:F:179:PHE:CE1	2.35	0.61
2:H:107:LEU:HB3	2:H:150:VAL:HG12	1.82	0.61
2:I:101:GLU:HG3	2:I:102:ARG:N	2.16	0.61
2:I:111:ASN:ND2	2:I:114:CYS:HB2	2.16	0.61
2:K:50:SER:HB3	2:K:54:GLY:H	1.64	0.61
1:A:257:ALA:HB1	1:A:261:MET:HE2	1.82	0.61
2:L:128:ARG:NH2	5:L:2008:HOH:O	2.34	0.61
1:D:75:ASP:OD2	1:D:77:ALA:HB3	2.01	0.61
1:E:267:LEU:O	1:E:269:ARG:N	2.34	0.61
2:H:1:MET:CE	2:H:91:VAL:HG12	2.31	0.61
2:I:76:LEU:HD22	2:I:103:ILE:CD1	2.30	0.61
2:I:48:LEU:HD21	2:I:58:LEU:HD11	1.82	0.60
2:G:129:LYS:HD3	5:G:2030:HOH:O	2.00	0.60
2:I:104:ASP:O	2:I:106:VAL:HG23	2.01	0.60
2:I:15:GLY:O	2:I:86:ILE:HA	2.01	0.60
1:A:17:ARG:HD2	1:A:179:PHE:CD1	2.36	0.60
2:L:99:LEU:CD1	2:L:129:LYS:HB2	2.31	0.60
1:D:287:GLN:NE2	5:D:1010:HOH:O	2.34	0.60
1:E:167:ARG:HG2	5:E:1026:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:130:ARG:CZ	2:L:135:ALA:HB2	2.32	0.60
1:F:267:LEU:O	1:F:269:ARG:N	2.34	0.60
1:F:309:VAL:HG23	5:F:1026:HOH:O	2.02	0.60
2:I:137:LYS:HB2	2:I:144:GLU:HG3	1.84	0.60
2:I:56:LYS:HG2	2:I:57:ASP:H	1.67	0.59
1:C:75:ASP:OD2	1:C:77:ALA:HB3	2.01	0.59
2:L:65:PHE:H	2:L:65:PHE:HD1	1.49	0.59
1:D:189:PRO:HB3	1:D:246:GLN:NE2	2.17	0.59
1:A:202:LEU:HD22	1:A:207:ILE:HG21	1.83	0.59
2:G:130:ARG:CZ	2:G:135:ALA:HB2	2.32	0.59
2:H:91:VAL:HG13	2:H:91:VAL:O	2.03	0.59
1:B:243:VAL:HG13	1:B:244:LYS:CD	2.32	0.59
2:G:19:ASP:OD2	2:G:20:HIS:N	2.35	0.59
1:D:106:HIS:ND1	1:D:107:PRO:HD2	2.17	0.59
2:H:92:VAL:HG23	2:H:93:GLY:N	2.18	0.59
2:I:19:ASP:OD1	2:I:58:LEU:HD22	2.02	0.59
1:C:1:ALA:HA	1:C:306:ARG:HG2	1.84	0.59
2:G:110:PRO:HD2	2:G:145:PHE:CE2	2.37	0.59
2:H:80:GLN:NE2	2:H:80:GLN:H	2.00	0.59
1:D:243:VAL:HG13	1:D:244:LYS:CD	2.33	0.58
2:I:102:ARG:NH2	2:I:139:LYS:HD3	2.18	0.58
1:A:254:LEU:HD22	1:A:261:MET:CE	2.33	0.58
2:J:111:ASN:HD22	2:J:114:CYS:HB2	1.67	0.58
2:J:115:ILE:HG23	2:J:119:GLU:HG3	1.85	0.58
2:J:12:ILE:HD11	2:J:62:GLU:CB	2.32	0.58
2:K:128:ARG:NH1	2:K:128:ARG:HB3	2.15	0.58
2:L:58:LEU:O	2:L:59:ILE:HG13	2.03	0.58
1:B:220:ALA:HB2	1:B:256:ASN:HD22	1.67	0.58
1:D:140:LEU:C	1:D:140:LEU:HD23	2.24	0.58
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.84	0.58
5:B:1053:HOH:O	2:H:139:LYS:CB	2.51	0.58
2:I:31:SER:O	2:I:34:LYS:HG3	2.03	0.58
1:D:261:MET:CE	1:D:282:HIS:HB3	2.33	0.58
2:H:111:ASN:HD22	2:H:112:SER:N	2.02	0.58
1:E:170:HIS:O	1:E:174:GLN:HG3	2.03	0.58
1:D:108:GLN:CB	2:J:115:ILE:HD12	2.33	0.58
2:K:67:SER:HB3	2:K:85:ARG:HH21	1.64	0.58
1:A:194:MET:SD	1:A:195:PRO:HD2	2.43	0.58
1:F:104:MET:HE1	1:F:112:ALA:HA	1.85	0.58
2:K:55:ARG:HG2	2:K:55:ARG:HH11	1.68	0.58
2:J:110:PRO:HD2	2:J:145:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:30:LEU:HD21	2:K:44:ILE:CD1	2.21	0.57
1:E:148:THR:HB	5:E:1050:HOH:O	2.03	0.57
1:F:121:ASN:HB3	5:F:1115:HOH:O	2.04	0.57
1:D:114:LEU:CD2	2:J:121:VAL:HG11	2.33	0.57
1:C:154:ASN:HA	1:C:181:GLY:O	2.04	0.57
2:H:67:SER:H	2:H:70:GLN:NE2	1.98	0.57
2:H:84:ASN:HB3	2:H:91:VAL:HG23	1.85	0.57
2:L:65:PHE:HD2	2:L:85:ARG:HD2	1.70	0.57
1:B:35:GLN:NE2	1:B:309:VAL:HG13	2.19	0.57
1:D:214:SER:OG	1:D:217:GLU:HG3	2.04	0.57
1:E:50:GLU:CD	1:E:234:ARG:HH22	2.07	0.57
1:E:80:SER:HB2	1:F:54:ARG:NH2	2.19	0.57
1:F:49:PHE:CE2	1:F:81:LEU:HD13	2.40	0.57
1:A:134:HIS:CE1	1:A:137:GLN:HB2	2.39	0.57
1:A:271:ASP:CG	1:A:271:ASP:O	2.40	0.57
1:E:240:TYR:O	1:E:243:VAL:HG12	2.05	0.57
2:G:13:LYS:HG3	2:G:89:TYR:CE1	2.39	0.57
2:H:119:GLU:HG3	2:H:120:PRO:HD2	1.87	0.57
2:I:43:THR:O	2:L:47:ASN:HB2	2.04	0.57
1:B:14:ASP:OD2	1:B:113:ARG:NH2	2.35	0.57
1:D:229:ARG:HE	1:D:268:PRO:HB2	1.68	0.57
2:I:22:PRO:HB2	2:I:25:ILE:HG13	1.87	0.57
2:L:87:ASP:CB	2:L:92:VAL:HG21	2.31	0.57
1:C:239:GLU:HA	5:C:1036:HOH:O	2.03	0.57
1:D:17:ARG:HD2	1:D:179:PHE:CD1	2.39	0.57
1:A:106:HIS:HE1	1:A:108:GLN:OE1	1.88	0.57
1:F:240:TYR:O	1:F:243:VAL:HG12	2.05	0.57
2:I:149:VAL:HG12	2:I:149:VAL:O	2.05	0.57
1:B:114:LEU:HD11	2:H:121:VAL:HG11	1.86	0.56
2:K:128:ARG:HH11	2:K:128:ARG:CB	2.14	0.56
1:A:257:ALA:CB	1:A:261:MET:CE	2.82	0.56
2:K:100:PRO:O	2:K:127:VAL:HB	2.06	0.56
2:L:46:LEU:HD22	2:L:57:ASP:HB3	1.86	0.56
1:B:137:GLN:HG2	1:B:168:THR:HG22	1.87	0.56
2:I:41:ARG:C	2:I:42:ILE:HD12	2.25	0.56
1:D:20:LEU:HD13	1:D:142:LEU:HD11	1.88	0.56
1:E:267:LEU:HD11	1:E:286:PHE:CD1	2.41	0.56
2:I:59:ILE:HD12	2:I:59:ILE:H	1.70	0.56
2:K:128:ARG:HH12	2:K:135:ALA:HB3	1.70	0.56
1:B:122:VAL:HB	5:B:1051:HOH:O	2.05	0.56
1:D:158:ALA:HB2	1:D:222:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:GLU:CD	1:F:234:ARG:HH22	2.09	0.56
2:L:8:GLN:O	2:L:10:GLU:HG3	2.05	0.56
1:E:140:LEU:C	1:E:140:LEU:HD23	2.26	0.55
2:G:40:GLN:HE22	2:G:63:ASN:HB2	1.70	0.55
2:K:71:VAL:HG12	2:K:97:PRO:HB3	1.88	0.55
2:G:112:SER:HA	2:G:117:HIS:HE2	1.72	0.55
2:K:104:ASP:O	2:K:105:ASN:HB2	2.05	0.55
2:K:130:ARG:CZ	2:K:135:ALA:HB2	2.36	0.55
1:B:17:ARG:HD2	1:B:179:PHE:CE1	2.41	0.55
1:E:192:LEU:HD11	1:E:242:ASN:HB3	1.89	0.55
2:K:18:ILE:HD11	2:K:66:LEU:HD11	1.88	0.55
1:A:80:SER:HB2	1:C:54:ARG:NH2	2.21	0.55
1:D:137:GLN:HG2	1:D:168:THR:HG22	1.88	0.55
1:B:81:LEU:HG	1:B:86:GLU:O	2.06	0.55
2:L:73:GLN:HE22	2:L:106:VAL:HG21	1.71	0.55
2:I:21:ILE:HG22	2:I:25:ILE:HB	1.88	0.55
1:C:81:LEU:HG	1:C:86:GLU:O	2.07	0.55
1:D:265:HIS:CD2	1:D:266:PRO:O	2.60	0.55
1:E:49:PHE:CE2	1:E:81:LEU:HD13	2.42	0.55
2:H:65:PHE:CE1	2:H:85:ARG:HG3	2.42	0.55
2:L:22:PRO:HD2	2:L:80:GLN:O	2.07	0.55
1:D:106:HIS:CG	1:D:107:PRO:HD2	2.42	0.55
1:D:81:LEU:HG	1:D:86:GLU:O	2.06	0.55
1:D:94:VAL:CG1	1:E:54:ARG:HG2	2.31	0.55
2:G:112:SER:HA	2:G:117:HIS:NE2	2.20	0.55
1:F:87:THR:HB	2:L:119:GLU:OE1	2.07	0.55
2:L:7:LEU:O	2:L:8:GLN:HB2	2.06	0.55
1:A:114:LEU:HD13	1:A:114:LEU:C	2.27	0.55
1:C:270:VAL:O	1:C:271:ASP:CG	2.46	0.55
1:B:170:HIS:O	1:B:174:GLN:HG3	2.07	0.54
1:D:154:ASN:HA	1:D:181:GLY:O	2.08	0.54
2:G:40:GLN:NE2	2:G:63:ASN:HB2	2.21	0.54
2:G:65:PHE:CD2	2:G:85:ARG:HD3	2.41	0.54
2:H:9:VAL:HG11	2:H:60:LYS:NZ	2.23	0.54
1:B:101:ALA:HB2	1:B:304:LEU:HD21	1.89	0.54
1:C:243:VAL:HG13	1:C:244:LYS:HD2	1.87	0.54
2:L:111:ASN:HB2	2:L:145:PHE:HZ	1.73	0.54
1:A:270:VAL:O	1:A:271:ASP:OD1	2.25	0.54
1:D:109:GLU:OE1	1:D:130:GLY:O	2.26	0.54
2:I:35:LEU:HD13	2:I:40:GLN:HG3	1.89	0.54
2:I:44:ILE:HA	2:L:46:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD21	1:B:288:GLN:HG2	1.88	0.54
1:B:240:TYR:HE1	5:B:1071:HOH:O	1.90	0.54
1:D:49:PHE:CE2	1:D:81:LEU:HD13	2.42	0.54
2:H:109:CYS:SG	2:H:111:ASN:HB3	2.47	0.54
2:G:134:ILE:N	2:G:134:ILE:HD12	2.23	0.54
1:D:54:ARG:CD	1:D:267:LEU:HB2	2.37	0.54
1:B:88:LEU:N	2:H:119:GLU:OE1	2.39	0.54
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.72	0.54
1:D:267:LEU:HD12	1:F:94:VAL:CG1	2.37	0.54
1:B:114:LEU:HD12	2:H:121:VAL:HG11	1.90	0.54
1:A:108:GLN:HG3	2:G:113:ASN:OD1	2.07	0.54
2:G:19:ASP:OD2	2:G:56:LYS:HE3	2.06	0.54
1:F:101:ALA:HB2	1:F:304:LEU:HD21	1.90	0.54
1:F:8:HIS:O	1:F:9:ILE:HD13	2.07	0.54
2:L:75:ALA:HB1	2:L:99:LEU:CD2	2.38	0.54
1:A:257:ALA:CB	1:A:261:MET:HE1	2.38	0.53
2:G:61:ILE:N	2:G:61:ILE:HD12	2.22	0.53
2:H:131:ALA:HA	5:H:2013:HOH:O	2.08	0.53
2:J:30:LEU:CD1	2:J:44:ILE:HD13	2.37	0.53
1:B:267:LEU:HD11	1:B:286:PHE:CD1	2.43	0.53
1:E:75:ASP:OD2	1:E:77:ALA:HB3	2.08	0.53
2:H:67:SER:OG	2:H:70:GLN:HG3	2.08	0.53
2:J:78:ALA:HB1	2:J:81:ALA:HB2	1.90	0.53
2:K:107:LEU:HD21	2:K:151:LEU:HD23	1.89	0.53
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.43	0.53
1:A:243:VAL:HG13	1:A:244:LYS:CD	2.38	0.53
2:G:14:ARG:HA	2:G:86:ILE:HG22	1.90	0.53
1:C:287:GLN:H	1:C:287:GLN:HE21	1.54	0.53
1:D:131:SER:HB3	1:D:234:ARG:HD3	1.89	0.53
2:H:22:PRO:O	2:H:25:ILE:HB	2.08	0.53
2:L:84:ASN:OD1	2:L:94:LYS:HG2	2.09	0.53
1:C:35:GLN:NE2	1:C:309:VAL:HG13	2.24	0.53
1:D:270:VAL:O	1:D:271:ASP:CG	2.47	0.53
1:D:94:VAL:HG22	1:E:267:LEU:HD12	1.89	0.53
1:E:35:GLN:HE22	1:E:309:VAL:HG13	1.71	0.53
1:F:261:MET:HG2	1:F:262:LYS:N	2.24	0.53
2:I:105:ASN:HB2	2:I:122:SER:HB3	1.90	0.53
1:A:15:LEU:O	1:A:178:LYS:HE3	2.08	0.53
2:J:111:ASN:ND2	2:J:114:CYS:HB2	2.23	0.53
1:A:237:PRO:HA	1:A:240:TYR:CZ	2.44	0.53
1:B:266:PRO:HB2	3:B:1002:PAL:H31	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LYS:NZ	5:C:1070:HOH:O	2.42	0.53
1:F:121:ASN:HA	5:F:1100:HOH:O	2.09	0.53
2:I:35:LEU:HD22	2:I:40:GLN:CG	2.38	0.53
2:L:29:LEU:HD21	2:L:77:TYR:HB3	1.90	0.53
1:B:267:LEU:HD11	1:B:286:PHE:CE1	2.44	0.52
1:B:60:GLU:HG2	1:B:63:MET:HE1	1.91	0.52
2:H:132:ASN:N	5:H:2013:HOH:O	2.30	0.52
2:H:31:SER:HB3	2:K:27:PHE:HZ	1.72	0.52
2:H:86:ILE:HG22	2:H:87:ASP:N	2.24	0.52
1:B:160:VAL:HB	1:B:227:MET:SD	2.49	0.52
2:I:66:LEU:HA	2:I:71:VAL:HB	1.91	0.52
1:C:52:SER:HB2	1:C:105:ARG:NH1	2.23	0.52
1:E:163:LEU:HG	1:E:188:ALA:HB2	1.91	0.52
2:K:7:LEU:HD12	2:K:10:GLU:OE2	2.10	0.52
2:K:9:VAL:HG12	2:K:60:LYS:NZ	2.24	0.52
1:B:59:PHE:CZ	1:B:136:THR:HG21	2.45	0.52
1:E:270:VAL:O	1:E:271:ASP:CG	2.47	0.52
1:F:94:VAL:HG23	1:F:95:ILE:N	2.24	0.52
2:I:132:ASN:O	2:I:133:ASP:HB3	2.10	0.52
2:K:21:ILE:HB	2:K:57:ASP:HB2	1.92	0.52
2:K:77:TYR:OH	2:K:151:LEU:HD22	2.09	0.52
2:K:82:THR:HG22	2:K:84:ASN:HD21	1.74	0.52
2:K:94:LYS:HB2	2:K:94:LYS:NZ	2.25	0.52
1:A:254:LEU:HD22	1:A:261:MET:HE1	1.90	0.52
1:D:215:ILE:HD11	1:D:227:MET:HE1	1.91	0.52
2:G:40:GLN:OE1	2:G:63:ASN:HB2	2.10	0.52
1:B:60:GLU:HG2	1:B:63:MET:CE	2.40	0.52
2:G:12:ILE:HG22	2:G:13:LYS:N	2.21	0.52
2:H:104:ASP:O	2:H:106:VAL:HG23	2.09	0.52
1:A:12:ILE:HG21	1:A:175:ALA:HB2	1.91	0.52
1:B:15:LEU:O	1:B:178:LYS:HE3	2.10	0.52
1:D:156:HIS:HD2	1:D:185:TYR:OH	1.91	0.52
1:D:59:PHE:O	1:D:63:MET:HG3	2.09	0.52
1:E:80:SER:HB2	1:F:54:ARG:HH22	1.75	0.52
2:L:30:LEU:HD11	2:L:46:LEU:HD11	1.90	0.52
2:L:72:ASP:HA	2:L:97:PRO:HB3	1.92	0.52
1:A:121:ASN:HA	5:A:1030:HOH:O	2.09	0.52
1:E:264:LEU:O	1:E:265:HIS:HB2	2.09	0.52
1:D:54:ARG:NH2	1:F:80:SER:HB2	2.25	0.52
1:C:265:HIS:HD2	1:C:267:LEU:HA	1.75	0.52
1:E:222:VAL:O	1:E:261:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ALA:N	2:J:115:ILE:HD13	2.25	0.52
2:J:58:LEU:HD21	2:J:60:LYS:HG3	1.92	0.52
1:E:38:LEU:HD11	1:E:305:ASN:ND2	2.25	0.51
1:F:17:ARG:HD2	1:F:179:PHE:CD1	2.44	0.51
2:G:111:ASN:O	2:G:117:HIS:NE2	2.39	0.51
1:A:114:LEU:CD2	2:G:121:VAL:HG11	2.40	0.51
1:D:166:GLY:O	1:D:169:VAL:HG22	2.09	0.51
2:I:20:HIS:N	2:I:56:LYS:HE3	2.25	0.51
1:A:265:HIS:O	1:A:266:PRO:O	2.28	0.51
1:D:266:PRO:HB2	3:D:1004:PAL:H31	1.93	0.51
2:J:106:VAL:O	2:J:107:LEU:HD23	2.11	0.51
2:L:105:ASN:OD1	2:L:122:SER:CB	2.51	0.51
1:E:94:VAL:HG23	1:E:95:ILE:N	2.25	0.51
2:H:67:SER:N	2:H:70:GLN:HE21	2.00	0.51
2:L:95:SER:O	2:L:97:PRO:HD3	2.11	0.51
1:C:120:GLY:N	5:C:1042:HOH:O	2.39	0.51
1:E:229:ARG:HD3	1:E:268:PRO:O	2.11	0.51
2:K:78:ALA:HB1	2:K:81:ALA:HB2	1.92	0.51
1:E:109:GLU:OE1	1:E:130:GLY:O	2.29	0.51
1:E:10:ILE:HD12	1:E:112:ALA:HB1	1.93	0.51
1:F:106:HIS:ND1	1:F:107:PRO:HD2	2.25	0.51
2:L:76:LEU:HG	2:L:134:ILE:HD12	1.93	0.51
2:L:66:LEU:HD13	2:L:70:GLN:O	2.11	0.51
1:A:265:HIS:CG	1:A:266:PRO:O	2.63	0.51
1:C:156:HIS:HD2	1:C:185:TYR:OH	1.93	0.51
1:F:136:THR:HG22	1:F:299:LEU:CD2	2.41	0.51
2:K:130:ARG:HE	2:K:135:ALA:HB2	1.73	0.51
1:B:78:ASN:ND2	5:B:1069:HOH:O	2.40	0.50
1:E:284:TRP:CG	1:E:287:GLN:HG3	2.46	0.50
1:F:237:PRO:HA	1:F:240:TYR:CZ	2.45	0.50
2:L:100:PRO:O	2:L:127:VAL:HG21	2.10	0.50
2:L:18:ILE:HB	2:L:84:ASN:HB2	1.92	0.50
1:B:121:ASN:HA	5:B:1077:HOH:O	2.12	0.50
1:C:31:LYS:HG3	1:C:294:PHE:CE1	2.46	0.50
1:F:108:GLN:HG3	2:L:113:ASN:ND2	2.25	0.50
2:H:86:ILE:HD13	2:H:91:VAL:HA	1.91	0.50
2:I:101:GLU:HG3	2:I:102:ARG:HG3	1.94	0.50
1:A:140:LEU:HD21	1:A:288:GLN:HG2	1.93	0.50
1:B:154:ASN:HA	1:B:181:GLY:O	2.10	0.50
2:L:128:ARG:CB	2:L:128:ARG:NH1	2.74	0.50
1:D:1:ALA:HA	1:D:306:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG11	1:E:54:ARG:HG3	1.93	0.50
1:B:49:PHE:HE2	1:B:81:LEU:HD13	1.76	0.50
1:D:111:ALA:HA	2:J:115:ILE:HG12	1.92	0.50
1:E:106:HIS:CG	1:E:107:PRO:HD2	2.46	0.50
1:F:131:SER:HB3	1:F:234:ARG:CD	2.41	0.50
2:I:125:PHE:HA	2:I:137:LYS:O	2.12	0.50
2:I:59:ILE:HD12	2:I:59:ILE:N	2.25	0.50
1:A:81:LEU:HA	1:A:86:GLU:CB	2.26	0.50
1:A:81:LEU:HD12	1:A:91:THR:OG1	2.12	0.50
1:C:50:GLU:CD	1:C:234:ARG:HH22	2.14	0.50
2:K:148:ASN:HA	5:K:2014:HOH:O	2.12	0.50
2:L:44:ILE:CG2	2:L:45:GLY:H	2.09	0.50
1:B:189:PRO:HB3	1:B:246:GLN:HE22	1.76	0.50
1:D:165:TYR:CE2	1:D:235:LEU:HD23	2.47	0.50
1:E:165:TYR:CE2	1:E:235:LEU:HD23	2.47	0.50
2:H:107:LEU:HB3	2:H:150:VAL:CG1	2.41	0.50
1:E:237:PRO:HA	1:E:240:TYR:CZ	2.45	0.50
1:D:80:SER:HB2	1:E:54:ARG:NH2	2.26	0.50
2:G:4:ASP:C	2:G:6:LYS:H	2.15	0.50
2:J:72:ASP:HB3	2:J:98:SER:O	2.11	0.50
2:L:101:GLU:CA	2:L:127:VAL:HG22	2.34	0.50
1:A:189:PRO:HB3	1:A:246:GLN:HE22	1.74	0.50
1:D:230:VAL:O	1:D:232:LYS:N	2.45	0.50
1:D:229:ARG:NE	1:D:268:PRO:HB2	2.27	0.50
2:G:2:THR:HG22	2:G:11:ALA:H	1.76	0.50
1:B:114:LEU:HD11	2:H:121:VAL:CG1	2.42	0.50
2:L:132:ASN:O	2:L:133:ASP:HB3	2.11	0.50
2:L:85:ARG:O	2:L:86:ILE:HD13	2.12	0.50
1:D:131:SER:HA	1:D:167:ARG:HB3	1.94	0.49
2:G:46:LEU:HA	2:G:57:ASP:OD1	2.12	0.49
2:L:46:LEU:HD23	2:L:58:LEU:H	1.77	0.49
1:B:165:TYR:O	1:B:231:GLN:HG3	2.12	0.49
1:C:137:GLN:HG2	1:C:168:THR:HG22	1.94	0.49
1:D:240:TYR:O	1:D:243:VAL:HG12	2.11	0.49
2:H:14:ARG:HA	2:H:87:ASP:HA	1.94	0.49
2:I:125:PHE:CE2	2:I:145:PHE:HZ	2.29	0.49
1:D:94:VAL:CG2	1:E:267:LEU:HD12	2.42	0.49
2:K:90:GLU:OE1	2:K:90:GLU:HA	2.11	0.49
1:E:161:GLY:O	1:E:188:ALA:HB2	2.12	0.49
2:G:21:ILE:HB	2:G:57:ASP:HB2	1.95	0.49
2:I:46:LEU:HD21	2:I:58:LEU:N	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HG	5:C:1011:HOH:O	2.12	0.49
1:D:114:LEU:HG	2:J:115:ILE:CG2	2.42	0.49
2:I:36:THR:HG22	2:I:37:GLU:HG3	1.93	0.49
2:L:136:LEU:N	2:L:145:PHE:O	2.44	0.49
2:L:8:GLN:HE22	2:L:48:LEU:HD13	1.78	0.49
1:B:189:PRO:HG2	1:B:192:LEU:HB2	1.95	0.49
1:C:189:PRO:HG2	1:C:192:LEU:HB2	1.94	0.49
1:F:81:LEU:HG	1:F:86:GLU:O	2.13	0.49
2:L:130:ARG:NE	2:L:135:ALA:HB2	2.28	0.49
2:H:103:ILE:O	2:H:103:ILE:HG23	2.13	0.49
2:L:75:ALA:CB	2:L:99:LEU:HD23	2.43	0.49
1:B:284:TRP:CD2	1:B:287:GLN:HG3	2.47	0.49
1:C:187:ILE:HG12	1:C:212:HIS:HB2	1.94	0.49
1:C:243:VAL:HG13	1:C:244:LYS:CD	2.43	0.49
1:A:94:VAL:CG1	1:C:267:LEU:HD12	2.42	0.49
1:C:267:LEU:O	1:C:269:ARG:N	2.46	0.49
1:D:189:PRO:HB3	1:D:246:GLN:HE22	1.76	0.49
2:J:8:GLN:HB2	5:J:2024:HOH:O	2.12	0.49
2:L:78:ALA:HB1	2:L:81:ALA:HB2	1.95	0.49
2:H:21:ILE:HB	2:H:57:ASP:HB2	1.95	0.49
1:C:109:GLU:OE2	2:I:113:ASN:HB3	2.12	0.49
2:L:99:LEU:HD12	2:L:129:LYS:HB2	1.94	0.49
1:B:244:LYS:HB3	5:B:1100:HOH:O	2.12	0.48
1:E:227:MET:HB2	1:E:265:HIS:HD2	1.77	0.48
2:G:34:LYS:HB3	2:G:37:GLU:OE2	2.13	0.48
2:G:13:LYS:O	2:G:86:ILE:HG22	2.12	0.48
1:D:27:ALA:HA	1:D:298:ALA:HB2	1.96	0.48
2:I:32:LEU:HD11	2:I:77:TYR:CE2	2.48	0.48
2:L:152:ALA:O	2:L:153:ASN:HB2	2.11	0.48
1:D:211:LEU:O	1:D:212:HIS:CG	2.67	0.48
1:D:261:MET:CE	1:D:282:HIS:CG	2.96	0.48
2:H:102:ARG:HG2	2:H:139:LYS:CE	2.43	0.48
5:B:1053:HOH:O	2:H:139:LYS:HB2	2.13	0.48
2:H:32:LEU:HD23	2:H:32:LEU:O	2.13	0.48
2:J:77:TYR:N	2:J:77:TYR:CD1	2.81	0.48
2:L:65:PHE:CD1	2:L:65:PHE:N	2.80	0.48
1:B:261:MET:HG2	1:B:262:LYS:N	2.27	0.48
1:D:261:MET:HE1	1:D:282:HIS:CG	2.49	0.48
1:E:1:ALA:HA	1:E:306:ARG:HG2	1.95	0.48
2:I:20:HIS:H	2:I:56:LYS:CE	2.25	0.48
1:A:114:LEU:HD13	1:A:114:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:TYR:O	1:B:243:VAL:HG12	2.14	0.48
1:F:81:LEU:HD12	1:F:91:THR:OG1	2.13	0.48
2:G:12:ILE:HG21	2:G:62:GLU:OE1	2.12	0.48
2:H:92:VAL:HG23	2:H:93:GLY:H	1.78	0.48
2:L:109:CYS:SG	2:L:111:ASN:HB3	2.54	0.48
2:L:128:ARG:CB	2:L:128:ARG:HH11	2.26	0.48
2:L:87:ASP:OD2	2:L:92:VAL:HG11	2.14	0.48
1:A:267:LEU:O	1:A:269:ARG:N	2.46	0.48
1:E:251:ALA:CB	1:E:276:ASP:OD2	2.62	0.48
2:K:107:LEU:HD13	2:K:150:VAL:HG11	1.96	0.48
2:I:44:ILE:HG12	2:L:48:LEU:CD2	2.43	0.48
1:A:191:ALA:O	1:A:192:LEU:HD23	2.13	0.48
1:A:229:ARG:NH1	1:A:233:GLU:OE1	2.40	0.48
1:A:81:LEU:HG	1:A:86:GLU:O	2.13	0.48
2:H:111:ASN:C	2:H:111:ASN:HD22	2.16	0.48
2:K:55:ARG:NH1	2:K:55:ARG:HG2	2.29	0.48
2:L:39:ASP:OD1	2:L:40:GLN:N	2.46	0.48
1:F:106:HIS:CG	1:F:107:PRO:HD2	2.49	0.48
2:H:1:MET:O	2:H:2:THR:HG23	2.14	0.48
1:A:54:ARG:HH21	1:B:80:SER:HB2	1.78	0.48
1:F:214:SER:OG	1:F:217:GLU:HG3	2.14	0.48
2:I:25:ILE:O	2:I:29:LEU:HB2	2.14	0.48
2:J:125:PHE:HA	2:J:137:LYS:O	2.13	0.48
1:B:267:LEU:HD12	1:C:94:VAL:HG11	1.92	0.48
1:E:31:LYS:HE2	1:E:294:PHE:CE2	2.49	0.48
2:H:111:ASN:HB3	2:H:114:CYS:HB2	1.95	0.48
2:I:10:GLU:CG	2:I:11:ALA:N	2.72	0.48
1:C:219:MET:HE3	1:C:254:LEU:HD23	1.96	0.47
1:D:141:ASP:OD1	1:D:288:GLN:NE2	2.47	0.47
1:F:122:VAL:HB	5:F:1054:HOH:O	2.14	0.47
1:F:45:ALA:HB2	1:F:99:VAL:HG11	1.96	0.47
2:J:103:ILE:HD11	2:J:106:VAL:CG2	2.44	0.47
2:L:38:THR:O	2:L:39:ASP:HB2	2.14	0.47
1:B:270:VAL:HG12	1:B:270:VAL:O	2.14	0.47
1:C:17:ARG:HD2	1:C:179:PHE:CE1	2.49	0.47
2:H:79:PRO:HD2	2:H:80:GLN:HE22	1.79	0.47
5:F:1097:HOH:O	2:L:120:PRO:HG2	2.13	0.47
1:F:250:ARG:HH11	1:F:250:ARG:HG2	1.79	0.47
2:L:102:ARG:O	2:L:103:ILE:HD13	2.14	0.47
1:D:160:VAL:HB	1:D:227:MET:SD	2.54	0.47
2:J:50:SER:HB2	2:J:56:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1034:HOH:O	2:K:143:LYS:HE2	2.13	0.47
1:B:287:GLN:NE2	1:B:287:GLN:H	2.11	0.47
1:C:60:GLU:HG2	1:C:70:VAL:HG11	1.96	0.47
1:D:131:SER:HB3	1:D:234:ARG:CD	2.44	0.47
2:H:134:ILE:H	2:H:147:HIS:CD2	2.31	0.47
1:E:109:GLU:HG3	2:K:111:ASN:HD21	1.80	0.47
1:B:237:PRO:HA	1:B:240:TYR:CZ	2.49	0.47
1:F:52:SER:HB2	1:F:105:ARG:NH1	2.29	0.47
2:G:17:VAL:HG23	2:G:86:ILE:CD1	2.44	0.47
5:B:1053:HOH:O	2:H:139:LYS:HB3	2.12	0.47
2:J:19:ASP:OD2	2:J:20:HIS:N	2.41	0.47
2:J:40:GLN:OE1	2:J:63:ASN:HB2	2.15	0.47
2:K:131:ALA:HA	5:K:2019:HOH:O	2.14	0.47
1:B:156:HIS:HD2	1:B:185:TYR:OH	1.97	0.47
1:B:165:TYR:CE2	1:B:235:LEU:HD23	2.48	0.47
1:D:160:VAL:HG22	1:D:187:ILE:HB	1.96	0.47
2:H:14:ARG:CA	2:H:87:ASP:HA	2.44	0.47
2:H:19:ASP:OD1	2:H:20:HIS:N	2.44	0.47
2:G:146:SER:O	2:G:149:VAL:HG22	2.15	0.47
2:H:124:SER:OG	2:H:139:LYS:HG3	2.15	0.47
2:I:16:THR:HG22	2:I:17:VAL:N	2.29	0.47
2:K:14:ARG:HA	2:K:86:ILE:O	2.14	0.47
2:L:76:LEU:HD12	2:L:147:HIS:CG	2.49	0.47
1:D:267:LEU:HD12	1:F:94:VAL:HG11	1.97	0.47
1:E:265:HIS:O	1:E:267:LEU:N	2.48	0.47
1:F:60:GLU:HG2	1:F:70:VAL:HG11	1.97	0.47
2:G:18:ILE:HA	2:G:82:THR:O	2.14	0.47
2:J:11:ALA:HB1	5:J:2038:HOH:O	2.15	0.47
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.96	0.47
1:D:45:ALA:HA	1:D:71:VAL:O	2.14	0.47
2:I:20:HIS:H	2:I:56:LYS:HE3	1.79	0.47
2:K:18:ILE:HD11	2:K:66:LEU:CD1	2.45	0.47
2:L:98:SER:O	2:L:99:LEU:HD23	2.14	0.47
1:B:250:ARG:HH11	1:B:250:ARG:HG2	1.80	0.47
1:F:1:ALA:HA	1:F:306:ARG:HG2	1.97	0.47
2:K:77:TYR:CZ	2:K:151:LEU:HD22	2.50	0.47
2:L:3:HIS:O	2:L:9:VAL:HG22	2.15	0.47
1:B:87:THR:HB	2:H:119:GLU:OE1	2.15	0.46
1:D:12:ILE:HG13	1:D:171:SER:HB3	1.96	0.46
1:E:159:MET:HE2	1:E:172:LEU:CD2	2.40	0.46
1:C:131:SER:HB3	1:C:234:ARG:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASN:OD1	1:F:75:ASP:HB2	2.15	0.46
1:F:86:GLU:N	5:F:1062:HOH:O	2.47	0.46
2:K:84:ASN:N	2:K:84:ASN:ND2	2.60	0.46
1:B:270:VAL:O	1:B:271:ASP:CG	2.53	0.46
1:D:137:GLN:NE2	1:D:140:LEU:HD22	2.30	0.46
2:L:25:ILE:HD12	2:L:25:ILE:N	2.29	0.46
1:A:54:ARG:CD	1:A:267:LEU:HB2	2.43	0.46
1:B:165:TYR:CD2	1:B:235:LEU:HD23	2.51	0.46
1:C:226:TYR:CZ	1:C:266:PRO:HD3	2.51	0.46
1:D:20:LEU:HD13	1:D:142:LEU:CD1	2.45	0.46
2:I:45:GLY:H	2:L:46:LEU:H	1.64	0.46
2:I:18:ILE:HA	2:I:83:VAL:HG12	1.96	0.46
1:A:17:ARG:HD2	1:A:179:PHE:CE1	2.51	0.46
1:A:238:SER:HA	1:E:241:ALA:HA	1.98	0.46
2:G:52:GLU:O	2:G:53:MET:HG2	2.16	0.46
1:B:109:GLU:CD	2:H:113:ASN:HD22	2.19	0.46
1:E:108:GLN:HG3	2:K:113:ASN:ND2	2.29	0.46
1:D:12:ILE:HG21	1:D:175:ALA:HB2	1.98	0.46
1:A:162:ASP:OD1	1:A:162:ASP:C	2.54	0.46
2:G:8:GLN:HB3	2:G:48:LEU:HD22	1.97	0.46
2:G:102:ARG:HG2	2:G:104:ASP:OD2	2.15	0.46
2:G:50:SER:HB2	2:G:56:LYS:HG2	1.98	0.46
2:I:48:LEU:CD1	2:I:58:LEU:HG	2.39	0.46
2:K:12:ILE:HG12	2:K:13:LYS:N	2.31	0.46
1:B:130:GLY:O	1:B:131:SER:HB3	2.16	0.46
1:D:17:ARG:HD2	1:D:179:PHE:CE1	2.51	0.46
2:G:85:ARG:C	2:G:86:ILE:HD12	2.36	0.46
2:I:38:THR:O	2:I:40:GLN:NE2	2.49	0.46
2:J:21:ILE:HB	2:J:57:ASP:HB2	1.97	0.46
1:E:94:VAL:HG11	1:F:267:LEU:HD12	1.96	0.45
2:L:43:THR:HG22	2:L:60:LYS:HB2	1.98	0.45
1:F:109:GLU:HG3	2:L:111:ASN:HD21	1.82	0.45
2:K:7:LEU:HB2	2:K:10:GLU:OE1	2.17	0.45
2:L:90:GLU:HG2	2:L:91:VAL:H	1.81	0.45
1:B:1:ALA:HA	1:B:306:ARG:HG2	1.97	0.45
1:E:81:LEU:HG	1:E:86:GLU:O	2.17	0.45
1:F:108:GLN:HE21	2:L:113:ASN:HD21	1.63	0.45
2:H:9:VAL:HG11	2:H:60:LYS:HZ3	1.79	0.45
2:L:109:CYS:HA	2:L:110:PRO:HD3	1.85	0.45
2:L:40:GLN:HA	5:L:2015:HOH:O	2.16	0.45
2:G:44:ILE:HB	2:J:44:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:17:VAL:HG23	2:G:86:ILE:HD13	1.98	0.45
2:H:30:LEU:HD13	2:H:59:ILE:CD1	2.45	0.45
2:K:107:LEU:HD22	2:K:150:VAL:HG12	1.97	0.45
1:B:17:ARG:O	1:B:17:ARG:HG3	2.15	0.45
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.51	0.45
2:H:119:GLU:HG3	2:H:120:PRO:CD	2.46	0.45
1:C:10:ILE:HD12	1:C:112:ALA:HB1	1.99	0.45
1:E:52:SER:HB2	1:E:105:ARG:NH1	2.32	0.45
2:J:4:ASP:OD2	2:J:7:LEU:HB2	2.17	0.45
2:K:94:LYS:CB	2:K:94:LYS:NZ	2.79	0.45
1:B:37:GLU:OE2	1:B:40:LYS:HD2	2.17	0.45
1:C:136:THR:HA	1:C:139:LEU:HD12	1.99	0.45
1:E:160:VAL:HG22	1:E:187:ILE:HB	1.99	0.45
1:E:50:GLU:HB3	1:E:105:ARG:HG2	1.99	0.45
1:F:50:GLU:HB3	1:F:105:ARG:HG2	1.97	0.45
2:J:7:LEU:CD2	2:J:48:LEU:HB3	2.37	0.45
2:L:107:LEU:HA	2:L:152:ALA:HA	1.98	0.45
2:L:24:GLN:C	2:L:25:ILE:HD12	2.37	0.45
1:C:271:ASP:OD1	1:C:271:ASP:C	2.56	0.45
1:E:307:ASP:HA	5:E:1045:HOH:O	2.17	0.45
1:E:94:VAL:CG1	1:F:267:LEU:CD1	2.95	0.45
1:F:265:HIS:HD2	1:F:267:LEU:HA	1.81	0.45
2:I:102:ARG:HH21	2:I:139:LYS:HD3	1.81	0.45
2:L:74:LEU:HG	5:L:2016:HOH:O	2.16	0.45
1:C:48:PHE:HB2	1:C:74:SER:HA	1.99	0.45
2:G:99:LEU:HD12	2:G:100:PRO:HD2	1.98	0.45
2:I:17:VAL:HG13	2:I:60:LYS:HG2	1.99	0.45
2:J:128:ARG:O	2:J:134:ILE:HG23	2.17	0.45
2:K:16:THR:HG1	2:K:65:PHE:HA	1.80	0.45
2:K:30:LEU:HD13	2:K:59:ILE:HD13	1.99	0.45
1:B:189:PRO:HB3	1:B:246:GLN:NE2	2.32	0.45
1:E:121:ASN:HB3	5:E:1016:HOH:O	2.17	0.45
1:E:162:ASP:OD1	1:E:162:ASP:C	2.55	0.45
2:J:50:SER:O	2:J:54:GLY:N	2.49	0.45
2:L:63:ASN:O	2:L:64:THR:C	2.55	0.45
1:C:178:LYS:NZ	5:C:1084:HOH:O	2.50	0.44
1:C:234:ARG:HG2	1:C:234:ARG:HH11	1.81	0.44
1:D:266:PRO:HG2	5:D:1034:HOH:O	2.17	0.44
1:E:17:ARG:HD2	1:E:179:PHE:CE1	2.52	0.44
5:E:1007:HOH:O	1:F:269:ARG:HG2	2.16	0.44
2:G:86:ILE:N	2:G:86:ILE:HD12	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:LEU:O	2:L:145:PHE:N	2.31	0.44
2:L:59:ILE:HG22	2:L:60:LYS:N	2.32	0.44
2:L:90:GLU:HG2	2:L:91:VAL:N	2.31	0.44
1:D:267:LEU:HD23	1:D:267:LEU:HA	1.72	0.44
1:E:271:ASP:OD1	1:E:271:ASP:C	2.55	0.44
1:E:26:THR:HB	1:E:298:ALA:HB1	1.99	0.44
2:J:139:LYS:O	2:J:139:LYS:HG2	2.16	0.44
2:J:72:ASP:OD1	2:J:98:SER:HB3	2.16	0.44
1:B:245:ALA:HB3	1:B:271:ASP:OD1	2.17	0.44
1:B:2:ASN:HB2	1:B:308:LEU:HD21	1.99	0.44
1:C:58:SER:OG	1:C:296:ARG:NH1	2.49	0.44
1:F:265:HIS:O	1:F:267:LEU:N	2.51	0.44
2:G:65:PHE:HD2	2:G:85:ARG:HD3	1.80	0.44
2:J:6:LYS:O	2:J:6:LYS:HG3	2.18	0.44
2:L:111:ASN:ND2	2:L:141:CYS:SG	2.87	0.44
2:L:22:PRO:HA	2:L:55:ARG:O	2.17	0.44
1:E:251:ALA:HB3	1:E:276:ASP:OD2	2.18	0.44
1:F:267:LEU:O	1:F:268:PRO:C	2.53	0.44
1:A:75:ASP:OD2	1:A:77:ALA:HB3	2.18	0.44
1:B:104:MET:HE1	1:B:115:ALA:CB	2.48	0.44
1:D:216:GLU:HG3	5:D:1062:HOH:O	2.16	0.44
1:D:55:THR:O	1:D:59:PHE:HB2	2.17	0.44
1:F:163:LEU:HG	1:F:188:ALA:HB2	1.98	0.44
1:F:215:ILE:HG22	1:F:219:MET:HE2	2.00	0.44
2:I:59:ILE:CD1	2:I:59:ILE:H	2.29	0.44
2:I:7:LEU:HD13	2:L:9:VAL:HB	2.00	0.44
1:B:158:ALA:HB2	1:B:222:VAL:HG11	2.00	0.44
1:B:54:ARG:NH2	1:C:80:SER:HB2	2.32	0.44
1:D:162:ASP:C	1:D:162:ASP:OD1	2.56	0.44
1:D:78:ASN:OD1	1:E:75:ASP:HB2	2.18	0.44
1:F:106:HIS:ND1	1:F:107:PRO:CD	2.81	0.44
2:I:22:PRO:HB2	2:I:25:ILE:CG1	2.46	0.44
1:E:189:PRO:HB3	1:E:246:GLN:HE22	1.82	0.44
1:F:137:GLN:HG2	1:F:168:THR:CG2	2.46	0.44
1:F:8:HIS:C	1:F:9:ILE:HD13	2.38	0.44
2:L:137:LYS:HE3	2:L:142:GLU:O	2.17	0.44
1:A:187:ILE:HD11	1:A:218:VAL:HG21	2.00	0.44
1:A:60:GLU:HG2	1:A:70:VAL:HG11	2.00	0.44
1:C:267:LEU:HA	1:C:267:LEU:HD23	1.62	0.44
1:E:55:THR:O	1:E:59:PHE:HB2	2.18	0.44
2:H:137:LYS:NZ	2:H:142:GLU:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:99:LEU:HD22	2:L:134:ILE:CD1	2.48	0.44
1:B:65:ARG:HD3	5:B:1039:HOH:O	2.17	0.44
1:F:142:LEU:HD11	1:F:175:ALA:HB1	2.00	0.44
1:F:267:LEU:HD11	1:F:286:PHE:CE1	2.53	0.44
2:I:108:VAL:HG21	2:I:153:ASN:HB2	2.00	0.44
2:K:58:LEU:HD21	2:K:60:LYS:HE3	2.00	0.44
1:A:114:LEU:CD1	1:A:114:LEU:C	2.87	0.43
2:I:85:ARG:O	2:I:86:ILE:HB	2.18	0.43
1:A:9:ILE:HG13	1:A:299:LEU:HD11	2.01	0.43
1:C:131:SER:HB3	1:C:234:ARG:HD3	2.00	0.43
1:D:48:PHE:HB2	1:D:74:SER:HA	2.00	0.43
1:E:80:SER:CB	1:F:54:ARG:NH2	2.81	0.43
1:A:109:GLU:OE2	2:G:113:ASN:ND2	2.51	0.43
2:K:73:GLN:OE1	2:K:106:VAL:HG21	2.18	0.43
2:K:82:THR:HG22	2:K:84:ASN:ND2	2.34	0.43
1:B:265:HIS:C	1:B:266:PRO:O	2.48	0.43
1:C:53:THR:O	1:C:57:LEU:HB2	2.18	0.43
1:F:131:SER:HB3	1:F:234:ARG:HD2	1.99	0.43
2:G:102:ARG:HG2	2:G:103:ILE:N	2.33	0.43
2:I:136:LEU:O	2:I:144:GLU:HA	2.17	0.43
2:I:1:MET:HB2	2:I:3:HIS:CE1	2.52	0.43
2:K:9:VAL:C	2:K:10:GLU:HG3	2.38	0.43
1:A:94:VAL:HG23	1:A:95:ILE:N	2.34	0.43
1:D:160:VAL:HA	1:D:187:ILE:O	2.19	0.43
1:E:119:SER:O	1:E:120:GLY:C	2.56	0.43
1:E:192:LEU:HD11	1:E:242:ASN:CB	2.48	0.43
2:I:15:GLY:CA	2:I:62:GLU:HA	2.36	0.43
2:K:99:LEU:HA	2:K:100:PRO:HD3	1.81	0.43
2:L:46:LEU:CD2	2:L:57:ASP:HB3	2.47	0.43
2:L:88:ASN:OD1	2:L:89:TYR:HD1	2.01	0.43
1:D:255:HIS:ND1	1:D:256:ASN:N	2.67	0.43
1:D:271:ASP:OD1	1:D:271:ASP:C	2.57	0.43
1:E:38:LEU:CD1	1:E:305:ASN:ND2	2.82	0.43
1:E:86:GLU:N	5:E:1021:HOH:O	2.51	0.43
2:G:95:SER:O	2:G:96:ARG:C	2.57	0.43
1:A:50:GLU:CD	1:A:234:ARG:HH22	2.22	0.43
2:G:36:THR:O	2:G:38:THR:N	2.50	0.43
2:L:104:ASP:HA	2:L:124:SER:HA	2.00	0.43
1:A:10:ILE:HD12	1:A:112:ALA:HB1	1.99	0.43
1:D:114:LEU:HD21	2:J:121:VAL:HG11	2.00	0.43
1:D:13:ASN:HA	1:D:13:ASN:HD22	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ASP:OD1	1:E:288:GLN:NE2	2.51	0.43
2:H:111:ASN:O	2:H:117:HIS:CE1	2.71	0.43
2:I:18:ILE:O	2:I:58:LEU:HA	2.17	0.43
2:K:5:ASN:O	2:K:6:LYS:HB2	2.18	0.43
2:K:9:VAL:HG11	2:K:58:LEU:HD23	2.01	0.43
2:L:128:ARG:HB3	2:L:128:ARG:CZ	2.48	0.43
2:L:81:ALA:H	2:L:96:ARG:HH12	1.58	0.43
1:A:229:ARG:HD3	1:A:268:PRO:O	2.19	0.43
1:A:284:TRP:O	1:A:288:GLN:HB2	2.18	0.43
1:A:140:LEU:CD2	1:A:288:GLN:HG2	2.49	0.43
1:D:111:ALA:HB2	2:J:115:ILE:CD1	2.47	0.43
1:E:230:VAL:O	1:E:232:LYS:N	2.52	0.43
2:H:65:PHE:CD1	2:H:85:ARG:HG3	2.54	0.43
2:K:73:GLN:CD	2:K:106:VAL:HG21	2.38	0.43
2:L:68:GLU:O	2:L:71:VAL:HG12	2.19	0.43
1:D:30:LEU:CD2	1:D:309:VAL:HG11	2.49	0.43
1:F:52:SER:HB2	1:F:105:ARG:HH11	1.84	0.43
2:G:125:PHE:HA	2:G:137:LYS:O	2.18	0.43
1:F:310:LEU:N	5:F:1046:HOH:O	2.52	0.42
2:J:110:PRO:HD2	2:J:145:PHE:CD2	2.53	0.42
2:L:105:ASN:O	2:L:106:VAL:C	2.56	0.42
2:L:107:LEU:HD23	2:L:152:ALA:HB2	2.00	0.42
2:L:107:LEU:HD23	2:L:152:ALA:HA	2.01	0.42
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.00	0.42
2:I:29:LEU:HD11	2:I:74:LEU:CD2	2.49	0.42
2:I:9:VAL:CG1	2:I:47:ASN:HD22	2.31	0.42
2:J:103:ILE:HD11	2:J:106:VAL:HG22	2.00	0.42
2:J:136:LEU:HD12	2:J:150:VAL:HG21	2.01	0.42
2:L:72:ASP:C	2:L:74:LEU:H	2.22	0.42
1:C:96:SER:HB2	5:C:1042:HOH:O	2.19	0.42
1:D:165:TYR:CD2	1:D:235:LEU:HD23	2.54	0.42
1:F:250:ARG:HG2	1:F:250:ARG:NH1	2.34	0.42
2:L:99:LEU:CD2	2:L:134:ILE:HD11	2.49	0.42
1:A:223:ASP:O	1:A:261:MET:HA	2.19	0.42
1:C:170:HIS:O	1:C:174:GLN:HG3	2.19	0.42
1:D:120:GLY:O	1:D:121:ASN:CG	2.57	0.42
1:A:266:PRO:HB2	3:A:1001:PAL:H31	2.02	0.42
1:A:54:ARG:HH22	1:B:86:GLU:CD	2.22	0.42
1:E:229:ARG:NE	3:E:1005:PAL:O4	2.52	0.42
1:F:219:MET:HE3	1:F:254:LEU:HD23	2.01	0.42
2:I:56:LYS:CE	2:I:58:LEU:HD21	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:84:ASN:OD1	2:J:94:LYS:HE2	2.20	0.42
2:K:94:LYS:HB2	2:K:94:LYS:HZ2	1.84	0.42
2:L:137:LYS:HE3	2:L:137:LYS:HB2	1.80	0.42
2:I:44:ILE:HG12	2:L:48:LEU:HD23	2.01	0.42
1:E:214:SER:OG	1:E:217:GLU:HG3	2.20	0.42
1:E:267:LEU:HA	1:E:267:LEU:HD23	1.55	0.42
2:I:110:PRO:HD2	2:I:145:PHE:CE1	2.55	0.42
1:D:134:HIS:HB2	1:D:167:ARG:HG3	2.01	0.42
1:D:31:LYS:HG3	1:D:294:PHE:CE1	2.55	0.42
1:F:81:LEU:HD23	5:F:1084:HOH:O	2.19	0.42
2:G:129:LYS:HB2	2:G:129:LYS:NZ	2.35	0.42
1:A:136:THR:HG22	1:A:299:LEU:CD2	2.49	0.42
1:C:134:HIS:CD2	1:C:168:THR:HG22	2.54	0.42
1:E:164:LYS:HA	1:E:195:PRO:HD3	2.01	0.42
2:G:73:GLN:HB2	2:G:106:VAL:HG21	2.02	0.42
2:H:50:SER:OG	2:H:53:MET:HB2	2.19	0.42
2:I:56:LYS:CG	2:I:57:ASP:H	2.32	0.42
2:K:70:GLN:HB3	2:K:73:GLN:H	1.85	0.42
1:A:101:ALA:HB2	1:A:304:LEU:HD21	2.01	0.42
1:E:94:VAL:HG12	1:F:267:LEU:HD12	2.01	0.42
2:J:111:ASN:O	2:J:117:HIS:NE2	2.44	0.42
2:J:119:GLU:HA	2:J:120:PRO:HD3	1.86	0.42
2:K:70:GLN:HB3	2:K:73:GLN:HG3	2.01	0.42
1:A:54:ARG:NH2	1:B:80:SER:HB2	2.35	0.42
1:D:134:HIS:CE1	1:D:137:GLN:HB2	2.55	0.42
2:H:23:ALA:O	2:H:24:GLN:HB2	2.20	0.42
2:L:64:THR:O	2:L:64:THR:HG23	2.20	0.42
1:A:265:HIS:O	1:A:266:PRO:C	2.58	0.41
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.63	0.41
1:A:270:VAL:O	1:A:272:GLU:OE1	2.38	0.41
1:A:61:THR:O	1:A:65:ARG:HG2	2.20	0.41
1:A:54:ARG:NH1	1:B:86:GLU:OE2	2.49	0.41
1:D:153:ASP:HB2	1:D:180:ASP:O	2.20	0.41
1:D:75:ASP:HB2	1:F:78:ASN:OD1	2.20	0.41
1:E:138:THR:O	1:E:142:LEU:HG	2.20	0.41
2:L:100:PRO:O	2:L:127:VAL:CG2	2.67	0.41
2:L:137:LYS:HB3	2:L:144:GLU:HG3	2.02	0.41
2:L:44:ILE:CG2	2:L:45:GLY:N	2.76	0.41
1:A:42:LYS:HE3	5:A:1054:HOH:O	2.20	0.41
1:D:27:ALA:CA	1:D:298:ALA:HB2	2.50	0.41
1:E:161:GLY:O	1:E:188:ALA:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ASP:HB2	1:E:230:VAL:HA	2.02	0.41
2:G:22:PRO:HG3	2:G:80:GLN:OE1	2.19	0.41
2:K:34:LYS:HE2	2:K:37:GLU:CD	2.41	0.41
2:K:86:ILE:HG22	2:K:87:ASP:N	2.34	0.41
1:A:96:SER:O	1:A:122:VAL:HG21	2.20	0.41
1:A:80:SER:O	1:A:84:LYS:HB2	2.21	0.41
1:B:104:MET:HE1	1:B:115:ALA:HB2	2.02	0.41
1:F:114:LEU:HD13	1:F:114:LEU:C	2.40	0.41
2:G:132:ASN:O	2:G:133:ASP:HB2	2.21	0.41
2:J:94:LYS:O	2:J:95:SER:HB3	2.20	0.41
2:L:21:ILE:C	2:L:23:ALA:H	2.23	0.41
1:D:162:ASP:HB2	1:D:230:VAL:HA	2.03	0.41
1:F:13:ASN:HA	1:F:13:ASN:HD22	1.62	0.41
1:F:156:HIS:HD2	1:F:185:TYR:OH	2.03	0.41
2:L:135:ALA:HB1	2:L:144:GLU:HG2	2.03	0.41
2:L:72:ASP:HA	2:L:97:PRO:CB	2.50	0.41
1:C:165:TYR:CE2	1:C:235:LEU:HD23	2.55	0.41
1:C:45:ALA:HB2	1:C:99:VAL:HG11	2.02	0.41
1:D:120:GLY:O	1:D:121:ASN:OD1	2.39	0.41
2:I:10:GLU:CA	2:I:44:ILE:HD12	2.47	0.41
2:I:21:ILE:CB	2:I:57:ASP:HB2	2.35	0.41
2:I:21:ILE:HD12	2:I:57:ASP:HB2	2.02	0.41
2:J:102:ARG:HH11	2:J:102:ARG:HG2	1.85	0.41
2:L:146:SER:O	2:L:148:ASN:N	2.53	0.41
1:A:48:PHE:CE2	1:A:56:ARG:HB2	2.56	0.41
1:B:192:LEU:HD11	1:B:242:ASN:CB	2.48	0.41
1:F:81:LEU:HD23	1:F:81:LEU:O	2.21	0.41
2:L:117:HIS:O	2:L:118:ALA:HB2	2.20	0.41
1:C:138:THR:O	1:C:142:LEU:HG	2.20	0.41
2:G:40:GLN:CD	2:G:63:ASN:HB2	2.40	0.41
2:L:139:LYS:HE2	2:L:140:TYR:CZ	2.55	0.41
2:L:61:ILE:HG22	2:L:62:GLU:N	2.35	0.41
1:B:121:ASN:HB2	5:B:1066:HOH:O	2.21	0.41
1:C:140:LEU:C	1:C:140:LEU:HD23	2.41	0.41
1:E:227:MET:HE3	5:E:1032:HOH:O	2.20	0.41
1:F:150:GLY:O	1:F:151:ARG:HB3	2.20	0.41
2:J:86:ILE:HD13	2:J:91:VAL:HA	2.03	0.41
1:B:268:PRO:HD3	3:B:1002:PAL:H1P1	2.02	0.41
1:B:17:ARG:NH1	1:B:17:ARG:HG2	2.35	0.41
1:F:161:GLY:O	1:F:163:LEU:HG	2.21	0.41
2:G:2:THR:HG22	2:G:11:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:56:LYS:CG	2:I:57:ASP:N	2.82	0.41
1:A:274:ALA:CB	1:A:276:ASP:OD1	2.69	0.41
1:E:52:SER:HB2	1:E:105:ARG:HH11	1.86	0.41
1:F:21:ASN:HA	1:F:21:ASN:HD22	1.74	0.41
1:F:54:ARG:HD3	1:F:267:LEU:HB2	2.02	0.41
2:H:84:ASN:HB3	2:H:91:VAL:CG2	2.51	0.41
2:I:55:ARG:NH1	2:L:40:GLN:NE2	2.69	0.41
2:J:4:ASP:OD1	2:J:7:LEU:HD12	2.21	0.41
1:E:109:GLU:HG3	2:K:141:CYS:HB2	2.03	0.41
2:L:35:LEU:HD23	2:L:35:LEU:HA	1.90	0.41
1:A:284:TRP:HA	1:A:287:GLN:OE1	2.21	0.41
1:D:50:GLU:CD	1:D:234:ARG:HH22	2.24	0.41
2:H:66:LEU:HA	2:H:70:GLN:NE2	2.36	0.41
2:K:7:LEU:HB2	2:K:10:GLU:CD	2.41	0.41
2:L:76:LEU:CD1	2:L:134:ILE:HB	2.51	0.41
1:E:246:GLN:HB2	1:E:246:GLN:HE21	1.68	0.40
2:G:135:ALA:O	2:G:136:LEU:HD23	2.21	0.40
2:G:110:PRO:HG3	2:G:150:VAL:HA	2.01	0.40
2:G:149:VAL:CG2	2:G:150:VAL:N	2.84	0.40
2:H:42:ILE:HB	2:K:46:LEU:HB2	2.03	0.40
2:J:58:LEU:CD2	2:J:60:LYS:HG3	2.51	0.40
2:K:145:PHE:CD1	2:K:145:PHE:N	2.88	0.40
1:D:42:LYS:HA	1:D:100:ASP:OD2	2.22	0.40
1:D:140:LEU:HD12	1:D:292:GLY:CA	2.51	0.40
1:F:109:GLU:OE2	2:L:113:ASN:OD1	2.39	0.40
2:G:108:VAL:HG12	2:G:152:ALA:O	2.21	0.40
2:G:112:SER:CA	2:G:117:HIS:HE2	2.33	0.40
2:H:109:CYS:CB	2:H:138:CYS:SG	3.01	0.40
2:H:92:VAL:CG2	2:H:93:GLY:N	2.84	0.40
1:B:227:MET:O	1:B:266:PRO:HD2	2.22	0.40
1:D:108:GLN:HG3	2:J:113:ASN:HD21	1.83	0.40
2:G:102:ARG:HD3	2:G:104:ASP:OD2	2.22	0.40
2:G:134:ILE:HD13	2:G:147:HIS:CE1	2.56	0.40
2:G:149:VAL:HG23	2:G:150:VAL:N	2.36	0.40
2:I:20:HIS:ND1	2:I:56:LYS:HE3	2.35	0.40
2:K:42:ILE:HG12	2:K:61:ILE:HG23	2.04	0.40
2:L:25:ILE:HG21	2:L:77:TYR:O	2.21	0.40
2:L:18:ILE:HB	2:L:84:ASN:HD22	1.85	0.40
1:B:250:ARG:NH1	1:B:250:ARG:HG2	2.36	0.40
2:I:10:GLU:HA	2:I:44:ILE:CD1	2.44	0.40
2:J:130:ARG:CD	2:J:135:ALA:HB2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:LEU:HD21	2:J:60:LYS:CE	2.47	0.40
2:K:147:HIS:O	2:K:151:LEU:HG	2.21	0.40
1:B:35:GLN:HE22	1:B:309:VAL:HG13	1.84	0.40
1:C:13:ASN:HA	1:C:13:ASN:HD22	1.61	0.40
1:D:35:GLN:HE22	1:D:309:VAL:HG13	1.81	0.40
1:E:165:TYR:CD2	1:E:235:LEU:HD23	2.56	0.40
2:J:73:GLN:HE22	2:J:103:ILE:HD12	1.86	0.40
1:D:114:LEU:HD22	2:J:121:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	278 (90%)	25 (8%)	5 (2%)	9	8
1	B	308/310 (99%)	288 (94%)	15 (5%)	5 (2%)	9	8
1	C	308/310 (99%)	284 (92%)	21 (7%)	3 (1%)	15	16
1	D	308/310 (99%)	276 (90%)	28 (9%)	4 (1%)	12	11
1	E	308/310 (99%)	281 (91%)	22 (7%)	5 (2%)	9	8
1	F	308/310 (99%)	281 (91%)	23 (8%)	4 (1%)	12	11
2	G	151/153 (99%)	127 (84%)	19 (13%)	5 (3%)	4	1
2	H	151/153 (99%)	132 (87%)	18 (12%)	1 (1%)	22	25
2	I	151/153 (99%)	110 (73%)	31 (20%)	10 (7%)	1	0
2	J	151/153 (99%)	129 (85%)	19 (13%)	3 (2%)	7	5
2	K	151/153 (99%)	127 (84%)	22 (15%)	2 (1%)	12	11
2	L	151/153 (99%)	88 (58%)	49 (32%)	14 (9%)	0	0
All	All	2754/2778 (99%)	2401 (87%)	292 (11%)	61 (2%)	6	4

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	117	HIS
2	I	22	PRO
2	I	34	LYS
2	I	69	ASP
2	L	7	LEU
2	L	69	ASP
2	L	118	ALA
1	A	85	GLY
1	A	120	GLY
1	B	85	GLY
1	B	130	GLY
1	C	85	GLY
1	C	219	MET
1	D	120	GLY
1	E	85	GLY
1	E	120	GLY
1	E	130	GLY
1	F	219	MET
2	G	51	GLY
2	G	52	GLU
2	I	38	THR
2	I	149	VAL
2	J	14	ARG
2	K	14	ARG
2	L	35	LEU
2	L	106	VAL
2	L	147	HIS
1	B	240	TYR
1	D	231	GLN
1	F	85	GLY
1	F	130	GLY
1	F	267	LEU
2	I	8	GLN
2	K	8	GLN
2	L	44	ILE
2	L	105	ASN
1	B	76	SER
1	D	85	GLY
1	E	267	LEU
2	L	47	ASN
2	L	73	GLN
1	B	267	LEU

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Mol	Chain	Res	Type
1	E	76	SER
2	G	117	HIS
2	I	72	ASP
2	I	105	ASN
2	J	95	SER
2	L	22	PRO
2	L	38	THR
2	L	97	PRO
1	A	270	VAL
1	D	219	MET
2	I	86	ILE
2	L	131	ALA
2	G	96	ARG
1	A	266	PRO
1	C	130	GLY
1	A	267	LEU
2	I	93	GLY
2	G	97	PRO
2	J	115	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	261/261 (100%)	253 (97%)	8 (3%)	40	52
1	B	261/261 (100%)	252 (97%)	9 (3%)	37	48
1	C	261/261 (100%)	251 (96%)	10 (4%)	33	43
1	D	261/261 (100%)	254 (97%)	7 (3%)	44	57
1	E	261/261 (100%)	252 (97%)	9 (3%)	37	48
1	F	261/261 (100%)	253 (97%)	8 (3%)	40	52
2	G	137/137 (100%)	134 (98%)	3 (2%)	52	64
2	H	137/137 (100%)	132 (96%)	5 (4%)	35	46
2	I	137/137 (100%)	136 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	137/137 (100%)	132 (96%)	5 (4%)	35	46
2	K	137/137 (100%)	132 (96%)	5 (4%)	35	46
2	L	137/137 (100%)	135 (98%)	2 (2%)	65	76
All	All	2388/2388 (100%)	2316 (97%)	72 (3%)	41	52

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	59	PHE
1	A	109	GLU
1	A	140	LEU
1	A	233	GLU
1	A	265	HIS
1	A	271	ASP
1	A	285	TYR
1	B	13	ASN
1	B	17	ARG
1	B	59	PHE
1	B	131	SER
1	B	140	LEU
1	B	233	GLU
1	B	271	ASP
1	B	285	TYR
1	B	287	GLN
1	C	13	ASN
1	C	17	ARG
1	C	59	PHE
1	C	104	MET
1	C	109	GLU
1	C	134	HIS
1	C	140	LEU
1	C	233	GLU
1	C	271	ASP
1	C	287	GLN
1	D	13	ASN
1	D	59	PHE
1	D	140	LEU
1	D	233	GLU
1	D	271	ASP
1	D	285	TYR

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Mol	Chain	Res	Type
1	D	287	GLN
1	E	13	ASN
1	E	59	PHE
1	E	109	GLU
1	E	131	SER
1	E	140	LEU
1	E	233	GLU
1	E	271	ASP
1	E	285	TYR
1	E	287	GLN
1	F	13	ASN
1	F	59	PHE
1	F	134	HIS
1	F	140	LEU
1	F	233	GLU
1	F	271	ASP
1	F	285	TYR
1	F	287	GLN
2	G	108	VAL
2	G	141	CYS
2	G	147	HIS
2	H	38	THR
2	H	80	GLN
2	H	111	ASN
2	H	138	CYS
2	H	147	HIS
2	I	147	HIS
2	J	77	TYR
2	J	101	GLU
2	J	103	ILE
2	J	104	ASP
2	J	146	SER
2	K	30	LEU
2	K	39	ASP
2	K	84	ASN
2	K	88	ASN
2	K	101	GLU
2	L	133	ASP
2	L	137	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	21	ASN
1	A	35	GLN
1	A	156	HIS
1	A	246	GLN
1	A	291	ASN
1	B	13	ASN
1	B	21	ASN
1	B	35	GLN
1	B	156	HIS
1	B	242	ASN
1	B	246	GLN
1	B	287	GLN
1	B	291	ASN
1	C	13	ASN
1	C	21	ASN
1	C	35	GLN
1	C	137	GLN
1	C	156	HIS
1	C	246	GLN
1	C	287	GLN
1	C	291	ASN
1	C	297	GLN
1	D	21	ASN
1	D	35	GLN
1	D	137	GLN
1	D	156	HIS
1	D	246	GLN
1	D	287	GLN
1	D	291	ASN
1	D	297	GLN
1	D	305	ASN
1	E	13	ASN
1	E	21	ASN
1	E	35	GLN
1	E	156	HIS
1	E	246	GLN
1	E	291	ASN
1	E	297	GLN
1	E	305	ASN
1	F	13	ASN
1	F	21	ASN
1	F	35	GLN

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Mol	Chain	Res	Type
1	F	137	GLN
1	F	156	HIS
1	F	242	ASN
1	F	246	GLN
1	F	287	GLN
1	F	291	ASN
1	F	297	GLN
2	G	47	ASN
2	G	63	ASN
2	G	84	ASN
2	G	147	HIS
2	G	148	ASN
2	H	70	GLN
2	H	84	ASN
2	H	88	ASN
2	H	111	ASN
2	H	113	ASN
2	H	117	HIS
2	H	147	HIS
2	H	148	ASN
2	I	3	HIS
2	I	47	ASN
2	I	63	ASN
2	I	111	ASN
2	I	132	ASN
2	I	147	HIS
2	I	148	ASN
2	I	153	ASN
2	J	84	ASN
2	J	113	ASN
2	J	147	HIS
2	K	20	HIS
2	K	47	ASN
2	K	63	ASN
2	K	73	GLN
2	K	84	ASN
2	K	88	ASN
2	K	113	ASN
2	K	147	HIS
2	L	40	GLN
2	L	63	ASN
2	L	73	GLN

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Mol	Chain	Res	Type
2	L	113	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PAL	B	1002	-	9,15,15	2.54	4 (44%)	11,21,21	1.71	2 (18%)
3	PAL	F	1006	-	9,15,15	2.52	5 (55%)	11,21,21	1.62	2 (18%)
3	PAL	E	1005	-	9,15,15	1.98	4 (44%)	11,21,21	2.07	2 (18%)
3	PAL	A	1001	-	9,15,15	2.67	5 (55%)	11,21,21	1.53	2 (18%)
3	PAL	D	1004	-	9,15,15	2.42	4 (44%)	11,21,21	1.80	2 (18%)
3	PAL	C	1003	-	9,15,15	2.36	5 (55%)	11,21,21	1.59	2 (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	PAL	B	1002	-	-	2/11/17/17	-
3	PAL	F	1006	-	-	2/11/17/17	-
3	PAL	E	1005	-	-	2/11/17/17	-
3	PAL	A	1001	-	-	0/11/17/17	-
3	PAL	D	1004	-	-	2/11/17/17	-
3	PAL	C	1003	-	-	3/11/17/17	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	PAL	C3-C2	4.92	1.60	1.53
3	A	1001	PAL	C3-C2	4.82	1.60	1.53
3	F	1006	PAL	C3-C2	4.44	1.59	1.53
3	D	1004	PAL	C3-C2	4.27	1.59	1.53
3	C	1003	PAL	C3-C2	3.71	1.58	1.53
3	A	1001	PAL	C2-N2	-3.62	1.41	1.46
3	C	1003	PAL	C2-N2	-3.47	1.42	1.46
3	D	1004	PAL	C2-N2	-3.38	1.42	1.46
3	F	1006	PAL	C2-N2	-3.20	1.42	1.46
3	B	1002	PAL	C2-N2	-3.11	1.42	1.46
3	A	1001	PAL	P-C1P	3.01	1.84	1.79
3	D	1004	PAL	P-C1P	2.98	1.84	1.79
3	F	1006	PAL	P-O1P	-2.96	1.44	1.50
3	E	1005	PAL	P-O1P	-2.87	1.44	1.50
3	E	1005	PAL	P-C1P	2.80	1.84	1.79
3	B	1002	PAL	P-O1P	-2.76	1.44	1.50
3	C	1003	PAL	P-O2P	-2.58	1.49	1.54
3	E	1005	PAL	C3-C2	2.54	1.57	1.53
3	F	1006	PAL	P-O2P	-2.46	1.49	1.54
3	B	1002	PAL	P-C1P	2.43	1.83	1.79
3	A	1001	PAL	C1-N2	-2.36	1.28	1.34
3	A	1001	PAL	P-O1P	-2.33	1.45	1.50
3	F	1006	PAL	C1-N2	-2.31	1.29	1.34
3	D	1004	PAL	P-O1P	-2.31	1.45	1.50
3	C	1003	PAL	P-C1P	2.25	1.83	1.79
3	C	1003	PAL	P-O1P	-2.13	1.45	1.50
3	E	1005	PAL	C2-N2	-2.05	1.43	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1005	PAL	C2-N2-C1	5.81	132.57	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1004	PAL	C2-N2-C1	4.49	130.48	123.33
3	F	1006	PAL	C2-N2-C1	4.01	129.71	123.33
3	B	1002	PAL	C2-N2-C1	3.76	129.31	123.33
3	A	1001	PAL	C2-N2-C1	3.40	128.75	123.33
3	B	1002	PAL	C1P-C1-N2	3.36	118.39	115.19
3	C	1003	PAL	C2-N2-C1	3.33	128.63	123.33
3	C	1003	PAL	C1P-C1-N2	2.87	117.92	115.19
3	D	1004	PAL	C1P-C1-N2	2.76	117.82	115.19
3	E	1005	PAL	C1P-C1-N2	2.58	117.65	115.19
3	A	1001	PAL	C1P-C1-N2	2.41	117.49	115.19
3	F	1006	PAL	C1P-C1-N2	2.32	117.40	115.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1005	PAL	C4-C2-N2-C1
3	B	1002	PAL	C3-C2-N2-C1
3	F	1006	PAL	C3-C2-N2-C1
3	E	1005	PAL	C3-C2-N2-C1
3	D	1004	PAL	C3-C2-N2-C1
3	D	1004	PAL	C4-C2-N2-C1
3	B	1002	PAL	C4-C2-N2-C1
3	F	1006	PAL	C4-C2-N2-C1
3	C	1003	PAL	C3-C2-N2-C1
3	C	1003	PAL	C4-C2-N2-C1
3	C	1003	PAL	C1-C1P-P-O3P

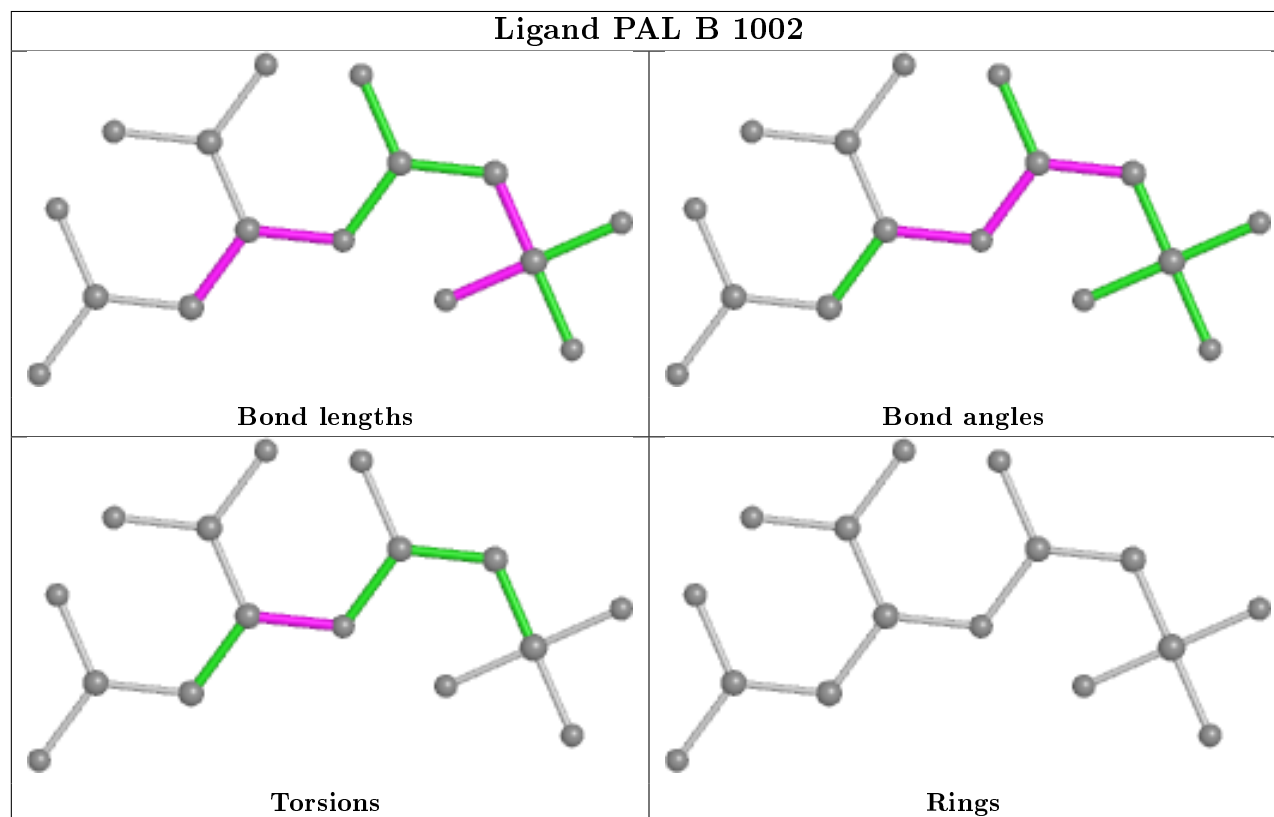
There are no ring outliers.

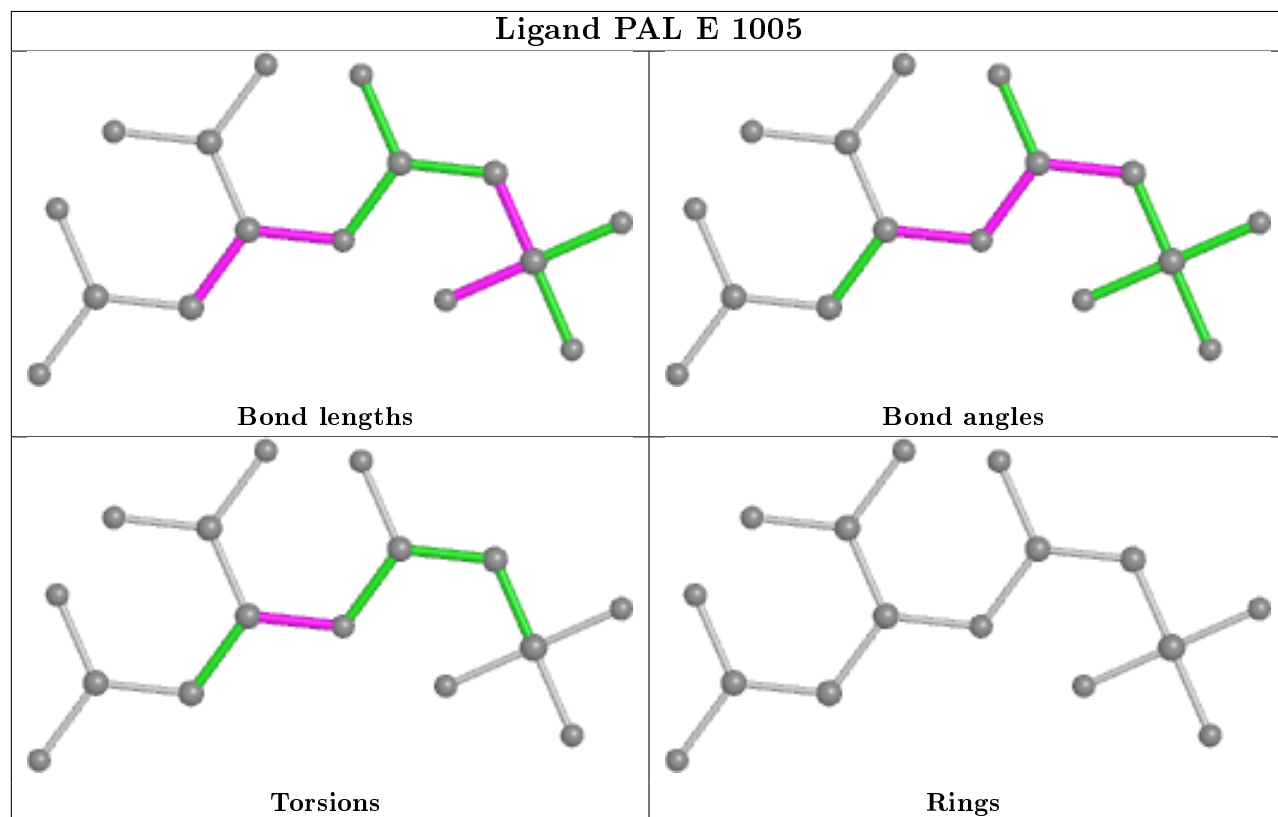
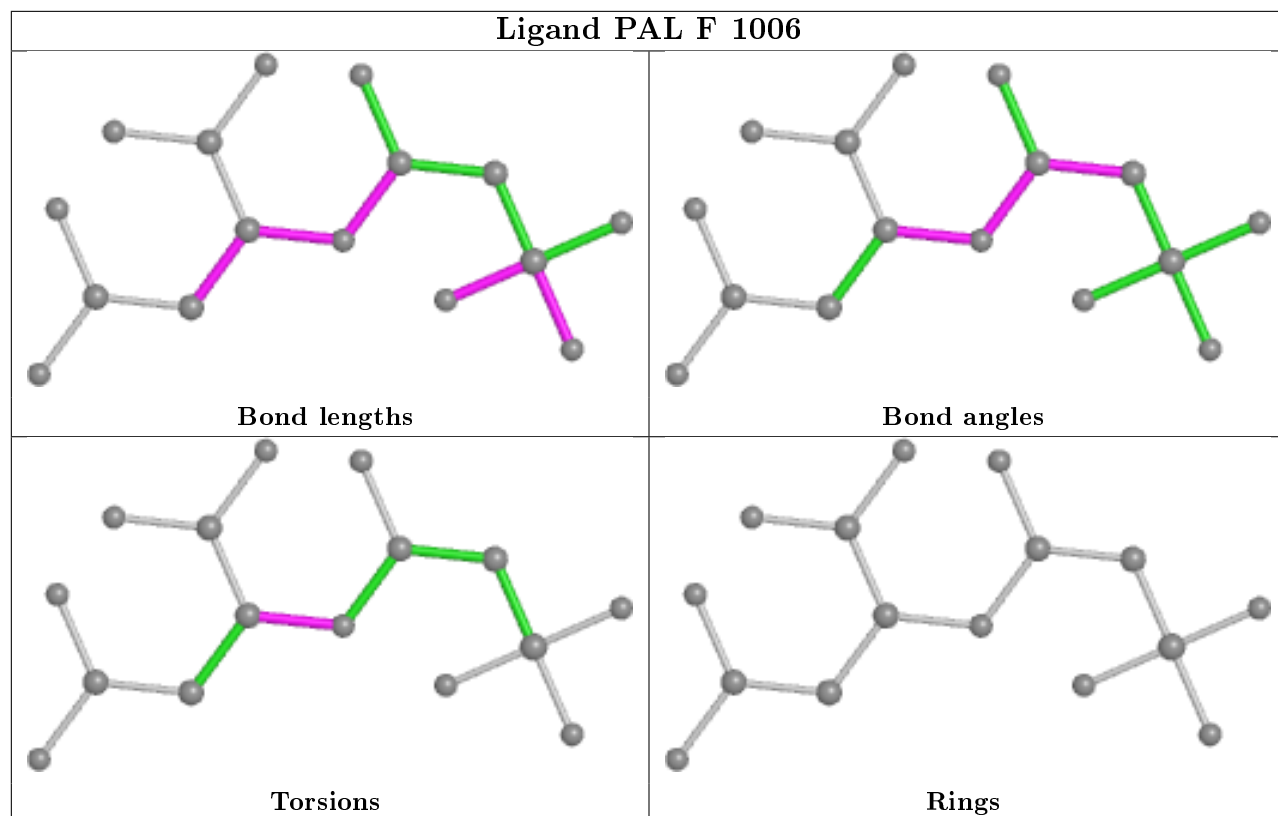
4 monomers are involved in 5 short contacts:

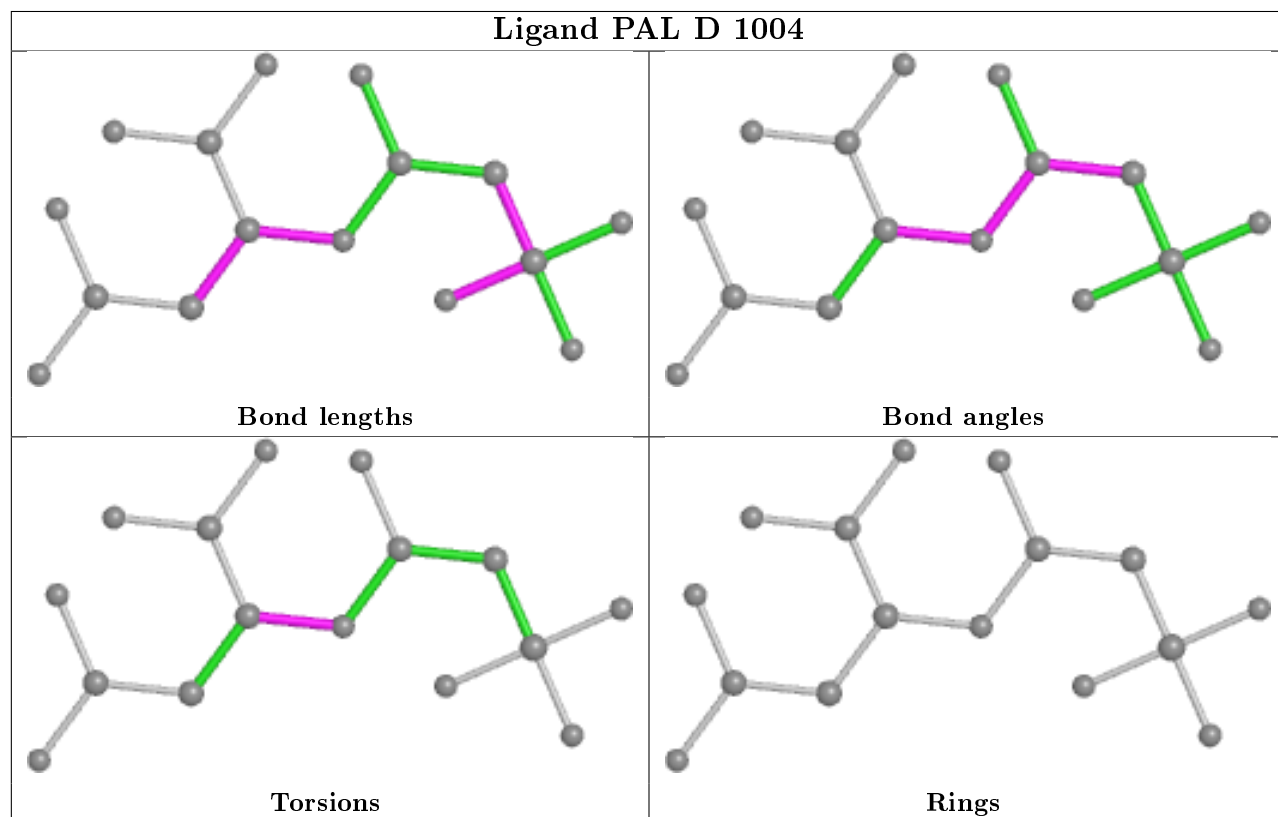
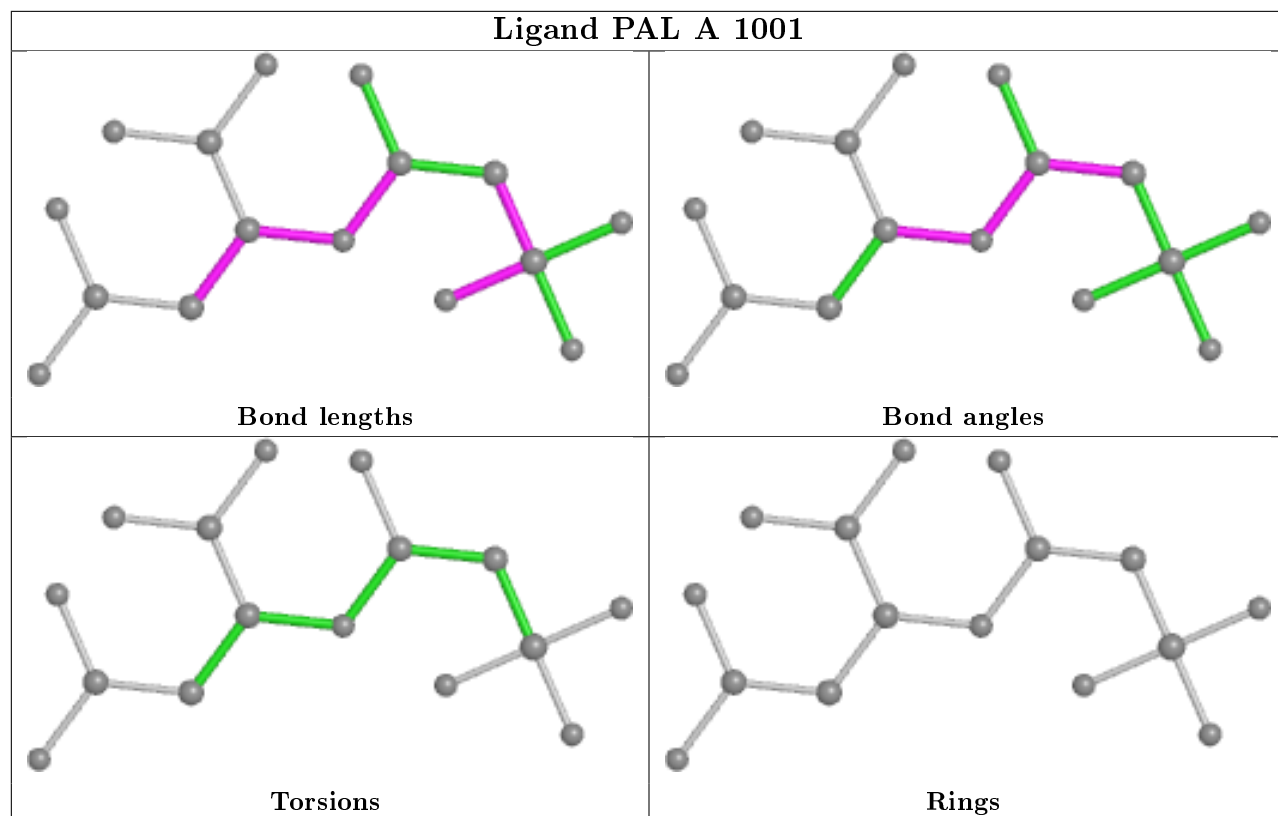
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	PAL	2	0
3	E	1005	PAL	1	0
3	A	1001	PAL	1	0
3	D	1004	PAL	1	0

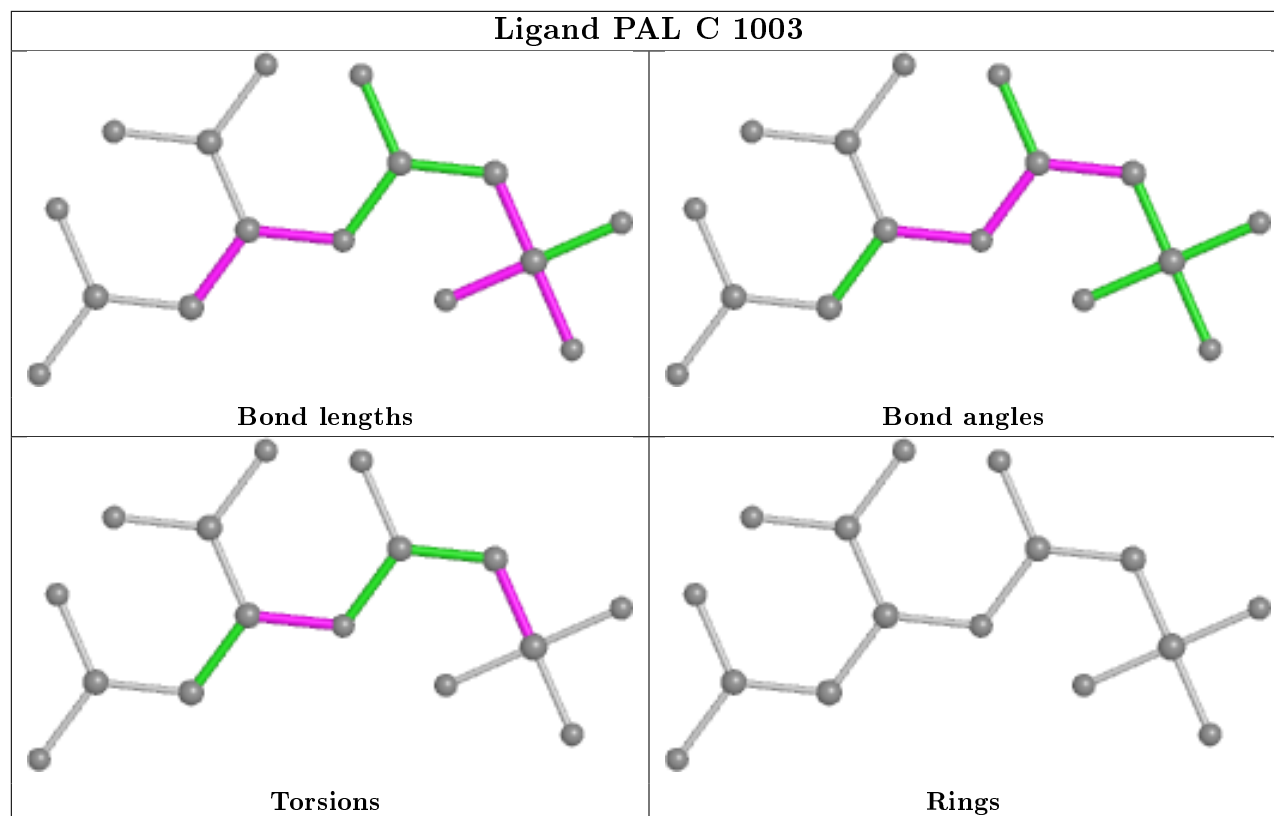
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	310/310 (100%)	1.85	120 (38%) 0 0	26, 41, 87, 123	0
1	B	310/310 (100%)	1.83	103 (33%) 0 0	23, 45, 101, 117	0
1	C	310/310 (100%)	2.01	136 (43%) 0 0	26, 50, 92, 116	0
1	D	310/310 (100%)	2.26	159 (51%) 0 0	32, 56, 99, 131	0
1	E	310/310 (100%)	2.49	174 (56%) 0 0	32, 58, 104, 126	0
1	F	310/310 (100%)	1.93	127 (40%) 0 0	31, 45, 94, 129	0
2	G	153/153 (100%)	2.46	72 (47%) 0 0	40, 60, 140, 153	0
2	H	153/153 (100%)	2.08	62 (40%) 0 0	36, 58, 134, 147	0
2	I	153/153 (100%)	5.00	123 (80%) 0 0	45, 125, 154, 163	0
2	J	153/153 (100%)	1.89	48 (31%) 0 0	38, 58, 133, 156	0
2	K	153/153 (100%)	2.87	87 (56%) 0 0	48, 74, 148, 169	0
2	L	153/153 (100%)	5.50	134 (87%) 0 0	49, 134, 157, 171	0
All	All	2778/2778 (100%)	2.47	1345 (48%) 0 0	23, 55, 139, 171	0

All (1345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	54	GLY	18.1
2	L	8	GLN	15.4
2	J	2	THR	14.3
2	I	54	GLY	13.9
2	I	11	ALA	12.9
1	F	309	VAL	12.6
2	I	89	TYR	12.3
2	I	151	LEU	12.1
2	I	86	ILE	11.9
1	D	79	THR	11.7
2	L	15	GLY	11.5

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASP	11.5
1	E	81	LEU	11.4
2	L	69	ASP	10.9
1	A	85	GLY	10.9
2	I	38	THR	10.8
2	L	38	THR	10.8
2	L	53	MET	10.7
2	L	50	SER	10.7
2	K	1	MET	10.6
2	G	2	THR	10.6
2	L	89	TYR	10.5
2	K	7	LEU	10.5
2	G	9	VAL	10.4
1	E	243	VAL	10.3
2	I	51	GLY	10.2
2	H	7	LEU	10.2
2	I	63	ASN	10.2
2	L	3	HIS	10.1
2	I	36	THR	10.1
2	I	15	GLY	10.1
2	L	132	ASN	10.1
1	A	81	LEU	10.0
1	D	236	ASP	9.9
2	I	14	ARG	9.9
1	F	81	LEU	9.8
2	J	7	LEU	9.7
2	K	132	ASN	9.6
1	B	237	PRO	9.5
2	K	3	HIS	9.5
2	K	9	VAL	9.4
2	L	1	MET	9.3
2	L	2	THR	9.3
2	L	49	PRO	9.2
2	L	7	LEU	9.2
2	I	98	SER	9.2
2	L	65	PHE	9.1
2	I	57	ASP	9.0
2	L	35	LEU	9.0
2	L	12	ILE	9.0
2	L	61	ILE	9.0
2	I	3	HIS	9.0
2	I	64	THR	8.9

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Mol	Chain	Res	Type	RSRZ
2	K	5	ASN	8.9
2	K	50	SER	8.8
2	I	66	LEU	8.8
2	H	4	ASP	8.8
2	I	65	PHE	8.8
2	I	84	ASN	8.8
1	A	79	THR	8.7
2	I	67	SER	8.8
2	I	88	ASN	8.7
1	E	237	PRO	8.7
2	L	76	LEU	8.7
2	L	22	PRO	8.6
2	I	69	ASP	8.6
2	L	96	ARG	8.6
2	L	36	THR	8.6
2	L	71	VAL	8.5
1	C	81	LEU	8.5
2	L	66	LEU	8.5
2	K	6	LYS	8.5
2	I	39	ASP	8.5
2	H	10	GLU	8.4
2	L	34	LYS	8.4
2	L	6	LYS	8.3
1	D	80	SER	8.3
1	E	236	ASP	8.3
2	L	105	ASN	8.3
2	L	77	TYR	8.3
2	L	86	ILE	8.3
2	I	80	GLN	8.2
2	L	91	VAL	8.1
2	I	43	THR	8.1
2	L	67	SER	8.1
2	I	7	LEU	8.1
1	B	81	LEU	8.0
2	H	3	HIS	8.0
2	L	51	GLY	8.0
2	I	12	ILE	8.0
2	H	5	ASN	7.9
2	L	4	ASP	7.9
2	L	90	GLU	7.9
2	I	40	GLN	7.9
2	L	88	ASN	7.9

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Mol	Chain	Res	Type	RSRZ
2	L	42	ILE	7.9
2	K	2	THR	7.8
2	I	68	GLU	7.8
2	I	70	GLN	7.7
2	L	92	VAL	7.7
2	L	80	GLN	7.7
2	L	52	GLU	7.7
2	L	133	ASP	7.7
2	L	11	ALA	7.6
2	L	25	ILE	7.6
2	L	98	SER	7.5
2	I	73	GLN	7.5
2	G	7	LEU	7.5
2	I	92	VAL	7.5
2	G	93	GLY	7.5
1	D	310	LEU	7.5
2	L	39	ASP	7.4
2	L	14	ARG	7.4
2	I	71	VAL	7.4
2	I	5	ASN	7.4
1	C	255	HIS	7.4
1	B	79	THR	7.3
2	H	2	THR	7.3
2	L	131	ALA	7.2
1	B	243	VAL	7.2
1	E	85	GLY	7.2
2	I	1	MET	7.2
1	F	243	VAL	7.2
2	I	91	VAL	7.2
2	J	9	VAL	7.2
2	K	10	GLU	7.2
2	K	68	GLU	7.2
2	L	5	ASN	7.2
2	I	152	ALA	7.2
2	J	4	ASP	7.1
2	L	33	PHE	7.1
1	C	236	ASP	7.1
2	G	87	ASP	7.1
2	I	23	ALA	7.1
1	D	81	LEU	7.0
2	L	27	PHE	7.0
2	G	88	ASN	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	7.0
2	K	152	ALA	7.0
2	I	85	ARG	6.9
2	L	100	PRO	6.9
2	I	30	LEU	6.9
2	I	32	LEU	6.9
2	L	10	GLU	6.9
1	C	237	PRO	6.8
1	F	237	PRO	6.8
1	A	236	ASP	6.8
2	L	9	VAL	6.8
2	G	153	ASN	6.8
2	L	153	ASN	6.8
1	C	77	ALA	6.7
2	L	82	THR	6.7
2	L	75	ALA	6.7
2	L	72	ASP	6.7
2	L	79	PRO	6.7
2	I	31	SER	6.7
2	I	47	ASN	6.6
2	L	70	GLN	6.6
1	E	33	ASN	6.6
2	L	84	ASN	6.6
1	E	310	LEU	6.6
2	I	2	THR	6.6
2	K	54	GLY	6.6
2	I	90	GLU	6.6
2	G	6	LYS	6.6
2	J	1	MET	6.6
2	L	18	ILE	6.5
2	G	10	GLU	6.5
2	K	70	GLN	6.5
1	C	80	SER	6.5
1	E	255	HIS	6.5
2	K	153	ASN	6.4
2	L	87	ASP	6.4
2	J	153	ASN	6.4
1	E	82	GLY	6.4
2	I	95	SER	6.3
2	I	6	LYS	6.3
2	I	17	VAL	6.3
2	L	60	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
2	I	35	LEU	6.3
2	G	8	GLN	6.3
2	L	78	ALA	6.2
2	H	11	ALA	6.2
2	G	92	VAL	6.2
2	G	96	ARG	6.2
2	I	49	PRO	6.2
2	I	4	ASP	6.2
2	I	72	ASP	6.1
1	E	280	THR	6.1
2	L	148	ASN	6.1
2	L	64	THR	6.1
1	C	310	LEU	6.1
1	E	309	VAL	6.1
1	F	241	ALA	6.1
2	L	83	VAL	6.0
2	I	52	GLU	6.0
2	L	63	ASN	6.0
1	F	240	TYR	6.0
1	E	190	ASP	6.0
2	I	79	PRO	6.0
1	E	79	THR	6.0
2	G	133	ASP	6.0
2	H	1	MET	6.0
2	G	3	HIS	6.0
2	L	47	ASN	5.9
2	L	57	ASP	5.9
2	I	37	GLU	5.9
2	I	42	ILE	5.9
1	F	242	ASN	5.9
2	I	133	ASP	5.9
1	E	307	ASP	5.8
2	I	41	ARG	5.8
2	L	40	GLN	5.8
2	I	93	GLY	5.8
2	L	37	GLU	5.8
2	I	149	VAL	5.7
2	J	132	ASN	5.7
2	I	53	MET	5.7
2	L	68	GLU	5.7
1	D	30	LEU	5.6
1	D	280	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	267	LEU	5.6
2	L	17	VAL	5.6
2	H	88	ASN	5.6
1	E	120	GLY	5.6
1	D	255	HIS	5.6
1	A	78	ASN	5.6
1	C	79	THR	5.6
2	I	19	ASP	5.6
1	D	32	ALA	5.6
1	F	79	THR	5.6
2	L	95	SER	5.6
1	E	1	ALA	5.5
2	L	55	ARG	5.5
2	K	67	SER	5.5
2	I	33	PHE	5.5
2	I	48	LEU	5.5
2	K	148	ASN	5.4
1	A	84	LYS	5.4
2	G	67	SER	5.4
2	L	19	ASP	5.4
2	G	95	SER	5.4
2	I	153	ASN	5.4
2	H	6	LYS	5.4
2	I	81	ALA	5.4
1	F	85	GLY	5.3
1	A	190	ASP	5.3
2	I	25	ILE	5.3
1	A	237	PRO	5.3
2	I	96	ARG	5.3
2	G	152	ALA	5.3
2	J	3	HIS	5.3
2	I	59	ILE	5.3
2	I	9	VAL	5.3
1	C	252	SER	5.3
1	C	189	PRO	5.3
2	G	151	LEU	5.3
2	L	46	LEU	5.3
2	K	52	GLU	5.3
2	I	34	LYS	5.3
2	K	4	ASP	5.2
2	L	43	THR	5.2
1	E	140	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	57	LEU	5.2
1	D	240	TYR	5.2
2	I	18	ILE	5.2
2	L	13	LYS	5.2
1	E	202	LEU	5.2
2	I	13	LYS	5.1
2	H	87	ASP	5.1
1	D	84	LYS	5.1
2	G	132	ASN	5.1
1	E	241	ALA	5.1
2	L	97	PRO	5.1
1	E	121	ASN	5.1
2	J	8	GLN	5.1
2	G	1	MET	5.1
1	D	94	VAL	5.1
2	J	10	GLU	5.1
1	E	252	SER	5.1
2	G	97	PRO	5.0
1	E	214	SER	5.0
2	I	61	ILE	5.0
1	E	20	LEU	5.0
1	C	82	GLY	5.0
1	D	252	SER	5.0
2	J	98	SER	5.0
1	E	242	ASN	5.0
2	K	53	MET	5.0
2	L	93	GLY	5.0
2	L	23	ALA	4.9
1	A	310	LEU	4.9
1	D	237	PRO	4.9
1	E	276	ASP	4.9
2	L	21	ILE	4.9
2	I	146	SER	4.9
1	D	176	LEU	4.9
1	E	139	LEU	4.9
2	K	8	GLN	4.9
2	L	104	ASP	4.9
1	D	76	SER	4.9
1	F	80	SER	4.9
2	I	83	VAL	4.9
1	B	240	TYR	4.9
2	I	26	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	267	LEU	4.9
2	I	150	VAL	4.9
2	H	153	ASN	4.9
2	K	100	PRO	4.9
2	L	147	HIS	4.9
1	D	77	ALA	4.9
2	G	131	ALA	4.9
1	B	267	LEU	4.9
1	D	195	PRO	4.9
1	A	255	HIS	4.9
1	B	255	HIS	4.9
2	L	20	HIS	4.9
1	A	80	SER	4.9
2	I	10	GLU	4.8
1	D	202	LEU	4.8
1	B	252	SER	4.8
2	I	74	LEU	4.8
1	E	238	SER	4.8
1	E	30	LEU	4.8
1	F	308	LEU	4.8
2	I	147	HIS	4.8
1	E	216	GLU	4.8
1	B	215	ILE	4.8
1	D	82	GLY	4.7
2	K	98	SER	4.7
2	J	133	ASP	4.7
2	K	51	GLY	4.7
2	L	62	GLU	4.7
1	B	190	ASP	4.7
1	F	236	ASP	4.7
1	D	243	VAL	4.7
1	E	144	THR	4.7
1	B	84	LYS	4.7
2	I	75	ALA	4.7
2	K	11	ALA	4.7
2	L	134	ILE	4.7
2	I	50	SER	4.7
2	I	82	THR	4.7
1	C	20	LEU	4.7
1	C	202	LEU	4.7
2	H	67	SER	4.6
1	D	216	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
2	I	97	PRO	4.6
2	I	46	LEU	4.6
2	L	94	LYS	4.6
2	K	151	LEU	4.6
2	L	146	SER	4.6
1	D	95	ILE	4.6
1	E	154	ASN	4.6
2	L	16	THR	4.6
2	K	101	GLU	4.6
1	B	33	ASN	4.6
1	F	190	ASP	4.6
2	J	6	LYS	4.6
2	L	151	LEU	4.6
2	H	9	VAL	4.5
2	K	55	ARG	4.5
2	L	130	ARG	4.5
2	L	138	CYS	4.5
1	D	276	ASP	4.5
1	E	169	VAL	4.5
1	C	280	THR	4.5
1	B	242	ASN	4.5
1	F	267	LEU	4.5
2	K	66	LEU	4.5
1	C	241	ALA	4.5
1	D	33	ASN	4.5
2	G	11	ALA	4.5
2	L	74	LEU	4.5
2	K	79	PRO	4.5
1	E	145	ILE	4.5
1	A	57	LEU	4.5
2	L	30	LEU	4.5
2	G	99	LEU	4.5
1	C	15	LEU	4.4
1	E	136	THR	4.4
2	I	62	GLU	4.4
1	D	20	LEU	4.4
2	H	98	SER	4.4
1	F	83	LYS	4.4
2	G	98	SER	4.4
1	E	80	SER	4.4
1	E	95	ILE	4.4
1	D	279	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	85	GLY	4.4
1	D	172	LEU	4.4
2	I	24	GLN	4.4
1	C	214	SER	4.4
1	C	216	GLU	4.4
1	D	244	LYS	4.3
2	L	81	ALA	4.3
1	D	57	LEU	4.3
1	F	57	LEU	4.3
1	D	309	VAL	4.3
1	A	267	LEU	4.3
2	I	76	LEU	4.3
2	H	65	PHE	4.3
1	D	190	ASP	4.3
2	K	147	HIS	4.3
2	J	149	VAL	4.3
2	K	111	ASN	4.3
1	E	244	LYS	4.3
1	B	20	LEU	4.3
2	L	48	LEU	4.3
2	G	117	HIS	4.3
1	B	245	ALA	4.3
2	G	5	ASN	4.3
2	K	133	ASP	4.2
1	E	266	PRO	4.2
1	C	57	LEU	4.2
2	I	29	LEU	4.2
2	K	75	ALA	4.2
1	D	277	VAL	4.2
1	B	241	ALA	4.2
1	E	279	LYS	4.2
1	F	48	PHE	4.2
1	B	75	ASP	4.2
1	E	206	GLY	4.2
2	J	5	ASN	4.2
1	E	32	ALA	4.2
1	F	102	ILE	4.1
1	B	142	LEU	4.1
1	B	202	LEU	4.1
1	E	264	LEU	4.1
1	F	202	LEU	4.1
1	E	12	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	206	GLY	4.1
1	E	198	ILE	4.1
1	A	48	PHE	4.1
1	D	48	PHE	4.1
1	D	145	ILE	4.1
1	D	242	ASN	4.1
1	C	243	VAL	4.1
1	E	172	LEU	4.1
2	L	85	ARG	4.1
1	B	80	SER	4.1
1	E	240	TYR	4.1
1	B	83	LYS	4.1
1	B	256	ASN	4.1
2	K	146	SER	4.0
2	K	96	ARG	4.0
2	J	67	SER	4.0
2	K	80	GLN	4.0
2	H	138	CYS	4.0
1	D	85	GLY	4.0
1	C	242	ASN	4.0
1	E	201	MET	4.0
1	C	276	ASP	4.0
1	E	137	GLN	4.0
1	E	142	LEU	4.0
1	E	176	LEU	4.0
1	E	55	THR	4.0
1	A	216	GLU	4.0
2	K	118	ALA	4.0
2	J	130	ARG	4.0
1	E	74	SER	4.0
1	A	219	MET	4.0
1	E	293	ILE	4.0
2	G	39	ASP	4.0
2	G	94	LYS	4.0
1	E	268	PRO	4.0
1	C	85	GLY	4.0
1	F	39	LEU	3.9
2	I	148	ASN	4.0
2	H	90	GLU	3.9
2	L	121	VAL	3.9
1	B	238	SER	3.9
1	F	73	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	140	LEU	3.9
1	D	299	LEU	3.9
1	F	142	LEU	3.9
2	I	27	PHE	3.9
2	L	32	LEU	3.9
1	F	293	ILE	3.9
2	J	118	ALA	3.9
1	D	200	ASP	3.9
2	K	122	SER	3.9
2	L	99	LEU	3.9
1	C	251	ALA	3.9
2	H	118	ALA	3.9
2	G	148	ASN	3.9
1	D	74	SER	3.9
2	H	89	TYR	3.9
2	I	132	ASN	3.9
1	C	169	VAL	3.9
2	G	74	LEU	3.9
1	A	120	GLY	3.9
2	I	105	ASN	3.9
1	D	47	CYS	3.9
2	K	121	VAL	3.9
2	L	24	GLN	3.9
1	D	307	ASP	3.8
1	F	94	VAL	3.8
1	B	15	LEU	3.8
1	E	260	ASN	3.8
2	L	59	ILE	3.8
2	H	50	SER	3.8
1	C	142	LEU	3.8
2	J	50	SER	3.8
1	D	83	LYS	3.8
2	G	13	LYS	3.8
1	E	217	GLU	3.8
2	I	20	HIS	3.8
1	A	76	SER	3.8
1	B	78	ASN	3.8
1	E	218	VAL	3.8
1	F	71	VAL	3.8
1	F	76	SER	3.8
2	H	15	GLY	3.8
1	B	121	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	217	GLU	3.8
2	K	39	ASP	3.8
2	J	11	ALA	3.7
2	I	21	ILE	3.7
2	H	8	GLN	3.7
1	D	238	SER	3.7
1	C	257	ALA	3.7
1	D	72	GLY	3.7
1	C	240	TYR	3.7
1	A	92	ILE	3.7
1	E	83	LYS	3.7
2	H	39	ASP	3.7
2	I	22	PRO	3.7
1	C	198	ILE	3.7
1	A	300	LEU	3.7
1	E	138	THR	3.7
2	I	131	ALA	3.7
1	D	73	PHE	3.7
2	G	4	ASP	3.7
2	J	146	SER	3.7
1	A	243	VAL	3.7
1	F	74	SER	3.7
1	F	310	LEU	3.7
2	G	90	GLU	3.7
2	J	111	ASN	3.6
2	I	87	ASP	3.6
1	A	241	ALA	3.6
1	B	77	ALA	3.6
1	F	59	PHE	3.6
2	J	12	ILE	3.6
1	D	103	VAL	3.6
1	A	252	SER	3.6
1	C	266	PRO	3.6
1	E	153	ASP	3.6
1	B	172	LEU	3.6
1	B	216	GLU	3.6
1	E	103	VAL	3.6
2	K	30	LEU	3.6
1	A	280	THR	3.6
1	C	1	ALA	3.6
1	E	259	ALA	3.6
1	A	215	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	49	PRO	3.6
1	B	244	LYS	3.6
2	G	51	GLY	3.6
2	H	92	VAL	3.6
1	C	190	ASP	3.6
1	F	18	ASP	3.6
2	I	16	THR	3.6
2	H	95	SER	3.5
1	E	75	ASP	3.5
1	E	257	ALA	3.5
2	J	114	CYS	3.5
1	F	103	VAL	3.5
1	F	244	LYS	3.5
1	D	136	THR	3.5
1	F	280	THR	3.5
1	F	215	ILE	3.5
1	D	253	ASP	3.5
1	C	173	THR	3.5
1	B	94	VAL	3.5
1	F	46	SER	3.5
2	G	149	VAL	3.5
1	D	256	ASN	3.5
1	C	172	LEU	3.5
1	E	15	LEU	3.5
1	E	254	LEU	3.5
2	J	151	LEU	3.5
2	L	135	ALA	3.5
1	C	94	VAL	3.5
1	A	59	PHE	3.5
1	A	242	ASN	3.5
1	A	139	LEU	3.5
1	D	142	LEU	3.5
1	E	300	LEU	3.5
2	L	122	SER	3.5
1	A	140	LEU	3.5
2	I	109	CYS	3.5
2	L	41	ARG	3.5
1	B	307	ASP	3.5
1	E	76	SER	3.5
1	E	71	VAL	3.5
2	G	91	VAL	3.5
1	D	29	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	58	LEU	3.4
1	B	175	ALA	3.4
1	D	28	ALA	3.4
2	L	28	LYS	3.4
1	A	124	VAL	3.4
1	C	144	THR	3.4
1	A	266	PRO	3.4
1	C	196	GLN	3.4
1	A	95	ILE	3.4
2	K	25	ILE	3.4
2	K	104	ASP	3.4
1	A	138	THR	3.4
1	C	33	ASN	3.4
1	F	307	ASP	3.4
1	D	15	LEU	3.4
1	A	127	ALA	3.4
1	D	24	LEU	3.4
1	F	114	LEU	3.4
1	A	121	ASN	3.4
1	D	104	MET	3.4
1	C	139	LEU	3.4
1	D	46	SER	3.4
1	E	4	LEU	3.4
1	F	4	LEU	3.4
1	E	303	VAL	3.4
2	L	129	LYS	3.4
2	H	63	ASN	3.3
1	B	235	LEU	3.3
1	D	241	ALA	3.3
2	H	72	ASP	3.3
1	E	115	ALA	3.3
1	D	146	GLN	3.3
1	D	239	GLU	3.3
1	C	71	VAL	3.3
1	D	71	VAL	3.3
1	D	264	LEU	3.3
1	E	253	ASP	3.3
1	C	95	ILE	3.3
1	E	226	TYR	3.3
2	I	101	GLU	3.3
1	C	121	ASN	3.3
1	D	271	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	254	LEU	3.3
1	F	172	LEU	3.3
1	D	275	THR	3.3
2	J	115	ILE	3.3
1	D	121	ASN	3.3
1	C	238	SER	3.3
1	E	53	THR	3.3
1	E	77	ALA	3.3
1	F	95	ILE	3.3
1	C	213	SER	3.3
1	B	293	ILE	3.3
1	D	59	PHE	3.3
1	D	102	ILE	3.3
1	F	92	ILE	3.3
1	A	82	GLY	3.3
2	K	102	ARG	3.3
2	L	31	SER	3.3
1	A	103	VAL	3.3
1	D	23	VAL	3.3
2	I	100	PRO	3.2
1	C	215	ILE	3.2
1	E	48	PHE	3.2
2	K	134	ILE	3.2
1	E	84	LYS	3.2
1	D	34	PRO	3.2
1	F	270	VAL	3.2
1	C	254	LEU	3.2
1	E	212	HIS	3.2
1	A	256	ASN	3.2
1	C	32	ALA	3.2
2	L	102	ARG	3.2
2	L	128	ARG	3.2
1	C	256	ASN	3.2
2	J	105	ASN	3.2
2	K	88	ASN	3.2
1	B	91	THR	3.2
1	C	253	ASP	3.2
2	G	147	HIS	3.2
1	F	136	THR	3.2
1	C	73	PHE	3.2
2	H	86	ILE	3.2
1	C	83	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	G	89	TYR	3.2
1	B	140	LEU	3.2
1	A	102	ILE	3.2
1	B	95	ILE	3.2
1	C	48	PHE	3.2
1	A	276	ASP	3.2
1	B	169	VAL	3.2
2	G	150	VAL	3.2
1	D	300	LEU	3.2
1	D	127	ALA	3.2
1	F	252	SER	3.2
1	F	276	ASP	3.2
1	D	246	GLN	3.2
1	E	256	ASN	3.2
1	E	205	LYS	3.2
1	A	202	LEU	3.2
1	B	71	VAL	3.2
1	E	127	ALA	3.1
1	F	199	LEU	3.2
2	G	86	ILE	3.1
1	C	244	LYS	3.1
2	K	149	VAL	3.1
2	G	104	ASP	3.1
1	A	214	SER	3.1
1	E	130	GLY	3.1
2	J	113	ASN	3.1
2	I	55	ARG	3.1
2	G	138	CYS	3.1
1	B	176	LEU	3.1
1	E	18	ASP	3.1
1	E	94	VAL	3.1
1	F	77	ALA	3.1
2	I	99	LEU	3.1
1	F	72	GLY	3.1
1	F	238	SER	3.1
2	L	125	PHE	3.1
2	K	72	ASP	3.1
2	K	20	HIS	3.1
2	K	90	GLU	3.1
1	F	139	LEU	3.1
1	D	270	VAL	3.1
1	F	82	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	127	VAL	3.1
1	B	102	ILE	3.1
1	C	12	ILE	3.1
1	E	73	PHE	3.1
1	F	84	LYS	3.1
1	D	75	ASP	3.1
2	J	104	ASP	3.1
2	G	68	GLU	3.1
1	E	21	ASN	3.1
2	H	66	LEU	3.1
1	C	279	LYS	3.1
1	A	260	ASN	3.1
1	B	82	GLY	3.1
1	A	74	SER	3.1
1	C	125	LEU	3.1
1	C	235	LEU	3.1
1	F	169	VAL	3.1
2	K	127	VAL	3.1
1	A	104	MET	3.0
1	B	226	TYR	3.0
2	K	89	TYR	3.0
2	L	111	ASN	3.0
1	B	57	LEU	3.0
1	C	46	SER	3.0
1	C	91	THR	3.0
1	D	53	THR	3.0
1	F	216	GLU	3.0
1	C	130	GLY	3.0
1	E	72	GLY	3.0
2	K	117	HIS	3.0
2	I	104	ASP	3.0
1	E	219	MET	3.0
2	L	73	GLN	3.0
1	A	259	ALA	3.0
1	B	300	LEU	3.0
1	D	61	THR	3.0
1	E	87	THR	3.0
1	F	75	ASP	3.0
2	H	29	LEU	3.0
1	F	104	MET	3.0
1	E	59	PHE	3.0
2	L	56	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	46	SER	3.0
1	B	299	LEU	3.0
1	F	32	ALA	3.0
1	F	125	LEU	3.0
2	L	136	LEU	3.0
1	B	198	ILE	3.0
1	D	22	LEU	3.0
1	F	266	PRO	3.0
1	F	47	CYS	3.0
1	C	145	ILE	3.0
2	K	12	ILE	3.0
2	K	95	SER	3.0
1	A	20	LEU	3.0
1	B	125	LEU	3.0
1	B	139	LEU	3.0
1	D	139	LEU	3.0
1	D	189	PRO	3.0
1	A	261	MET	2.9
1	A	125	LEU	2.9
1	D	274	ALA	2.9
2	H	70	GLN	2.9
2	I	111	ASN	2.9
1	A	18	ASP	2.9
1	A	293	ILE	2.9
1	C	59	PHE	2.9
1	E	215	ILE	2.9
2	G	12	ILE	2.9
2	J	23	ALA	2.9
1	C	102	ILE	2.9
2	J	148	ASN	2.9
1	A	47	CYS	2.9
1	E	299	LEU	2.9
2	H	141	CYS	2.9
1	E	134	HIS	2.9
1	A	23	VAL	2.9
1	E	306	ARG	2.9
2	L	103	ILE	2.9
1	E	180	ASP	2.9
1	A	66	LEU	2.9
1	C	30	LEU	2.9
1	E	24	LEU	2.9
1	E	25	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	155	LEU	2.9
1	F	264	LEU	2.9
1	D	4	LEU	2.9
1	F	196	GLN	2.9
1	C	84	LYS	2.9
2	I	28	LYS	2.9
2	I	77	TYR	2.9
1	C	270	VAL	2.9
2	L	149	VAL	2.9
1	E	2	ASN	2.9
1	F	78	ASN	2.9
1	E	143	PHE	2.9
1	B	266	PRO	2.9
1	C	17	ARG	2.9
1	A	172	LEU	2.9
1	B	264	LEU	2.9
1	F	138	THR	2.9
2	K	136	LEU	2.9
1	B	43	VAL	2.8
1	E	63	MET	2.8
2	H	91	VAL	2.8
2	I	45	GLY	2.8
1	A	83	LYS	2.8
1	D	92	ILE	2.8
1	F	300	LEU	2.8
1	E	78	ASN	2.8
2	I	112	SER	2.8
1	C	103	VAL	2.8
1	F	218	VAL	2.8
1	B	220	ALA	2.8
1	D	193	ALA	2.8
2	I	138	CYS	2.8
1	C	299	LEU	2.8
2	H	69	ASP	2.8
1	F	16	SER	2.8
2	K	123	SER	2.8
2	L	45	GLY	2.8
2	K	150	VAL	2.8
1	B	61	THR	2.8
1	F	127	ALA	2.8
1	C	176	LEU	2.8
1	F	15	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	30	LEU	2.8
2	G	29	LEU	2.8
2	K	109	CYS	2.8
1	C	104	MET	2.8
1	A	71	VAL	2.8
1	A	303	VAL	2.8
1	C	221	GLU	2.8
1	E	23	VAL	2.8
1	A	55	THR	2.8
1	A	279	LYS	2.8
2	J	117	HIS	2.8
2	G	72	ASP	2.8
1	A	44	ILE	2.8
1	B	280	THR	2.8
1	D	55	THR	2.8
2	L	118	ALA	2.8
1	B	24	LEU	2.8
1	C	300	LEU	2.8
1	D	254	LEU	2.8
1	F	140	LEU	2.8
2	H	112	SER	2.8
2	J	112	SER	2.8
1	D	153	ASP	2.8
2	G	70	GLN	2.8
1	A	295	ALA	2.8
1	C	92	ILE	2.8
1	F	87	THR	2.8
2	H	93	GLY	2.8
1	A	15	LEU	2.8
1	A	30	LEU	2.8
1	D	125	LEU	2.8
1	D	235	LEU	2.8
1	E	22	LEU	2.8
1	E	159	MET	2.8
1	C	239	GLU	2.7
2	K	114	CYS	2.7
1	A	12	ILE	2.7
2	H	13	LYS	2.7
2	H	30	LEU	2.7
2	K	74	LEU	2.7
1	F	296	ARG	2.7
1	A	153	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	219	MET	2.7
1	B	157	VAL	2.7
1	C	309	VAL	2.7
1	F	23	VAL	2.7
1	D	91	THR	2.7
1	D	179	PHE	2.7
1	E	245	ALA	2.7
1	E	247	PHE	2.7
2	I	118	ALA	2.7
1	A	299	LEU	2.7
1	C	267	LEU	2.7
1	E	46	SER	2.7
2	K	46	LEU	2.7
1	C	268	PRO	2.7
1	F	268	PRO	2.7
1	F	155	LEU	2.7
2	G	69	ASP	2.7
1	E	47	CYS	2.7
1	A	63	MET	2.7
1	C	120	GLY	2.7
1	E	56	ARG	2.7
1	A	136	THR	2.7
1	B	295	ALA	2.7
2	I	78	ALA	2.7
1	E	308	LEU	2.7
2	K	42	ILE	2.7
2	L	29	LEU	2.7
1	B	17	ARG	2.7
2	K	82	THR	2.7
1	D	215	ILE	2.7
1	E	235	LEU	2.7
2	J	147	HIS	2.7
1	E	181	GLY	2.7
1	D	63	MET	2.7
1	F	63	MET	2.7
1	C	23	VAL	2.7
1	A	25	ALA	2.7
1	C	61	THR	2.7
1	E	16	SER	2.7
1	F	274	ALA	2.7
1	C	88	LEU	2.7
2	I	60	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	76	SER	2.6
1	C	210	SER	2.6
1	F	144	THR	2.6
2	K	131	ALA	2.6
1	D	155	LEU	2.6
1	E	39	LEU	2.6
2	J	51	GLY	2.6
1	C	246	GLN	2.6
2	I	8	GLN	2.6
1	E	296	ARG	2.6
1	D	138	THR	2.6
1	D	168	THR	2.6
1	E	28	ALA	2.6
2	K	138	CYS	2.6
1	B	144	THR	2.6
1	C	55	THR	2.6
1	E	148	THR	2.6
2	L	145	PHE	2.6
1	F	159	MET	2.6
1	D	16	SER	2.6
2	G	146	SER	2.6
1	A	169	VAL	2.6
1	C	206	GLY	2.6
1	C	220	ALA	2.6
1	F	88	LEU	2.6
2	K	119	GLU	2.6
1	F	120	GLY	2.6
1	A	26	THR	2.6
1	A	4	LEU	2.6
1	A	22	LEU	2.6
1	B	145	ILE	2.6
1	F	145	ILE	2.6
2	J	90	GLU	2.6
1	A	226	TYR	2.6
1	D	150	GLY	2.6
1	D	278	ASP	2.6
1	E	19	ASP	2.6
1	D	43	VAL	2.6
1	E	277	VAL	2.6
1	A	189	PRO	2.6
1	C	155	LEU	2.6
1	E	104	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	203	ASP	2.6
1	A	240	TYR	2.6
1	C	138	THR	2.5
1	D	157	VAL	2.5
1	E	275	THR	2.5
1	B	59	PHE	2.5
1	D	98	TYR	2.5
1	C	168	THR	2.5
1	D	218	VAL	2.5
1	E	135	PRO	2.5
1	C	114	LEU	2.5
1	D	293	ILE	2.5
1	B	130	GLY	2.5
1	F	64	HIS	2.5
1	B	98	TYR	2.5
1	C	124	VAL	2.5
1	A	217	GLU	2.5
1	D	66	LEU	2.5
1	D	88	LEU	2.5
1	E	60	GLU	2.5
1	C	271	ASP	2.5
2	G	63	ASN	2.5
1	E	301	ALA	2.5
1	E	197	TYR	2.5
1	F	275	THR	2.5
2	G	64	THR	2.5
1	B	88	LEU	2.5
1	C	22	LEU	2.5
2	H	113	ASN	2.5
1	D	137	GLN	2.5
1	D	27	ALA	2.5
1	D	251	ALA	2.5
1	D	301	ALA	2.5
1	E	91	THR	2.5
1	E	168	THR	2.5
1	F	189	PRO	2.5
1	D	166	GLY	2.5
1	E	125	LEU	2.5
1	A	239	GLU	2.5
1	B	119	SER	2.5
1	C	184	PHE	2.5
1	E	207	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	49	PHE	2.5
2	K	59	ILE	2.5
1	C	201	MET	2.5
2	H	14	ARG	2.5
2	J	53	MET	2.5
2	I	94	LYS	2.5
1	E	203	ASP	2.5
1	D	130	GLY	2.5
1	B	4	LEU	2.5
2	L	150	VAL	2.5
1	F	214	SER	2.5
1	A	112	ALA	2.5
1	D	78	ASN	2.5
1	E	292	GLY	2.5
1	A	264	LEU	2.4
1	C	140	LEU	2.4
1	C	192	LEU	2.4
2	G	80	GLN	2.4
2	K	48	LEU	2.4
1	C	293	ILE	2.4
1	F	143	PHE	2.4
1	D	201	MET	2.4
2	J	72	ASP	2.4
1	E	34	PRO	2.4
1	F	2	ASN	2.4
1	C	137	GLN	2.4
1	D	56	ARG	2.4
2	K	71	VAL	2.4
1	D	159	MET	2.4
1	B	281	PRO	2.4
1	D	31	LYS	2.4
1	E	246	GLN	2.4
2	G	14	ARG	2.4
1	A	53	THR	2.4
1	A	115	ALA	2.4
1	C	87	THR	2.4
1	D	283	ALA	2.4
1	E	61	THR	2.4
1	A	309	VAL	2.4
2	H	68	GLU	2.4
2	H	83	VAL	2.4
2	J	68	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	187	ILE	2.4
1	F	44	ILE	2.4
2	H	109	CYS	2.4
1	F	13	ASN	2.4
1	D	266	PRO	2.4
2	L	117	HIS	2.4
1	F	61	THR	2.4
1	E	239	GLU	2.4
1	F	157	VAL	2.4
2	I	106	VAL	2.4
1	A	145	ILE	2.4
1	B	104	MET	2.4
1	C	207	ILE	2.4
2	G	25	ILE	2.4
2	G	134	ILE	2.4
2	H	105	ASN	2.4
1	F	135	PRO	2.4
2	I	114	CYS	2.4
1	D	204	GLU	2.4
1	C	26	THR	2.4
1	C	295	ALA	2.4
1	D	26	THR	2.4
1	E	173	THR	2.4
2	J	131	ALA	2.4
1	D	18	ASP	2.4
1	A	39	LEU	2.4
1	A	88	LEU	2.4
1	D	211	LEU	2.4
1	E	305	ASN	2.4
2	L	44	ILE	2.4
1	D	184	PHE	2.4
1	E	179	PHE	2.4
1	A	77	ALA	2.4
1	A	180	ASP	2.4
1	C	47	CYS	2.4
1	E	158	ALA	2.4
1	F	111	ALA	2.4
1	C	136	THR	2.4
1	D	196	GLN	2.4
1	A	128	GLY	2.4
1	F	239	GLU	2.4
1	B	12	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	159	MET	2.4
1	C	63	MET	2.4
1	D	64	HIS	2.4
1	E	223	ASP	2.4
1	F	295	ALA	2.4
2	K	130	ARG	2.4
1	D	87	THR	2.4
2	G	16	THR	2.4
1	E	213	SER	2.4
1	B	308	LEU	2.4
1	D	152	LEU	2.4
1	C	260	ASN	2.3
1	D	120	GLY	2.3
1	A	134	HIS	2.3
1	B	253	ASP	2.3
2	H	134	ILE	2.3
1	D	226	TYR	2.3
2	L	152	ALA	2.3
1	A	176	LEU	2.3
1	A	270	VAL	2.3
2	H	114	CYS	2.3
1	A	296	ARG	2.3
1	E	281	PRO	2.3
1	A	273	ILE	2.3
1	F	224	ILE	2.3
1	A	58	SER	2.3
1	E	210	SER	2.3
1	A	114	LEU	2.3
1	B	30	LEU	2.3
1	F	20	LEU	2.3
1	F	163	LEU	2.3
2	G	66	LEU	2.3
1	A	253	ASP	2.3
1	E	70	VAL	2.3
1	C	205	LYS	2.3
1	E	184	PHE	2.3
1	C	259	ALA	2.3
1	F	226	TYR	2.3
2	G	23	ALA	2.3
1	F	55	THR	2.3
1	A	221	GLU	2.3
1	B	66	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	221	GLU	2.3
1	F	304	LEU	2.3
1	F	137	GLN	2.3
2	G	28	LYS	2.3
2	I	56	LYS	2.3
1	A	277	VAL	2.3
1	C	70	VAL	2.3
1	F	198	ILE	2.3
1	D	247	PHE	2.3
2	G	65	PHE	2.3
1	A	16	SER	2.3
1	C	127	ALA	2.3
1	D	25	ALA	2.3
1	D	45	ALA	2.3
1	E	111	ALA	2.3
1	F	45	ALA	2.3
1	F	245	ALA	2.3
2	I	141	CYS	2.3
2	J	78	ALA	2.3
2	J	138	CYS	2.3
1	A	168	THR	2.3
2	H	52	GLU	2.3
2	H	54	GLY	2.3
2	K	105	ASN	2.3
1	B	32	ALA	2.3
1	D	214	SER	2.3
1	F	166	GLY	2.3
2	H	51	GLY	2.3
1	E	174	GLN	2.3
2	H	57	ASP	2.3
1	B	152	LEU	2.3
1	E	199	LEU	2.3
2	K	29	LEU	2.3
1	F	60	GLU	2.3
1	A	94	VAL	2.3
1	D	234	ARG	2.3
1	F	43	VAL	2.3
2	G	85	ARG	2.3
1	D	2	ASN	2.3
1	E	178	LYS	2.3
1	D	62	SER	2.3
1	D	207	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	2.3
1	B	48	PHE	2.3
1	D	295	ALA	2.3
1	B	136	THR	2.3
1	F	168	THR	2.3
1	D	192	LEU	2.3
1	D	199	LEU	2.3
1	D	154	ASN	2.2
1	D	169	VAL	2.2
1	F	121	ASN	2.2
2	L	108	VAL	2.2
1	A	75	ASP	2.2
2	K	112	SER	2.2
1	C	28	ALA	2.2
1	C	112	ALA	2.2
2	H	61	ILE	2.2
1	A	24	LEU	2.2
1	A	142	LEU	2.2
1	E	211	LEU	2.2
2	G	136	LEU	2.2
2	H	48	LEU	2.2
1	B	303	VAL	2.2
1	C	218	VAL	2.2
1	E	58	SER	2.2
1	D	224	ILE	2.2
1	E	112	ALA	2.2
2	I	145	PHE	2.2
2	I	102	ARG	2.2
1	E	152	LEU	2.2
1	A	137	GLN	2.2
1	B	239	GLU	2.2
2	J	69	ASP	2.2
1	A	70	VAL	2.2
1	B	218	VAL	2.2
1	C	43	VAL	2.2
1	F	70	VAL	2.2
2	G	114	CYS	2.2
2	J	122	SER	2.2
2	L	137	LYS	2.2
1	E	251	ALA	2.2
1	C	179	PHE	2.2
1	B	260	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	135	PRO	2.2
1	F	128	GLY	2.2
2	L	26	GLY	2.2
1	B	74	SER	2.2
2	G	50	SER	2.2
1	B	47	CYS	2.2
1	D	44	ILE	2.2
2	K	44	ILE	2.2
2	K	78	ALA	2.2
1	E	31	LYS	2.2
2	G	35	LEU	2.2
2	G	100	PRO	2.2
2	H	133	ASP	2.2
1	F	277	VAL	2.2
1	F	101	ALA	2.2
2	H	78	ALA	2.2
2	H	38	THR	2.2
1	B	268	PRO	2.2
1	F	299	LEU	2.2
2	K	22	PRO	2.2
1	D	306	ARG	2.2
2	I	123	SER	2.2
1	B	23	VAL	2.2
1	B	137	GLN	2.2
1	D	149	GLN	2.2
1	F	124	VAL	2.2
2	H	71	VAL	2.2
1	A	289	ALA	2.2
1	B	127	ALA	2.2
2	G	75	ALA	2.2
2	K	103	ILE	2.2
1	C	39	LEU	2.2
1	C	66	LEU	2.2
2	J	66	LEU	2.2
2	K	99	LEU	2.2
1	A	213	SER	2.2
1	D	19	ASP	2.1
1	E	124	VAL	2.1
1	F	303	VAL	2.1
2	G	83	VAL	2.1
1	B	92	ILE	2.1
1	B	120	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	102	ILE	2.1
2	J	38	THR	2.1
2	J	110	PRO	2.1
1	A	238	SER	2.1
2	H	40	GLN	2.1
1	C	75	ASP	2.1
1	C	197	TYR	2.1
1	E	141	ASP	2.1
1	E	271	ASP	2.1
1	C	277	VAL	2.1
1	E	284	TRP	2.1
1	F	1	ALA	2.1
1	C	44	ILE	2.1
1	D	40	LYS	2.1
1	E	92	ILE	2.1
2	G	79	PRO	2.1
2	L	115	ILE	2.1
1	B	39	LEU	2.1
2	K	32	LEU	2.1
1	B	213	SER	2.1
1	C	153	ASP	2.1
1	A	33	ASN	2.1
1	C	98	TYR	2.1
1	E	295	ALA	2.1
1	F	176	LEU	2.1
2	K	76	LEU	2.1
1	E	194	MET	2.1
1	B	177	ALA	2.1
1	C	25	ALA	2.1
1	B	195	PRO	2.1
1	E	228	THR	2.1
1	F	173	THR	2.1
1	C	4	LEU	2.1
1	C	199	LEU	2.1
1	C	264	LEU	2.1
1	A	119	SER	2.1
2	K	93	GLY	2.1
1	B	138	THR	2.1
1	C	204	GLU	2.1
1	D	167	ARG	2.1
1	F	91	THR	2.1
2	J	59	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	61	ILE	2.1
1	D	49	PHE	2.1
1	E	66	LEU	2.1
2	G	30	LEU	2.1
2	H	46	LEU	2.1
1	A	257	ALA	2.1
1	C	274	ALA	2.1
1	F	27	ALA	2.1
2	G	77	TYR	2.1
1	F	22	LEU	2.1
2	K	31	SER	2.1
1	C	287	GLN	2.1
1	A	298	ALA	2.0
1	E	3	PRO	2.0
2	K	23	ALA	2.0
1	D	70	VAL	2.0
1	E	270	VAL	2.0
1	A	9	ILE	2.0
1	B	285	TYR	2.0
1	D	114	LEU	2.0
1	E	45	ALA	2.0
2	H	64	THR	2.0
1	B	214	SER	2.0
1	A	10	ILE	2.0
2	H	58	LEU	2.0
1	D	175	ALA	2.0
1	F	255	HIS	2.0
2	L	109	CYS	2.0
1	B	309	VAL	2.0
1	C	24	LEU	2.0
2	H	21	ILE	2.0
1	E	231	GLN	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 carbohydrates in this entry.

6.4 Ligands

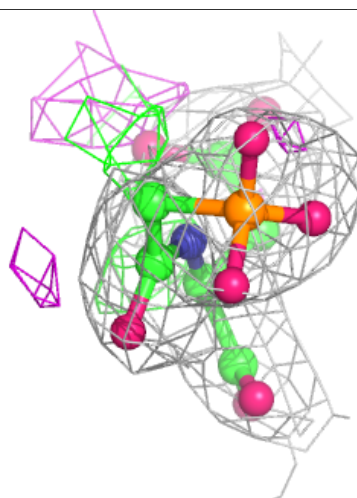
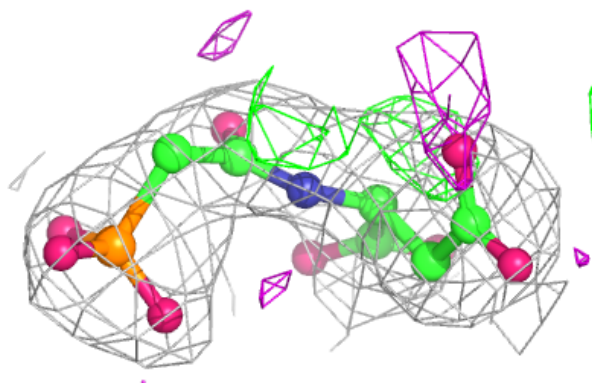
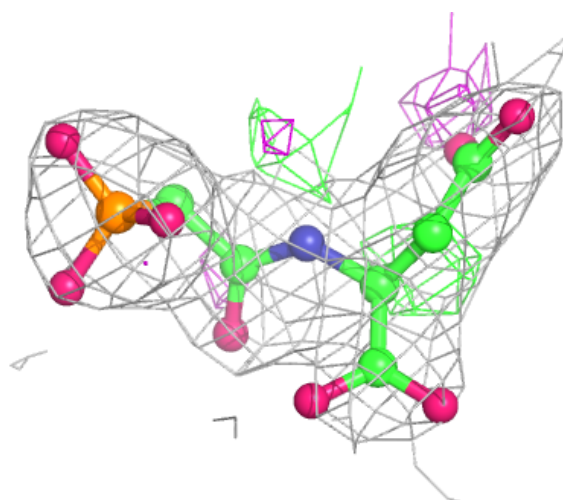
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	L	2006	1/1	0.89	0.08	53,53,53,53	0
3	PAL	E	1005	16/16	0.92	0.31	43,59,68,71	0
3	PAL	A	1001	16/16	0.94	0.26	36,44,48,49	0
3	PAL	D	1004	16/16	0.95	0.24	39,49,59,61	0
3	PAL	B	1002	16/16	0.95	0.25	35,45,53,57	0
3	PAL	C	1003	16/16	0.96	0.24	36,50,60,60	0
3	PAL	F	1006	16/16	0.97	0.21	35,45,57,59	0
4	ZN	G	2002	1/1	0.97	0.12	48,48,48,48	0
4	ZN	H	2001	1/1	0.98	0.08	50,50,50,50	0
4	ZN	J	2004	1/1	0.99	0.07	52,52,52,52	0
4	ZN	K	2005	1/1	0.99	0.08	53,53,53,53	0
4	ZN	I	2003	1/1	0.99	0.06	51,51,51,51	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.

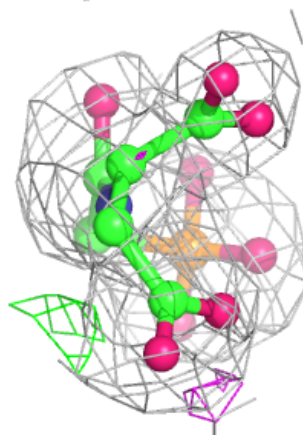
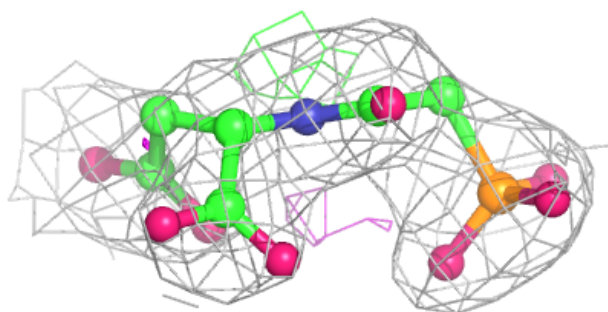
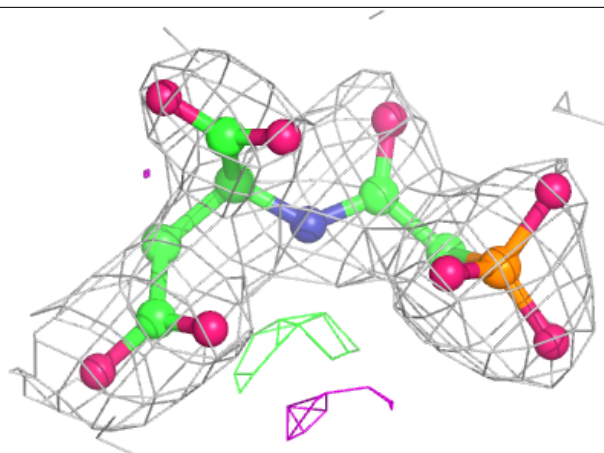
Electron density around PAL E 1005:

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



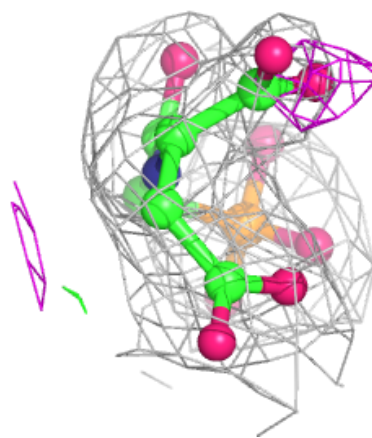
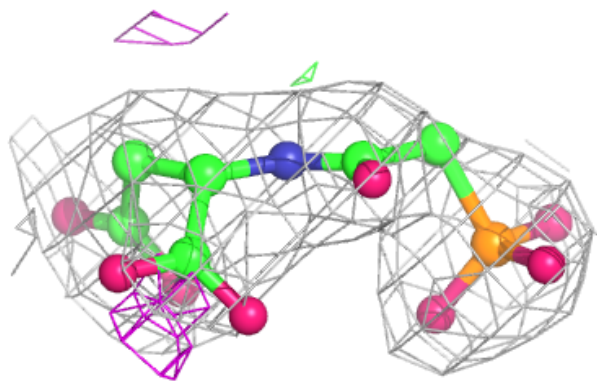
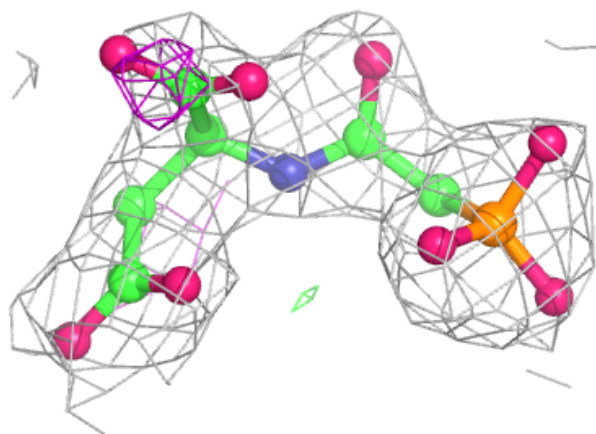
Electron density around PAL A 1001:

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



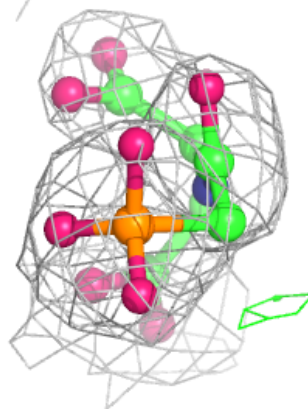
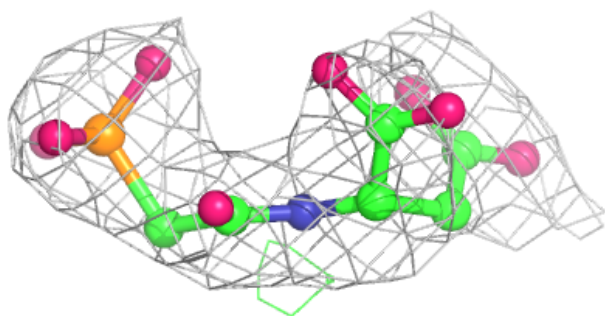
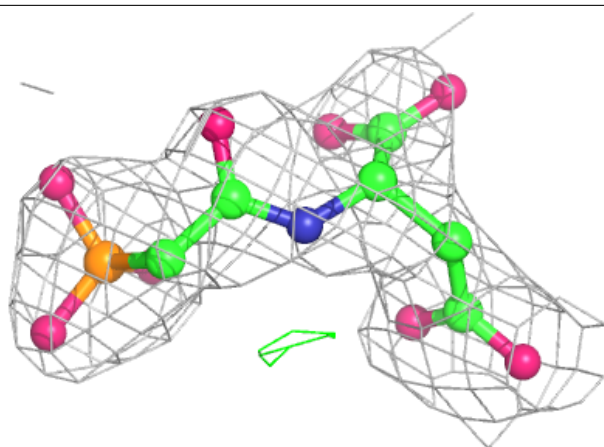
Electron density around PAL D 1004:

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



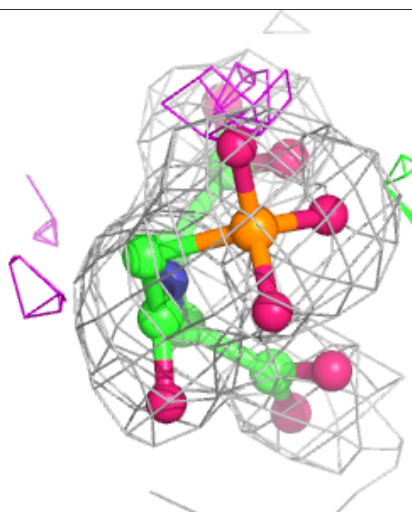
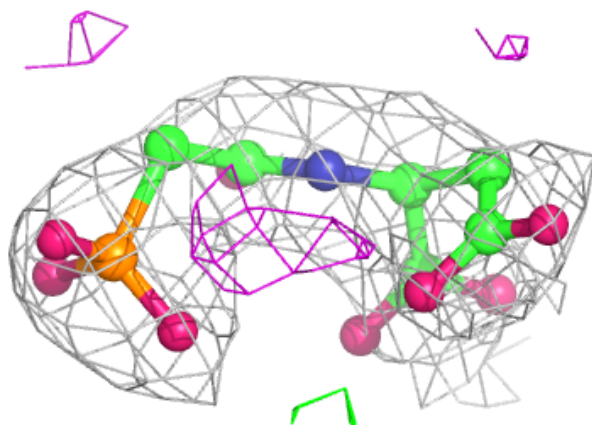
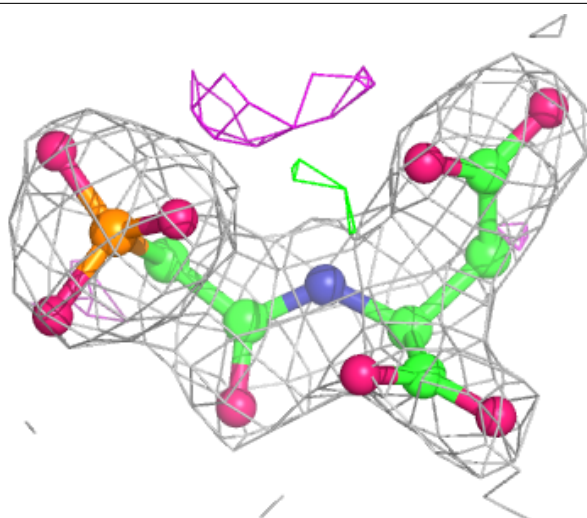
Electron density around PAL B 1002:

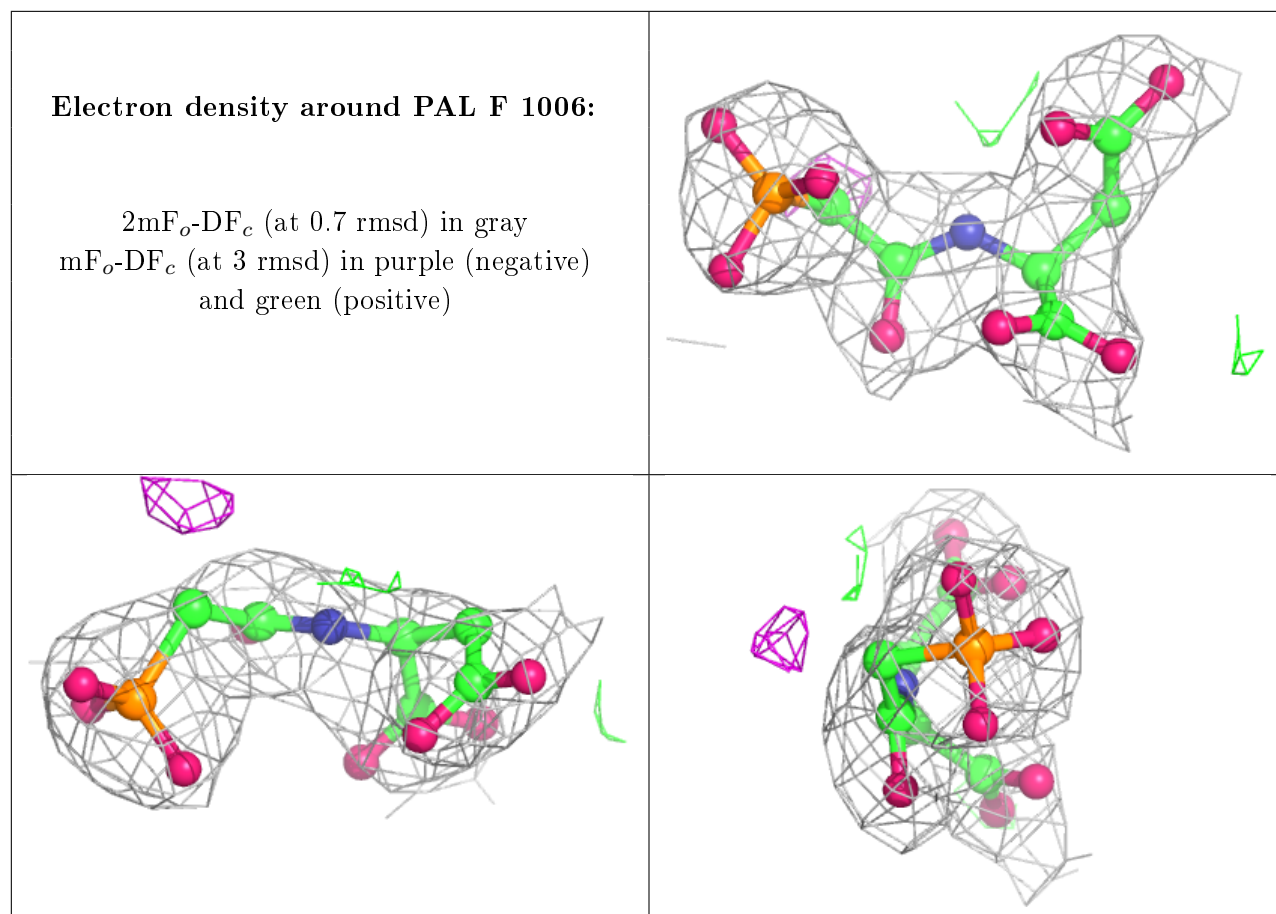
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAL C 1003:

$2mF_o-DF_c$ (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.