



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:22 AM UTC

PDB ID : 1Q95 / pdb_00001q95
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

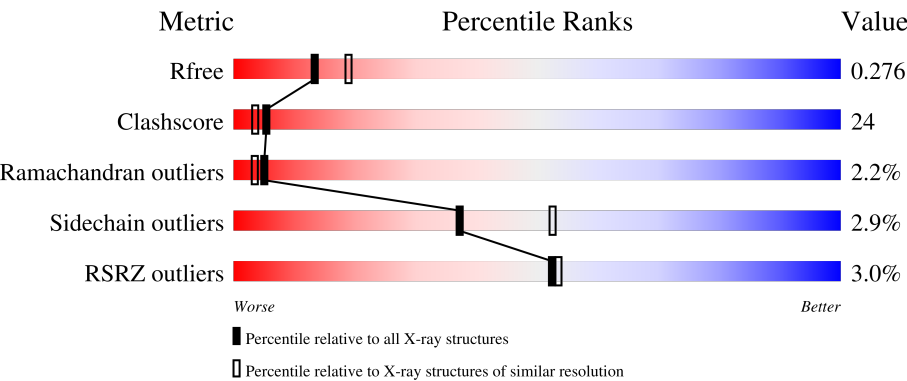
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	310	2% 66% 28% 5% .
1	B	310	2% 68% 27% 5% .
1	C	310	67% 29% .
1	D	310	% 64% 31% 5% .
1	E	310	3% 65% 31% .

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Mol	Chain	Length	Quality of chain
1	F	310	2%68%28%.
2	G	153	3%51%44%5%.
2	H	153	%52%44%.
2	I	153	8%48%46%5%.
2	J	153	2%54%42%5%.
2	K	153	%50%43%7%.
2	L	153	18%24%66%10%.

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.

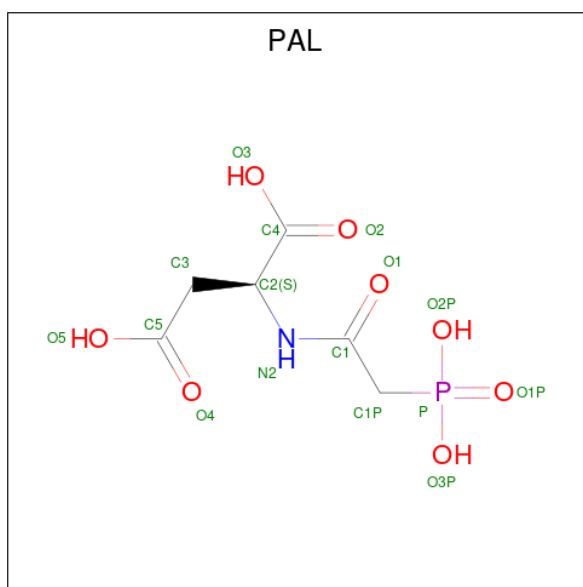
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

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 (CCD ID: PAL) (formula: $C_6H_{10}NO_8P$).



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 (CCD ID: ZN) (formula: Zn).

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

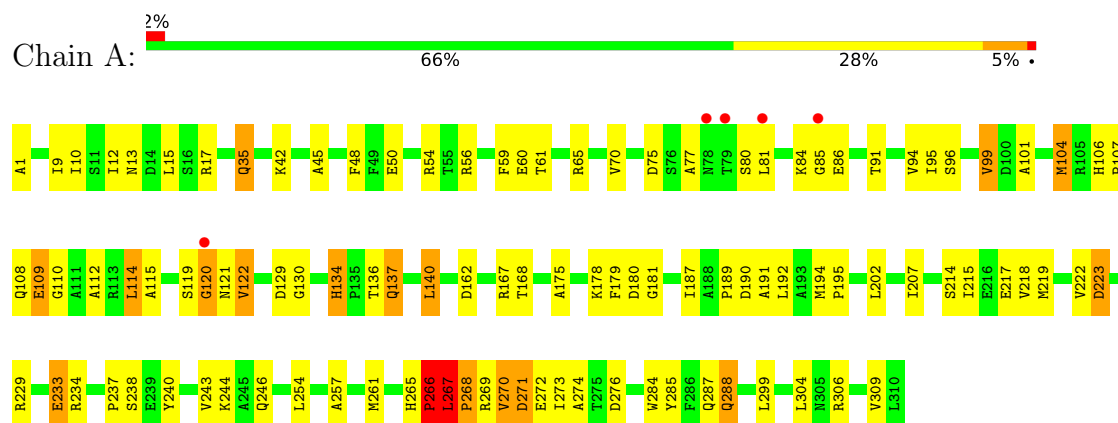
- Molecule 5 is water.

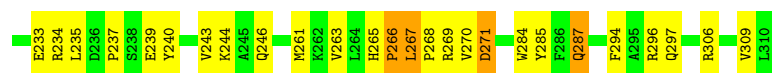
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total 122	O 122	0	0
5	B	120	Total 120	O 120	0	0
5	C	99	Total 99	O 99	0	0
5	D	70	Total 70	O 70	0	0
5	E	72	Total 72	O 72	0	0
5	F	128	Total 128	O 128	0	0
5	G	49	Total 49	O 49	0	0
5	H	45	Total 45	O 45	0	0
5	I	25	Total 25	O 25	0	0
5	J	41	Total 41	O 41	0	0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

3 Residue-property plots

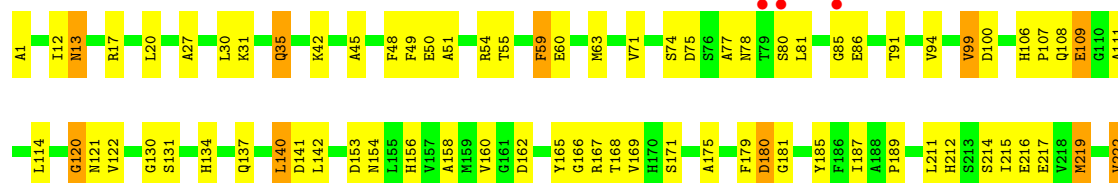
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Aspartate carbamoyltransferase catalytic chain

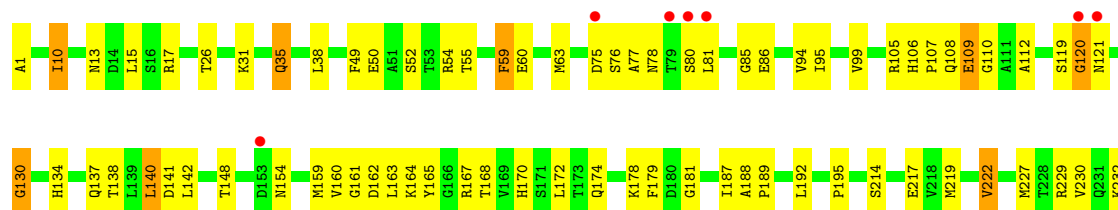




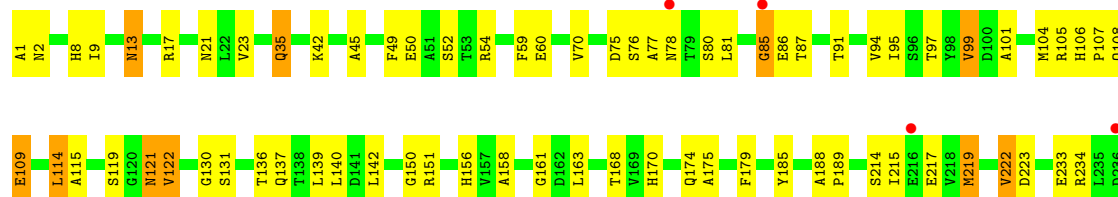
• Molecule 1: Aspartate carbamoyltransferase catalytic chain



• Molecule 1: Aspartate carbamoyltransferase catalytic chain

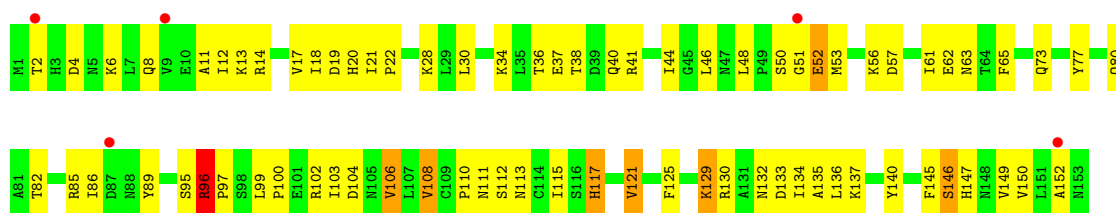


• Molecule 1: Aspartate carbamoyltransferase catalytic chain

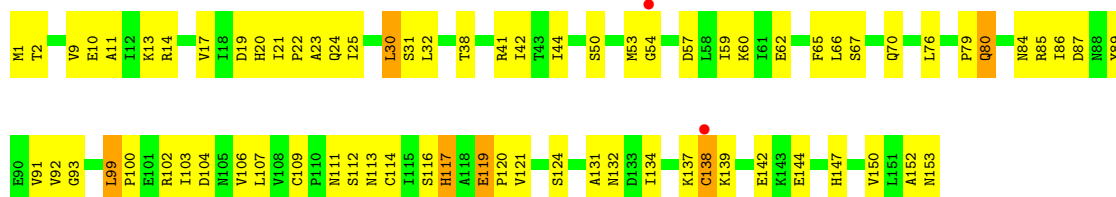


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

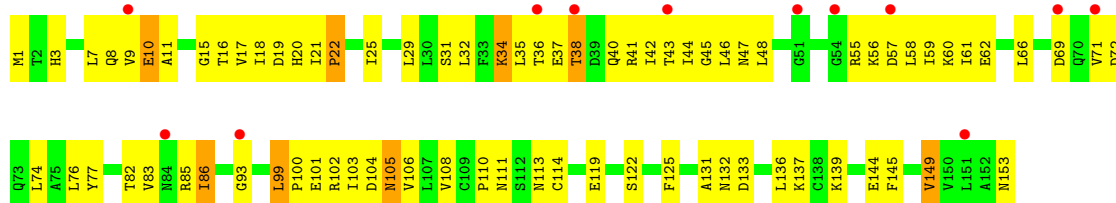




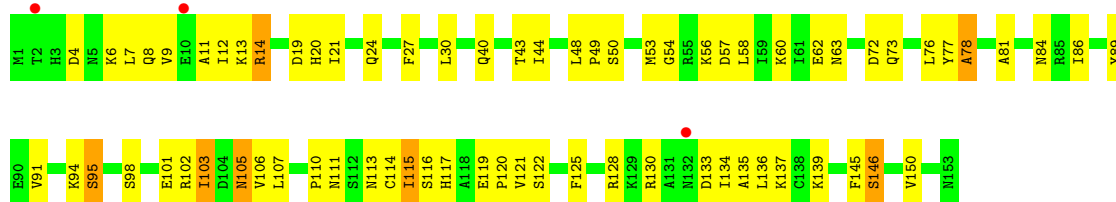
• Molecule 2: Aspartate carbamoyltransferase regulatory chain



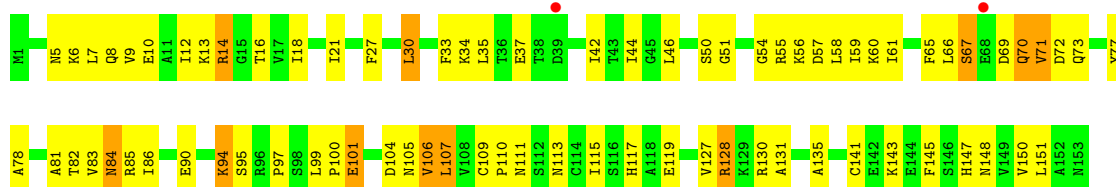
• Molecule 2: Aspartate carbamoyltransferase regulatory chain



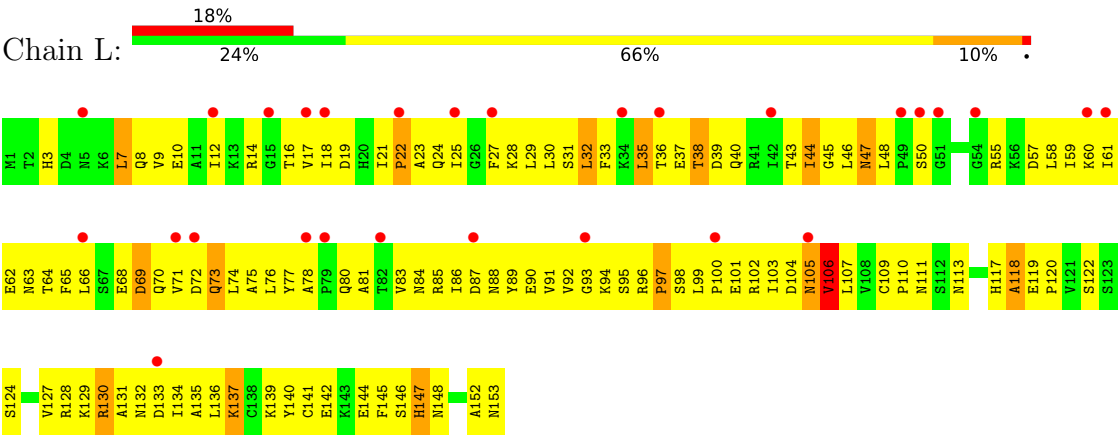
• Molecule 2: Aspartate carbamoyltransferase regulatory chain



• 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 8.00 – 2.46	Depositor EDS
% Data completeness (in resolution range)	84.7 (8.00-2.46) 82.0 (8.00-2.46)	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 0.236 , 0.276	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)	0.40 , 73.4	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	0.91	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	0.57	2/2461 (0.1%)	1.20	21/3339 (0.6%)
1	B	0.50	0/2461	1.08	15/3339 (0.4%)
1	C	0.47	0/2461	1.03	14/3339 (0.4%)
1	D	0.45	0/2461	1.02	13/3339 (0.4%)
1	E	0.44	0/2461	1.03	13/3339 (0.4%)
1	F	0.47	0/2461	1.04	16/3339 (0.5%)
2	G	0.45	0/1219	1.00	7/1647 (0.4%)
2	H	0.43	0/1219	0.93	5/1647 (0.3%)
2	I	0.37	0/1219	0.94	4/1647 (0.2%)
2	J	0.43	0/1219	0.92	3/1647 (0.2%)
2	K	0.42	0/1219	1.09	15/1647 (0.9%)
2	L	0.38	0/1219	1.03	6/1647 (0.4%)
All	All	0.46	2/22080 (0.0%)	1.04	132/29916 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	LEU	C-O	6.72	1.32	1.24
1	A	267	LEU	CA-C	-6.27	1.45	1.52

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	CA-C-N	-20.89	89.75	120.46
1	A	267	LEU	C-N-CA	-20.89	89.75	120.46
1	B	267	LEU	CA-C-N	-12.21	104.58	119.84
1	B	267	LEU	C-N-CA	-12.21	104.58	119.84
1	C	267	LEU	N-CA-C	11.72	135.71	109.81
1	D	266	PRO	N-CA-C	-11.63	92.99	111.14
1	C	266	PRO	N-CA-C	-11.63	93.12	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	105	ASN	N-CA-C	11.25	126.42	112.47
2	K	71	VAL	N-CA-C	-11.10	97.22	111.09
1	F	267	LEU	N-CA-C	10.57	133.16	109.81
1	B	267	LEU	N-CA-C	10.49	133.00	109.81
1	D	267	LEU	N-CA-C	10.46	132.93	109.81
1	B	266	PRO	N-CA-C	-10.27	95.42	111.34
1	E	267	LEU	N-CA-C	9.85	131.58	109.81
1	C	267	LEU	CA-C-N	-9.48	107.99	119.84
1	C	267	LEU	C-N-CA	-9.48	107.99	119.84
1	D	267	LEU	CA-C-N	-9.48	108.00	119.84
1	D	267	LEU	C-N-CA	-9.48	108.00	119.84
1	E	267	LEU	CA-C-N	-9.33	108.18	119.84
1	E	267	LEU	C-N-CA	-9.33	108.18	119.84
1	A	134	HIS	CA-C-N	8.88	128.47	119.24
1	A	134	HIS	C-N-CA	8.88	128.47	119.24
1	A	267	LEU	N-CA-C	8.56	128.74	109.81
1	B	99	VAL	N-CA-C	8.46	121.30	109.29
1	F	35	GLN	CA-C-N	8.21	129.00	119.47
1	F	35	GLN	C-N-CA	8.21	129.00	119.47
1	A	266	PRO	N-CA-C	-8.11	95.75	112.47
1	E	35	GLN	CA-C-N	8.07	129.92	119.84
1	E	35	GLN	C-N-CA	8.07	129.92	119.84
1	F	267	LEU	CA-C-N	-8.04	109.78	119.84
1	F	267	LEU	C-N-CA	-8.04	109.78	119.84
1	C	122	VAL	N-CA-C	-7.86	98.96	107.77
1	E	134	HIS	CA-C-N	7.67	127.22	119.24
1	E	134	HIS	C-N-CA	7.67	127.22	119.24
2	G	96	ARG	CA-C-N	7.64	129.40	119.84
2	G	96	ARG	C-N-CA	7.64	129.40	119.84
1	D	122	VAL	N-CA-C	-7.63	99.03	107.73
1	F	266	PRO	N-CA-C	-7.35	97.33	112.47
1	A	268	PRO	N-CA-C	-7.31	98.22	110.21
2	L	36	THR	N-CA-C	7.27	122.17	109.96
1	E	222	VAL	N-CA-C	7.15	118.33	108.89
1	C	35	GLN	CA-C-N	7.10	126.78	119.82
1	C	35	GLN	C-N-CA	7.10	126.78	119.82
1	C	99	VAL	N-CA-C	7.08	119.34	109.29
2	K	69	ASP	N-CA-C	-6.99	104.67	112.57
2	G	106	VAL	N-CA-C	6.92	122.12	112.50
2	K	51	GLY	N-CA-C	-6.89	105.17	113.99
1	E	99	VAL	N-CA-C	6.83	118.88	109.46
1	E	266	PRO	N-CA-C	-6.71	98.64	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	GLN	CA-C-N	6.70	128.21	119.84
1	B	35	GLN	C-N-CA	6.70	128.21	119.84
1	D	99	VAL	N-CA-C	6.66	118.65	109.46
1	F	222	VAL	N-CA-C	6.62	118.61	109.80
1	F	99	VAL	N-CA-C	6.54	118.48	109.46
1	B	222	VAL	N-CA-C	6.51	117.98	109.58
1	A	35	GLN	CA-C-N	6.51	127.98	119.84
1	A	35	GLN	C-N-CA	6.51	127.98	119.84
1	F	121	ASN	N-CA-C	6.49	120.52	112.47
1	B	10	ILE	N-CA-C	6.44	117.10	111.56
1	A	122	VAL	N-CA-C	-6.43	101.71	107.56
1	B	181	GLY	N-CA-C	6.42	123.79	114.10
1	C	180	ASP	N-CA-C	6.35	119.49	109.96
1	A	99	VAL	N-CA-C	6.33	118.28	109.29
1	C	222	VAL	N-CA-C	6.19	117.57	109.58
1	F	122	VAL	N-CA-C	-6.17	100.86	107.77
1	A	222	VAL	N-CA-C	6.13	118.46	109.63
1	B	122	VAL	N-CA-C	-6.08	100.96	107.77
1	D	35	GLN	CA-C-N	5.98	127.32	119.84
1	D	35	GLN	C-N-CA	5.98	127.32	119.84
1	C	223	ASP	N-CA-C	-5.96	105.66	113.12
2	K	106	VAL	N-CA-C	5.96	116.62	110.36
2	K	117	HIS	N-CA-C	5.85	117.52	111.03
1	F	223	ASP	N-CA-C	-5.83	106.30	113.41
1	E	10	ILE	N-CA-C	5.81	116.56	111.56
1	A	223	ASP	N-CA-C	-5.80	105.86	113.12
1	B	223	ASP	N-CA-C	-5.74	106.41	113.41
1	D	223	ASP	N-CA-C	-5.72	106.43	113.41
1	F	2	ASN	CA-C-N	5.61	125.28	119.56
1	F	2	ASN	C-N-CA	5.61	125.28	119.56
1	D	180	ASP	N-CA-C	5.60	119.05	110.20
2	I	119	GLU	CA-C-N	5.57	126.81	119.84
2	I	119	GLU	C-N-CA	5.57	126.81	119.84
1	C	121	ASN	N-CA-C	5.57	119.37	112.47
2	K	67	SER	N-CA-C	-5.56	107.04	113.88
2	K	119	GLU	N-CA-C	5.56	118.95	110.50
1	D	272	GLU	N-CA-C	-5.55	105.38	111.82
2	K	109	CYS	CA-C-N	5.53	125.18	119.05
2	K	109	CYS	C-N-CA	5.53	125.18	119.05
1	F	97	THR	N-CA-C	-5.52	106.59	113.38
2	K	107	LEU	N-CA-C	5.51	117.64	110.53
2	L	130	ARG	N-CA-C	5.48	115.63	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	37	GLU	N-CA-C	-5.47	99.39	108.75
2	L	32	LEU	N-CA-C	5.44	119.00	111.71
2	L	27	PHE	N-CA-C	-5.44	107.21	112.97
1	B	40	LYS	N-CA-C	5.43	120.33	111.37
1	F	272	GLU	N-CA-C	-5.41	105.55	111.82
2	K	119	GLU	CA-C-N	5.39	126.58	119.84
2	K	119	GLU	C-N-CA	5.39	126.58	119.84
2	K	101	GLU	N-CA-C	-5.34	106.26	112.89
1	B	180	ASP	N-CA-C	5.33	118.63	110.20
2	G	140	TYR	CA-C-N	-5.31	112.78	122.38
2	G	140	TYR	C-N-CA	-5.31	112.78	122.38
2	I	99	LEU	CA-C-N	5.26	125.55	119.92
2	I	99	LEU	C-N-CA	5.26	125.55	119.92
1	A	180	ASP	N-CA-C	5.26	118.26	110.48
1	C	297	GLN	N-CA-C	-5.22	105.50	111.14
2	H	119	GLU	CA-C-N	5.21	126.36	119.84
2	H	119	GLU	C-N-CA	5.21	126.36	119.84
1	F	297	GLN	N-CA-C	-5.21	105.49	111.07
2	G	146	SER	N-CA-C	-5.21	101.97	110.20
2	K	70	GLN	N-CA-C	5.21	121.90	110.80
2	J	78	ALA	CA-C-N	5.17	124.80	119.05
2	J	78	ALA	C-N-CA	5.17	124.80	119.05
1	A	273	ILE	CB-CA-C	-5.17	104.52	110.41
2	H	116	SER	N-CA-C	5.17	119.05	112.34
1	A	104	MET	N-CA-C	5.14	117.20	109.23
1	A	137	GLN	N-CA-C	-5.13	105.77	111.36
1	A	288	GLN	N-CA-C	-5.12	104.97	111.11
1	C	47	CYS	N-CA-C	5.10	117.23	107.75
2	K	95	SER	N-CA-C	5.09	116.57	108.79
1	A	266	PRO	CA-C-N	-5.08	109.40	121.80
1	A	266	PRO	C-N-CA	-5.08	109.40	121.80
1	A	181	GLY	N-CA-C	5.07	120.88	113.48
1	D	51	ALA	N-CA-C	5.07	116.83	110.24
2	G	121	VAL	N-CA-C	5.07	116.01	108.46
2	H	99	LEU	CA-C-N	5.06	125.53	120.52
2	H	99	LEU	C-N-CA	5.06	125.53	120.52
1	E	219	MET	N-CA-C	5.04	118.21	111.75
2	L	33	PHE	N-CA-C	5.03	121.51	110.80
1	B	287	GLN	N-CA-C	-5.02	106.42	112.54
1	D	222	VAL	N-CA-C	5.02	116.69	109.51
1	E	10	ILE	CB-CA-C	-5.01	106.68	111.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	94	0
1	B	2415	0	2422	109	0
1	C	2415	0	2422	72	0
1	D	2415	0	2422	123	0
1	E	2415	0	2422	99	0
1	F	2415	0	2422	102	0
2	G	1201	0	1219	67	0
2	H	1201	0	1219	83	0
2	I	1201	0	1219	91	0
2	J	1201	0	1219	76	0
2	K	1201	0	1219	76	0
2	L	1201	0	1219	139	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
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	7	0
5	D	70	0	0	4	0
5	E	72	0	0	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	26	0	0	2	0
5	L	25	0	0	6	0
All	All	22620	0	21882	1050	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 24.

All (1050) 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
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
1:E:159:MET:HE2	1:E:172:LEU:HD23	1.41	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
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:B:60:GLU:HA	1:B:63:MET:HE3	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:119:SER:C	5:C:1042:HOH:O	2.23	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
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
1:B:60:GLU:HA	1:B:63:MET:HE2	1.66	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
1:B:254:LEU:HD22	1:B:261:MET:HE1	1.67	0.76
1:A:265:HIS:C	1:A:266:PRO:O	2.23	0.76
2:I:108:VAL:HG21	2:I:153:ASN:HD22	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:SER:C	5:B:1051:HOH:O	2.27	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
1:D:254:LEU:HD22	1:D:261:MET:HE1	1.69	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: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
2:J:105:ASN:OD1	2:J:122:SER:HB3	1.88	0.72
1:F:287:GLN:H	1:F:287:GLN:HE21	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:7:LEU:HD23	2:J:49:PRO:HD2	1.71	0.71
2:J:58:LEU:HD21	2:J:60:LYS:HE3	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:13:LYS:HB2	2:J:89:TYR:CZ	2.25	0.71
2:J:84:ASN:HD21	2:J:94:LYS:CD	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:F:287:GLN:NE2	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:F:119:SER:C	5:F:1054:HOH:O	2.33	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
1:A:257:ALA:HB1	1:A:261:MET:HE2	1.75	0.69
2:L:50:SER:HA	2:L:55:ARG:HA	1.73	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
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
2:K:83:VAL:C	2:K:84:ASN:HD22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:MET:HE2	1:B:282:HIS:ND1	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:49:PHE:HE2	1:F:81:LEU:HD13	1.59	0.67
1:F:189:PRO:HB3	1:F:246:GLN:NE2	2.10	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:HD22	2:K:84:ASN:N	1.93	0.66
1:E:140:LEU:HD21	1:E:288:GLN:HG2	1.76	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:E:60:GLU:HA	1:E:63:MET:HE3	1.75	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:B:114:LEU:CD1	2:H:121:VAL:HG11	2.25	0.65
1:D:49:PHE:HE2	1:D:81:LEU:HD13	1.61	0.65
2:I:9:VAL:HG13	2:I:47:ASN:HB2	1.77	0.65
2:I:10:GLU:CG	2:I:11:ALA:H	2.06	0.65
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:D:215:ILE:HD11	1:D:227:MET:HE1	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:PRO:HA	1:F:240:TYR:CE2	2.32	0.64
2:H:30:LEU:HD21	2:H:44:ILE:CD1	2.25	0.64
2:H:152:ALA:O	2:H:153:ASN:HB2	1.96	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:229:ARG:HD3	1:C:268:PRO:O	1.98	0.64
1:C:240:TYR:O	1:C:243:VAL:HG12	1.97	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:D:140:LEU:C	1:D:140:LEU:HD23	2.24	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
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:D:261:MET:HE2	1:D:282:HIS:CG	2.35	0.62
1:F:81:LEU:HD22	5:F:1029:HOH:O	1.99	0.62
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:42:LYS:HE3	5:F:1086:HOH:O	1.99	0.62
1:F:284:TRP:CD2	1:F:287:GLN:HG3	2.34	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:A:215:ILE:HG22	1:A:219:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:CD	1:E:234:ARG:HH22	2.07	0.62
1:A:271:ASP:O	1:A:271:ASP:CG	2.40	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:75:ASP:OD2	1:F:77:ALA:HB3	2.00	0.61
1:F:267:LEU:HD11	1:F:286:PHE:CD1	2.34	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:41:ARG:C	2:I:42:ILE:HD12	2.25	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:E:159:MET:HE2	1:E:172:LEU:CD2	2.25	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:15:GLY:O	2:I:86:ILE:HA	2.01	0.60
2:I:104:ASP:O	2:I:106:VAL:HG23	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
1:E:140:LEU:C	1:E:140:LEU:HD23	2.26	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASP:OD2	1:C:77:ALA:HB3	2.01	0.59
1:F:50:GLU:CD	1:F:234:ARG:HH22	2.09	0.59
2:L:65:PHE:HD1	2:L:65:PHE:H	1.49	0.59
1:A:114:LEU:HD13	1:A:114:LEU:C	2.27	0.59
1:C:270:VAL:O	1:C:271:ASP:CG	2.46	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:12:ILE:HD11	2:J:62:GLU:CB	2.32	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:K:128:ARG:HB3	2:K:128:ARG:NH1	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: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:D:108:GLN:CB	2:J:115:ILE:HD12	2.33	0.58
1:E:170:HIS:O	1:E:174:GLN:HG3	2.03	0.58
2:K:67:SER:HB3	2:K:85:ARG:HH21	1.64	0.58
1:D:60:GLU:HA	1:D:63:MET:HE3	1.84	0.58
1:A:194:MET:SD	1:A:195:PRO:HD2	2.43	0.58
1:E:270:VAL:O	1:E:271:ASP:CG	2.47	0.58
2:K:55:ARG:HH11	2:K:55:ARG:HG2	1.68	0.58
2:J:110:PRO:HD2	2:J:145:PHE:CE2	2.39	0.58
1:D:270:VAL:O	1:D:271:ASP:CG	2.47	0.57
2:K:30:LEU:HD21	2:K:44:ILE:CD1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:104:MET:HE1	1:A:115:ALA:HB2	1.87	0.56
1:A:257:ALA:CB	1:A:261:MET:CE	2.82	0.56
1:B:137:GLN:HG2	1:B:168:THR:HG22	1.87	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: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
1:A:254:LEU:HD22	1:A:261:MET:HE1	1.86	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
2:L:8:GLN:O	2:L:10:GLU:HG3	2.05	0.56
2:G:40:GLN:HE22	2:G:63:ASN:HB2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:215:ILE:HG22	1:D:219:MET:HE2	1.87	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:C:50:GLU:CD	1:C:234:ARG:HH22	2.14	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
1:D:106:HIS:CG	1:D:107:PRO:HD2	2.42	0.55
1:F:87:THR:HB	2:L:119:GLU:OE1	2.07	0.55
2:G:112:SER:HA	2:G:117:HIS:NE2	2.20	0.55
2:L:7:LEU:O	2:L:8:GLN:HB2	2.06	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
1:B:140:LEU:HD21	1:B:288:GLN:HG2	1.88	0.54
1:B:219:MET:HE3	1:B:253:ASP:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:CYS:SG	2:H:111:ASN:HB3	2.47	0.54
2:G:134:ILE:HD12	2:G:134:ILE:N	2.23	0.54
1:B:88:LEU:N	2:H:119:GLU:OE1	2.39	0.54
1:D:54:ARG:CD	1:D:267:LEU:HB2	2.37	0.54
1:B:114:LEU:HD12	2:H:121:VAL:HG11	1.90	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: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:8:HIS:O	1:F:9:ILE:HD13	2.07	0.54
1:F:101:ALA:HB2	1:F:304:LEU:HD21	1.90	0.54
2:L:75:ALA:HB1	2:L:99:LEU:CD2	2.38	0.54
2:G:61:ILE:HD12	2:G:61:ILE:N	2.22	0.53
1:B:104:MET:HE1	1:B:115:ALA:CB	2.38	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
1:F:254:LEU:HD22	1:F:261:MET:HE1	1.91	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
1:C:261:MET:HE1	1:C:263:VAL:CG2	2.39	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:G:4:ASP:C	2:G:6:LYS:H	2.15	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: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
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
1:F:261:MET:HG2	1:F:262:LYS:N	2.24	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
1:F:121:ASN:HA	5:F:1100:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:31:SER:HB3	2:K:27:PHE:HZ	1.72	0.52
2:H:132:ASN:N	5:H:2013:HOH:O	2.30	0.52
2:H:86:ILE:HG22	2:H:87:ASP:N	2.24	0.52
2:H:111:ASN:HD22	2:H:111:ASN:C	2.16	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
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:D:261:MET:HE3	1:D:282:HIS:HB3	1.92	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
1:F:94:VAL:HG23	1:F:95:ILE:N	2.24	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:59:PHE:O	1:D:63:MET:HG3	2.09	0.52
1:D:156:HIS:HD2	1:D:185:TYR:OH	1.91	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:D:54:ARG:NH2	1:F:80:SER:HB2	2.25	0.52
1:E:264:LEU:O	1:E:265:HIS:HB2	2.09	0.52
1:C:265:HIS:HD2	1:C:267:LEU:HA	1.75	0.52
1:D:111:ALA:N	2:J:115:ILE:HD13	2.25	0.52
1:E:222:VAL:O	1:E:261:MET:HG3	2.10	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:A:114:LEU:CD2	2:G:121:VAL:HG11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:270:VAL:O	1:B:271:ASP:CG	2.53	0.51
1:C:261:MET:HE1	1:C:263:VAL:HG22	1.92	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:B:60:GLU:HG2	1:B:63:MET:HE1	1.93	0.51
1:B:104:MET:HE1	1:B:115:ALA:HB2	1.93	0.51
1:B:109:GLU:CD	2:H:113:ASN:HD22	2.19	0.51
1:E:10:ILE:HD12	1:E:112:ALA:HB1	1.93	0.51
1:E:109:GLU:OE1	1:E:130:GLY:O	2.29	0.51
1:F:104:MET:HE1	1:F:115:ALA:CB	2.40	0.51
1:F:106:HIS:ND1	1:F:107:PRO:HD2	2.25	0.51
2:L:66:LEU:HD13	2:L:70:GLN:O	2.11	0.51
2:L:76:LEU:HG	2:L:134:ILE:HD12	1.93	0.51
1:A:162:ASP:OD1	1:A:162:ASP:C	2.54	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:18:ILE:HB	2:L:84:ASN:HB2	1.92	0.50
2:L:100:PRO:O	2:L:127:VAL:HG21	2.10	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:G:85:ARG:C	2:G:86:ILE:HD12	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	2:L:128:ARG:CB	2.74	0.50
1:D:1:ALA:HA	1:D:306:ARG:HG2	1.93	0.50
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:59:ILE:HD12	2:I:59:ILE:N	2.25	0.50
2:I:125:PHE:HA	2:I:137:LYS:O	2.12	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
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:D:80:SER:HB2	1:E:54:ARG:NH2	2.26	0.50
1:E:237:PRO:HA	1:E:240:TYR:CZ	2.45	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:B:114:LEU:HD11	2:H:121:VAL:CG1	2.42	0.50
1:D:229:ARG:NE	1:D:268:PRO:HB2	2.27	0.50
1:D:230:VAL:O	1:D:232:LYS:N	2.45	0.50
2:G:2:THR:HG22	2:G:11:ALA:H	1.76	0.50
2:L:24:GLN:C	2:L:25:ILE:HD12	2.37	0.50
2:L:85:ARG:O	2:L:86:ILE:HD13	2.12	0.50
2:L:132:ASN:O	2:L:133:ASP:HB3	2.11	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:C:271:ASP:OD1	1:C:271:ASP:C	2.56	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
2:K:94:LYS:HB2	2:K:94:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:CG2	1:E:267:LEU:HD12	2.42	0.49
2:K:90:GLU:HA	2:K:90:GLU:OE1	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
2:L:63:ASN:O	2:L:64:THR:C	2.55	0.49
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
1:E:162:ASP:OD1	1:E:162:ASP:C	2.55	0.49
2:I:36:THR:HG22	2:I:37:GLU:HG3	1.93	0.49
2:L:8:GLN:HE22	2:L:48:LEU:HD13	1.78	0.49
2:L:136:LEU:N	2:L:145:PHE:O	2.44	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
1:E:271:ASP:OD1	1:E:271:ASP:C	2.55	0.49
1:F:267:LEU:O	1:F:268:PRO:C	2.53	0.49
2:H:103:ILE:HG23	2:H:103:ILE:O	2.13	0.49
2:L:75:ALA:CB	2:L:99:LEU:HD23	2.43	0.49
1:A:94:VAL:CG1	1:C:267:LEU:HD12	2.42	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: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
1:C:109:GLU:OE2	2:I:113:ASN:HB3	2.12	0.49
2:H:21:ILE:HB	2:H:57:ASP:HB2	1.95	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
1:F:8:HIS:C	1:F:9:ILE:HD13	2.38	0.48
2:G:13:LYS:O	2:G:86:ILE:HG22	2.12	0.48
2:G:34:LYS:HB3	2:G:37:GLU:OE2	2.13	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
5:B:1053:HOH:O	2:H:139:LYS:HB2	2.13	0.48
1:D:162:ASP:C	1:D:162:ASP:OD1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:LEU:HD23	2:H:32:LEU:O	2.13	0.48
2:H:102:ARG:HG2	2:H:139:LYS:CE	2.43	0.48
2:J:77:TYR:CD1	2:J:77:TYR:N	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: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
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:87:ASP:OD2	2:L:92:VAL:HG11	2.14	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
1:A:114:LEU:C	1:A:114:LEU:CD1	2.87	0.48
1:A:267:LEU:O	1:A:269:ARG:N	2.46	0.48
1:D:215:ILE:CD1	1:D:227:MET:HE1	2.43	0.48
1:E:251:ALA:CB	1:E:276:ASP:OD2	2.62	0.48
2:I:44:ILE:HG12	2:L:48:LEU:CD2	2.43	0.48
2:K:107:LEU:HD13	2:K:150:VAL:HG11	1.96	0.48
1:A:81:LEU:HG	1:A:86:GLU:O	2.13	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:E:119:SER:O	1:E:120:GLY:C	2.56	0.48
2:K:55:ARG:HG2	2:K:55:ARG:NH1	2.29	0.48
2:L:39:ASP:OD1	2:L:40:GLN:N	2.46	0.48
1:B:265:HIS:C	1:B:266:PRO:O	2.48	0.48
1:F:106:HIS:CG	1:F:107:PRO:HD2	2.49	0.48
2:G:95:SER:O	2:G:96:ARG:C	2.57	0.48
2:H:1:MET:O	2:H:2:THR:HG23	2.14	0.48
1:A:50:GLU:CD	1:A:234:ARG:HH22	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASP:OD1	1:D:288:GLN:NE2	2.47	0.47
1:D:271:ASP:C	1:D:271:ASP:OD1	2.57	0.47
1:F:45:ALA:HB2	1:F:99:VAL:HG11	1.96	0.47
1:F:122:VAL:HB	5:F:1054:HOH:O	2.14	0.47
2:J:103:ILE:HD11	2:J:106:VAL:CG2	2.44	0.47
2:K:9:VAL:C	2:K:10:GLU:HG3	2.38	0.47
2:L:38:THR:O	2:L:39:ASP:HB2	2.14	0.47
1:B:270:VAL:O	1:B:270:VAL:HG12	2.14	0.47
1:C:17:ARG:HD2	1:C:179:PHE:CE1	2.49	0.47
5:F:1097:HOH:O	2:L:120:PRO:HG2	2.13	0.47
2:H:79:PRO:HD2	2:H:80:GLN:HE22	1.79	0.47
1:D:120:GLY:O	1:D:121:ASN:CG	2.57	0.47
1:F:250:ARG:HH11	1:F:250:ARG:HG2	1.79	0.47
2:K:73:GLN:CD	2:K:106:VAL:HG21	2.38	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
5:E:1034:HOH:O	2:K:143:LYS:HE2	2.13	0.47
2:J:50:SER:HB2	2:J:56:LYS:HG2	1.96	0.47
2:L:105:ASN:O	2:L:106:VAL:C	2.56	0.47
1:B:287:GLN:H	1:B:287:GLN:NE2	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
1:E:109:GLU:HG3	2:K:111:ASN:HD21	1.80	0.47
2:H:134:ILE:H	2:H:147:HIS:CD2	2.31	0.47
1:B:237:PRO:HA	1:B:240:TYR:CZ	2.49	0.47
5:B:1053:HOH:O	2:H:139:LYS:HB3	2.12	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
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:A:54:ARG:HH22	1:B:86:GLU:CD	2.22	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:G:146:SER:O	2:G:149:VAL:HG22	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:B:250:ARG:HH11	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:C:131:SER:HB3	1:C:234:ARG:CD	2.45	0.46
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:A:265:HIS:O	1:A:266:PRO:C	2.58	0.46
1:D:137:GLN:NE2	1:D:140:LEU:HD22	2.30	0.46
2:L:21:ILE:C	2:L:23:ALA:H	2.23	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:18:ILE:HA	2:I:83:VAL:HG12	1.96	0.46
2:I:45:GLY:H	2:L:46:LEU:H	1.64	0.46
2:K:34:LYS:HE2	2:K:37:GLU:CD	2.41	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
1:A:257:ALA:CB	1:A:261:MET:HE2	2.45	0.46
1:E:108:GLN:HG3	2:K:113:ASN:ND2	2.29	0.46
1:F:114:LEU:HD13	1:F:114:LEU:C	2.40	0.46
2:G:52:GLU:O	2:G:53:MET:HG2	2.16	0.46
2:H:1:MET:HE3	2:H:91:VAL:HG12	1.97	0.46
1:D:12:ILE:HG21	1:D:175:ALA:HB2	1.98	0.46
2:L:72:ASP:C	2:L:74:LEU:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:8:GLN:HB3	2:G:48:LEU:HD22	1.97	0.46
2:G:40:GLN:CD	2:G:63:ASN:HB2	2.40	0.46
1:C:140:LEU:C	1:C:140:LEU:HD23	2.41	0.46
2:G:50:SER:HB2	2:G:56:LYS:HG2	1.98	0.46
2:G:102:ARG:HG2	2:G:104:ASP:OD2	2.15	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:A:257:ALA:CB	1:A:261:MET:HE1	2.46	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: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
1:F:215:ILE:HG22	1:F:219:MET:HE2	1.98	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:D:50:GLU:CD	1:D:234:ARG:HH22	2.24	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:K:7:LEU:HB2	2:K:10:GLU:CD	2.41	0.45
2:L:40:GLN:HA	5:L:2015:HOH:O	2.16	0.45
2:L:109:CYS:HA	2:L:110:PRO:HD3	1.85	0.45
2:G:17:VAL:HG23	2:G:86:ILE:HD13	1.98	0.45
2:G:44:ILE:HB	2:J:44:ILE:HB	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:HG3	1:B:17:ARG:O	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:NZ	2:K:94:LYS:CB	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:50:GLU:HB3	1:E:105:ARG:HG2	1.99	0.45
1:E:160:VAL:HG22	1:E:187:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:94:VAL:CG1	1:F:267:LEU:CD1	2.95	0.45
1:E:307:ASP:HA	5:E:1045:HOH:O	2.17	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:B:265:HIS:O	1:B:266:PRO:C	2.58	0.45
1:E:121:ASN:HB3	5:E:1016:HOH:O	2.17	0.45
2:J:50:SER:O	2:J:54:GLY:N	2.49	0.45
1:A:267:LEU:O	1:A:268:PRO:C	2.43	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:HD12	2:G:86:ILE: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
2:L:136:LEU:O	2:L:145:PHE:N	2.31	0.44
1:D:267:LEU:HD23	1:D:267:LEU:HA	1.72	0.44
1:E:26:THR:HB	1:E:298:ALA:HB1	1.99	0.44
2:J:72:ASP:OD1	2:J:98:SER:HB3	2.16	0.44
2:J:139:LYS:O	2:J:139:LYS:HG2	2.16	0.44
1:B:2:ASN:HB2	1:B:308:LEU:HD21	1.99	0.44
1:B:245:ALA:HB3	1:B:271:ASP:OD1	2.17	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:22:PRO:HA	2:L:55:ARG:O	2.17	0.44
2:L:111:ASN:ND2	2:L:141:CYS:SG	2.87	0.44
1:E:251:ALA:HB3	1:E:276:ASP:OD2	2.18	0.44
1:A:75:ASP:OD2	1:A:77:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:THR:O	1:D:59:PHE:HB2	2.17	0.44
1:D:216:GLU:HG3	5:D:1062:HOH:O	2.16	0.44
1:F:163:LEU:HG	1:F:188:ALA:HB2	1.98	0.44
2:I:7:LEU:HD13	2:L:9:VAL:HB	2.00	0.44
2:I:59:ILE:H	2:I:59:ILE:CD1	2.29	0.44
1:B:54:ARG:NH2	1:C:80:SER:HB2	2.32	0.44
1:B:158:ALA:HB2	1:B:222:VAL:HG11	2.00	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:G:4:ASP:C	2:G:6:LYS:N	2.76	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
2:L:137:LYS:HE3	2:L:142:GLU:O	2.17	0.44
1:A:60:GLU:HG2	1:A:70:VAL:HG11	2.00	0.44
1:A:119:SER:O	1:A:120:GLY:C	2.61	0.44
1:A:187:ILE:HD11	1:A:218:VAL:HG21	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
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
2:G:52:GLU:C	2:G:53:MET:HG2	2.42	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:A:109:GLU:OE2	2:G:113:ASN:ND2	2.51	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
2:H:50:SER:HB3	2:H:54:GLY:C	2.43	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: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:1:MET:HB2	2:I:3:HIS:CE1	2.52	0.43
2:I:136:LEU:O	2:I:144:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG23	1:A:95:ILE:N	2.34	0.43
1:B:140:LEU:C	1:B:140:LEU:HD23	2.43	0.43
1:D:160:VAL:HA	1:D:187:ILE:O	2.19	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:J:20:HIS:O	2:J:53:MET:HE1	2.18	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: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
1:D:233:GLU:CD	1:D:233:GLU:H	2.26	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:C:215:ILE:HG22	1:C:219:MET:HE2	2.01	0.43
1:D:13:ASN:HD22	1:D:13:ASN:HA	1.57	0.43
1:D:114:LEU:HD21	2:J:121:VAL:HG11	2.00	0.43
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:81:ALA:H	2:L:96:ARG:HH12	1.58	0.43
2:L:128:ARG:HB3	2:L:128:ARG:CZ	2.48	0.43
1:A:229:ARG:HD3	1:A:268:PRO:O	2.19	0.43
1:A:140:LEU:CD2	1:A:288:GLN:HG2	2.49	0.43
1:A:284:TRP:O	1:A:288:GLN:HB2	2.18	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: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:A:129:ASP:O	1:A:129:ASP:CG	2.62	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.00	0.42
2:I:9:VAL:CG1	2:I:47:ASN:HD22	2.31	0.42
2:I:29:LEU:HD11	2:I:74:LEU:CD2	2.49	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:N	2.77	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:95:SER:C	2:L:97:PRO:HD3	2.45	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:A:266:PRO:HB2	3:A:1001:PAL:H31	2.02	0.42
1:E:229:ARG:NE	3:E:1005:PAL:O4	2.52	0.42
2:I:44:ILE:HG12	2:L:48:LEU:HD23	2.01	0.42
2:I:56:LYS:CE	2:I:58:LEU:HD21	2.44	0.42
2:J:84:ASN:OD1	2:J:94:LYS:HE2	2.20	0.42
2:L:137:LYS:HE3	2:L:137:LYS:HB2	1.80	0.42
1:B:81:LEU:C	1:B:81:LEU:HD23	2.45	0.42
1:B:261:MET:HE2	1:B:282:HIS:CG	2.54	0.42
1:E:214:SER:OG	1:E:217:GLU:HG3	2.20	0.42
1:E:267:LEU:HD23	1:E:267:LEU:HA	1.55	0.42
2:I:110:PRO:HD2	2:I:145:PHE:CE1	2.55	0.42
1:D:31:LYS:HG3	1:D:294:PHE:CE1	2.55	0.42
1:D:134:HIS:HB2	1:D:167:ARG:HG3	2.01	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:B:75:ASP:C	1:B:77:ALA:H	2.28	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:J:114:CYS:O	2:J:115:ILE:C	2.63	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:D:261:MET:HE2	1:D:282:HIS:ND1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:ARG:NH1	1:B:86:GLU:OE2	2.49	0.41
1:A:61:THR:O	1:A:65:ARG:HG2	2.20	0.41
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.63	0.41
1:A:270:VAL:O	1:A:272:GLU:OE1	2.38	0.41
1:D:75:ASP:HB2	1:F:78:ASN:OD1	2.20	0.41
1:D:153:ASP:HB2	1:D:180:ASP:O	2.20	0.41
1:E:138:THR:O	1:E:142:LEU:HG	2.20	0.41
2:J:115:ILE:O	2:J:116:SER:C	2.63	0.41
2:L:44:ILE:CG2	2:L:45:GLY:N	2.76	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
1:A:42:LYS:HE3	5:A:1054:HOH:O	2.20	0.41
1:C:162:ASP:OD1	1:C:162:ASP:C	2.63	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
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
1:A:80:SER:O	1:A:84:LYS:HB2	2.21	0.41
1:A:96:SER:O	1:A:122:VAL:HG21	2.20	0.41
1:D:131:SER:C	1:D:167:ARG:HB3	2.46	0.41
1:F:270:VAL:O	1:F:271:ASP:CG	2.63	0.41
2:G:132:ASN:O	2:G:133:ASP:HB2	2.21	0.41
2:H:111:ASN:ND2	2:H:111:ASN:C	2.78	0.41
2:J:94:LYS:O	2:J:95:SER:HB3	2.20	0.41
2:L:12:ILE:C	2:L:14:ARG:H	2.28	0.41
1:A:110:GLY:C	2:G:115:ILE:HG21	2.45	0.41
1:D:162:ASP:HB2	1:D:230:VAL:HA	2.03	0.41
1:F:13:ASN:HD22	1:F:13:ASN:HA	1.62	0.41
1:F:156:HIS:HD2	1:F:185:TYR:OH	2.03	0.41
2:L:72:ASP:HA	2:L:97:PRO:CB	2.50	0.41
2:L:135:ALA:HB1	2:L:144:GLU:HG2	2.03	0.41
1:C:45:ALA:HB2	1:C:99:VAL:HG11	2.02	0.41
1:C:165:TYR:CE2	1:C:235:LEU:HD23	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:70:GLN:C	2:K:72:ASP:N	2.72	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:60:GLU:CA	1:B:63:MET:HE2	2.44	0.41
1:B:192:LEU:HD11	1:B:242:ASN:CB	2.48	0.41
1:E:75:ASP:C	1:E:77:ALA:H	2.29	0.41
1:F:81:LEU:HD23	1:F:81:LEU:O	2.21	0.41
1:A:189:PRO:O	1:A:190:ASP:C	2.64	0.41
1:B:271:ASP:OD1	1:B:271:ASP:C	2.63	0.41
1:C:138:THR:O	1:C:142:LEU:HG	2.20	0.41
2:L:139:LYS:HE2	2:L:140:TYR:CZ	2.55	0.41
1:B:121:ASN:HB2	5:B:1066:HOH:O	2.21	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:A:274:ALA:CB	1:A:276:ASP:OD1	2.69	0.41
1:B:17:ARG:NH1	1:B:17:ARG:HG2	2.35	0.41
1:B:268:PRO:HD3	3:B:1002:PAL:H1P1	2.02	0.41
1:E:52:SER:HB2	1:E:105:ARG:HH11	1.86	0.41
1:E:109:GLU:HG3	2:K:141:CYS:HB2	2.03	0.41
1:E:110:GLY:C	2:K:115:ILE:HG21	2.46	0.41
1:F:21:ASN:HD22	1:F:21:ASN:HA	1.74	0.41
1:F:54:ARG:HD3	1:F:267:LEU:HB2	2.02	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
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:I:56:LYS:CG	2:I:57:ASP:N	2.82	0.41
2:J:4:ASP:OD1	2:J:7:LEU:HD12	2.21	0.41
2:J:58:LEU:C	2:J:58:LEU:HD23	2.45	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:C:265:HIS:O	1:C:266:PRO:C	2.64	0.41
2:H:66:LEU:HA	2:H:70:GLN:NE2	2.36	0.41
2:I:60:LYS:C	2:I:61:ILE:HG13	2.46	0.41
2:L:76:LEU:CD1	2:L:134:ILE:HB	2.51	0.41
1:E:246:GLN:HE21	1:E:246:GLN:HB2	1.68	0.40
2:G:110:PRO:HG3	2:G:150:VAL:HA	2.01	0.40
2:G:135:ALA:O	2:G:136:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:149:VAL:CG2	2:G:150:VAL:N	2.84	0.40
2:H:1:MET:HE3	2:H:91:VAL:H	1.86	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
2:L:61:ILE:HG22	2:L:62:GLU:N	2.35	0.40
2:L:117:HIS:O	2:L:118:ALA:HB2	2.20	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:92:VAL:CG2	2:H:93:GLY:N	2.84	0.40
2:H:109:CYS:CB	2:H:138:CYS:SG	3.01	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:18:ILE:HB	2:L:84:ASN:HD22	1.85	0.40
2:L:25:ILE:HG21	2:L:77:TYR:O	2.21	0.40
1:B:250:ARG:HG2	1:B:250:ARG:NH1	2.36	0.40
2:I:10:GLU:HA	2:I:44:ILE:CD1	2.44	0.40
2:J:58:LEU:HD21	2:J:60:LYS:CE	2.47	0.40
2:J:130:ARG:CD	2:J:135:ALA:HB2	2.49	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:HD22	1:C:13:ASN:HA	1.61	0.40
1:D:35:GLN:HE22	1:D:309:VAL:HG13	1.81	0.40
1:D:81:LEU:C	1:D:81:LEU:HD23	2.47	0.40
1:D:114:LEU:HD22	2:J:121:VAL:HG11	2.02	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

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%)	7	7
1	B	308/310 (99%)	288 (94%)	15 (5%)	5 (2%)	7	7
1	C	308/310 (99%)	284 (92%)	21 (7%)	3 (1%)	12	14
1	D	308/310 (99%)	276 (90%)	28 (9%)	4 (1%)	9	9
1	E	308/310 (99%)	281 (91%)	22 (7%)	5 (2%)	7	7
1	F	308/310 (99%)	281 (91%)	23 (8%)	4 (1%)	9	9
2	G	151/153 (99%)	127 (84%)	19 (13%)	5 (3%)	3	1
2	H	151/153 (99%)	132 (87%)	18 (12%)	1 (1%)	18	24
2	I	151/153 (99%)	110 (73%)	31 (20%)	10 (7%)	1	0
2	J	151/153 (99%)	129 (85%)	19 (13%)	3 (2%)	6	4
2	K	151/153 (99%)	127 (84%)	22 (15%)	2 (1%)	9	9
2	L	151/153 (99%)	88 (58%)	49 (32%)	14 (9%)	0	0
All	All	2754/2778 (99%)	2401 (87%)	292 (11%)	61 (2%)	5	3

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	35	50
1	B	261/261 (100%)	251 (96%)	10 (4%)	29	43
1	C	261/261 (100%)	251 (96%)	10 (4%)	29	43
1	D	261/261 (100%)	253 (97%)	8 (3%)	35	50
1	E	261/261 (100%)	254 (97%)	7 (3%)	39	54
1	F	261/261 (100%)	253 (97%)	8 (3%)	35	50
2	G	137/137 (100%)	135 (98%)	2 (2%)	57	70
2	H	137/137 (100%)	132 (96%)	5 (4%)	31	45
2	I	137/137 (100%)	136 (99%)	1 (1%)	76	84
2	J	137/137 (100%)	133 (97%)	4 (3%)	37	52
2	K	137/137 (100%)	132 (96%)	5 (4%)	31	45
2	L	137/137 (100%)	135 (98%)	2 (2%)	57	70
All	All	2388/2388 (100%)	2318 (97%)	70 (3%)	37	52

All (70) 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

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Mol	Chain	Res	Type
1	A	114	LEU
1	A	140	LEU
1	A	233	GLU
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	267	LEU
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	125	LEU
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	109	GLU
1	D	140	LEU
1	D	233	GLU
1	D	237	PRO
1	D	271	ASP
1	D	287	GLN
1	E	13	ASN
1	E	59	PHE
1	E	109	GLU
1	E	140	LEU
1	E	233	GLU
1	E	285	TYR
1	E	287	GLN
1	F	13	ASN
1	F	59	PHE

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Mol	Chain	Res	Type
1	F	109	GLU
1	F	114	LEU
1	F	140	LEU
1	F	233	GLU
1	F	271	ASP
1	F	287	GLN
2	G	108	VAL
2	G	129	LYS
2	H	30	LEU
2	H	38	THR
2	H	80	GLN
2	H	138	CYS
2	H	144	GLU
2	I	10	GLU
2	J	24	GLN
2	J	101	GLU
2	J	103	ILE
2	J	146	SER
2	K	30	LEU
2	K	84	ASN
2	K	94	LYS
2	K	101	GLU
2	K	128	ARG
2	L	106	VAL
2	L	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) 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	231	GLN
1	B	242	ASN
1	B	246	GLN

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Mol	Chain	Res	Type
1	B	287	GLN
1	B	291	ASN
1	C	13	ASN
1	C	21	ASN
1	C	35	GLN
1	C	156	HIS
1	C	246	GLN
1	C	287	GLN
1	C	291	ASN
1	C	297	GLN
1	D	6	GLN
1	D	21	ASN
1	D	35	GLN
1	D	156	HIS
1	D	246	GLN
1	D	265	HIS
1	D	287	GLN
1	D	291	ASN
1	D	297	GLN
1	D	305	ASN
1	E	6	GLN
1	E	13	ASN
1	E	21	ASN
1	E	35	GLN
1	E	146	GLN
1	E	154	ASN
1	E	156	HIS
1	E	174	GLN
1	E	196	GLN
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
1	F	64	HIS
1	F	146	GLN
1	F	156	HIS
1	F	196	GLN
1	F	246	GLN
1	F	287	GLN

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Mol	Chain	Res	Type
1	F	291	ASN
1	F	297	GLN
1	F	305	ASN
2	G	47	ASN
2	G	73	GLN
2	G	84	ASN
2	G	147	HIS
2	G	148	ASN
2	H	8	GLN
2	H	70	GLN
2	H	84	ASN
2	H	88	ASN
2	H	105	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	40	GLN
2	I	47	ASN
2	I	63	ASN
2	I	88	ASN
2	I	105	ASN
2	I	132	ASN
2	I	148	ASN
2	I	153	ASN
2	J	73	GLN
2	J	84	ASN
2	J	88	ASN
2	J	113	ASN
2	J	132	ASN
2	J	147	HIS
2	J	148	ASN
2	K	20	HIS
2	K	24	GLN
2	K	40	GLN
2	K	47	ASN
2	K	63	ASN
2	K	73	GLN
2	K	84	ASN
2	K	88	ASN

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Mol	Chain	Res	Type
2	K	113	ASN
2	L	40	GLN
2	L	73	GLN
2	L	84	ASN
2	L	111	ASN
2	L	113	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	F	1006	-	15,15,15	1.88	6 (40%)	20,21,21	1.72	5 (25%)
3	PAL	A	1001	-	15,15,15	2.00	6 (40%)	20,21,21	1.61	6 (30%)
3	PAL	B	1002	-	15,15,15	1.91	5 (33%)	20,21,21	1.82	6 (30%)
3	PAL	E	1005	-	15,15,15	1.70	5 (33%)	20,21,21	1.86	5 (25%)
3	PAL	D	1004	-	15,15,15	1.83	5 (33%)	20,21,21	1.80	6 (30%)
3	PAL	C	1003	-	15,15,15	1.82	6 (40%)	20,21,21	1.66	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PAL	F	1006	-	-	2/17/17/17	-
3	PAL	A	1001	-	-	2/17/17/17	-
3	PAL	B	1002	-	-	2/17/17/17	-
3	PAL	E	1005	-	-	3/17/17/17	-
3	PAL	D	1004	-	-	2/17/17/17	-
3	PAL	C	1003	-	-	3/17/17/17	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	PAL	C3-C2	3.29	1.60	1.53
3	A	1001	PAL	C3-C2	3.22	1.60	1.53
3	A	1001	PAL	P-C1P	3.11	1.84	1.79
3	D	1004	PAL	P-C1P	3.07	1.84	1.79
3	F	1006	PAL	P-O1P	-3.05	1.44	1.50
3	F	1006	PAL	C3-C2	2.97	1.59	1.53
3	E	1005	PAL	P-O1P	-2.96	1.44	1.50
3	E	1005	PAL	P-C1P	2.89	1.84	1.79
3	D	1004	PAL	C3-C2	2.87	1.59	1.53
3	B	1002	PAL	P-O1P	-2.84	1.44	1.50
3	A	1001	PAL	O4-C5	2.70	1.30	1.22
3	C	1003	PAL	P-O2P	-2.66	1.49	1.55
3	F	1006	PAL	P-O2P	-2.54	1.49	1.55
3	B	1002	PAL	P-C1P	2.51	1.83	1.79
3	C	1003	PAL	C3-C2	2.51	1.58	1.53
3	C	1003	PAL	O4-C5	2.45	1.30	1.22
3	A	1001	PAL	P-O1P	-2.40	1.45	1.50
3	D	1004	PAL	P-O1P	-2.38	1.45	1.50
3	A	1001	PAL	C1-N2	-2.38	1.28	1.34
3	F	1006	PAL	C1-N2	-2.33	1.29	1.34
3	C	1003	PAL	P-C1P	2.32	1.83	1.79
3	D	1004	PAL	O4-C5	2.32	1.29	1.22
3	D	1004	PAL	O2-C4	2.31	1.28	1.22
3	B	1002	PAL	O4-C5	2.31	1.29	1.22
3	A	1001	PAL	O2-C4	2.30	1.28	1.22
3	F	1006	PAL	O4-C5	2.25	1.29	1.22
3	C	1003	PAL	P-O1P	-2.20	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	PAL	O2-C4	2.16	1.28	1.22
3	B	1002	PAL	O2-C4	2.07	1.28	1.22
3	E	1005	PAL	O2-C4	2.05	1.28	1.22
3	E	1005	PAL	O4-C5	2.03	1.28	1.22
3	E	1005	PAL	P-O2P	-2.02	1.50	1.55
3	F	1006	PAL	O2-C4	2.00	1.28	1.22

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1005	PAL	C2-N2-C1	4.34	132.57	121.68
3	E	1005	PAL	C4-C2-N2	3.84	119.48	110.57
3	D	1004	PAL	C4-C2-N2	3.70	119.16	110.57
3	F	1006	PAL	C4-C2-N2	3.66	119.07	110.57
3	D	1004	PAL	C2-N2-C1	3.51	130.48	121.68
3	B	1002	PAL	C1P-C1-N2	3.36	118.39	115.19
3	B	1002	PAL	C4-C2-N2	3.26	118.13	110.57
3	F	1006	PAL	C2-N2-C1	3.20	129.71	121.68
3	B	1002	PAL	C2-N2-C1	3.04	129.31	121.68
3	A	1001	PAL	O3-C4-O2	-2.91	117.47	124.08
3	B	1002	PAL	O3-C4-O2	-2.89	117.51	124.08
3	C	1003	PAL	C4-C2-N2	2.89	117.27	110.57
3	C	1003	PAL	C1P-C1-N2	2.87	117.92	115.19
3	A	1001	PAL	C2-N2-C1	2.82	128.75	121.68
3	C	1003	PAL	C2-N2-C1	2.77	128.63	121.68
3	E	1005	PAL	O3-C4-O2	-2.76	117.81	124.08
3	D	1004	PAL	C1P-C1-N2	2.76	117.82	115.19
3	D	1004	PAL	O3-C4-O2	-2.71	117.94	124.08
3	C	1003	PAL	O3-C4-O2	-2.70	117.96	124.08
3	F	1006	PAL	O3-C4-O2	-2.68	118.01	124.08
3	E	1005	PAL	C1P-C1-N2	2.58	117.65	115.19
3	B	1002	PAL	C2-C3-C5	2.52	119.84	112.75
3	A	1001	PAL	O3-C4-C2	2.51	122.00	113.51
3	A	1001	PAL	C4-C2-N2	2.49	116.34	110.57
3	C	1003	PAL	O3-C4-C2	2.44	121.77	113.51
3	A	1001	PAL	C1P-C1-N2	2.41	117.49	115.19
3	F	1006	PAL	O3-C4-C2	2.36	121.49	113.51
3	B	1002	PAL	O3-C4-C2	2.35	121.45	113.51
3	F	1006	PAL	C1P-C1-N2	2.32	117.40	115.19
3	D	1004	PAL	O3-C4-C2	2.20	120.96	113.51
3	E	1005	PAL	O3-C4-C2	2.17	120.84	113.51
3	D	1004	PAL	C2-C3-C5	2.10	118.65	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PAL	C2-C3-C5	2.02	118.44	112.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

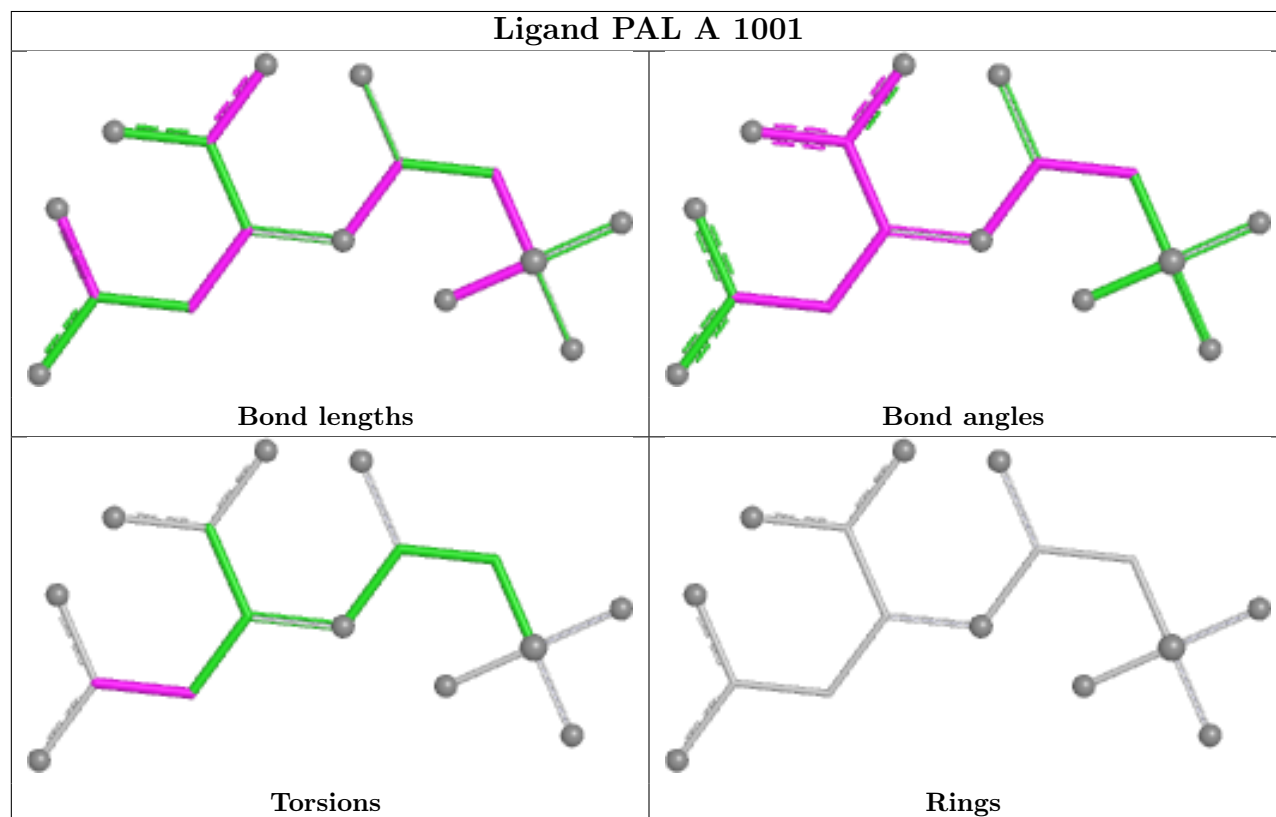
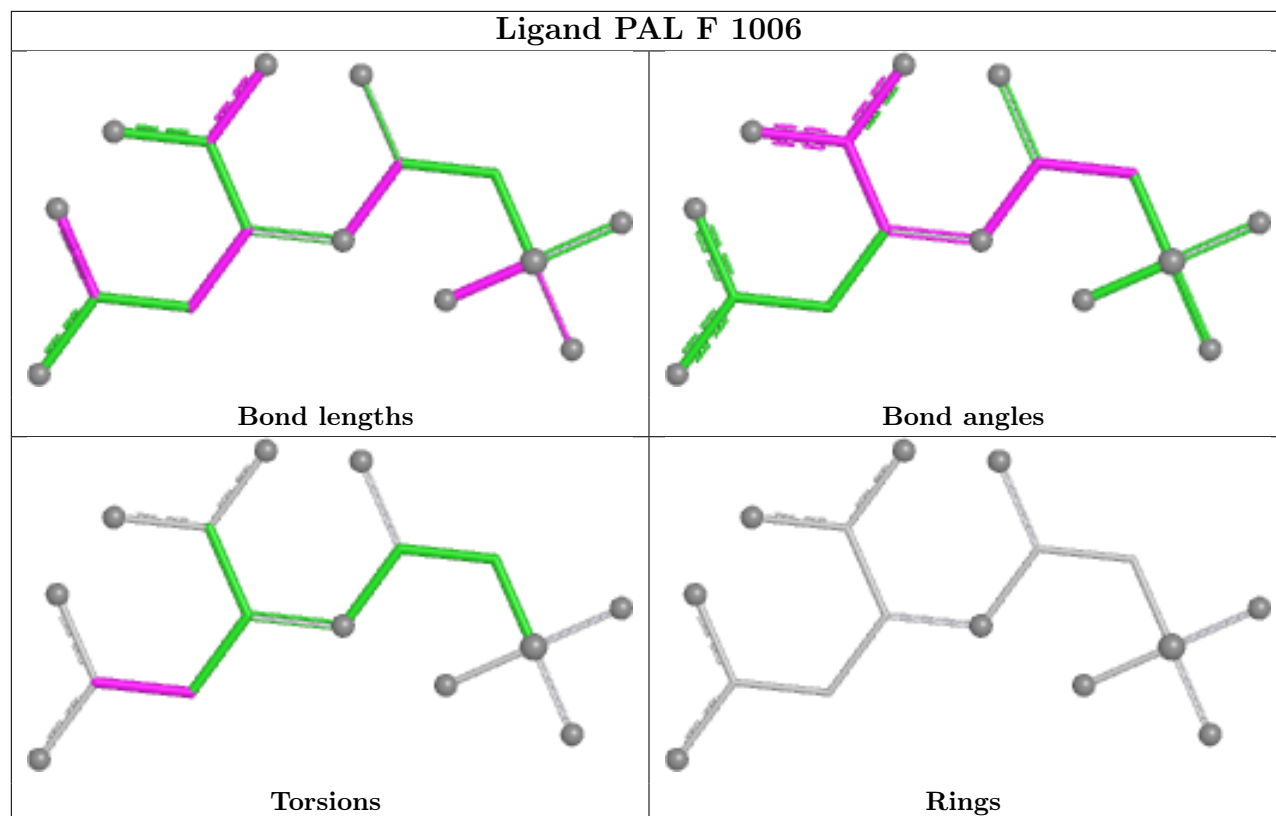
Mol	Chain	Res	Type	Atoms
3	A	1001	PAL	C2-C3-C5-O5
3	B	1002	PAL	C2-C3-C5-O5
3	C	1003	PAL	C2-C3-C5-O5
3	D	1004	PAL	C2-C3-C5-O5
3	E	1005	PAL	C2-C3-C5-O5
3	F	1006	PAL	C2-C3-C5-O5
3	E	1005	PAL	C2-C3-C5-O4
3	A	1001	PAL	C2-C3-C5-O4
3	B	1002	PAL	C2-C3-C5-O4
3	C	1003	PAL	C2-C3-C5-O4
3	D	1004	PAL	C2-C3-C5-O4
3	F	1006	PAL	C2-C3-C5-O4
3	E	1005	PAL	C4-C2-C3-C5
3	C	1003	PAL	C1-C1P-P-O3P

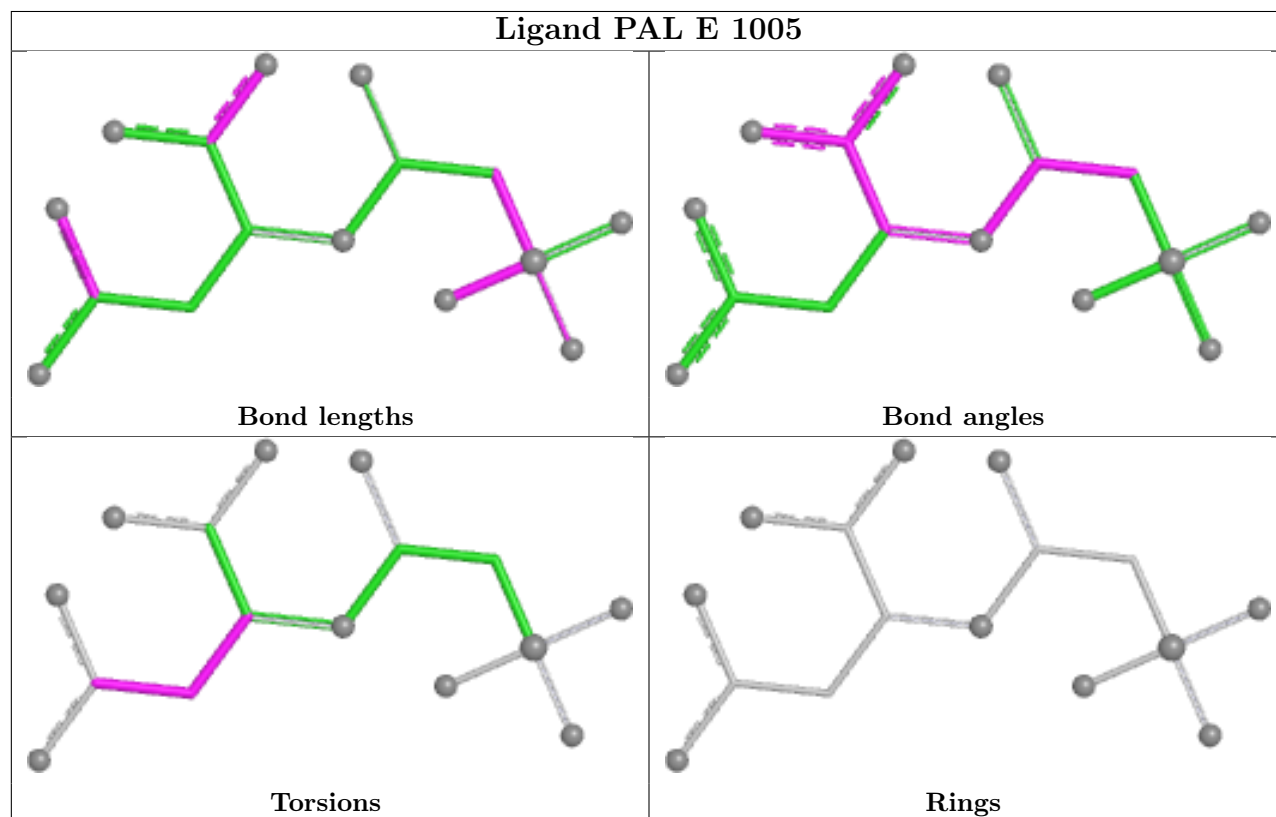
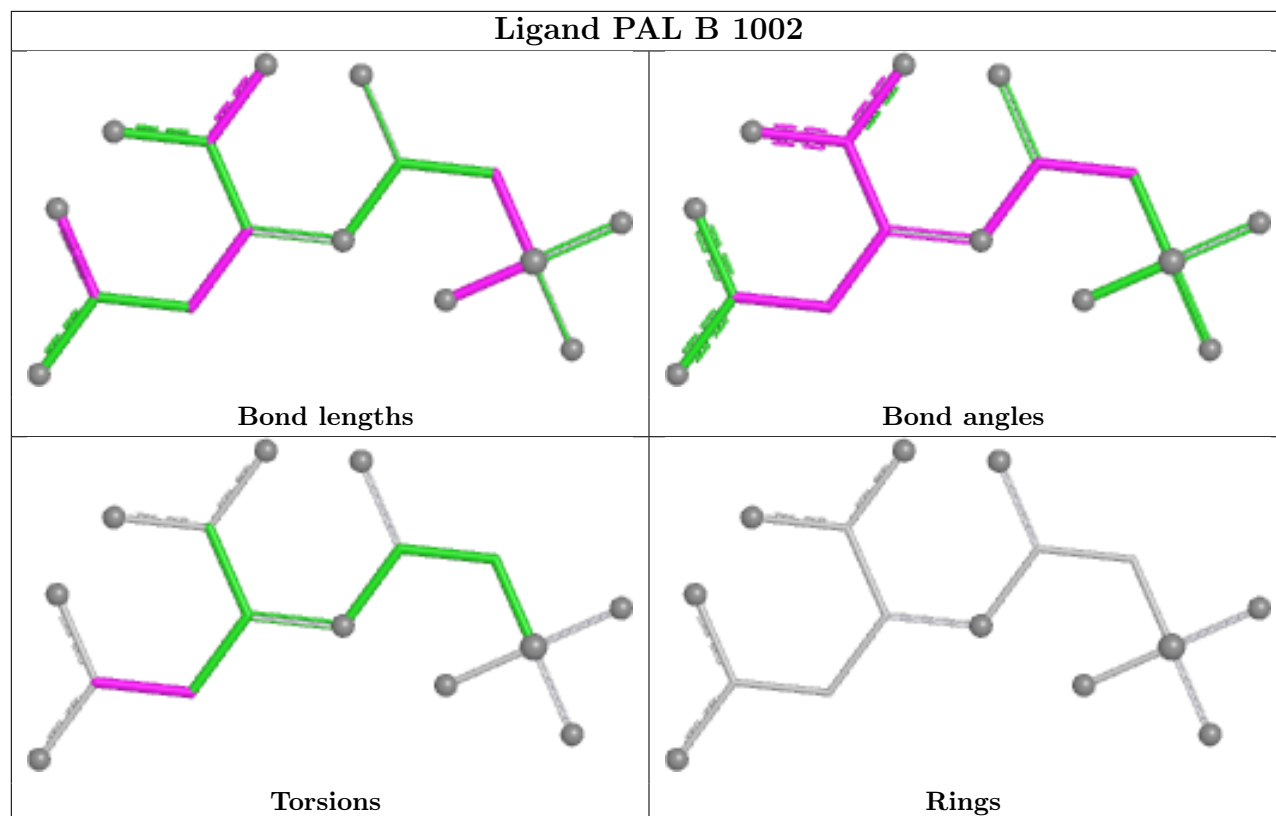
There are no ring outliers.

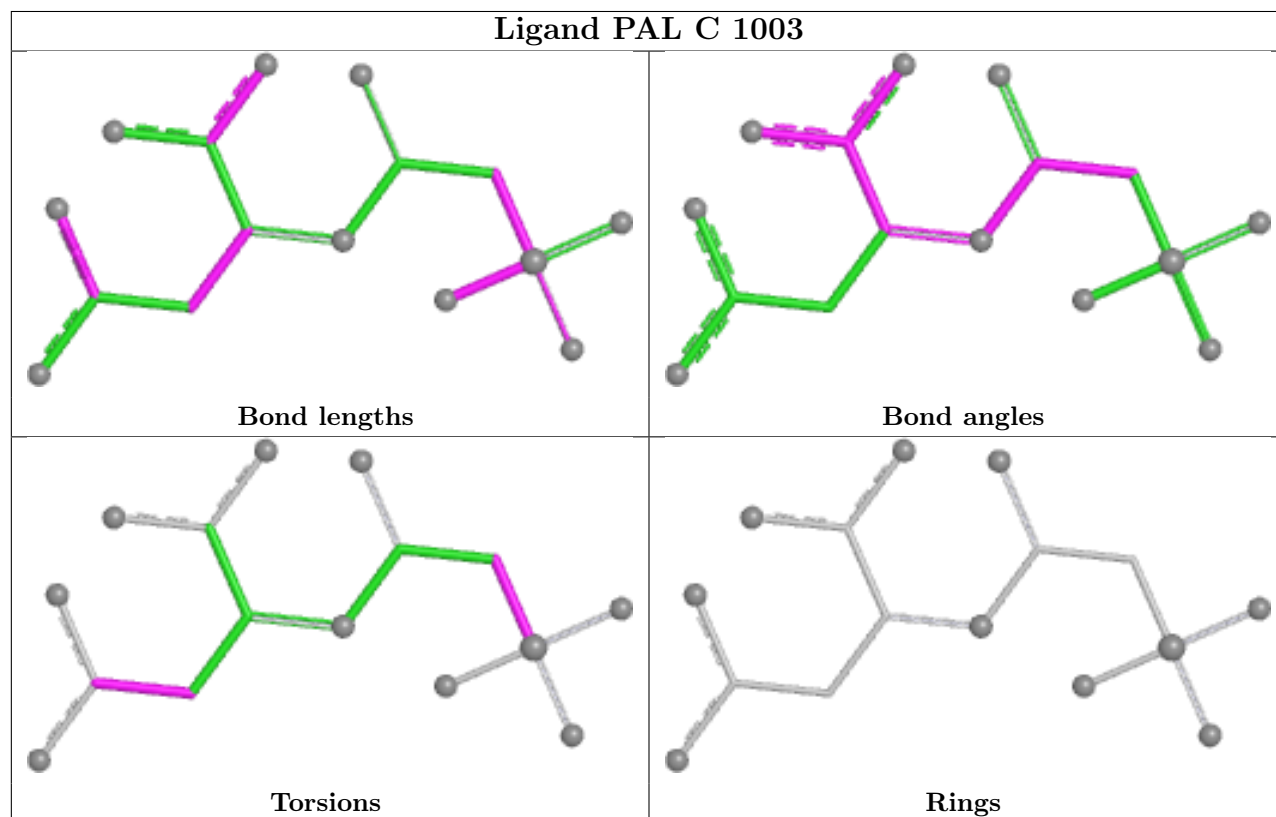
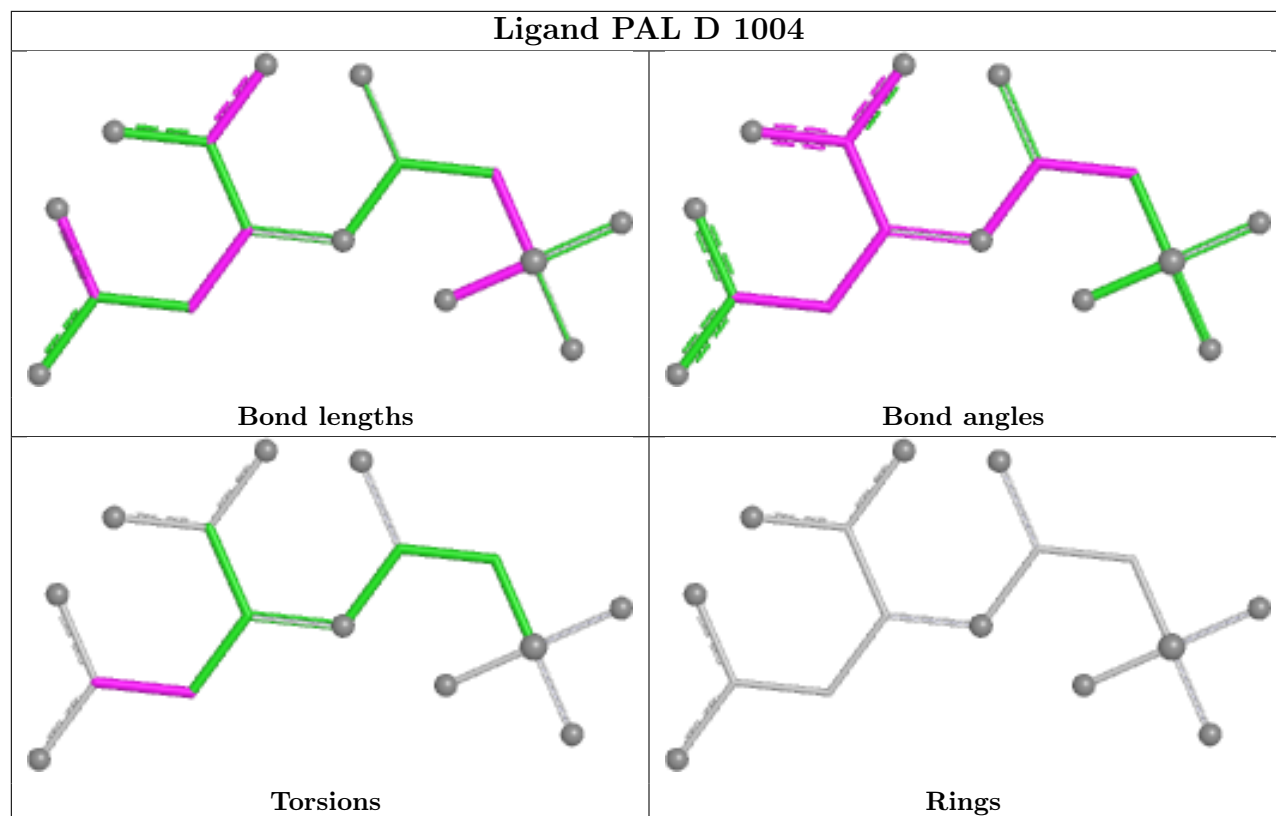
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PAL	1	0
3	B	1002	PAL	2	0
3	E	1005	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%)	-0.38	5 (1%) 70 73	26, 41, 86, 123	0
1	B	310/310 (100%)	-0.33	6 (1%) 66 67	23, 45, 101, 117	0
1	C	310/310 (100%)	-0.36	1 (0%) 90 91	26, 50, 92, 116	0
1	D	310/310 (100%)	-0.13	4 (1%) 75 77	32, 56, 99, 131	0
1	E	310/310 (100%)	-0.12	9 (2%) 53 55	32, 58, 104, 126	0
1	F	310/310 (100%)	-0.33	6 (1%) 66 67	31, 45, 94, 129	0
2	G	153/153 (100%)	0.01	5 (3%) 49 50	40, 60, 140, 153	0
2	H	153/153 (100%)	-0.10	2 (1%) 75 77	36, 58, 134, 147	0
2	I	153/153 (100%)	0.76	12 (7%) 19 16	45, 125, 154, 163	0
2	J	153/153 (100%)	-0.13	3 (1%) 65 66	38, 58, 133, 156	0
2	K	153/153 (100%)	0.15	2 (1%) 75 77	48, 74, 148, 169	0
2	L	153/153 (100%)	1.09	28 (18%) 3 2	49, 134, 157, 171	0
All	All	2778/2778 (100%)	-0.09	83 (2%) 52 53	23, 55, 139, 171	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	54	GLY	5.4
2	I	51	GLY	5.3
2	L	50	SER	5.0
1	B	236	ASP	5.0
1	A	85	GLY	4.5
1	D	79	THR	4.3
1	F	85	GLY	3.7
1	E	121	ASN	3.7
1	B	85	GLY	3.6
2	L	79	PRO	3.5
1	D	236	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	120	GLY	3.3
1	A	81	LEU	3.3
1	B	80	SER	3.2
2	L	61	ILE	3.1
1	A	79	THR	3.0
1	A	78	ASN	3.0
2	H	138	CYS	3.0
2	K	39	ASP	3.0
2	L	42	ILE	2.9
2	I	151	LEU	2.9
1	E	79	THR	2.9
1	E	81	LEU	2.9
2	L	5	ASN	2.8
1	F	267	LEU	2.8
2	G	152	ALA	2.8
1	E	80	SER	2.7
2	I	38	THR	2.7
2	J	2	THR	2.7
2	L	22	PRO	2.7
2	G	9	VAL	2.7
2	L	15	GLY	2.6
2	I	36	THR	2.6
1	E	267	LEU	2.5
2	L	100	PRO	2.5
2	L	78	ALA	2.5
1	D	85	GLY	2.5
1	F	216	GLU	2.5
1	E	153	ASP	2.4
2	I	84	ASN	2.4
2	H	54	GLY	2.4
2	I	57	ASP	2.4
2	L	12	ILE	2.4
2	G	2	THR	2.4
2	L	82	THR	2.3
2	L	25	ILE	2.3
1	B	75	ASP	2.3
1	E	75	ASP	2.3
2	L	17	VAL	2.3
1	B	79	THR	2.3
2	L	36	THR	2.3
2	I	93	GLY	2.3
2	L	133	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	132	ASN	2.3
1	A	120	GLY	2.3
2	L	60	LYS	2.3
2	I	43	THR	2.2
1	F	236	ASP	2.2
2	G	87	ASP	2.2
2	L	87	ASP	2.2
1	E	268	PRO	2.2
2	L	49	PRO	2.2
2	L	72	ASP	2.2
1	F	78	ASN	2.2
2	L	34	LYS	2.2
2	L	27	PHE	2.2
1	F	309	VAL	2.2
1	B	82	GLY	2.1
2	G	51	GLY	2.1
2	L	54	GLY	2.1
2	L	105	ASN	2.1
2	J	10	GLU	2.1
2	L	51	GLY	2.1
2	L	93	GLY	2.1
2	I	9	VAL	2.1
2	L	71	VAL	2.1
2	K	68	GLU	2.1
1	D	80	SER	2.1
2	I	69	ASP	2.0
2	I	71	VAL	2.0
2	L	66	LEU	2.0
2	L	18	ILE	2.0
1	C	75	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

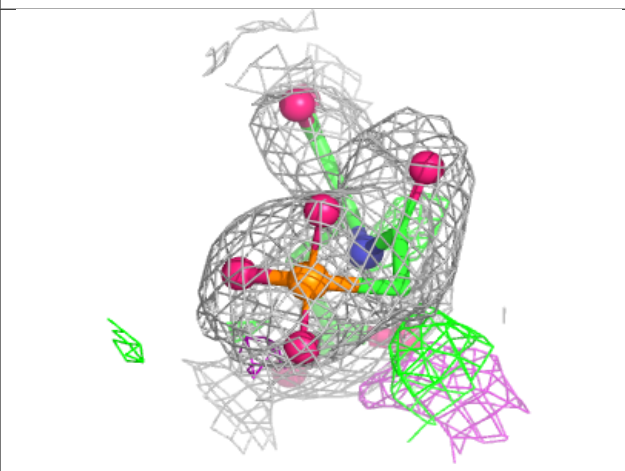
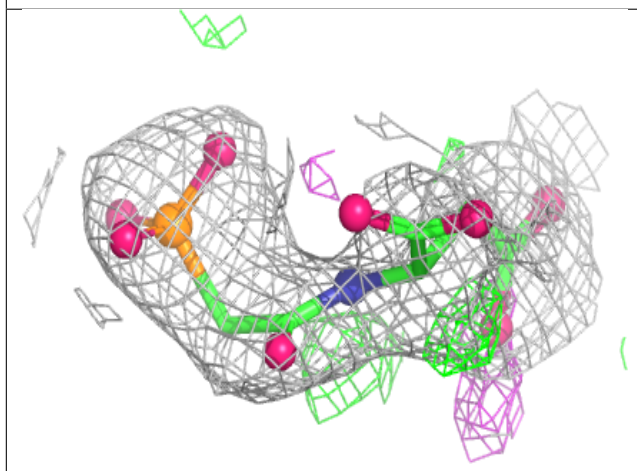
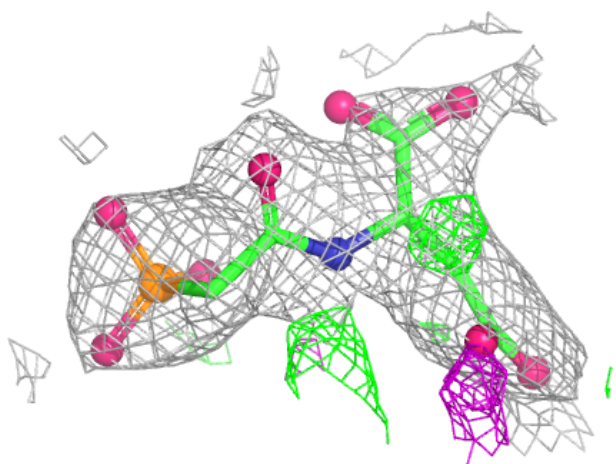
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	G	2002	1/1	0.82	0.07	48,48,48,48	0
4	ZN	H	2001	1/1	0.89	0.04	50,50,50,50	0
4	ZN	L	2006	1/1	0.89	0.04	53,53,53,53	0
3	PAL	E	1005	16/16	0.93	0.11	43,59,68,71	0
3	PAL	C	1003	16/16	0.95	0.08	36,50,60,60	0
3	PAL	D	1004	16/16	0.95	0.08	39,49,59,61	0
3	PAL	A	1001	16/16	0.96	0.08	36,44,48,49	0
3	PAL	B	1002	16/16	0.96	0.07	35,45,53,57	0
3	PAL	F	1006	16/16	0.97	0.07	35,45,57,59	0
4	ZN	J	2004	1/1	0.98	0.02	52,52,52,52	0
4	ZN	K	2005	1/1	0.98	0.02	53,53,53,53	0
4	ZN	I	2003	1/1	0.98	0.03	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.

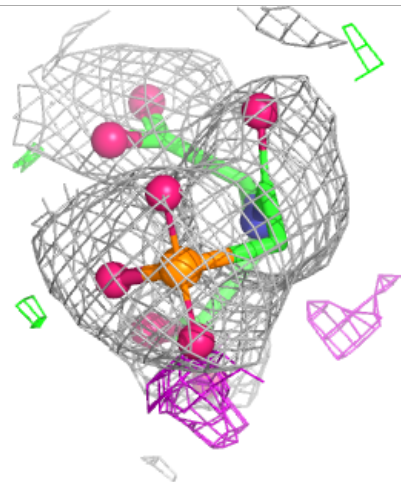
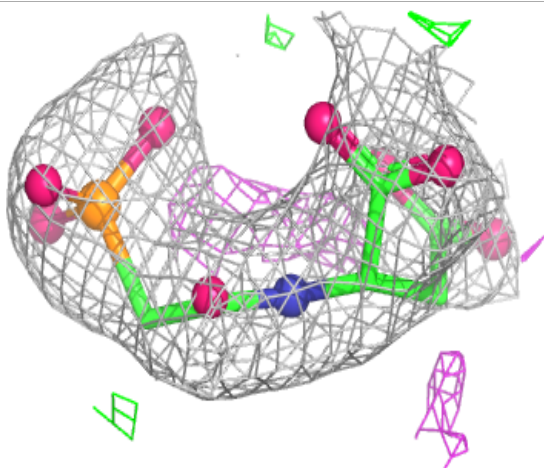
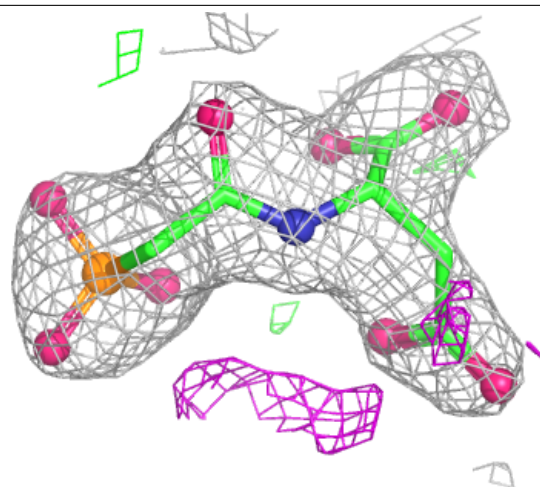
Electron density around PAL E 1005:

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



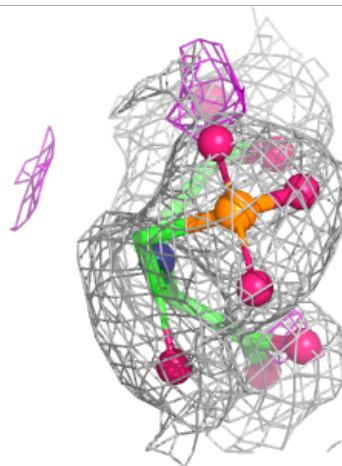
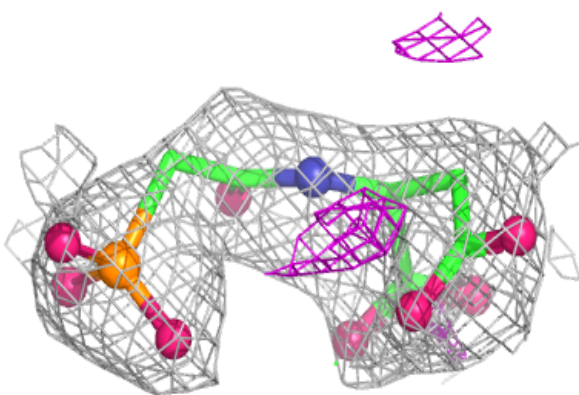
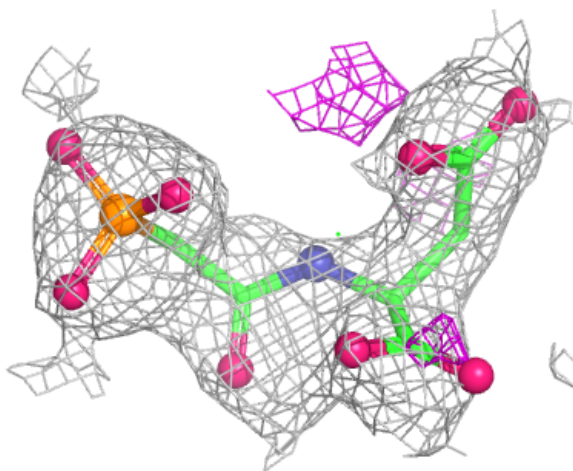
Electron density around PAL C 1003:

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



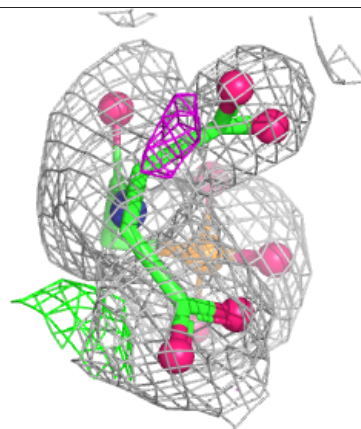
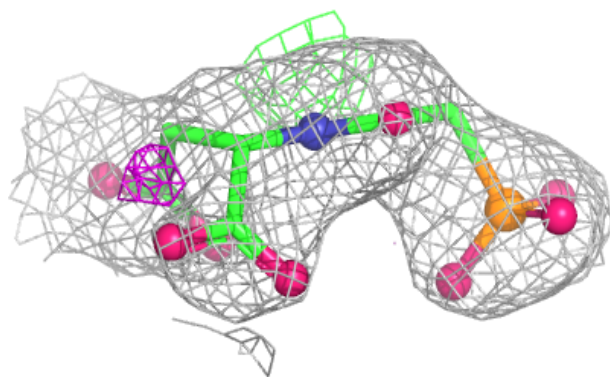
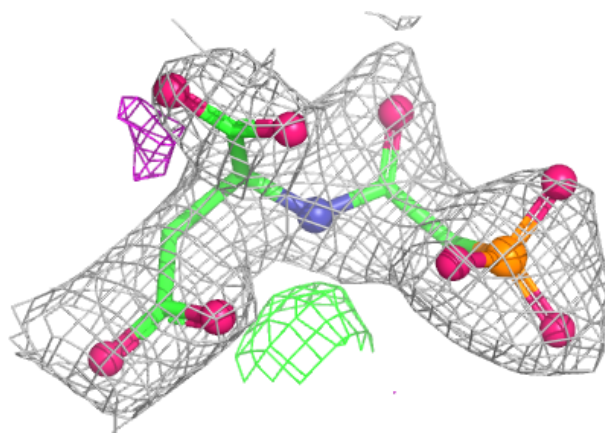
Electron density around PAL D 1004:

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



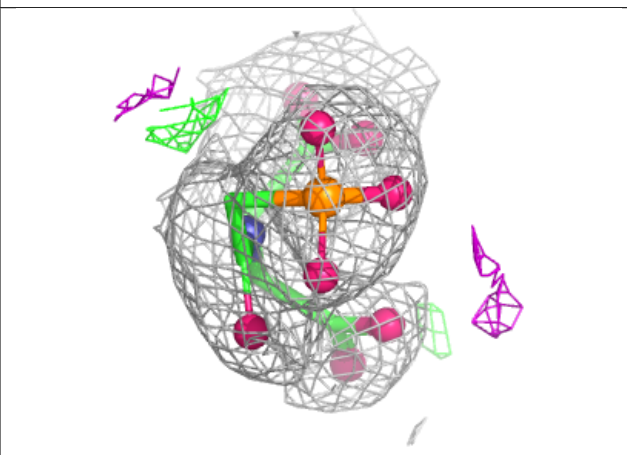
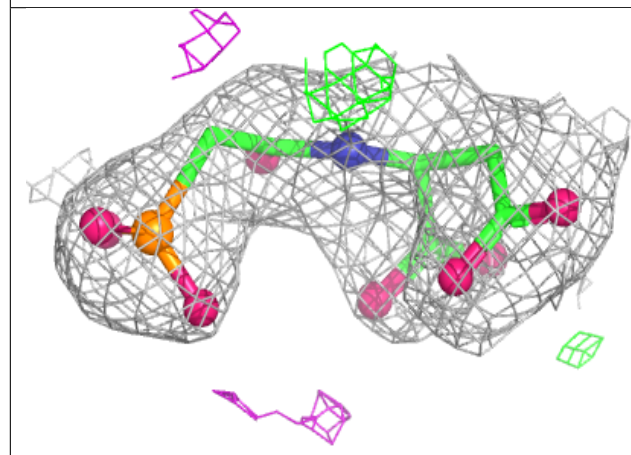
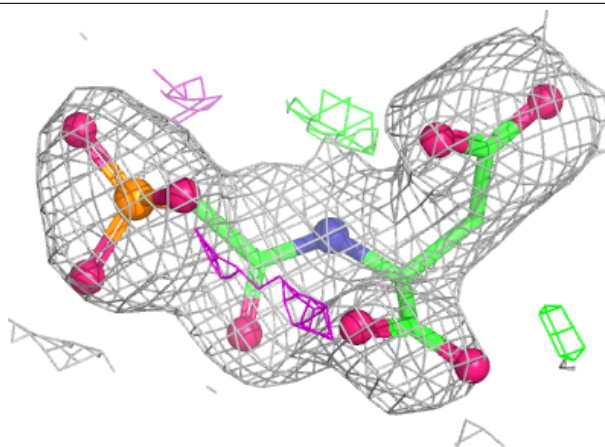
Electron density around PAL A 1001:

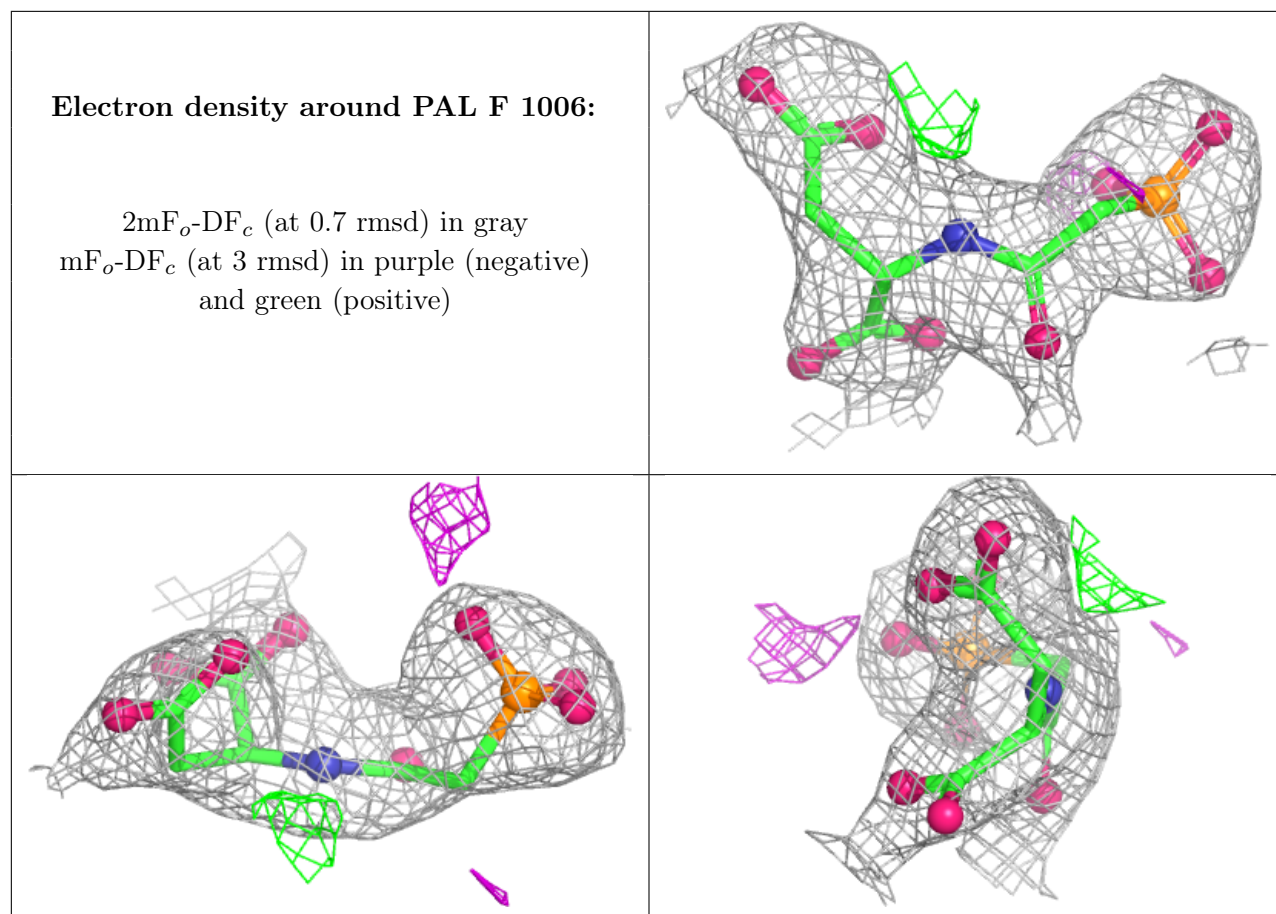
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAL 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.