



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:53 PM UTC

PDB ID : 2VF8 / pdb_00002vf8
Title : Crystal structure of UvrA2 from *Deinococcus radiodurans*
Authors : Timmins, J.; Gordon, E.; Caria, S.; Leonard, G.; Kuo, M.S.; Monchois, V.;
McSweeney, S.
Deposited on : 2007-10-31
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

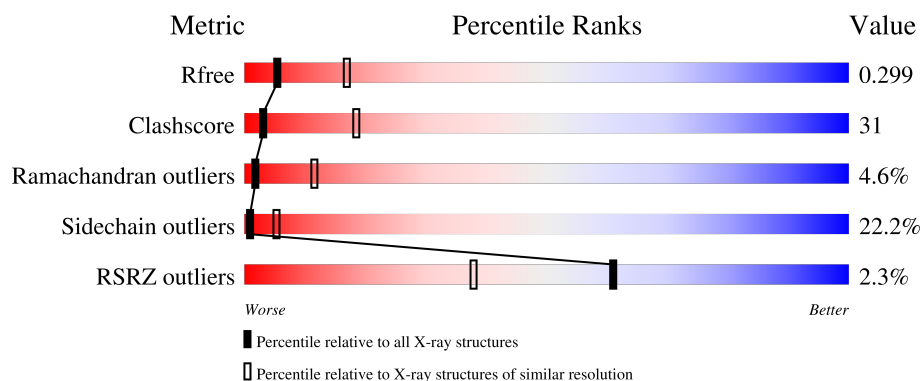
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	842	3% 43%38%14% . .
1	B	842	3% 40%42%15% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12843 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 EXCINUCLEASE ABC SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	806	Total	C	N	O	S	0	26	0
			6182	3879	1119	1165	19			
1	B	835	Total	C	N	O	S	0	26	0
			6402	4014	1154	1215	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	746	ARG	GLN	engineered mutation	UNP Q9RYW8
B	746	ARG	GLN	engineered mutation	UNP Q9RYW8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



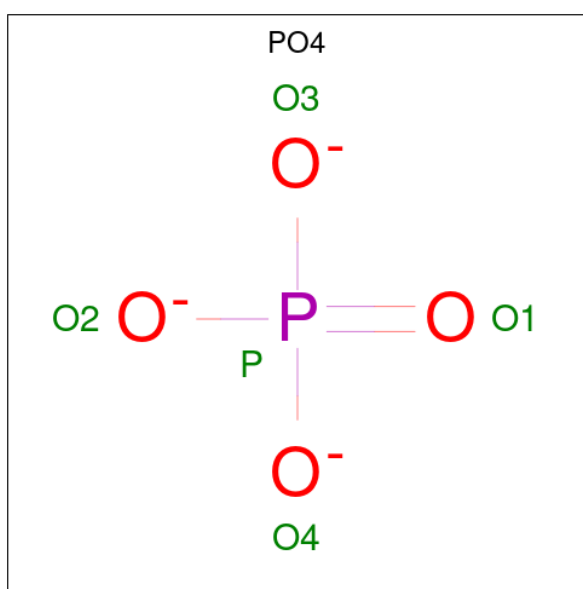
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	1
			5	4	1		
4	A	1	Total	O	S	0	1
			5	4	1		
4	A	1	Total	O	S	0	1
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	1
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	1
			5	4	1		
4	B	1	Total	O	S	0	1
			5	4	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	1
			5	4	1		

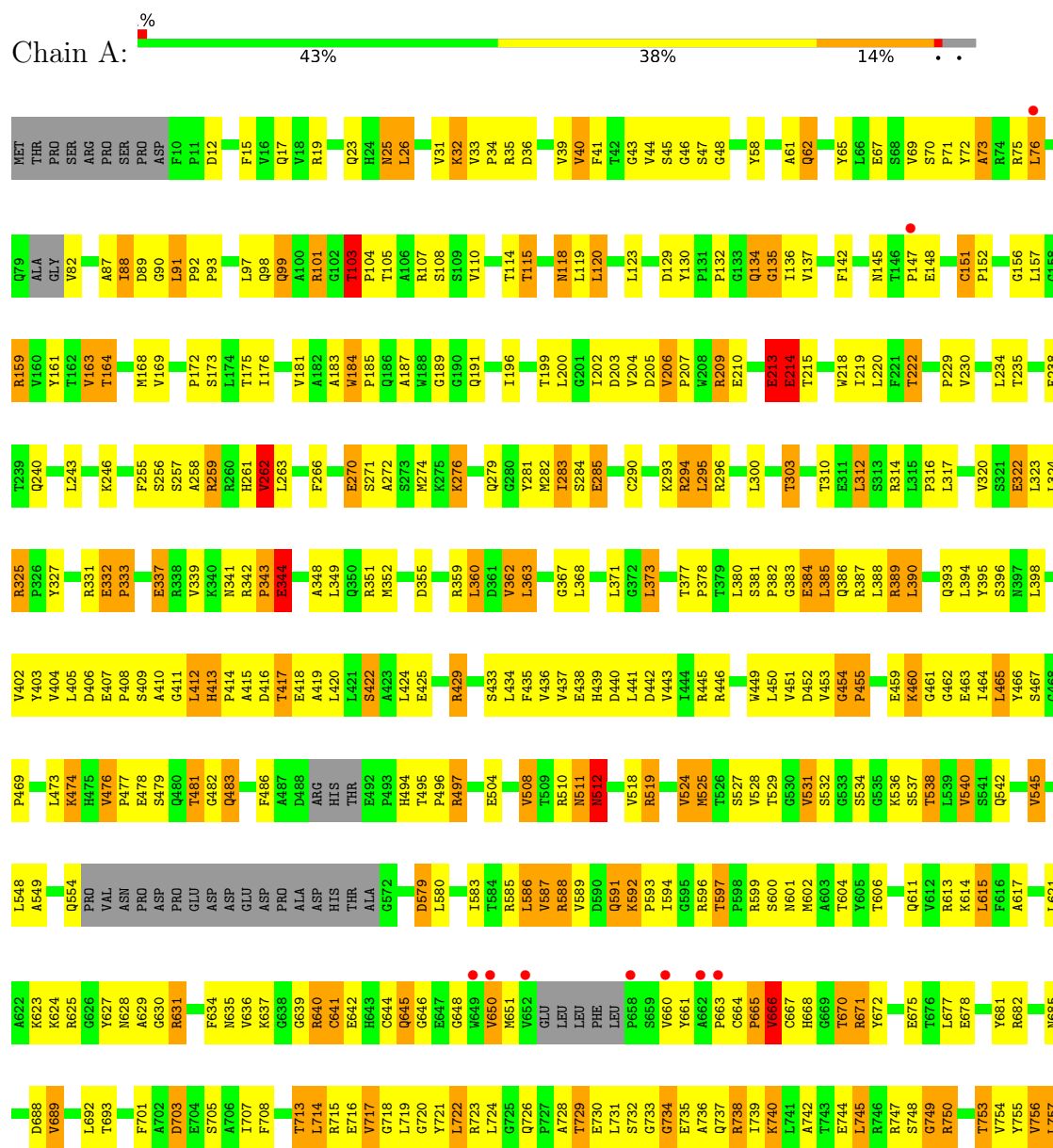
- Molecule 6 is water.

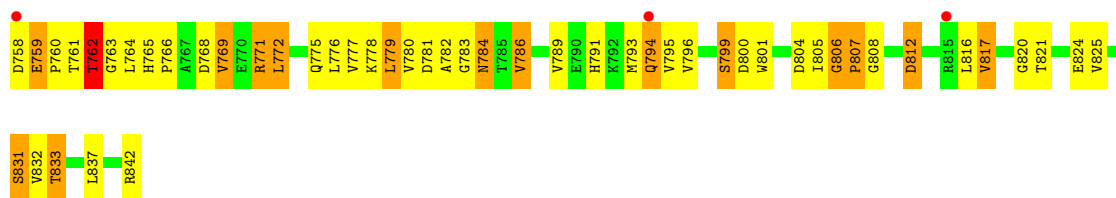
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	65	Total	O	0	0
			65	65		

3 Residue-property plots

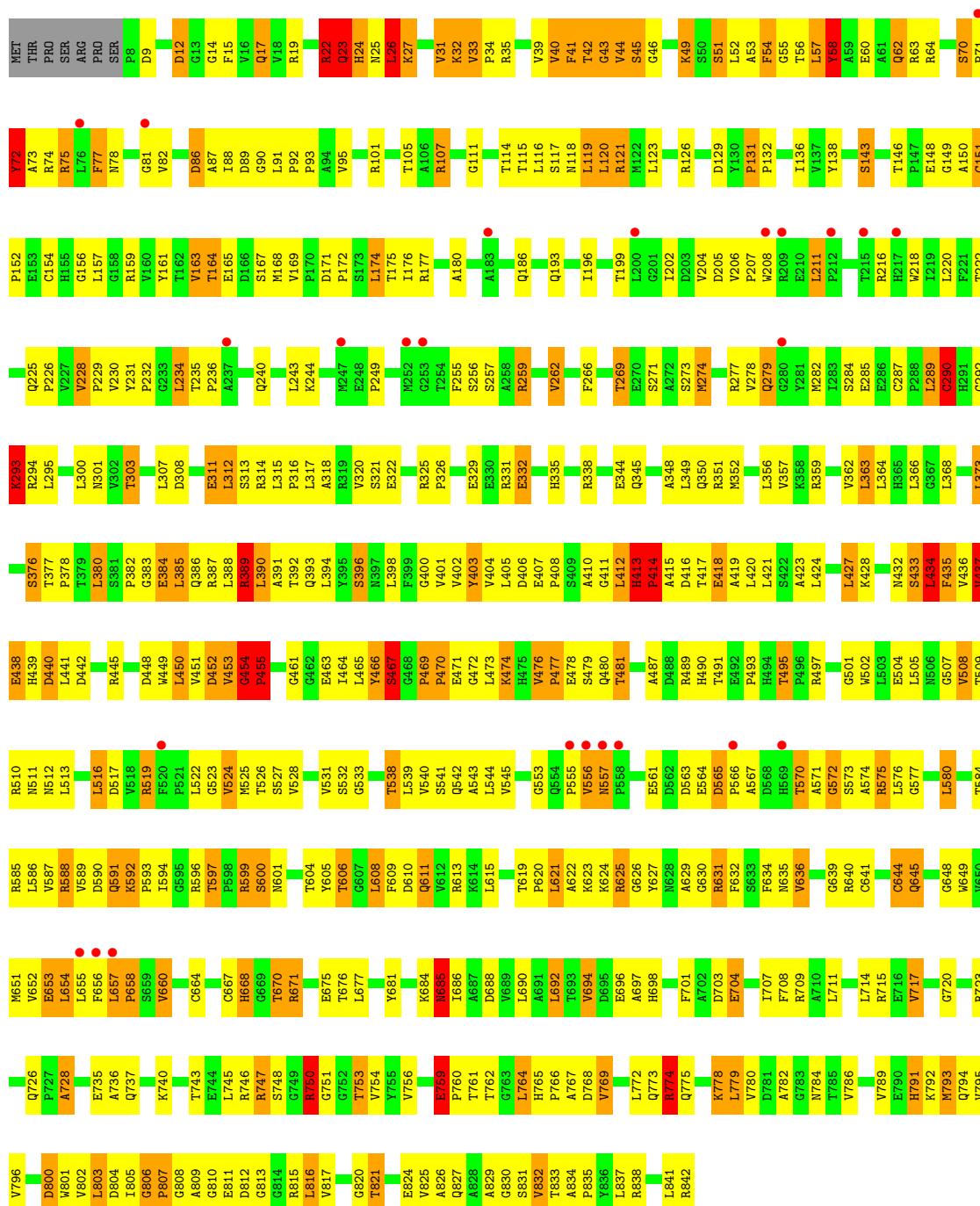
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: EXCINUCLEASE ABC SUBUNIT A





● Molecule 1: EXCINUCLEASE ABC SUBUNIT A



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.63Å 171.04Å 204.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.06 – 3.00 102.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (102.06-3.00) 95.9 (102.06-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.294 0.235 , 0.299	Depositor DCC
R_{free} test set	2543 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12843	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: PO4, SO4, ZN, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	7/6312 (0.1%)	1.22	28/8572 (0.3%)
1	B	1.23	39/6543 (0.6%)	1.35	79/8899 (0.9%)
All	All	1.12	46/12855 (0.4%)	1.29	107/17471 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	GLU	N-CA	19.95	1.69	1.46
1	A	270	GLU	CD-OE2	17.32	1.58	1.25
1	B	466	TYR	C-O	15.99	1.42	1.23
1	B	455	PRO	C-O	13.44	1.40	1.24
1	B	438	GLU	CA-C	13.11	1.68	1.52
1	B	44	VAL	CA-CB	-12.88	1.40	1.54
1	B	437	VAL	CA-C	-12.71	1.37	1.52
1	B	57	LEU	N-CA	10.86	1.60	1.46
1	B	44	VAL	CA-C	10.50	1.65	1.52
1	B	43	GLY	CA-C	10.35	1.65	1.52
1	A	270	GLU	CD-OE1	10.02	1.44	1.25
1	B	452	ASP	C-O	9.46	1.35	1.24
1	B	42	THR	C-N	9.25	1.44	1.32
1	B	452	ASP	CA-C	9.13	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	469	PRO	CA-CB	-8.99	1.45	1.53
1	B	434	LEU	C-N	8.30	1.45	1.33
1	B	454	GLY	N-CA	7.93	1.55	1.44
1	B	435	PHE	N-CA	-7.61	1.36	1.45
1	A	650	VAL	CA-CB	7.47	1.62	1.53
1	B	437	VAL	C-O	-7.35	1.14	1.24
1	B	23	GLN	CA-C	-7.22	1.43	1.52
1	B	22	ARG	N-CA	7.21	1.55	1.46
1	B	57	LEU	CA-C	6.80	1.61	1.52
1	A	276	LYS	CE-NZ	6.72	1.69	1.49
1	B	455	PRO	N-CD	-6.48	1.38	1.47
1	B	434	LEU	C-O	6.43	1.31	1.24
1	B	43	GLY	N-CA	-6.34	1.39	1.45
1	B	290	CYS	CB-SG	-6.34	1.60	1.81
1	B	467	SER	CA-CB	6.29	1.64	1.53
1	B	58	TYR	CA-CB	6.12	1.63	1.53
1	B	750	ARG	N-CA	5.88	1.49	1.46
1	B	403	TYR	N-CA	-5.87	1.38	1.46
1	B	433	SER	CA-C	-5.69	1.45	1.52
1	B	467	SER	CB-OG	5.65	1.53	1.42
1	A	540	VAL	CA-CB	-5.55	1.48	1.54
1	B	42	THR	N-CA	-5.53	1.39	1.45
1	B	452	ASP	CB-CG	-5.31	1.38	1.52
1	A	99[A]	GLN	CA-C	5.25	1.59	1.52
1	B	43	GLY	C-O	-5.22	1.17	1.23
1	B	22	ARG	CA-CB	5.19	1.60	1.52
1	B	832	VAL	CA-C	-5.18	1.46	1.53
1	B	556	VAL	CA-CB	5.10	1.60	1.54
1	B	405	LEU	CA-C	-5.07	1.46	1.52
1	A	666	VAL	CA-CB	5.07	1.60	1.54
1	B	82	VAL	CA-CB	5.01	1.60	1.54
1	B	45	SER	CB-OG	5.01	1.52	1.42

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	806	GLY	CA-C-N	13.69	136.95	119.84
1	A	806	GLY	C-N-CA	13.69	136.95	119.84
1	B	44	VAL	O-C-N	-11.79	109.95	122.57
1	B	413	HIS	CA-C-N	11.45	134.16	119.84
1	B	413	HIS	C-N-CA	11.45	134.16	119.84
1	A	631	ARG	N-CA-C	-10.71	99.60	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	GLY	CA-C-N	-9.06	109.32	119.28
1	B	454	GLY	C-N-CA	-9.06	109.32	119.28
1	B	453	VAL	N-CA-C	8.17	119.67	107.75
1	B	82	VAL	CA-C-N	-8.13	111.23	119.93
1	B	82	VAL	C-N-CA	-8.13	111.23	119.93
1	B	469	PRO	CA-C-N	8.12	130.00	119.84
1	B	469	PRO	C-N-CA	8.12	130.00	119.84
1	A	817	VAL	N-CA-C	7.81	118.61	110.72
1	B	42	THR	N-CA-C	7.75	122.09	109.85
1	A	511	ASN	CB-CA-C	-7.37	106.02	116.34
1	B	293	LYS	CA-C-N	-7.34	110.91	122.65
1	B	293	LYS	C-N-CA	-7.34	110.91	122.65
1	A	714	LEU	N-CA-C	-7.34	104.30	113.55
1	B	452	ASP	CB-CG-OD1	-7.27	101.69	118.40
1	B	454	GLY	CA-C-O	-7.11	111.35	121.52
1	B	750	ARG	N-CA-C	7.09	114.59	108.78
1	A	666	VAL	N-CA-C	6.91	118.96	111.77
1	B	435	PHE	CA-C-O	-6.72	113.51	121.11
1	B	121	ARG	N-CA-C	-6.72	103.88	111.07
1	B	592	LYS	CA-C-N	6.66	128.16	119.84
1	B	592	LYS	C-N-CA	6.66	128.16	119.84
1	A	786	VAL	N-CA-C	6.57	116.34	106.42
1	A	660	VAL	N-CA-C	6.50	118.76	108.89
1	A	419	ALA	N-CA-C	-6.44	104.34	111.36
1	B	293	LYS	N-CA-C	-6.42	102.03	110.43
1	B	45	SER	O-C-N	-6.38	114.98	122.89
1	B	86	ASP	N-CA-C	6.29	117.80	111.07
1	B	735	GLU	N-CA-C	-6.26	106.18	113.88
1	A	205	ASP	N-CA-C	6.23	119.91	112.93
1	B	750	ARG	CB-CA-C	-6.22	108.11	117.07
1	B	42	THR	CA-C-N	-6.22	113.56	122.64
1	B	42	THR	C-N-CA	-6.22	113.56	122.64
1	B	436	VAL	CG1-CB-CG2	6.19	124.42	110.80
1	A	413	HIS	CA-C-N	6.14	127.52	119.84
1	A	413	HIS	C-N-CA	6.14	127.52	119.84
1	B	432	ASN	N-CA-C	6.11	117.47	108.86
1	B	62	GLN	N-CA-C	6.08	117.58	111.07
1	B	466	TYR	O-C-N	6.06	128.86	123.41
1	B	434	LEU	CA-C-O	-5.98	114.37	120.71
1	B	436	VAL	CA-C-O	-5.98	113.30	120.78
1	B	441	LEU	N-CA-C	5.98	119.41	111.75
1	B	315	LEU	N-CA-C	5.97	118.66	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	PHE	N-CA-CB	-5.94	100.92	111.08
1	A	734	GLY	N-CA-C	-5.92	105.64	112.50
1	B	72	TYR	N-CA-C	-5.91	105.32	113.18
1	A	135	GLY	N-CA-C	5.87	127.09	113.18
1	B	466	TYR	N-CA-C	5.82	117.32	108.07
1	B	736	ALA	N-CA-C	-5.78	104.90	111.14
1	A	443	VAL	N-CA-C	-5.75	106.10	111.45
1	B	131	PRO	CA-C-N	5.75	127.02	119.84
1	B	131	PRO	C-N-CA	5.75	127.02	119.84
1	B	624	LYS	N-CA-C	5.72	117.19	111.07
1	B	477	PRO	CA-C-N	-5.70	112.06	122.38
1	B	477	PRO	C-N-CA	-5.70	112.06	122.38
1	B	791	HIS	N-CA-C	-5.68	106.22	114.12
1	B	23	GLN	CG-CD-NE2	-5.67	107.90	116.40
1	A	32	LYS	N-CA-C	-5.66	99.97	109.07
1	B	40	VAL	N-CA-CB	-5.63	102.21	111.44
1	B	295	LEU	N-CA-C	5.62	117.96	109.41
1	B	495	THR	CA-C-N	5.61	125.94	119.93
1	B	495	THR	C-N-CA	5.61	125.94	119.93
1	A	103	THR	CA-C-N	-5.52	115.07	120.98
1	A	103	THR	C-N-CA	-5.52	115.07	120.98
1	B	436	VAL	CA-C-N	-5.50	112.71	120.75
1	B	436	VAL	C-N-CA	-5.50	112.71	120.75
1	B	467	SER	N-CA-CB	5.37	119.57	110.49
1	A	222	THR	N-CA-C	5.35	118.56	110.64
1	A	47	SER	N-CA-C	5.35	117.19	111.36
1	A	580	LEU	N-CA-C	5.35	116.79	111.07
1	B	70	SER	CA-C-N	5.34	126.51	119.84
1	B	70	SER	C-N-CA	5.34	126.51	119.84
1	B	832	VAL	CB-CA-C	-5.33	104.14	111.65
1	B	33	VAL	CB-CA-C	-5.30	101.72	111.36
1	B	235	THR	CA-C-N	5.29	126.45	119.84
1	B	235	THR	C-N-CA	5.29	126.45	119.84
1	B	23	GLN	CG-CD-OE1	5.29	131.38	120.80
1	A	362	VAL	N-CA-C	-5.28	105.70	110.82
1	A	71	PRO	N-CA-C	-5.27	107.88	114.20
1	B	631	ARG	N-CA-C	-5.26	106.64	113.16
1	B	469	PRO	CB-CA-C	-5.23	106.47	111.39
1	B	389[A]	ARG	N-CA-C	-5.20	105.30	111.69
1	A	722	LEU	N-CA-C	5.16	118.23	109.76
1	B	111	GLY	N-CA-C	-5.16	106.46	113.37
1	B	448	ASP	N-CA-C	-5.16	107.54	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	VAL	CA-C-N	5.14	130.86	121.97
1	B	44	VAL	C-N-CA	5.14	130.86	121.97
1	B	522	LEU	N-CA-C	5.13	117.77	109.40
1	A	670	THR	N-CA-C	5.13	116.68	111.14
1	B	35	ARG	N-CA-CB	5.13	117.45	110.38
1	B	384	GLU	CA-C-N	-5.12	112.40	120.60
1	B	384	GLU	C-N-CA	-5.12	112.40	120.60
1	B	436	VAL	CA-CB-CG1	-5.12	101.70	110.40
1	A	627	TYR	N-CA-C	5.11	117.76	110.24
1	B	31	VAL	CB-CA-C	-5.11	101.87	110.71
1	B	41	PHE	CA-C-O	-5.11	114.70	120.32
1	B	87	ALA	N-CA-C	5.11	116.83	108.55
1	A	142	PHE	N-CA-C	-5.10	105.78	112.41
1	B	644	CYS	N-CA-C	-5.07	107.65	113.88
1	B	206	VAL	CA-C-N	5.03	126.13	119.84
1	B	206	VAL	C-N-CA	5.03	126.13	119.84
1	B	43	GLY	CA-C-O	5.02	127.41	122.14

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	GLY	Peptide
1	A	666	VAL	Peptide
1	A	806	GLY	Peptide
1	B	45	SER	Mainchain
1	B	455	PRO	Mainchain
1	B	565	ASP	Peptide
1	B	806	GLY	Peptide

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	6182	0	6036	384	0
1	B	6402	0	6222	409	0
2	A	54	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	54	0	24	10	0
3	A	2	0	0	0	0
3	B	2	0	0	1	0
4	A	15	0	0	0	0
4	B	25	0	0	0	0
5	B	5	0	0	0	0
6	A	37	0	0	5	0
6	B	65	0	0	9	0
All	All	12843	0	12306	793	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 31.

All (793) 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:A:276:LYS:CE	1:A:276:LYS:NZ	1.69	1.52
1:B:438:GLU:N	1:B:438:GLU:CA	1.69	1.51
1:A:759:GLU:OE2	1:A:791[A]:HIS:CD2	1.83	1.30
1:B:413:HIS:CE1	1:B:833:THR:HG22	1.77	1.19
1:B:413:HIS:HE1	1:B:833:THR:HG22	1.06	1.17
1:B:487:ALA:HB1	1:B:490:HIS:NE2	1.65	1.11
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.15	1.09
1:A:764:LEU:HD12	1:A:768:ASP:HB3	1.32	1.06
1:A:120:LEU:H	1:A:120:LEU:HD12	1.23	1.00
1:B:685:ASN:HD22	1:B:686:ILE:H	1.02	0.99
1:A:343:PRO:HD2	1:A:344:GLU:OE1	1.63	0.97
1:B:412:LEU:HD21	1:B:416:ASP:HB2	1.45	0.97
1:A:413:HIS:HE1	1:A:833:THR:HG22	1.27	0.96
1:B:196:ILE:HG23	1:B:228:VAL:HG21	1.48	0.96
1:A:452:ASP:OD1	1:A:481:THR:HG21	1.66	0.96
1:A:670:THR:HG21	1:A:677:LEU:HD11	1.47	0.96
1:A:418:GLU:OE1	1:A:446:ARG:NH2	1.98	0.95
1:A:592:LYS:HG3	1:A:593:PRO:HD2	1.47	0.94
1:A:804:ASP:HB3	1:A:817:VAL:HG23	1.48	0.93
1:A:386:GLN:NE2	1:A:406:ASP:H	1.65	0.93
1:A:753:THR:N	1:A:784:ASN:HD21	1.66	0.93
1:A:585:ARG:HB2	1:A:753:THR:HB	1.49	0.91
1:A:538:THR:HG23	2:A:1844:ADP:O2A	1.70	0.91
1:B:599:ARG:HH11	1:B:599:ARG:CG	1.82	0.91
1:A:753:THR:H	1:A:784:ASN:HD21	1.13	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:TYR:HB2	1:A:786:VAL:HG12	1.51	0.90
1:A:599:ARG:HD2	1:A:635:ASN:ND2	1.86	0.89
1:A:386:GLN:HE22	1:A:406:ASP:H	0.90	0.88
1:A:108:SER:O	1:A:377:THR:HG23	1.73	0.87
1:A:644:CYS:SG	1:A:648:GLY:N	2.47	0.87
1:B:287:CYS:SG	1:B:290:CYS:HB2	2.15	0.86
1:A:412:LEU:O	1:A:791[B]:HIS:HD2	1.57	0.86
1:A:46:GLY:O	2:A:1843:ADP:H5'2	1.76	0.86
1:A:670:THR:O	1:A:671:ARG:HB2	1.76	0.86
1:B:504:GLU:HB2	1:B:577:GLY:O	1.77	0.85
1:B:159:ARG:HD3	1:B:284:SER:OG	1.76	0.85
1:A:413:HIS:CE1	1:A:833:THR:HG22	2.10	0.84
1:B:599:ARG:HE	1:B:635:ASN:ND2	1.75	0.84
1:B:580:LEU:HD12	1:B:580:LEU:H	1.44	0.83
1:A:527:SER:HB3	1:A:796:VAL:HG22	1.60	0.83
1:B:759:GLU:CG	1:B:791:HIS:HD2	1.91	0.83
1:B:545:VAL:HG13	1:B:586:LEU:HD21	1.62	0.82
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.43	0.82
1:B:807:PRO:HG3	1:B:815[A]:ARG:NH1	1.93	0.82
1:A:120:LEU:HD12	1:A:120:LEU:N	1.93	0.82
1:A:199:THR:HG21	1:A:229:PRO:O	1.80	0.82
1:B:413:HIS:HD2	1:B:415:ALA:H	1.28	0.82
1:A:411:GLY:HA2	1:A:791[A]:HIS:CD2	2.14	0.81
1:B:759:GLU:CG	1:B:791:HIS:CD2	2.64	0.81
1:A:478:GLU:N	1:A:478:GLU:OE1	2.14	0.81
1:B:338:ARG:HH11	1:B:345:GLN:HE22	1.30	0.80
1:B:685:ASN:HD22	1:B:686:ILE:N	1.80	0.80
1:A:181:VAL:HG11	1:A:184:TRP:CE3	2.17	0.80
1:B:487:ALA:CB	1:B:490:HIS:NE2	2.43	0.80
1:B:599:ARG:HG2	1:B:599:ARG:NH1	1.97	0.79
1:A:615:LEU:HD11	1:A:681:TYR:CE1	2.16	0.79
1:A:804:ASP:OD2	1:A:831:SER:HB2	1.82	0.79
1:B:176:ILE:HD12	1:B:204:VAL:HA	1.65	0.79
1:A:670:THR:HG22	1:A:672:TYR:H	1.45	0.79
1:A:497:ARG:HH11	1:A:497:ARG:CG	1.96	0.78
1:A:750:ARG:HA	1:A:750:ARG:NH1	1.99	0.78
1:B:413:HIS:HE1	1:B:833:THR:CG2	1.94	0.78
1:A:589:VAL:HB	1:A:757:LEU:HB3	1.65	0.78
1:B:175:THR:HG23	1:B:205:ASP:HA	1.65	0.78
1:A:173:SER:HA	1:A:209:ARG:HD3	1.65	0.78
1:B:759:GLU:HG2	1:B:791:HIS:CD2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:THR:HG23	1:A:763:GLY:N	2.00	0.77
1:A:327:TYR:HA	1:A:332:GLU:HG2	1.66	0.77
1:A:386:GLN:HE22	1:A:406:ASP:N	1.75	0.76
1:A:438:GLU:HG3	1:A:440:ASP:H	1.50	0.76
1:B:163:VAL:HA	6:B:2011:HOH:O	1.84	0.76
1:A:373:LEU:HD23	1:A:373:LEU:H	1.50	0.76
1:A:762:THR:CG2	1:A:763:GLY:H	1.98	0.76
1:B:698:HIS:CD2	1:B:715:ARG:HD2	2.19	0.76
1:B:413:HIS:CD2	1:B:415:ALA:H	2.04	0.76
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.49	0.76
1:A:413:HIS:HE1	1:A:833:THR:CG2	1.97	0.76
1:B:538:THR:HG21	2:B:1844:ADP:H5'1	1.65	0.75
1:A:40:VAL:HG12	1:A:450:LEU:HD12	1.67	0.75
1:B:226:PRO:HD2	1:B:255:PHE:HB3	1.67	0.75
1:A:412:LEU:O	1:A:791[B]:HIS:CD2	2.39	0.75
1:B:737:GLN:HE22	1:B:760:PRO:HA	1.52	0.74
1:B:796:VAL:HG12	1:B:837:LEU:HD21	1.68	0.74
1:A:450:LEU:HG	1:A:451:VAL:N	2.02	0.74
1:A:599:ARG:CD	1:A:635:ASN:HD21	1.99	0.74
1:B:829:ALA:HA	6:B:2058:HOH:O	1.86	0.74
1:B:77:PHE:CZ	1:B:654:LEU:CB	2.71	0.73
1:B:380:LEU:HD23	1:B:385:LEU:HB3	1.69	0.73
1:B:508:VAL:HA	1:B:574:ALA:HB2	1.69	0.73
1:B:22:ARG:NH2	1:B:86:ASP:OD1	2.15	0.73
1:A:529:THR:HG22	1:A:796:VAL:HG21	1.70	0.72
1:A:599:ARG:CD	1:A:635:ASN:ND2	2.51	0.72
1:A:586:LEU:O	1:A:586:LEU:HG	1.88	0.72
1:A:642:GLU:OE1	1:A:642:GLU:HA	1.89	0.72
1:B:348:ALA:O	1:B:352:MET:HB2	1.89	0.72
1:B:320:VAL:HG21	1:B:373:LEU:HD21	1.70	0.72
1:B:454:GLY:HA2	1:B:463:GLU:HB2	1.72	0.72
1:B:77:PHE:CZ	1:B:654:LEU:HB3	2.25	0.71
1:A:511:ASN:HD22	1:A:538:THR:HG21	1.54	0.71
1:A:531:VAL:HG12	1:A:534:SER:HB3	1.72	0.71
1:A:641:CYS:SG	1:A:667:CYS:HB3	2.30	0.71
1:B:290:CYS:SG	1:B:293:LYS:O	2.48	0.71
1:A:602:MET:HG3	1:A:739:ILE:HD11	1.72	0.71
1:B:807:PRO:HD2	1:B:813:GLY:HA2	1.72	0.71
1:B:311:GLU:HG2	6:B:2018:HOH:O	1.90	0.71
1:A:25:ASN:H	1:A:25:ASN:HD22	1.39	0.70
1:A:719:LEU:HD22	1:A:722:LEU:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:O	1:B:467:SER:HA	1.91	0.70
1:B:49:LYS:HE3	1:B:439:HIS:NE2	2.06	0.70
1:A:425:GLU:HA	1:A:425:GLU:OE1	1.90	0.70
1:B:44:VAL:HG13	1:B:768:ASP:OD1	1.90	0.70
1:B:77:PHE:CE1	1:B:654:LEU:HB2	2.27	0.69
1:B:196:ILE:HG23	1:B:228:VAL:CG2	2.22	0.69
1:A:597:THR:HB	1:A:599:ARG:H	1.58	0.69
1:B:307:LEU:HB3	1:B:311:GLU:HB3	1.74	0.69
1:B:580:LEU:HD12	1:B:580:LEU:N	2.07	0.69
1:B:538:THR:CG2	2:B:1844:ADP:H5'1	2.23	0.69
1:B:580:LEU:H	1:B:580:LEU:CD1	2.05	0.69
1:A:759:GLU:OE2	1:A:791[A]:HIS:NE2	2.25	0.69
1:A:163:VAL:HG21	1:A:168:MET:HE3	1.75	0.69
1:A:762:THR:HG23	1:A:763:GLY:H	1.54	0.69
1:A:613:ARG:HH11	1:A:630:GLY:HA3	1.58	0.69
1:B:575:ARG:HH11	1:B:575:ARG:CG	2.06	0.69
1:A:367:GLY:HA2	6:A:2020:HOH:O	1.93	0.68
1:A:411:GLY:HA2	1:A:791[A]:HIS:NE2	2.07	0.68
1:B:773[A]:GLN:NE2	1:B:795:VAL:HG23	2.08	0.68
1:A:769:VAL:HG21	1:A:794:GLN:OE1	1.93	0.68
1:B:42:THR:OG1	1:B:452:ASP:OD1	2.10	0.68
1:A:344:GLU:HA	6:A:2016:HOH:O	1.94	0.68
1:A:466:TYR:OH	1:A:469:PRO:O	2.10	0.68
1:B:508:VAL:HA	1:B:574:ALA:CB	2.23	0.67
1:B:619:THR:HB	1:B:620:PRO:HD2	1.75	0.67
1:A:776:LEU:HA	1:A:779:LEU:HD22	1.76	0.67
1:B:146:THR:HB	1:B:148:GLU:OE2	1.94	0.67
1:B:386:GLN:HE22	1:B:406:ASP:H	1.43	0.67
1:B:453:VAL:O	1:B:454:GLY:O	2.13	0.67
1:A:764:LEU:CD1	1:A:768:ASP:HB3	2.19	0.67
1:A:295:LEU:HB2	1:A:300:LEU:CD1	2.25	0.67
1:B:412:LEU:CD2	1:B:416:ASP:HB2	2.23	0.66
1:B:759:GLU:HG3	1:B:791:HIS:CD2	2.30	0.66
1:A:675:GLU:O	1:A:678:GLU:N	2.27	0.66
1:A:747:ARG:O	1:A:749:GLY:N	2.27	0.66
1:A:762:THR:CG2	1:A:763:GLY:N	2.56	0.66
1:A:497:ARG:HG2	1:A:497:ARG:NH1	1.95	0.66
1:B:12:ASP:C	1:B:14:GLY:H	2.04	0.66
1:B:159:ARG:HB2	1:B:285:GLU:O	1.96	0.66
1:B:53:ALA:HA	1:B:57:LEU:HD12	1.77	0.66
1:B:290:CYS:HB3	1:B:292:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LEU:HD22	1:B:434:LEU:HD22	1.77	0.66
1:B:77:PHE:CZ	1:B:654:LEU:HB2	2.30	0.65
1:A:529:THR:CG2	1:A:796:VAL:HG21	2.25	0.65
1:A:670:THR:O	1:A:671:ARG:CB	2.44	0.65
1:A:613:ARG:HD2	1:A:630:GLY:HA2	1.79	0.65
1:A:646:GLY:O	1:A:671:ARG:HG2	1.97	0.65
1:A:235:THR:HG22	1:A:238:GLU:CD	2.22	0.65
1:B:599:ARG:HH11	1:B:599:ARG:HG3	1.62	0.65
1:A:393:GLN:HA	1:A:396:SER:HB3	1.79	0.65
1:A:413:HIS:HD2	1:A:415:ALA:H	1.42	0.65
1:A:266:PHE:CD1	1:A:282:MET:HE1	2.32	0.65
1:A:405:LEU:HB2	1:A:436:VAL:HG22	1.79	0.65
1:A:753:THR:N	1:A:784:ASN:ND2	2.44	0.64
1:B:807:PRO:HG3	1:B:815[A]:ARG:HH11	1.59	0.64
1:B:651:MET:HE3	1:B:653:GLU:HG2	1.78	0.64
1:B:622:ALA:HA	1:B:627:TYR:HB2	1.79	0.64
1:B:428:LYS:HB2	1:B:434:LEU:HD11	1.79	0.64
1:B:466:TYR:OH	1:B:472:GLY:HA3	1.97	0.64
1:B:211:LEU:O	1:B:216:ARG:HD3	1.98	0.64
1:B:801:TRP:CH2	1:B:820:GLY:HA2	2.33	0.64
1:B:385:LEU:HD12	1:B:385:LEU:H	1.63	0.64
1:A:322:GLU:HG3	1:A:325:ARG:HH21	1.63	0.63
1:B:90:GLY:O	1:B:92:PRO:HD3	1.99	0.63
1:B:600:SER:O	1:B:728:ALA:HB2	1.99	0.63
1:B:509:THR:HA	1:B:513:LEU:O	1.97	0.63
1:A:349:LEU:O	1:A:349:LEU:HD23	1.99	0.63
1:B:403:TYR:CE1	1:B:427:LEU:HD22	2.33	0.63
1:B:750:ARG:HB3	1:B:750:ARG:CZ	2.28	0.63
1:A:723:ARG:HB2	1:A:726:GLN:HB2	1.81	0.62
1:A:295:LEU:HB2	1:A:300:LEU:HD13	1.81	0.62
1:A:615:LEU:HD11	1:A:681:TYR:CD1	2.34	0.62
1:A:769:VAL:HG21	1:A:794:GLN:CD	2.23	0.62
1:A:235:THR:O	1:A:238:GLU:HG2	1.99	0.62
1:B:631:ARG:NH2	1:B:676:THR:OG1	2.28	0.62
1:B:176:ILE:HB	1:B:204:VAL:HG13	1.82	0.62
1:A:359:ARG:HH11	1:A:395:TYR:HD1	1.48	0.62
1:A:17:GLN:HE22	1:A:32:LYS:HB3	1.65	0.61
1:A:591[A]:GLN:OE1	1:A:762:THR:OG1	2.18	0.61
1:B:805:ILE:HG22	1:B:806:GLY:N	2.15	0.61
1:B:807:PRO:CD	1:B:813:GLY:HA2	2.30	0.61
1:A:25:ASN:ND2	2:A:1843:ADP:H4'	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:O	1:A:114:THR:HG23	2.00	0.61
1:A:776:LEU:HA	1:A:779:LEU:CD2	2.30	0.61
1:B:644:CYS:O	1:B:645:GLN:HB2	1.99	0.61
1:A:73:ALA:HA	1:A:76:LEU:HB2	1.82	0.61
1:B:403:TYR:CE1	1:B:427:LEU:CD2	2.84	0.61
1:A:672:TYR:HB2	1:A:677:LEU:HD21	1.82	0.61
1:A:807:PRO:HD2	1:A:812:ASP:O	1.99	0.61
1:A:271:SER:HB3	1:A:274:MET:HB3	1.83	0.61
1:A:599:ARG:HD2	1:A:635:ASN:HD22	1.64	0.61
1:B:49:LYS:CE	1:B:439:HIS:NE2	2.64	0.60
1:A:183:ALA:HA	1:A:281:TYR:CE2	2.36	0.60
1:A:383:GLY:O	1:A:384:GLU:C	2.43	0.60
1:B:597:THR:OG1	1:B:599:ARG:HB2	2.01	0.60
1:A:729:THR:O	1:A:730:GLU:HG3	2.01	0.60
1:B:222:THR:O	1:B:257:SER:OG	2.17	0.60
1:B:400:GLY:C	1:B:401:VAL:HG13	2.26	0.60
1:B:143:SER:O	1:B:149:GLY:HA3	2.02	0.60
1:B:388:LEU:O	1:B:391:ALA:HB3	2.02	0.60
1:A:103:THR:HG22	1:A:104:PRO:HD2	1.83	0.60
1:A:290:CYS:HB2	1:A:293:LYS:O	2.01	0.60
1:A:747:ARG:C	1:A:749:GLY:H	2.08	0.60
1:A:147:PRO:HG2	1:A:148:GLU:OE2	2.01	0.60
1:A:592:LYS:HG3	1:A:593:PRO:CD	2.27	0.60
1:B:538:THR:HG23	2:B:1844:ADP:O2A	2.02	0.60
1:A:734:GLY:HA2	1:A:762:THR:HG21	1.82	0.60
1:A:161:TYR:OH	1:A:279:GLN:HG2	2.01	0.60
1:B:599:ARG:NE	1:B:635:ASN:ND2	2.48	0.60
1:B:793:MET:HE1	1:B:833:THR:HB	1.84	0.60
1:A:164:THR:O	1:A:168:MET:HG3	2.01	0.59
1:B:231:TYR:HB2	1:B:234:LEU:HD11	1.84	0.59
1:B:657:LEU:HB2	1:B:658:PRO:HD2	1.84	0.59
1:A:524:VAL:HG13	1:A:800:ASP:HB2	1.84	0.59
1:B:613:ARG:HB3	1:B:629:ALA:HB1	1.84	0.59
1:A:455:PRO:HD2	1:A:461:GLY:HA2	1.82	0.59
1:A:176:ILE:HB	1:A:204:VAL:HG13	1.83	0.59
1:A:508:VAL:HG22	1:A:508:VAL:O	2.01	0.59
1:B:49:LYS:HG3	2:B:1843:ADP:O1B	2.03	0.59
1:B:491:THR:HG22	1:B:842:ARG:OXT	2.03	0.59
1:B:437:VAL:C	1:B:438:GLU:CA	2.71	0.59
1:B:694:VAL:HG12	1:B:720:GLY:HA2	1.85	0.59
1:B:714:LEU:O	1:B:717:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PRO:HG2	1:A:344:GLU:HG3	1.85	0.59
1:B:193:GLN:HE22	1:B:255:PHE:HA	1.67	0.59
1:B:313:SER:HA	1:B:373:LEU:HD23	1.83	0.59
1:B:807:PRO:HD2	1:B:812:ASP:O	2.02	0.59
1:A:527:SER:CB	1:A:796:VAL:HG22	2.31	0.59
1:A:398:LEU:HD23	1:B:64:ARG:HB3	1.85	0.58
1:A:613:ARG:HH11	1:A:630:GLY:CA	2.15	0.58
1:A:821:THR:OG1	1:A:824:GLU:HG3	2.03	0.58
1:B:294:ARG:NH2	6:B:2017:HOH:O	2.36	0.58
1:A:666:VAL:HG23	1:A:666:VAL:O	2.04	0.58
1:B:779:LEU:N	1:B:779:LEU:HD23	2.19	0.58
1:A:327:TYR:HA	1:A:332:GLU:CG	2.33	0.58
1:B:516:LEU:HD11	1:B:816:LEU:HB2	1.84	0.58
1:B:711:LEU:O	1:B:715:ARG:HG3	2.04	0.58
1:A:479:SER:O	1:A:482:GLY:N	2.36	0.58
1:B:553:GLY:O	1:B:555:PRO:HD3	2.03	0.58
1:A:93:PRO:HG2	1:B:93:PRO:HG2	1.86	0.57
1:A:807:PRO:HD2	1:A:808:GLY:H	1.68	0.57
1:A:312:LEU:HD11	1:A:320:VAL:HG13	1.86	0.57
1:A:454:GLY:O	1:A:465:LEU:HG	2.05	0.57
1:A:599:ARG:HD3	1:A:635:ASN:HD21	1.69	0.57
1:B:373:LEU:HD22	1:B:373:LEU:H	1.69	0.57
1:A:615:LEU:CD1	1:A:681:TYR:CD1	2.86	0.57
1:B:694:VAL:CG1	1:B:720:GLY:HA2	2.35	0.57
1:B:834:ALA:HB3	1:B:835:PRO:HD3	1.86	0.57
1:A:759:GLU:OE1	1:A:759:GLU:HA	2.03	0.57
1:A:644:CYS:C	1:A:646:GLY:N	2.60	0.57
1:B:563:ASP:HB3	1:B:564:GLU:HG2	1.86	0.57
1:A:588:ARG:HB2	1:A:588:ARG:CZ	2.34	0.57
1:B:363:LEU:O	1:B:368:LEU:HB2	2.05	0.57
1:A:343:PRO:HG2	1:A:344:GLU:H	1.69	0.57
1:A:418:GLU:CD	1:A:446:ARG:HH22	2.09	0.57
1:B:393:GLN:HA	1:B:393:GLN:NE2	2.20	0.56
1:A:781:ASP:C	1:A:783:GLY:H	2.13	0.56
1:B:631:ARG:O	1:B:639:GLY:HA3	2.06	0.56
1:A:61:ALA:HB2	1:A:91:LEU:HD13	1.87	0.56
1:A:148:GLU:OE2	1:A:148:GLU:N	2.30	0.56
1:A:717:VAL:HG13	1:A:738:ARG:HB3	1.86	0.56
1:B:163:VAL:HG21	1:B:262:VAL:HG11	1.87	0.56
1:A:450:LEU:HG	1:A:451:VAL:H	1.69	0.56
1:A:351:ARG:HD3	6:A:2017:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HB3	1:B:311:GLU:CB	2.35	0.56
1:A:587:VAL:HG22	1:A:755:TYR:CD2	2.41	0.56
6:A:2003:HOH:O	1:B:396:SER:HB2	2.04	0.56
1:A:644:CYS:HG	1:A:648:GLY:H	1.50	0.56
1:B:12:ASP:O	1:B:14:GLY:N	2.39	0.56
1:B:33:VAL:CG1	1:B:39:VAL:HG11	2.35	0.56
1:B:126[A]:ARG:HH21	1:B:138:TYR:HD1	1.53	0.56
1:B:826:ALA:HB2	1:B:837:LEU:HB3	1.88	0.56
1:A:728:ALA:HA	1:A:731:LEU:HD12	1.86	0.56
2:B:1843:ADP:PA	2:B:1843:ADP:H8	2.29	0.56
1:A:745:LEU:HD11	1:A:775:GLN:HB3	1.88	0.56
1:B:74:ARG:O	1:B:74:ARG:HD3	2.06	0.56
1:B:526:THR:HG23	1:B:801:TRP:HB3	1.88	0.56
1:A:602:MET:HG3	1:A:739:ILE:CD1	2.37	0.55
1:B:318:ALA:O	1:B:322:GLU:HG3	2.06	0.55
1:B:400:GLY:C	1:B:401:VAL:CG1	2.79	0.55
1:A:779:LEU:O	1:A:784:ASN:HB2	2.06	0.55
1:B:46:GLY:N	2:B:1843:ADP:O2B	2.40	0.55
1:B:366:LEU:O	1:B:368:LEU:N	2.39	0.55
1:B:533:GLY:N	2:B:1844:ADP:O1B	2.33	0.55
1:A:349:LEU:HD23	1:A:349:LEU:C	2.31	0.55
1:A:759:GLU:OE2	1:A:791[A]:HIS:HD2	1.76	0.55
1:B:174:LEU:HB2	1:B:180:ALA:HB2	1.88	0.55
1:A:753:THR:O	1:A:784:ASN:ND2	2.39	0.55
1:A:40:VAL:HA	1:A:436:VAL:O	2.07	0.55
1:B:23:GLN:HG3	1:B:24:HIS:N	2.23	0.54
1:B:652:VAL:C	1:B:654:LEU:H	2.14	0.54
1:B:759:GLU:HG3	1:B:791:HIS:HD2	1.65	0.54
1:A:120:LEU:N	1:A:120:LEU:CD1	2.67	0.54
1:A:176:ILE:HD12	1:A:204:VAL:HA	1.89	0.54
1:A:617:ALA:HB2	1:A:629:ALA:HA	1.90	0.54
1:B:42:THR:OG1	1:B:452:ASP:HA	2.07	0.54
1:A:152:PRO:HG3	1:A:296:ARG:HE	1.72	0.54
1:B:54:PHE:CZ	1:B:404:VAL:HG12	2.42	0.54
1:B:440:ASP:C	1:B:440:ASP:OD1	2.50	0.54
1:A:481:THR:HB	1:A:765:HIS:HE2	1.73	0.54
1:B:491:THR:C	1:B:493:PRO:HD3	2.32	0.54
1:B:619:THR:O	1:B:623:LYS:HD3	2.08	0.54
1:A:452:ASP:OD1	1:A:481:THR:CG2	2.49	0.54
1:A:587:VAL:CG2	1:A:755:TYR:CD2	2.91	0.54
1:B:119:LEU:HB3	1:B:356:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:HG22	1:B:464:ILE:O	2.07	0.54
1:B:805:ILE:CG2	1:B:806:GLY:N	2.71	0.54
1:A:689:VAL:O	1:A:692:LEU:HB2	2.07	0.53
1:B:377:THR:N	1:B:378:PRO:HD2	2.23	0.53
1:A:368:LEU:HB3	1:A:371:LEU:HD12	1.90	0.53
1:A:793:MET:O	1:A:794:GLN:C	2.52	0.53
1:A:438:GLU:HG3	1:A:439:HIS:N	2.22	0.53
1:A:451:VAL:HG22	1:A:467:SER:HB2	1.90	0.53
1:A:757:LEU:HD23	1:A:760:PRO:HG3	1.91	0.53
1:B:129:ASP:N	1:B:303:THR:O	2.40	0.53
1:B:473:LEU:HD12	1:B:476:VAL:CG2	2.39	0.53
1:B:74:ARG:HH12	1:B:78:ASN:HA	1.72	0.53
1:B:539:LEU:HG	1:B:539:LEU:O	2.09	0.53
1:B:648:GLY:C	1:B:649:TRP:CD1	2.86	0.53
1:A:322:GLU:HG3	1:A:325:ARG:NH2	2.24	0.53
1:B:159:ARG:HD3	1:B:284:SER:HG	1.71	0.53
1:B:609:PHE:O	1:B:610:ASP:C	2.50	0.53
1:A:234:LEU:HB3	1:A:238:GLU:HG3	1.91	0.52
1:A:719:LEU:HB3	1:A:722:LEU:HD12	1.89	0.52
1:A:218:TRP:O	1:A:222:THR:HG22	2.10	0.52
1:A:118:ASN:C	1:A:118:ASN:ND2	2.68	0.52
1:B:782:ALA:HB3	1:B:784:ASN:ND2	2.25	0.52
1:B:599:ARG:CG	1:B:599:ARG:NH1	2.48	0.52
1:B:538:THR:HA	1:B:542:GLN:HB2	1.92	0.52
1:B:577:GLY:HA2	1:B:580:LEU:HD11	1.91	0.52
1:A:650:VAL:HG21	1:A:665:PRO:HG3	1.91	0.51
1:B:385:LEU:HA	1:B:388:LEU:HB2	1.93	0.51
1:B:452:ASP:OD2	1:B:479:SER:HB2	2.09	0.51
1:B:466:TYR:CD2	1:B:467:SER:N	2.79	0.51
1:A:483:GLN:O	1:A:486:PHE:N	2.42	0.51
1:A:666:VAL:O	1:A:666:VAL:CG2	2.58	0.51
1:B:386:GLN:HE22	1:B:406:ASP:N	2.06	0.51
1:A:722:LEU:HD21	1:A:735:GLU:OE1	2.11	0.51
1:B:199:THR:HG21	1:B:229:PRO:O	2.08	0.51
1:A:473:LEU:HB3	1:A:486:PHE:HE2	1.75	0.51
1:B:32:LYS:HD3	6:B:2030:HOH:O	2.11	0.51
1:B:523:GLY:HA2	1:B:784:ASN:O	2.10	0.51
1:B:773[A]:GLN:CD	1:B:795:VAL:HG23	2.35	0.51
1:A:390:LEU:HD22	1:A:390:LEU:O	2.11	0.51
1:A:613:ARG:NH1	1:A:630:GLY:HA3	2.23	0.51
1:A:758[A]:ASP:OD2	1:A:759:GLU:N	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PRO:O	1:A:320:VAL:HG23	2.11	0.51
1:A:736:ALA:O	1:A:740:LYS:HD2	2.11	0.51
1:B:175:THR:HG22	1:B:177:ARG:H	1.75	0.51
1:A:181:VAL:HG13	1:A:184:TRP:HB2	1.93	0.51
1:B:383:GLY:HA3	1:B:387:ARG:NH2	2.26	0.51
1:B:440:ASP:OD1	1:B:442:ASP:N	2.44	0.51
1:A:123:LEU:C	1:A:123:LEU:HD23	2.36	0.51
1:B:150:ALA:HB1	1:B:156:GLY:HA3	1.92	0.51
1:B:556:VAL:O	1:B:557:ASN:CB	2.59	0.51
1:B:775:GLN:HE22	1:B:778:LYS:NZ	2.09	0.51
1:A:776:LEU:O	1:A:780:VAL:HG23	2.11	0.50
1:B:33:VAL:HG13	1:B:39:VAL:HG11	1.91	0.50
1:B:806:GLY:HA2	1:B:815[A]:ARG:H	1.75	0.50
1:A:716:GLU:C	1:A:718:GLY:H	2.19	0.50
1:A:39:VAL:HA	1:A:449:TRP:O	2.11	0.50
1:B:428:LYS:HB2	1:B:434:LEU:CD1	2.40	0.50
1:B:575:ARG:CG	1:B:575:ARG:NH1	2.72	0.50
1:B:667:CYS:HB2	1:B:670:THR:HG22	1.94	0.50
1:B:677:LEU:HA	1:B:685:ASN:HD21	1.76	0.50
1:B:524:VAL:HG13	1:B:800:ASP:HB2	1.92	0.50
1:B:805:ILE:CG2	1:B:806:GLY:H	2.25	0.50
1:A:23:GLN:O	1:A:26:LEU:HB2	2.12	0.50
1:A:414:PRO:HA	1:A:417:THR:CG2	2.41	0.50
1:A:631:ARG:O	1:A:639:GLY:HA3	2.11	0.50
1:A:441:LEU:O	1:A:445:ARG:HB2	2.12	0.50
1:B:62:GLN:O	1:B:63:ARG:C	2.55	0.50
1:A:271:SER:CB	1:A:274:MET:HB3	2.42	0.50
1:A:528:VAL:HG13	1:A:805:ILE:HD13	1.93	0.50
1:A:341:ASN:O	1:A:342:ARG:HG3	2.11	0.50
1:B:75:ARG:HH11	1:B:75:ARG:HB3	1.77	0.50
1:A:713:THR:HG21	1:A:742:ALA:O	2.12	0.49
1:B:413:HIS:CD2	1:B:413:HIS:C	2.89	0.49
1:B:588:ARG:NH1	1:B:588:ARG:HB2	2.27	0.49
1:B:575:ARG:HH11	1:B:575:ARG:HG2	1.77	0.49
1:A:420:LEU:C	1:A:422:SER:N	2.70	0.49
1:B:772:LEU:O	1:B:775:GLN:HB2	2.13	0.49
1:B:793:MET:HE3	1:B:837:LEU:HG	1.93	0.49
1:A:163:VAL:HG22	1:A:168:MET:CG	2.42	0.49
1:B:24:HIS:CE1	2:B:1843:ADP:C5	3.00	0.49
1:B:382:PRO:HA	1:B:385:LEU:CD1	2.43	0.49
1:A:525:MET:HG2	1:A:786:VAL:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PRO:HG3	1:B:301:ASN:HB3	1.94	0.49
1:B:269:THR:HG21	1:B:274:MET:HE3	1.95	0.49
1:B:528:VAL:HG21	1:B:540:VAL:HG21	1.95	0.49
1:A:380:LEU:HD23	1:A:385:LEU:HD13	1.95	0.49
1:A:640:ARG:HG2	1:A:640:ARG:HH11	1.77	0.49
1:A:750:ARG:HA	1:A:750:ARG:CZ	2.41	0.49
1:B:278:VAL:HG12	1:B:282:MET:HE2	1.94	0.49
1:B:636:VAL:O	1:B:640:ARG:HD3	2.13	0.49
1:B:838:ARG:HH11	1:B:838:ARG:HB3	1.76	0.49
1:B:504:GLU:CG	1:B:519:ARG:HG2	2.43	0.49
1:B:754:VAL:HG13	1:B:754:VAL:O	2.13	0.49
1:A:17:GLN:O	1:A:88:ILE:HA	2.12	0.49
1:B:387:ARG:NH2	1:B:410:ALA:O	2.46	0.49
1:B:806:GLY:HA2	1:B:815[B]:ARG:H	1.76	0.49
1:A:159:ARG:NH1	1:A:284:SER:HB3	2.28	0.48
1:A:677:LEU:HD22	1:A:685:ASN:HD22	1.78	0.48
1:B:507:GLY:N	1:B:517:ASP:OD2	2.46	0.48
1:A:43:GLY:C	1:A:765:HIS:HD2	2.20	0.48
1:A:440:ASP:OD1	1:A:442:ASP:HB2	2.13	0.48
1:A:775:GLN:HE22	1:A:778:LYS:NZ	2.11	0.48
1:A:156:GLY:O	1:A:294:ARG:HD2	2.14	0.48
1:A:765:HIS:ND1	1:A:766:PRO:HD2	2.28	0.48
1:B:156:GLY:O	1:B:294:ARG:HB3	2.13	0.48
1:B:575:ARG:HH11	1:B:575:ARG:HG3	1.76	0.48
1:B:656:PHE:CD1	1:B:657:LEU:HD23	2.49	0.48
1:B:657:LEU:CB	1:B:658:PRO:HD2	2.43	0.48
1:A:67:GLU:HB3	1:A:75:ARG:HD3	1.95	0.48
1:A:118:ASN:ND2	1:A:118:ASN:O	2.46	0.48
1:A:753:THR:H	1:A:784:ASN:ND2	1.94	0.48
1:B:398:LEU:HD22	1:B:401:VAL:HG11	1.94	0.48
1:B:561:GLU:HA	1:B:596:ARG:HH22	1.78	0.48
1:A:538:THR:CG2	2:A:1844:ADP:O2A	2.54	0.48
1:A:545:VAL:HG23	1:A:756:VAL:HG21	1.95	0.48
1:A:602:MET:O	1:A:606:THR:HG23	2.13	0.48
1:A:644:CYS:C	1:A:646:GLY:H	2.19	0.48
1:A:804:ASP:OD1	1:A:833:THR:CG2	2.62	0.48
1:B:407:GLU:HG2	1:B:410:ALA:HB2	1.94	0.48
1:B:588:ARG:HB2	1:B:588:ARG:HH11	1.77	0.48
1:A:130:TYR:HE2	1:A:137:VAL:HG23	1.79	0.48
1:A:717:VAL:CG1	1:A:738:ARG:HB3	2.43	0.48
1:B:25:ASN:O	1:B:26:LEU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PRO:HB3	1:B:478:GLU:HG3	1.95	0.48
1:B:533:GLY:HA3	1:B:809:ALA:HB1	1.96	0.48
1:B:540:VAL:O	1:B:545:VAL:HG23	2.14	0.48
1:B:821:THR:HG23	1:B:824:GLU:CD	2.39	0.48
1:A:168:MET:HE1	1:A:259:ARG:N	2.29	0.48
1:A:281:TYR:O	1:A:282:MET:HG2	2.13	0.48
1:A:390:LEU:HD11	1:A:424:LEU:HD23	1.95	0.48
1:B:385:LEU:HD12	1:B:385:LEU:N	2.27	0.48
1:B:408:PRO:HB2	1:B:420:LEU:HD11	1.96	0.48
1:A:90:GLY:O	1:A:92:PRO:HD3	2.13	0.48
1:A:412:LEU:HD12	1:A:417:THR:HA	1.96	0.48
1:B:218:TRP:O	1:B:222:THR:HG22	2.14	0.48
1:B:811:GLU:HB2	6:B:2019:HOH:O	2.12	0.48
1:B:510:ARG:HD2	1:B:572:GLY:O	2.14	0.47
1:B:765:HIS:HD1	1:B:767:ALA:H	1.62	0.47
1:B:765:HIS:ND1	1:B:766:PRO:HD2	2.29	0.47
1:A:266:PHE:CE1	1:A:282:MET:HE1	2.50	0.47
1:A:343:PRO:CG	1:A:344:GLU:H	2.27	0.47
1:A:407:GLU:C	1:A:409:SER:H	2.22	0.47
1:A:713:THR:CG2	1:A:742:ALA:O	2.62	0.47
1:A:801:TRP:CZ3	1:A:820:GLY:HA2	2.49	0.47
1:B:12:ASP:C	1:B:14:GLY:N	2.70	0.47
1:B:150:ALA:HB1	1:B:156:GLY:CA	2.45	0.47
1:B:262:VAL:HG22	1:B:278:VAL:HG13	1.96	0.47
1:B:287:CYS:HG	3:B:1845:ZN:ZN	1.27	0.47
1:A:156:GLY:O	1:A:294:ARG:HB3	2.14	0.47
1:B:417:THR:O	1:B:418:GLU:C	2.55	0.47
1:B:510:ARG:HB2	1:B:570:THR:HG21	1.95	0.47
1:B:692:LEU:HD23	1:B:697:ALA:HA	1.96	0.47
1:A:159:ARG:HH11	1:A:284:SER:HB3	1.78	0.47
1:A:455:PRO:HD2	1:A:460:LYS:O	2.14	0.47
1:A:549:ALA:HB1	1:A:554:GLN:HG2	1.96	0.47
1:B:49:LYS:CG	2:B:1843:ADP:O1B	2.63	0.47
1:B:95:VAL:O	1:B:403:TYR:HA	2.14	0.47
1:B:317:LEU:CD2	1:B:373:LEU:HD13	2.43	0.47
1:B:470:PRO:O	1:B:472:GLY:N	2.48	0.47
1:A:454:GLY:HA2	1:A:461:GLY:C	2.40	0.47
1:A:601:ASN:OD1	1:A:724:LEU:O	2.32	0.47
1:A:703:ASP:OD2	1:A:703:ASP:N	2.47	0.47
1:B:77:PHE:HZ	1:B:654:LEU:HB3	1.78	0.47
1:A:87:ALA:C	1:A:88:ILE:HG12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213[A]:GLU:HG3	1:A:214[A]:GLU:HG3	1.96	0.47
1:A:348:ALA:O	1:A:352:MET:HG3	2.15	0.47
1:A:716:GLU:C	1:A:718:GLY:N	2.71	0.47
1:B:167:SER:OG	1:B:168:MET:N	2.48	0.47
1:B:402:VAL:HG13	1:B:433:SER:HB2	1.96	0.47
1:B:745:LEU:HD21	1:B:775:GLN:HE21	1.79	0.47
1:B:793:MET:CE	1:B:833:THR:HB	2.45	0.47
1:B:403:TYR:CE1	1:B:427:LEU:HD21	2.50	0.47
1:A:585:ARG:HB2	1:A:753:THR:CB	2.32	0.47
1:B:204:VAL:HG12	1:B:204:VAL:O	2.14	0.47
1:B:802:VAL:HB	1:B:825:VAL:HG21	1.96	0.47
1:A:360:LEU:O	1:A:363:LEU:HB2	2.16	0.46
1:B:753:THR:HG23	1:B:784:ASN:OD1	2.15	0.46
1:A:70:SER:C	1:A:72:TYR:N	2.73	0.46
1:A:719:LEU:C	1:A:721:TYR:H	2.22	0.46
1:B:545:VAL:CG1	1:B:586:LEU:HD21	2.40	0.46
1:B:651:MET:HG2	1:B:652:VAL:H	1.80	0.46
1:B:652:VAL:HG22	1:B:660:VAL:O	2.15	0.46
1:A:58:TYR:CZ	1:A:62:GLN:HG2	2.50	0.46
1:A:359:ARG:O	1:A:360:LEU:C	2.58	0.46
1:A:393:GLN:OE1	1:A:403:TYR:HE2	1.98	0.46
1:B:17:GLN:O	1:B:88:ILE:HA	2.15	0.46
1:B:512:ASN:HD21	1:B:810:GLY:HA2	1.80	0.46
1:B:157:LEU:O	1:B:294:ARG:HD2	2.16	0.46
1:A:35:ARG:O	1:A:36:ASP:HB2	2.15	0.46
1:B:670:THR:C	1:B:671:ARG:HG3	2.41	0.46
1:A:759:GLU:OE1	1:A:759:GLU:CA	2.63	0.46
1:A:640:ARG:HA	1:A:672:TYR:HA	1.98	0.46
1:B:43:GLY:C	1:B:765:HIS:HD2	2.23	0.46
1:A:196:ILE:HG21	1:A:255:PHE:HB2	1.97	0.46
1:A:807:PRO:CD	1:A:808:GLY:H	2.29	0.46
1:B:685:ASN:ND2	1:B:686:ILE:H	1.87	0.46
1:B:764:LEU:HB3	1:B:769:VAL:HG12	1.97	0.46
1:A:70:SER:C	1:A:72:TYR:H	2.23	0.46
1:A:97:LEU:HD12	1:A:405:LEU:HD21	1.98	0.46
1:A:114:THR:C	1:A:115:THR:HG23	2.41	0.46
1:A:271:SER:HB3	1:A:274:MET:CB	2.46	0.46
1:A:373:LEU:H	1:A:373:LEU:CD2	2.25	0.46
1:B:41:PHE:N	1:B:41:PHE:CD2	2.81	0.46
1:B:454:GLY:O	1:B:455:PRO:C	2.55	0.46
1:B:685:ASN:HB3	1:B:688:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLN:OE1	1:A:62:GLN:HA	2.16	0.45
1:A:393:GLN:OE1	1:A:403:TYR:CE2	2.69	0.45
1:B:123:LEU:HD23	1:B:123:LEU:C	2.40	0.45
1:B:34:PRO:HD3	1:B:449:TRP:CG	2.51	0.45
1:B:411:GLY:HA2	1:B:791:HIS:CD2	2.51	0.45
1:B:664:CYS:O	1:B:668:HIS:HA	2.17	0.45
1:B:698:HIS:CD2	1:B:715:ARG:CD	2.97	0.45
1:B:804:ASP:OD1	1:B:833:THR:CG2	2.65	0.45
1:A:585:ARG:CB	1:A:753:THR:HB	2.34	0.45
1:A:640:ARG:HG2	1:A:640:ARG:NH1	2.31	0.45
1:B:151:CYS:HA	1:B:152:PRO:HD3	1.77	0.45
1:B:175:THR:HG22	1:B:177:ARG:N	2.32	0.45
1:B:747:ARG:NH1	6:B:2049:HOH:O	2.49	0.45
1:A:266:PHE:CG	1:A:282:MET:HE1	2.51	0.45
1:A:403:TYR:HB2	1:A:434:LEU:CD2	2.46	0.45
1:A:733:GLY:HA2	1:A:736:ALA:HB3	1.98	0.45
1:B:70:SER:C	1:B:72:TYR:H	2.24	0.45
1:B:120:LEU:HD12	1:B:120:LEU:C	2.42	0.45
1:B:775:GLN:HE22	1:B:778:LYS:HZ3	1.64	0.45
1:B:794:GLN:HA	6:B:2054:HOH:O	2.16	0.45
1:A:39:VAL:HG22	1:A:449:TRP:HB3	1.99	0.45
1:B:423:ALA:O	1:B:427:LEU:HB2	2.17	0.45
1:B:625:ARG:O	1:B:627:TYR:N	2.50	0.45
1:B:703:ASP:OD2	1:B:703:ASP:N	2.48	0.45
1:A:148:GLU:H	1:A:148:GLU:CD	2.21	0.45
1:A:185:PRO:HB2	1:A:189:GLY:HA3	1.99	0.45
1:B:15:PHE:CD2	1:B:32:LYS:HG3	2.51	0.45
1:B:222:THR:O	1:B:257:SER:CB	2.64	0.45
1:B:597:THR:HG1	1:B:599:ARG:HB2	1.80	0.45
1:A:203:ASP:OD2	1:A:206:VAL:HG22	2.17	0.45
1:B:577:GLY:CA	1:B:580:LEU:HD11	2.45	0.45
1:B:750:ARG:HB2	1:B:751:GLY:H	1.46	0.45
1:A:15:PHE:HA	1:A:34:PRO:HA	1.99	0.45
1:A:44:VAL:HG12	1:A:45:SER:O	2.17	0.45
1:A:413:HIS:CG	1:A:414:PRO:HD2	2.52	0.45
1:B:585:ARG:HB2	1:B:753:THR:HB	1.99	0.45
1:A:164:THR:HG23	1:A:283:ILE:HD11	1.99	0.44
1:A:801:TRP:CH2	1:A:820:GLY:HA2	2.51	0.44
1:B:60:GLU:HG2	1:B:88:ILE:HD12	1.98	0.44
1:B:231:TYR:CE1	1:B:249:PRO:HA	2.52	0.44
1:B:575:ARG:NH1	1:B:575:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HD3	1:A:730:GLU:O	2.17	0.44
1:A:461:GLY:O	1:A:463:GLU:N	2.50	0.44
1:A:473:LEU:O	1:A:476:VAL:HG22	2.17	0.44
1:B:107:ARG:NH2	1:B:565:ASP:HB3	2.32	0.44
1:B:202:ILE:O	1:B:204:VAL:HG23	2.17	0.44
1:B:701:PHE:HD2	1:B:704:GLU:HG3	1.82	0.44
1:A:402:VAL:HG13	1:A:433:SER:HB3	1.99	0.44
1:A:719:LEU:HD22	1:A:722:LEU:CD1	2.46	0.44
1:B:312:LEU:HD22	1:B:320:VAL:HG22	2.00	0.44
1:B:419:ALA:O	1:B:420:LEU:C	2.57	0.44
1:B:808:GLY:N	1:B:812:ASP:O	2.50	0.44
1:A:310:THR:O	1:A:314:ARG:HG2	2.18	0.44
1:A:511:ASN:HB3	1:A:512:ASN:H	1.63	0.44
1:A:587:VAL:HG21	1:A:744:GLU:HG3	1.99	0.44
1:A:634:PHE:CD1	1:A:634:PHE:C	2.96	0.44
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.75	0.44
1:B:590:ASP:OD1	1:B:592:LYS:HB2	2.17	0.44
1:B:630:GLY:H	1:B:632:PHE:H	1.64	0.44
1:B:782:ALA:HB3	1:B:784:ASN:HD22	1.82	0.44
1:A:537:SER:OG	2:A:1844:ADP:O2B	2.22	0.44
1:B:177:ARG:NH2	1:B:205:ASP:OD2	2.49	0.44
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.27	0.44
1:B:435:PHE:CD1	1:B:435:PHE:N	2.84	0.44
1:B:452:ASP:OD1	1:B:481:THR:HG21	2.18	0.44
1:B:703:ASP:HB3	6:B:2046:HOH:O	2.17	0.44
1:B:820:GLY:HA3	1:B:824:GLU:OE1	2.18	0.44
1:B:841:LEU:O	1:B:842:ARG:C	2.61	0.44
1:A:634:PHE:O	1:A:640:ARG:NH1	2.51	0.44
1:A:732:SER:HB3	1:A:735:GLU:OE2	2.18	0.44
1:B:332:GLU:HG3	1:B:335:HIS:HB2	1.99	0.44
1:B:387:ARG:O	1:B:391:ALA:HB2	2.18	0.44
1:B:761:THR:HA	1:B:764:LEU:HD22	2.00	0.44
1:A:159:ARG:NH2	1:A:285:GLU:HA	2.33	0.44
1:A:331:ARG:O	1:A:333:PRO:HD3	2.18	0.44
1:A:504:GLU:HG2	1:A:519:ARG:HG3	1.99	0.44
1:B:19:ARG:NH2	1:B:89:ASP:OD2	2.45	0.44
1:B:266:PHE:HE1	1:B:279:GLN:HE22	1.63	0.44
1:B:383:GLY:CA	1:B:387:ARG:NH2	2.81	0.44
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.57	0.44
1:B:428:LYS:CB	1:B:434:LEU:HD11	2.46	0.44
1:A:337:GLU:O	1:A:341:ASN:ND2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD12	1:A:476:VAL:HG21	1.99	0.43
1:A:510:ARG:O	1:A:511:ASN:HB2	2.17	0.43
1:B:41:PHE:CD1	1:B:53:ALA:HB2	2.53	0.43
1:B:413:HIS:HA	1:B:414:PRO:HD2	1.57	0.43
1:B:466:TYR:CD2	1:B:466:TYR:C	2.96	0.43
1:B:504:GLU:HG3	1:B:519:ARG:HG2	1.99	0.43
1:B:601:ASN:OD1	1:B:601:ASN:C	2.61	0.43
1:B:831:SER:HB3	1:B:834:ALA:HB2	2.00	0.43
1:A:675:GLU:O	1:A:678:GLU:HB2	2.19	0.43
1:B:606:THR:HG1	1:B:608:LEU:H	1.66	0.43
1:A:25:ASN:HD22	1:A:25:ASN:N	2.13	0.43
1:A:412:LEU:HD22	1:A:412:LEU:HA	1.91	0.43
1:B:511:ASN:HD22	1:B:538:THR:HB	1.83	0.43
1:B:611:GLN:HB3	1:B:707:ILE:HD11	2.00	0.43
1:B:817:VAL:HG21	1:B:830:GLY:O	2.17	0.43
1:A:134:GLN:HE21	1:A:134:GLN:C	2.27	0.43
1:A:373:LEU:HD23	1:A:373:LEU:N	2.26	0.43
1:B:350:GLN:CD	1:B:350:GLN:C	2.86	0.43
1:A:41:PHE:HB2	1:A:437:VAL:HA	2.00	0.43
1:A:99[A]:GLN:HE22	1:A:105:THR:HG23	1.82	0.43
1:A:404:VAL:C	1:A:405:LEU:HD12	2.44	0.43
1:B:594:ILE:HB	1:B:605:TYR:CD1	2.53	0.43
1:A:207:PRO:O	1:A:210:GLU:HB2	2.18	0.43
1:A:651:MET:HB2	1:A:661:TYR:HE2	1.84	0.43
1:B:70:SER:O	1:B:72:TYR:N	2.46	0.43
1:B:473:LEU:HD12	1:B:473:LEU:HA	1.67	0.43
1:B:804:ASP:OD1	1:B:833:THR:HG23	2.19	0.43
1:A:416:ASP:C	1:A:418:GLU:N	2.76	0.43
1:A:719:LEU:O	1:A:721:TYR:N	2.51	0.43
1:B:487:ALA:CB	1:B:490:HIS:CE1	3.01	0.43
1:B:801:TRP:CZ3	1:B:820:GLY:HA2	2.53	0.43
1:A:19:ARG:NH2	1:A:89:ASP:OD2	2.52	0.43
1:B:118:ASN:HA	1:B:121:ARG:NH1	2.33	0.43
1:B:402:VAL:HG11	1:B:435:PHE:CE2	2.54	0.43
1:A:701:PHE:O	1:A:708:PHE:HB2	2.18	0.43
1:A:701:PHE:CD2	1:A:707:ILE:HG21	2.54	0.43
1:B:803:LEU:HD12	1:B:803:LEU:HA	1.69	0.43
1:A:181:VAL:HG11	1:A:184:TRP:HE3	1.75	0.42
1:A:677:LEU:HD22	1:A:685:ASN:ND2	2.34	0.42
1:A:681:TYR:O	1:A:682:ARG:C	2.62	0.42
1:A:685:ASN:OD1	1:A:688:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:TYR:HB2	1:B:404:VAL:HG21	2.01	0.42
1:B:417:THR:O	1:B:420:LEU:N	2.52	0.42
1:A:796:VAL:O	1:A:799:SER:HB2	2.20	0.42
1:B:70:SER:O	1:B:73:ALA:N	2.49	0.42
1:B:599:ARG:NH2	1:B:645:GLN:O	2.52	0.42
1:B:723:ARG:HB2	1:B:726:GLN:HB2	2.00	0.42
1:A:17:GLN:HB3	1:A:89:ASP:HB2	2.01	0.42
1:A:163:VAL:HG22	1:A:168:MET:HG2	2.01	0.42
1:A:262:VAL:HG12	1:A:263:LEU:N	2.33	0.42
1:A:717:VAL:HG12	1:A:719:LEU:HG	2.01	0.42
1:A:775:GLN:NE2	1:A:778:LYS:NZ	2.67	0.42
1:B:27:LYS:HD3	1:B:461:GLY:O	2.19	0.42
1:B:464:ILE:O	1:B:465:LEU:C	2.63	0.42
1:A:169:VAL:HG23	1:A:169:VAL:O	2.19	0.42
1:A:279:GLN:CG	1:A:282:MET:HE3	2.50	0.42
1:A:474:LYS:HG3	1:A:486:PHE:CE1	2.55	0.42
1:A:536:LYS:HD2	1:A:789:VAL:HG13	2.01	0.42
1:A:651:MET:HB2	1:A:661:TYR:CE2	2.54	0.42
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.72	0.42
1:B:652:VAL:C	1:B:654:LEU:N	2.76	0.42
1:B:657:LEU:O	1:B:658:PRO:C	2.62	0.42
1:A:390:LEU:C	1:A:390:LEU:CD2	2.92	0.42
1:B:114:THR:HA	1:B:392:THR:OG1	2.19	0.42
1:B:449:TRP:CZ3	1:B:469:PRO:HD3	2.55	0.42
1:B:463:GLU:C	1:B:464:ILE:HD12	2.43	0.42
1:B:589:VAL:HG12	1:B:737:GLN:HG2	2.01	0.42
1:A:41:PHE:HE2	1:A:435:PHE:HB3	1.84	0.42
1:A:481:THR:HB	1:A:765:HIS:NE2	2.35	0.42
1:A:528:VAL:HG21	1:A:540:VAL:HG21	2.01	0.42
1:A:644:CYS:O	1:A:645:GLN:C	2.62	0.42
1:A:579:ASP:OD1	1:A:579:ASP:N	2.51	0.42
1:B:26:LEU:HD21	1:B:52:LEU:HB2	2.01	0.42
1:B:681:TYR:N	1:B:684:LYS:O	2.46	0.42
1:A:413:HIS:CD2	1:A:415:ALA:H	2.30	0.42
1:A:349:LEU:C	1:A:349:LEU:CD2	2.92	0.42
1:A:390:LEU:O	1:A:390:LEU:CD2	2.67	0.42
1:A:418:GLU:O	1:A:418:GLU:HG3	2.20	0.42
1:A:476:VAL:HA	1:A:477:PRO:HD2	1.80	0.42
1:B:49:LYS:NZ	2:B:1843:ADP:O1B	2.50	0.42
1:B:350:GLN:OE1	1:B:351:ARG:N	2.53	0.42
1:B:690:LEU:HD23	1:B:690:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:NH2	1:A:410:ALA:O	2.53	0.41
1:A:390:LEU:HD22	1:A:390:LEU:C	2.45	0.41
1:A:538:THR:HA	1:A:542:GLN:HB2	2.01	0.41
1:A:717:VAL:HG13	1:A:738:ARG:HD2	2.02	0.41
1:A:114:THR:CG2	1:A:388:LEU:HD22	2.51	0.41
1:A:151:CYS:HA	1:A:152:PRO:HD3	1.88	0.41
1:A:759:GLU:CD	1:A:791[A]:HIS:CD2	2.83	0.41
1:B:161:TYR:CE2	1:B:284:SER:HB2	2.55	0.41
1:B:402:VAL:HG11	1:B:435:PHE:CZ	2.55	0.41
1:A:48:GLY:C	1:A:453:VAL:HG11	2.45	0.41
1:A:159:ARG:CZ	1:A:285:GLU:HA	2.50	0.41
1:A:168:MET:HE1	1:A:258:ALA:C	2.45	0.41
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.87	0.41
1:A:587:VAL:HG21	1:A:755:TYR:CD2	2.56	0.41
1:B:164:THR:O	1:B:165:GLU:C	2.63	0.41
1:B:293:LYS:HE3	1:B:308:ASP:OD2	2.20	0.41
1:B:390:LEU:HD22	1:B:394:LEU:HD11	2.02	0.41
1:B:565:ASP:O	1:B:567:ALA:N	2.53	0.41
1:B:74:ARG:CD	1:B:74:ARG:C	2.94	0.41
1:B:116:LEU:O	1:B:117:SER:C	2.62	0.41
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.89	0.41
1:A:276:LYS:NZ	1:A:276:LYS:CD	2.68	0.41
1:A:382:PRO:HG3	1:A:591[A]:GLN:NE2	2.35	0.41
1:A:548:LEU:HA	1:A:548:LEU:HD23	1.76	0.41
1:B:451:VAL:HA	1:B:466:TYR:O	2.20	0.41
1:B:599:ARG:NE	1:B:635:ASN:HD21	2.17	0.41
1:B:619:THR:HB	1:B:620:PRO:CD	2.47	0.41
1:A:494:HIS:O	1:A:496:PRO:HD3	2.20	0.41
1:B:74:ARG:HD3	1:B:74:ARG:C	2.46	0.41
1:B:107:ARG:CZ	1:B:376:SER:OG	2.69	0.41
1:A:129:ASP:HB2	1:A:303:THR:HG22	2.03	0.41
1:A:602:MET:HE2	1:A:724:LEU:HA	2.02	0.41
1:A:631:ARG:HG3	1:A:631:ARG:HH11	1.86	0.41
1:A:737:GLN:HE22	1:A:762:THR:HB	1.86	0.41
1:B:24:HIS:ND1	1:B:51:SER:OG	2.54	0.41
1:B:580:LEU:N	1:B:580:LEU:CD1	2.74	0.41
1:A:152:PRO:HG3	1:A:296:ARG:HH21	1.86	0.41
1:B:269:THR:HB	1:B:271:SER:HB3	2.01	0.41
1:B:366:LEU:HD23	1:B:387:ARG:HG2	2.03	0.41
1:B:438:GLU:HA	1:B:438:GLU:OE2	2.21	0.41
1:A:91:LEU:HA	1:A:92:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:O	1:A:219:ILE:HG13	2.20	0.41
1:A:408:PRO:HB2	1:A:420:LEU:HD11	2.02	0.41
1:A:420:LEU:C	1:A:422:SER:H	2.28	0.41
1:A:420:LEU:O	1:A:422:SER:N	2.54	0.41
1:B:22:ARG:HH22	1:B:86:ASP:CG	2.17	0.41
1:B:325:ARG:N	1:B:326:PRO:HD2	2.36	0.41
1:B:329:GLU:OE1	1:B:331:ARG:NH1	2.54	0.41
1:B:385:LEU:CD1	1:B:385:LEU:N	2.83	0.41
1:B:466:TYR:CG	1:B:467:SER:N	2.89	0.41
1:B:542:GLN:O	1:B:543:ALA:C	2.64	0.41
1:B:601:ASN:ND2	1:B:634:PHE:CZ	2.88	0.41
1:A:256:SER:O	1:A:257:SER:C	2.63	0.41
1:B:22:ARG:O	1:B:23:GLN:O	2.39	0.41
1:B:362:VAL:O	1:B:363:LEU:C	2.60	0.41
1:B:491:THR:O	1:B:493:PRO:HD3	2.20	0.41
1:B:571:ALA:O	1:B:572:GLY:C	2.64	0.41
1:B:621:LEU:HD13	1:B:621:LEU:HA	1.97	0.41
1:A:327:TYR:CA	1:A:332:GLU:HG2	2.43	0.40
1:B:154:CYS:HB3	1:B:287:CYS:SG	2.61	0.40
1:B:208:TRP:HZ2	1:B:220:LEU:HD22	1.86	0.40
1:B:592:LYS:HA	1:B:593:PRO:HD2	1.84	0.40
1:B:232:PRO:O	1:B:234:LEU:HD23	2.20	0.40
1:B:413:HIS:CD2	1:B:414:PRO:N	2.89	0.40
1:B:476:VAL:O	1:B:477:PRO:C	2.63	0.40
1:B:497:ARG:HB2	1:B:524:VAL:HG22	2.04	0.40
1:B:501:GLY:O	1:B:502:TRP:CD1	2.75	0.40
1:B:841:LEU:HD23	1:B:841:LEU:HA	1.71	0.40
1:A:377:THR:N	1:A:378:PRO:CD	2.84	0.40
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.93	0.40
1:A:784:ASN:HD22	1:A:784:ASN:HA	1.56	0.40
1:B:171:ASP:HA	1:B:172:PRO:HD3	1.85	0.40
1:A:473:LEU:O	1:A:476:VAL:CG2	2.69	0.40
1:B:196:ILE:HG21	1:B:255:PHE:HB2	2.03	0.40
1:B:501:GLY:O	1:B:502:TRP:CG	2.75	0.40
1:B:544:LEU:O	1:B:544:LEU:HG	2.21	0.40
1:B:692:LEU:HG	1:B:696:GLU:HB3	2.03	0.40
1:A:65:TYR:CE2	1:A:69:VAL:HG21	2.56	0.40
1:A:103:THR:CG2	1:A:104:PRO:HD2	2.51	0.40
1:B:168:MET:HE1	1:B:259:ARG:N	2.36	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	797/842 (95%)	652 (82%)	110 (14%)	35 (4%)	2	12
1	B	834/842 (99%)	675 (81%)	119 (14%)	40 (5%)	2	11
All	All	1631/1684 (97%)	1327 (81%)	229 (14%)	75 (5%)	2	11

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213[A]	GLU
1	A	214[A]	GLU
1	A	262	VAL
1	A	455	PRO
1	A	663	PRO
1	A	665	PRO
1	A	748	SER
1	A	762	THR
1	A	807	PRO
1	B	23	GLN
1	B	55	GLY
1	B	454	GLY
1	B	557	ASN
1	B	566	PRO
1	B	645	GLN
1	B	685	ASN
1	B	807	PRO
1	A	135	GLY
1	A	272	ALA
1	A	343	PRO
1	A	462	GLY
1	A	512	ASN
1	A	705	SER
1	A	749	GLY
1	B	259	ARG

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Mol	Chain	Res	Type
1	B	418	GLU
1	B	471[A]	GLU
1	B	489	ARG
1	B	653	GLU
1	B	671	ARG
1	B	675	GLU
1	B	774[A]	ARG
1	A	187	ALA
1	A	344	GLU
1	A	459[A]	GLU
1	A	782	ALA
1	B	81	GLY
1	B	236	PRO
1	B	384	GLU
1	B	470	PRO
1	B	572	GLY
1	B	658	PRO
1	B	668	HIS
1	A	261	HIS
1	A	317	LEU
1	A	384	GLU
1	A	645	GLN
1	A	759	GLU
1	A	794	GLN
1	B	26	LEU
1	B	58	TYR
1	B	273	SER
1	B	704	GLU
1	B	728	ALA
1	B	759	GLU
1	A	132	PRO
1	A	333	PRO
1	A	474	LYS
1	A	637	LYS
1	A	668	HIS
1	A	671	ARG
1	A	720	GLY
1	B	24	HIS
1	B	71	PRO
1	B	101	ARG
1	B	207	PRO
1	B	708	PHE

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Mol	Chain	Res	Type
1	A	73	ALA
1	B	12	ASP
1	B	54	PHE
1	B	77	PHE
1	B	414	PRO
1	B	626	GLY
1	B	132	PRO
1	A	172	PRO

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	652/683 (96%)	505 (78%)	147 (22%)	1	5
1	B	676/683 (99%)	529 (78%)	147 (22%)	1	6
All	All	1328/1366 (97%)	1034 (78%)	294 (22%)	1	5

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	25	ASN
1	A	26	LEU
1	A	31	VAL
1	A	33	VAL
1	A	40	VAL
1	A	62	GLN
1	A	76	LEU
1	A	82	VAL
1	A	88	ILE
1	A	91	LEU
1	A	98	GLN
1	A	101	ARG
1	A	103	THR
1	A	107	ARG

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Mol	Chain	Res	Type
1	A	115	THR
1	A	118	ASN
1	A	119	LEU
1	A	120	LEU
1	A	134	GLN
1	A	136	ILE
1	A	145	ASN
1	A	151	CYS
1	A	157	LEU
1	A	159	ARG
1	A	163	VAL
1	A	164	THR
1	A	175	THR
1	A	184	TRP
1	A	191	GLN
1	A	200	LEU
1	A	202	ILE
1	A	206	VAL
1	A	209	ARG
1	A	213[A]	GLU
1	A	214[A]	GLU
1	A	220	LEU
1	A	230	VAL
1	A	243	LEU
1	A	246	LYS
1	A	259	ARG
1	A	262	VAL
1	A	270	GLU
1	A	283	ILE
1	A	285	GLU
1	A	294	ARG
1	A	295	LEU
1	A	303	THR
1	A	312	LEU
1	A	322	GLU
1	A	323	LEU
1	A	324	LEU
1	A	325	ARG
1	A	332	GLU
1	A	337	GLU
1	A	339	VAL
1	A	344	GLU

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Mol	Chain	Res	Type
1	A	355	ASP
1	A	360	LEU
1	A	362	VAL
1	A	363	LEU
1	A	373	LEU
1	A	381	SER
1	A	385	LEU
1	A	389	ARG
1	A	390	LEU
1	A	412	LEU
1	A	417	THR
1	A	422	SER
1	A	429[A]	ARG
1	A	460	LYS
1	A	464	ILE
1	A	465	LEU
1	A	476	VAL
1	A	481	THR
1	A	483	GLN
1	A	495	THR
1	A	497	ARG
1	A	508	VAL
1	A	512	ASN
1	A	518	VAL
1	A	519	ARG
1	A	524	VAL
1	A	525	MET
1	A	531	VAL
1	A	532	SER
1	A	538	THR
1	A	545	VAL
1	A	579	ASP
1	A	583	ILE
1	A	586	LEU
1	A	587	VAL
1	A	588	ARG
1	A	591[A]	GLN
1	A	592	LYS
1	A	594	ILE
1	A	596	ARG
1	A	597	THR
1	A	600	SER

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Mol	Chain	Res	Type
1	A	604	THR
1	A	611	GLN
1	A	614	LYS
1	A	615	LEU
1	A	621	LEU
1	A	623	LYS
1	A	624	LYS
1	A	625	ARG
1	A	628	ASN
1	A	636	VAL
1	A	640	ARG
1	A	641	CYS
1	A	664	CYS
1	A	666	VAL
1	A	689	VAL
1	A	693	THR
1	A	703	ASP
1	A	713	THR
1	A	714	LEU
1	A	715	ARG
1	A	717	VAL
1	A	729	THR
1	A	738	ARG
1	A	740	LYS
1	A	745	LEU
1	A	750	ARG
1	A	753	THR
1	A	754	VAL
1	A	756	VAL
1	A	757	LEU
1	A	761	THR
1	A	762	THR
1	A	769	VAL
1	A	771[A]	ARG
1	A	772	LEU
1	A	777	VAL
1	A	779	LEU
1	A	784	ASN
1	A	795	VAL
1	A	799	SER
1	A	812	ASP
1	A	816	LEU

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Mol	Chain	Res	Type
1	A	825	VAL
1	A	831	SER
1	A	832	VAL
1	A	833	THR
1	A	837	LEU
1	A	842	ARG
1	B	9	ASP
1	B	17	GLN
1	B	22	ARG
1	B	26	LEU
1	B	27	LYS
1	B	31	VAL
1	B	32	LYS
1	B	40	VAL
1	B	49	LYS
1	B	51	SER
1	B	56	THR
1	B	72	TYR
1	B	75	ARG
1	B	91	LEU
1	B	105	THR
1	B	107	ARG
1	B	115	THR
1	B	119	LEU
1	B	120	LEU
1	B	136	ILE
1	B	143	SER
1	B	151	CYS
1	B	163	VAL
1	B	164	THR
1	B	169	VAL
1	B	174	LEU
1	B	186	GLN
1	B	211	LEU
1	B	225	GLN
1	B	228	VAL
1	B	230	VAL
1	B	234	LEU
1	B	243	LEU
1	B	244[A]	LYS
1	B	256	SER
1	B	262	VAL

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Mol	Chain	Res	Type
1	B	269	THR
1	B	274	MET
1	B	277	ARG
1	B	279	GLN
1	B	289	LEU
1	B	290	CYS
1	B	293	LYS
1	B	300	LEU
1	B	303	THR
1	B	311	GLU
1	B	312	LEU
1	B	314	ARG
1	B	321	SER
1	B	332	GLU
1	B	344	GLU
1	B	349	LEU
1	B	357	VAL
1	B	359	ARG
1	B	363	LEU
1	B	364	LEU
1	B	373	LEU
1	B	376	SER
1	B	380	LEU
1	B	385	LEU
1	B	389[A]	ARG
1	B	390	LEU
1	B	396	SER
1	B	412	LEU
1	B	413	HIS
1	B	414	PRO
1	B	421	LEU
1	B	427	LEU
1	B	434	LEU
1	B	437	VAL
1	B	440	ASP
1	B	445	ARG
1	B	450	LEU
1	B	467	SER
1	B	474	LYS
1	B	476	VAL
1	B	480	GLN
1	B	481	THR

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Mol	Chain	Res	Type
1	B	495	THR
1	B	505	LEU
1	B	508	VAL
1	B	516	LEU
1	B	519	ARG
1	B	524	VAL
1	B	525	MET
1	B	527	SER
1	B	531	VAL
1	B	532	SER
1	B	538	THR
1	B	541	SER
1	B	570	THR
1	B	573	SER
1	B	575	ARG
1	B	576	LEU
1	B	580	LEU
1	B	584	THR
1	B	587	VAL
1	B	588	ARG
1	B	591[A]	GLN
1	B	597	THR
1	B	599	ARG
1	B	600	SER
1	B	604	THR
1	B	606	THR
1	B	608	LEU
1	B	611	GLN
1	B	615	LEU
1	B	621	LEU
1	B	625	ARG
1	B	636	VAL
1	B	641	CYS
1	B	654	LEU
1	B	655	LEU
1	B	657	LEU
1	B	660	VAL
1	B	670	THR
1	B	685	ASN
1	B	692	LEU
1	B	694	VAL
1	B	709	ARG

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Mol	Chain	Res	Type
1	B	717	VAL
1	B	740	LYS
1	B	743	THR
1	B	746	ARG
1	B	747	ARG
1	B	748	SER
1	B	750	ARG
1	B	753	THR
1	B	756	VAL
1	B	759	GLU
1	B	762	THR
1	B	764	LEU
1	B	769	VAL
1	B	774[A]	ARG
1	B	778	LYS
1	B	779	LEU
1	B	780	VAL
1	B	786	VAL
1	B	789	VAL
1	B	792	LYS
1	B	793	MET
1	B	800	ASP
1	B	803	LEU
1	B	816	LEU
1	B	821	THR
1	B	827	GLN
1	B	832	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	25	ASN
1	A	78	ASN
1	A	98	GLN
1	A	118	ASN
1	A	134	GLN
1	A	191	GLN
1	A	192	ASN
1	A	240[A]	GLN
1	A	335	HIS
1	A	386	GLN

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Mol	Chain	Res	Type
1	A	413	HIS
1	A	432	ASN
1	A	483	GLN
1	A	511	ASN
1	A	512	ASN
1	A	515	ASN
1	A	551	HIS
1	A	582	GLN
1	A	628	ASN
1	A	635	ASN
1	A	673	ASN
1	A	737	GLN
1	A	775	GLN
1	A	784	ASN
1	B	186	GLN
1	B	192	ASN
1	B	217	HIS
1	B	345	GLN
1	B	386	GLN
1	B	413	HIS
1	B	511	ASN
1	B	512	ASN
1	B	557	ASN
1	B	582	GLN
1	B	591[A]	GLN
1	B	628	ASN
1	B	635	ASN
1	B	645	GLN
1	B	668	HIS
1	B	685	ASN
1	B	737	GLN
1	B	773[A]	GLN
1	B	775	GLN
1	B	791	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
4	SO4	A	1847[A]	-	4,4,4	0.22	0	6,6,6	0.42	0
2	ADP	A	1844	-	28,29,29	1.48	5 (17%)	43,45,45	2.24	17 (39%)
2	ADP	A	1843	-	28,29,29	1.49	5 (17%)	43,45,45	1.70	10 (23%)
4	SO4	B	1851[A]	-	4,4,4	0.31	0	6,6,6	0.35	0
2	ADP	B	1843	-	28,29,29	1.76	5 (17%)	43,45,45	1.97	10 (23%)
4	SO4	B	1849	-	4,4,4	0.29	0	6,6,6	0.32	0
4	SO4	B	1850[A]	-	4,4,4	0.30	0	6,6,6	0.20	0
5	PO4	B	1852[A]	-	4,4,4	0.73	0	6,6,6	0.74	0
2	ADP	B	1844	-	28,29,29	1.60	5 (17%)	43,45,45	2.07	12 (27%)
4	SO4	A	1848[A]	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SO4	A	1849[A]	-	4,4,4	0.28	0	6,6,6	0.20	0
4	SO4	B	1847	-	4,4,4	0.34	0	6,6,6	0.32	0
4	SO4	B	1848[A]	-	4,4,4	0.39	0	6,6,6	0.13	0

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
2	ADP	B	1843	-	-	2/16/32/32	0/3/3/3
2	ADP	B	1844	-	-	5/16/32/32	0/3/3/3
2	ADP	A	1844	-	-	0/16/32/32	0/3/3/3
2	ADP	A	1843	-	-	2/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1843	ADP	C5-C4	5.62	1.49	1.39
2	A	1843	ADP	C5-C4	4.95	1.47	1.39
2	B	1844	ADP	C5-C4	4.03	1.46	1.39
2	B	1843	ADP	PA-O3A	3.95	1.63	1.59
2	A	1844	ADP	C5-C4	3.92	1.46	1.39
2	B	1844	ADP	C5-N7	-3.80	1.32	1.39
2	A	1844	ADP	C5-C6	3.20	1.49	1.41
2	B	1844	ADP	C8-N9	-3.17	1.32	1.37
2	B	1843	ADP	C5-N7	-2.89	1.33	1.39
2	A	1843	ADP	C5-N7	-2.68	1.34	1.39
2	A	1844	ADP	C8-N7	2.44	1.36	1.31
2	B	1843	ADP	C8-N7	2.42	1.36	1.31
2	A	1843	ADP	C8-N7	2.41	1.36	1.31
2	B	1844	ADP	O4'-C4'	-2.23	1.40	1.45
2	A	1844	ADP	C4-N9	-2.17	1.33	1.37
2	A	1843	ADP	C4-N9	-2.10	1.33	1.37
2	B	1843	ADP	C4-N3	2.07	1.38	1.34
2	A	1843	ADP	C5-C6	2.07	1.46	1.41
2	B	1844	ADP	C5-C6	2.06	1.46	1.41
2	A	1844	ADP	C8-N9	-2.04	1.34	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1843	ADP	N3-C4-N9	5.77	136.98	127.17
2	B	1844	ADP	C5-C4-N3	-5.76	118.78	126.72
2	B	1843	ADP	C5-C4-N3	-5.41	119.27	126.72
2	A	1844	ADP	C4-N9-C8	5.34	111.34	105.74
2	B	1844	ADP	N3-C4-N9	5.07	135.79	127.17
2	A	1844	ADP	C5-C4-N3	-4.79	120.12	126.72
2	A	1843	ADP	C5-C4-N3	-4.69	120.25	126.72
2	A	1844	ADP	N3-C4-N9	4.50	134.82	127.17
2	A	1844	ADP	N3-C2-N1	-4.23	122.17	128.58
2	A	1843	ADP	N3-C4-N9	4.21	134.32	127.17
2	A	1844	ADP	C2-N3-C4	4.18	122.04	111.83
2	B	1843	ADP	N6-C6-N1	3.99	127.26	118.38
2	B	1843	ADP	N3-C2-N1	-3.73	122.94	128.58
2	B	1844	ADP	O4'-C1'-N9	-3.69	101.00	108.09
2	B	1844	ADP	C4-C5-N7	-3.64	106.42	110.58
2	B	1844	ADP	N3-C2-N1	-3.56	123.19	128.58
2	A	1843	ADP	N3-C2-N1	-3.51	123.26	128.58
2	B	1844	ADP	C2-N3-C4	3.44	120.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1844	ADP	C4-N9-C8	3.44	109.35	105.74
2	B	1843	ADP	C2-N3-C4	3.34	120.00	111.83
2	B	1844	ADP	C5-N7-C8	3.30	108.63	103.45
2	A	1844	ADP	C4-C5-N7	-3.15	106.98	110.58
2	A	1844	ADP	N9-C8-N7	-3.14	109.47	113.94
2	A	1844	ADP	C6-C5-N7	3.13	138.13	132.09
2	B	1843	ADP	O3B-PB-O2B	3.08	119.34	107.80
2	B	1843	ADP	C5-C6-N6	-3.06	115.70	123.29
2	A	1843	ADP	C2-N3-C4	2.99	119.14	111.83
2	A	1844	ADP	O3'-C3'-C4'	-2.96	102.57	111.08
2	A	1843	ADP	C4-N9-C8	2.96	108.84	105.74
2	A	1843	ADP	C2-N1-C6	2.88	123.47	118.73
2	A	1844	ADP	O2A-PA-O5'	2.71	119.83	107.57
2	B	1844	ADP	N9-C8-N7	-2.69	110.12	113.94
2	A	1844	ADP	O3B-PB-O1B	2.60	120.98	110.83
2	B	1843	ADP	C4-N9-C8	2.59	108.46	105.74
2	B	1843	ADP	O4'-C1'-N9	-2.56	103.17	108.09
2	B	1843	ADP	C2-N1-C6	2.52	122.87	118.73
2	A	1844	ADP	O4'-C1'-N9	-2.44	103.40	108.09
2	A	1843	ADP	C4-C5-N7	-2.43	107.81	110.58
2	A	1844	ADP	C2'-C3'-C4'	2.41	107.27	102.61
2	A	1844	ADP	O3B-PB-O3A	-2.40	96.58	104.64
2	A	1843	ADP	N6-C6-N1	2.36	123.63	118.38
2	A	1844	ADP	C5-N7-C8	2.36	107.16	103.45
2	B	1844	ADP	O4'-C4'-C5'	-2.32	101.91	109.33
2	B	1844	ADP	O2B-PB-O1B	2.30	119.78	110.83
2	A	1844	ADP	C4-N9-C1'	-2.29	121.27	126.63
2	A	1844	ADP	O3B-PB-O2B	2.19	116.02	107.80
2	B	1844	ADP	O3A-PA-O1A	2.07	116.94	110.70
2	A	1843	ADP	O2A-PA-O1A	2.05	121.98	112.44
2	A	1843	ADP	C5-N7-C8	2.02	106.63	103.45

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1843	ADP	C5'-O5'-PA-O2A
2	B	1844	ADP	C5'-O5'-PA-O3A
2	A	1843	ADP	O4'-C4'-C5'-O5'
2	B	1844	ADP	O4'-C4'-C5'-O5'
2	B	1844	ADP	C3'-C4'-C5'-O5'
2	A	1843	ADP	C3'-C4'-C5'-O5'

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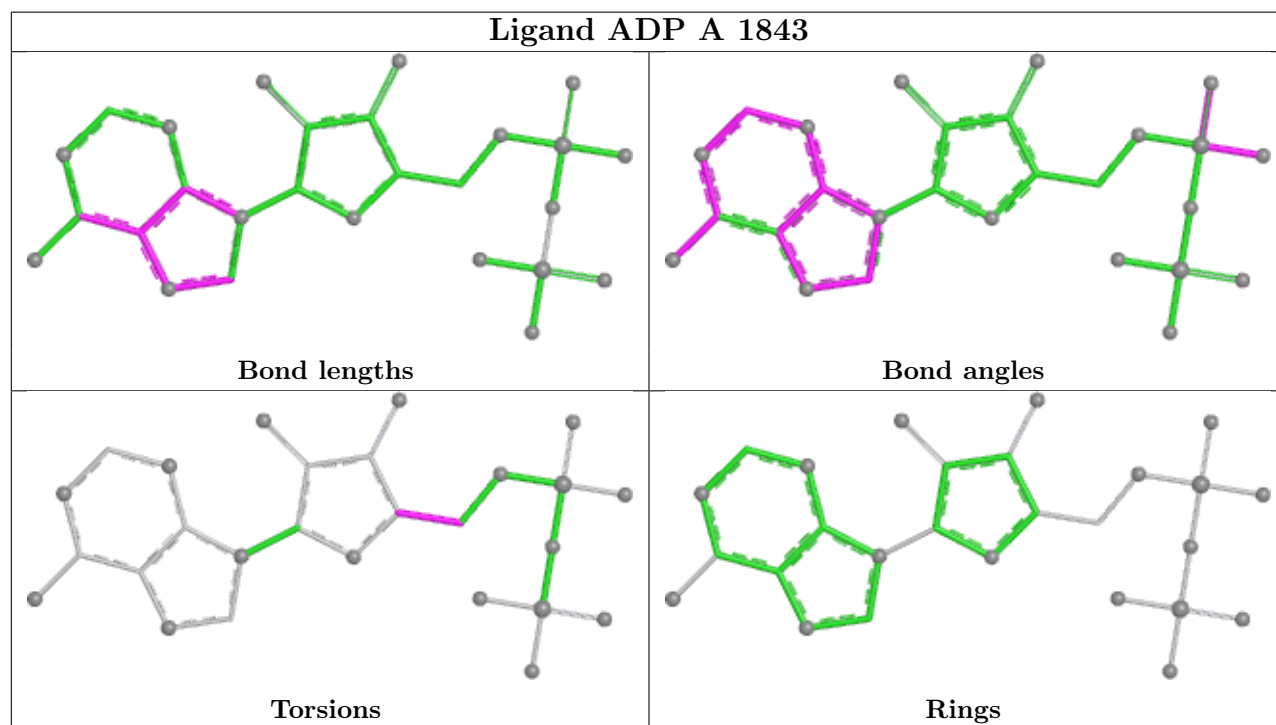
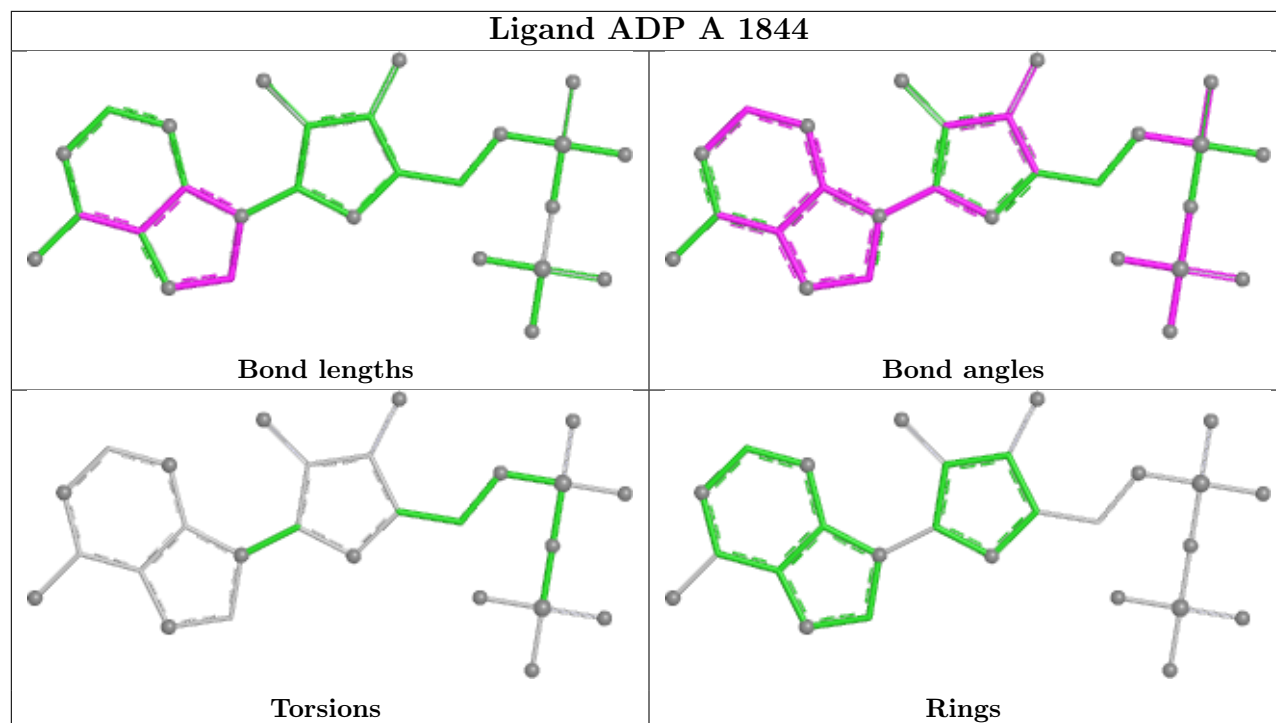
Mol	Chain	Res	Type	Atoms
2	B	1843	ADP	C5'-O5'-PA-O1A
2	B	1844	ADP	C5'-O5'-PA-O1A
2	B	1844	ADP	PB-O3A-PA-O1A

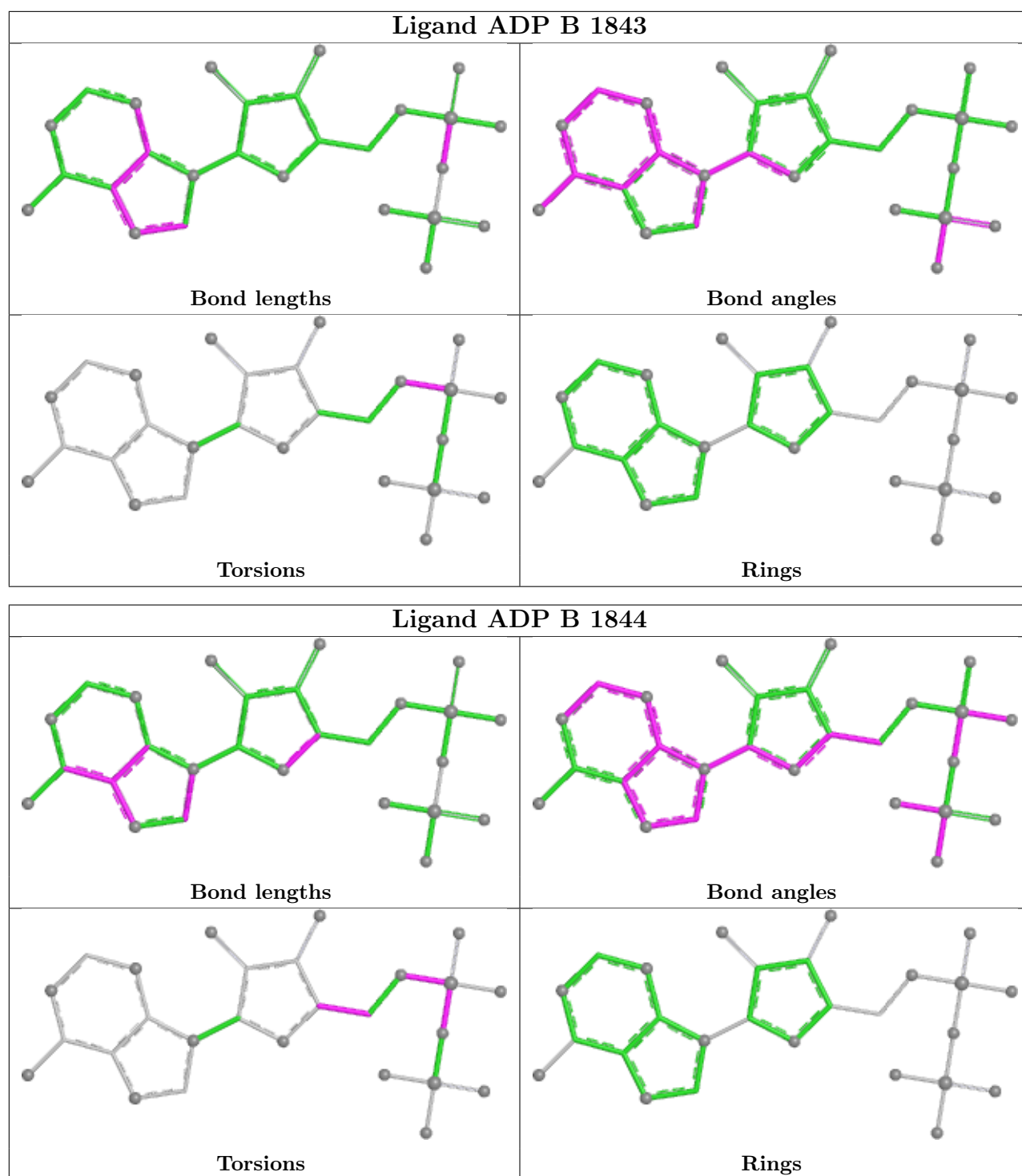
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1844	ADP	3	0
2	A	1843	ADP	2	0
2	B	1843	ADP	6	0
2	B	1844	ADP	4	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	806/842 (95%)	-0.02	12 (1%)	72 49	33, 64, 92, 111	5 (0%)
1	B	835/842 (99%)	0.09	25 (2%)	52 30	32, 64, 97, 134	5 (0%)
All	All	1641/1684 (97%)	0.04	37 (2%)	61 38	32, 64, 95, 134	10 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	652	VAL	5.0
1	A	662	ALA	4.0
1	A	660	VAL	3.5
1	B	208	TRP	3.5
1	B	556	VAL	3.4
1	A	658	PRO	3.3
1	B	657	LEU	3.2
1	A	650	VAL	3.0
1	A	758[A]	ASP	2.9
1	B	656	PHE	2.8
1	B	558	PRO	2.8
1	A	815[A]	ARG	2.8
1	B	252	MET	2.7
1	B	217	HIS	2.7
1	B	215	THR	2.6
1	B	200	LEU	2.6
1	B	569	HIS	2.6
1	B	253	GLY	2.5
1	B	247[A]	MET	2.5
1	B	183	ALA	2.5
1	B	566	PRO	2.5
1	B	76	LEU	2.5
1	B	520	PHE	2.4
1	B	71	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	237	ALA	2.4
1	B	655	LEU	2.4
1	B	81	GLY	2.3
1	A	794	GLN	2.3
1	B	555	PRO	2.3
1	B	557	ASN	2.2
1	A	649	TRP	2.2
1	A	663	PRO	2.1
1	B	280	GLY	2.1
1	A	147	PRO	2.1
1	A	76	LEU	2.0
1	B	209	ARG	2.0
1	B	212	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	1848[A]	5/5	0.63	0.17	93,93,94,95	5
4	SO4	B	1851[A]	5/5	0.65	0.15	98,98,100,100	5
4	SO4	A	1849[A]	5/5	0.75	0.24	89,90,90,91	5
4	SO4	B	1849	5/5	0.84	0.21	93,94,95,96	0
4	SO4	B	1848[A]	5/5	0.84	0.16	95,95,95,95	5
4	SO4	B	1850[A]	5/5	0.88	0.12	80,81,82,82	5
4	SO4	A	1847[A]	5/5	0.91	0.11	87,88,88,88	5
4	SO4	B	1847	5/5	0.92	0.08	90,91,91,91	0
5	PO4	B	1852[A]	5/5	0.92	0.14	85,86,86,86	5
3	ZN	A	1846	1/1	0.94	0.16	106,106,106,106	1

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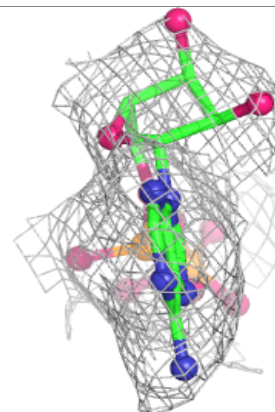
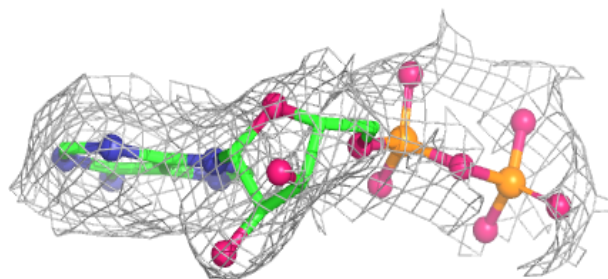
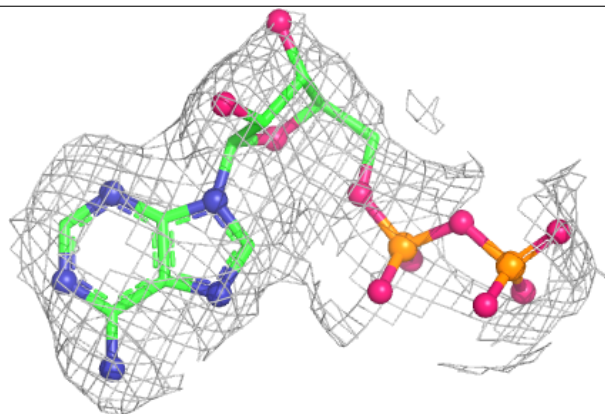
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1843	27/27	0.96	0.07	67,71,77,77	0
2	ADP	B	1843	27/27	0.97	0.07	53,57,58,59	0
2	ADP	B	1844	27/27	0.97	0.06	49,55,57,59	0
2	ADP	A	1844	27/27	0.98	0.06	31,47,51,51	0
3	ZN	A	1845	1/1	0.99	0.07	80,80,80,80	1
3	ZN	B	1845	1/1	0.99	0.10	44,44,44,44	1
3	ZN	B	1846	1/1	0.99	0.10	87,87,87,87	1

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

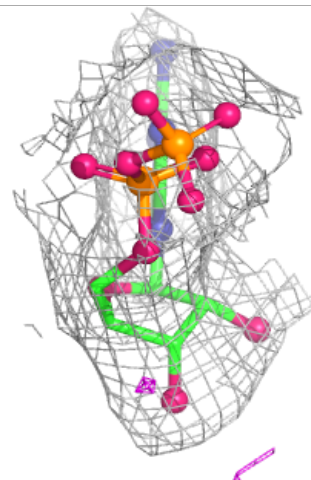
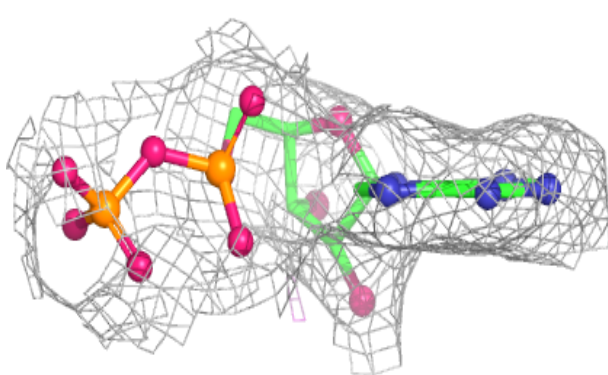
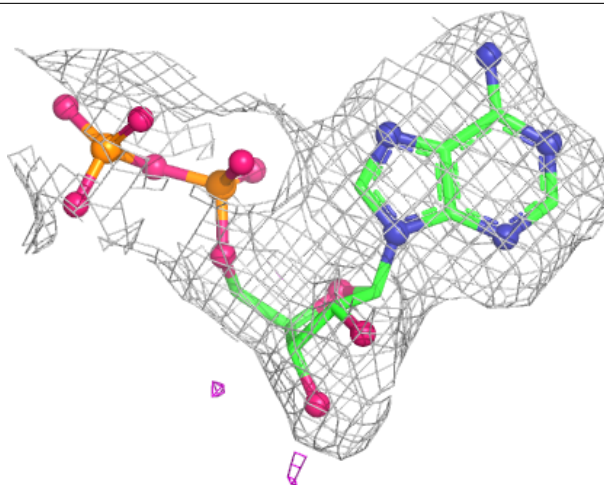
Electron density around ADP A 1843:

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



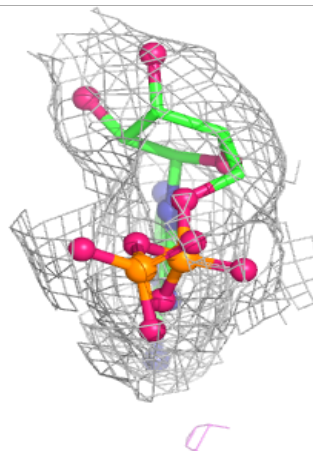
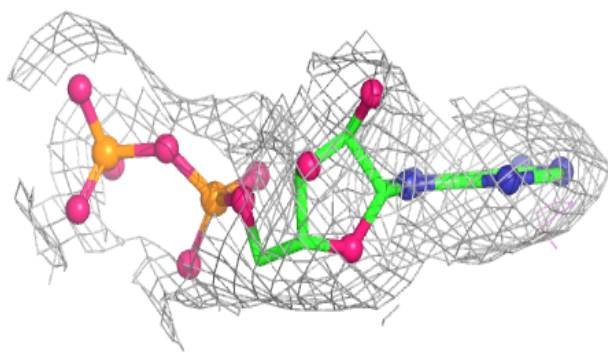
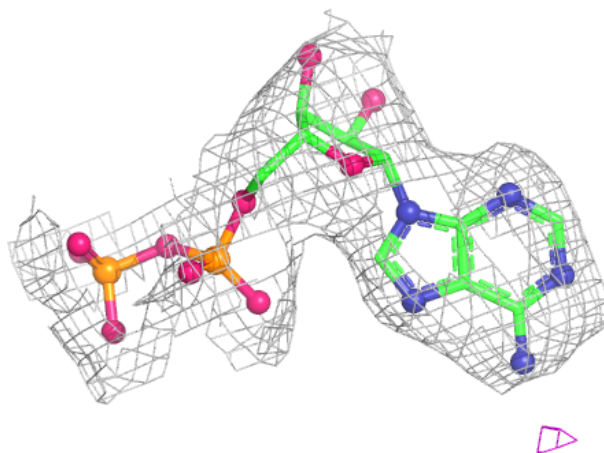
Electron density around ADP B 1843:

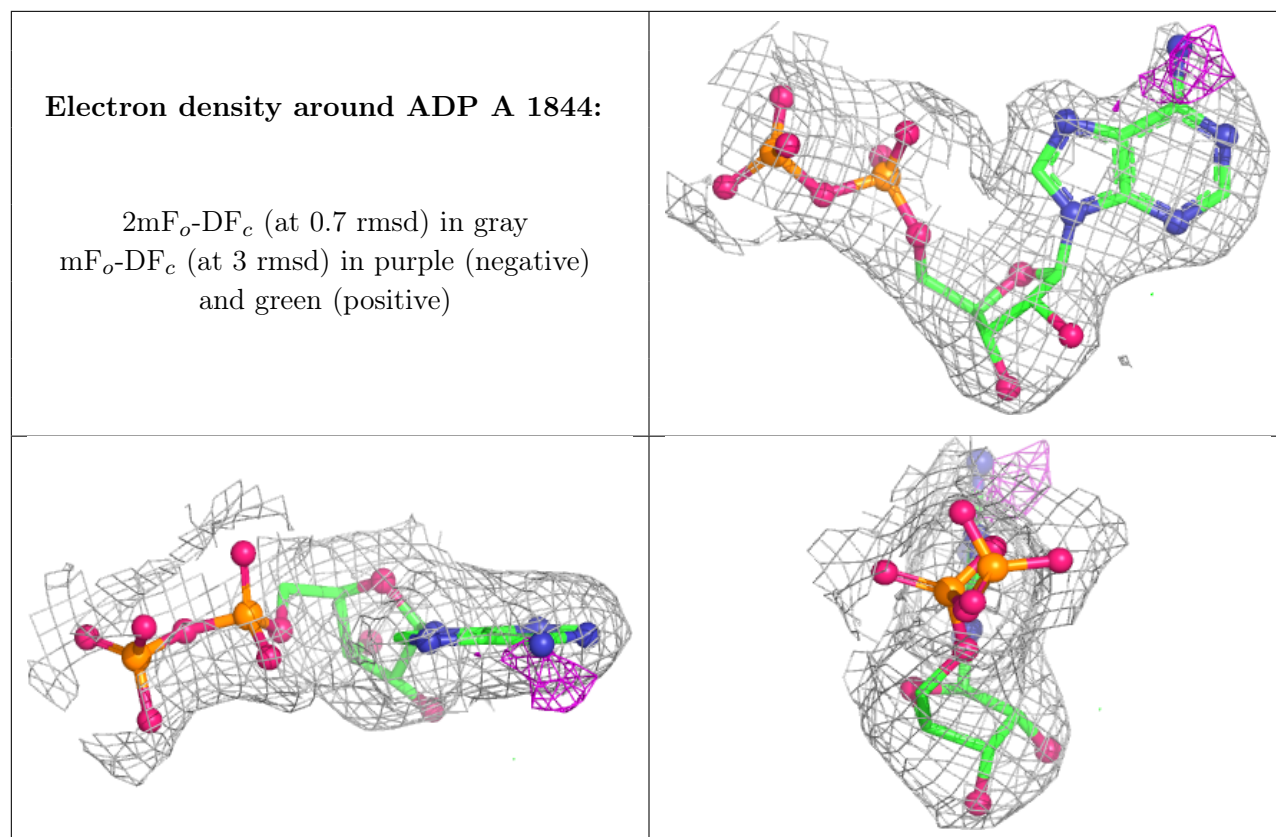
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP B 1844:

$2mF_o-DF_c$ (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.