



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:23 PM UTC

PDB ID : 2AWO / pdb_00002awo
Title : Crystal structure of the ADP-Mg-bound E. Coli MALK (Crystallized with ADP-Mg)
Authors : Lu, G.; Westbrook, J.M.; Davidson, A.L.; Chen, J.
Deposited on : 2005-09-01
Resolution : 2.80 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

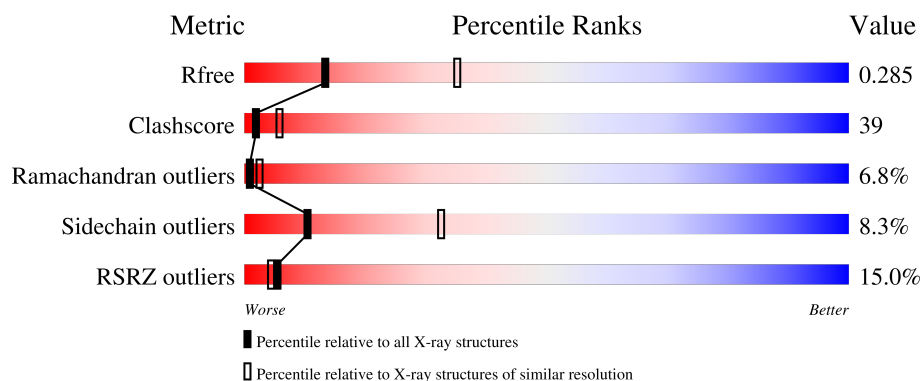
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	381	14% 40% 45% 10% • •
1	B	381	8% 45% 43% 9% • •
1	C	381	20% 40% 44% 10% • 5%
1	D	381	12% 39% 31% 7% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11005 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 Maltose/maltodextrin import ATP-binding protein malK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2882	1822	516	531	13			
1	B	374	Total	C	N	O	S	0	0	0
			2893	1828	518	534	13			
1	C	363	Total	C	N	O	S	0	0	0
			2800	1765	504	518	13			
1	D	299	Total	C	N	O	S	0	0	0
			2318	1465	409	432	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	cloning artifact	UNP P68187
A	373	SER	-	cloning artifact	UNP P68187
A	374	ALA	-	cloning artifact	UNP P68187
A	375	SER	-	cloning artifact	UNP P68187
A	376	HIS	-	cloning artifact	UNP P68187
A	377	HIS	-	cloning artifact	UNP P68187
A	378	HIS	-	cloning artifact	UNP P68187
A	379	HIS	-	cloning artifact	UNP P68187
A	380	HIS	-	cloning artifact	UNP P68187
A	381	HIS	-	cloning artifact	UNP P68187
B	372	ALA	-	cloning artifact	UNP P68187
B	373	SER	-	cloning artifact	UNP P68187
B	374	ALA	-	cloning artifact	UNP P68187
B	375	SER	-	cloning artifact	UNP P68187
B	376	HIS	-	cloning artifact	UNP P68187
B	377	HIS	-	cloning artifact	UNP P68187
B	378	HIS	-	cloning artifact	UNP P68187
B	379	HIS	-	cloning artifact	UNP P68187
B	380	HIS	-	cloning artifact	UNP P68187
B	381	HIS	-	cloning artifact	UNP P68187
C	372	ALA	-	cloning artifact	UNP P68187

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	SER	-	cloning artifact	UNP P68187
C	374	ALA	-	cloning artifact	UNP P68187
C	375	SER	-	cloning artifact	UNP P68187
C	376	HIS	-	cloning artifact	UNP P68187
C	377	HIS	-	cloning artifact	UNP P68187
C	378	HIS	-	cloning artifact	UNP P68187
C	379	HIS	-	cloning artifact	UNP P68187
C	380	HIS	-	cloning artifact	UNP P68187
C	381	HIS	-	cloning artifact	UNP P68187
D	372	ALA	-	cloning artifact	UNP P68187
D	373	SER	-	cloning artifact	UNP P68187
D	374	ALA	-	cloning artifact	UNP P68187
D	375	SER	-	cloning artifact	UNP P68187
D	376	HIS	-	cloning artifact	UNP P68187
D	377	HIS	-	cloning artifact	UNP P68187
D	378	HIS	-	cloning artifact	UNP P68187
D	379	HIS	-	cloning artifact	UNP P68187
D	380	HIS	-	cloning artifact	UNP P68187
D	381	HIS	-	cloning artifact	UNP P68187

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

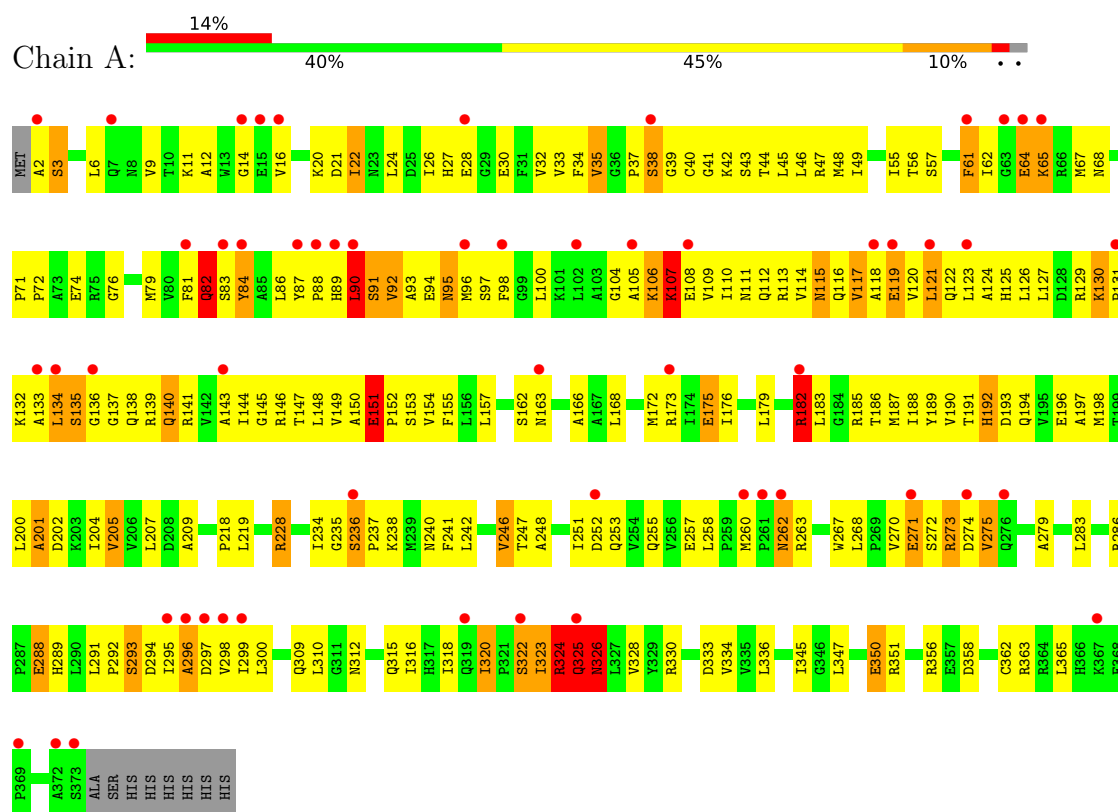


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

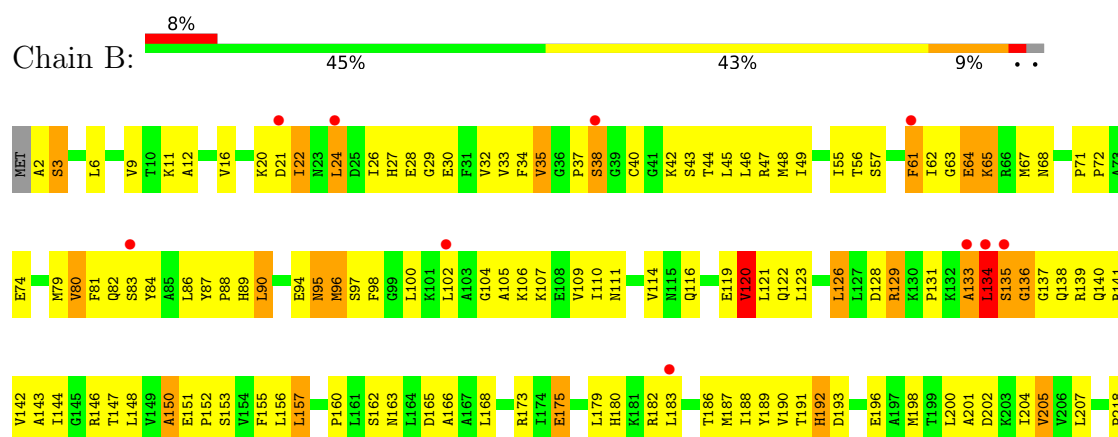
3 Residue-property plots

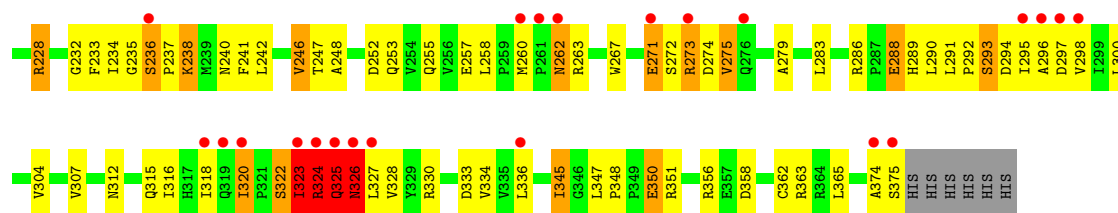
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Maltose/maltodextrin import ATP-binding protein malK

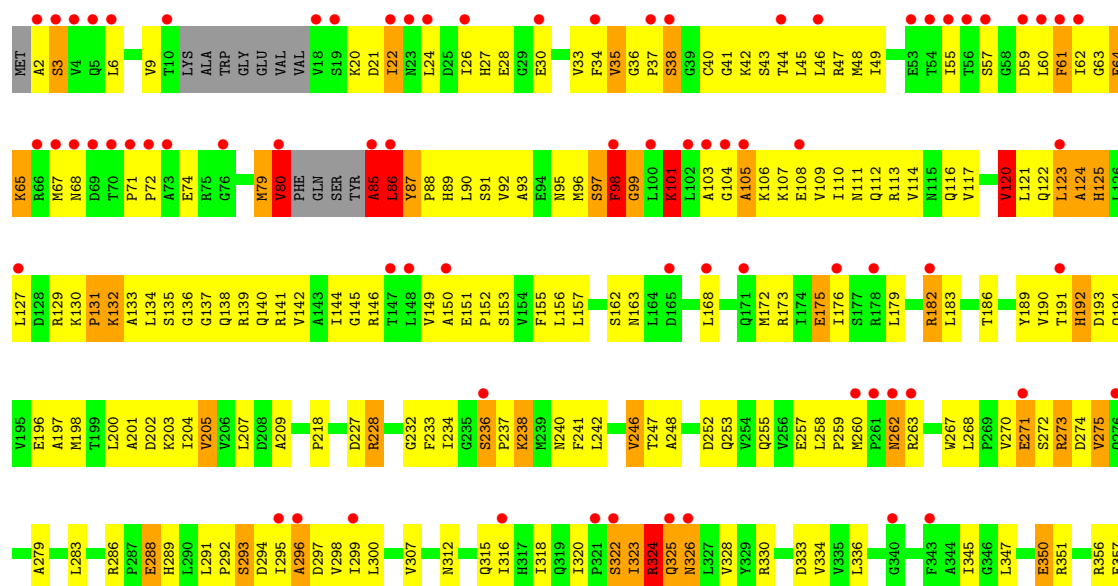


- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK

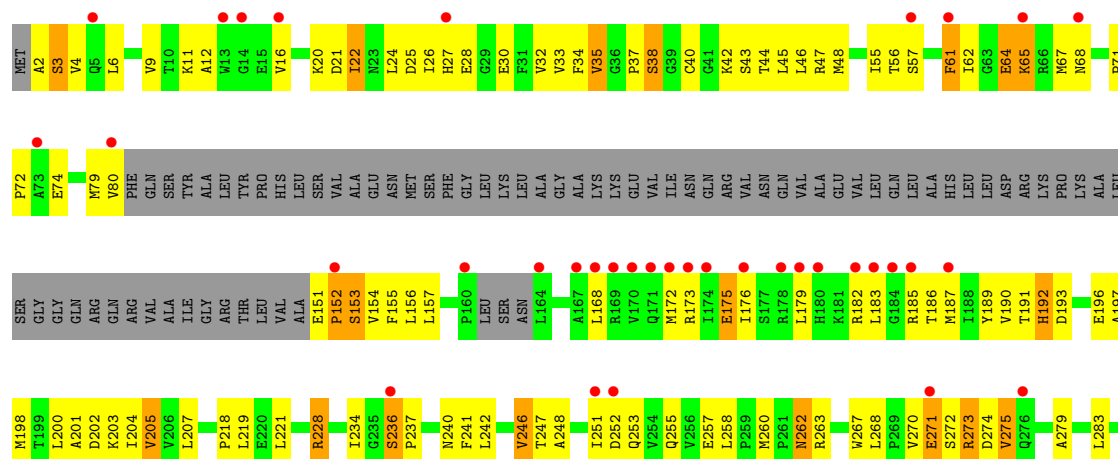


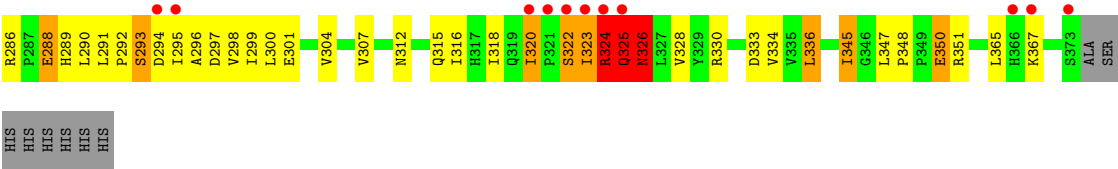


• Molecule 1: Maltose/maltodextrin import ATP-binding protein malK



• Molecule 1: Maltose/maltodextrin import ATP-binding protein malK





HIS
HIS
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HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.21Å 101.97Å 131.50Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	29.93 – 2.80 29.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.5 (29.93-2.80) 88.8 (29.93-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.277 0.245 , 0.285	Depositor DCC
R_{free} test set	2024 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11005	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG

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	0.82	3/2932 (0.1%)	1.26	32/3976 (0.8%)
1	B	1.06	2/2943 (0.1%)	1.22	23/3991 (0.6%)
1	C	1.43	5/2844 (0.2%)	1.34	28/3853 (0.7%)
1	D	0.95	1/2358 (0.0%)	1.23	15/3199 (0.5%)
All	All	1.09	11/11077 (0.1%)	1.26	98/15019 (0.7%)

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	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	LEU	N-CA	52.22	2.13	1.46
1	B	326	ASN	N-CA	47.04	2.06	1.46
1	C	87	TYR	N-CA	46.21	1.98	1.45
1	D	326	ASN	N-CA	39.04	1.96	1.46
1	A	326	ASN	N-CA	33.19	1.89	1.46
1	B	135	SER	N-CA	13.54	1.63	1.46
1	C	125	HIS	N-CA	10.06	1.59	1.46
1	A	83	SER	N-CA	9.59	1.58	1.46
1	A	107	LYS	N-CA	8.74	1.59	1.45
1	C	59	ASP	C-N	-8.33	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	MET	C-N	-6.31	1.24	1.33

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	LEU	CA-C-N	-25.07	84.16	120.51
1	C	86	LEU	C-N-CA	-25.07	84.16	120.51
1	B	326	ASN	N-CA-CB	-22.49	72.48	110.49
1	D	326	ASN	N-CA-CB	-20.57	75.73	110.49
1	A	326	ASN	N-CA-CB	-18.79	78.73	110.49
1	C	125	HIS	N-CA-CB	17.42	139.93	110.49
1	C	87	TYR	N-CA-C	16.26	128.30	109.60
1	A	107	LYS	N-CA-C	-15.96	91.24	114.39
1	D	324	ARG	NE-CZ-NH2	15.26	132.93	119.20
1	A	182	ARG	NE-CZ-NH2	15.10	132.79	119.20
1	B	325	GLN	CA-C-N	-14.33	94.17	121.54
1	B	325	GLN	C-N-CA	-14.33	94.17	121.54
1	A	182	ARG	NE-CZ-NH1	-14.21	107.29	121.50
1	D	324	ARG	NE-CZ-NH1	-14.14	107.36	121.50
1	C	86	LEU	N-CA-C	-14.13	80.71	110.80
1	A	182	ARG	CD-NE-CZ	13.59	143.43	124.40
1	D	324	ARG	CD-NE-CZ	13.46	143.25	124.40
1	D	325	GLN	CA-C-N	-13.25	96.23	121.54
1	D	325	GLN	C-N-CA	-13.25	96.23	121.54
1	D	326	ASN	N-CA-C	12.55	137.54	110.80
1	C	125	HIS	N-CA-C	-12.51	84.15	110.80
1	A	326	ASN	N-CA-C	12.33	137.06	110.80
1	A	325	GLN	CA-C-N	-12.11	98.41	121.54
1	A	325	GLN	C-N-CA	-12.11	98.41	121.54
1	B	326	ASN	N-CA-C	12.11	136.59	110.80
1	C	87	TYR	N-CA-CB	-11.51	92.83	109.75
1	A	202	ASP	N-CA-C	-11.47	99.42	113.41
1	B	202	ASP	N-CA-C	-11.46	99.43	113.41
1	D	202	ASP	N-CA-C	-11.40	99.50	113.41
1	B	135	SER	N-CA-CB	11.35	129.67	110.49
1	C	202	ASP	N-CA-C	-11.24	99.69	113.41
1	C	325	GLN	OE1-CD-NE2	-9.70	112.91	122.60
1	B	135	SER	N-CA-C	-9.22	91.16	110.80
1	A	201	ALA	N-CA-C	9.06	123.27	110.50
1	C	201	ALA	N-CA-C	9.05	123.26	110.50
1	D	201	ALA	N-CA-C	8.97	123.14	110.50
1	A	107	LYS	N-CA-CB	8.96	122.80	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ALA	N-CA-C	8.92	123.08	110.50
1	A	192	HIS	N-CA-C	-8.07	102.91	114.12
1	C	192	HIS	N-CA-C	-7.84	103.22	114.12
1	D	192	HIS	N-CA-C	-7.74	103.36	114.12
1	B	150	ALA	N-CA-C	-7.71	97.45	109.25
1	C	124	ALA	CA-C-N	-7.53	107.16	121.54
1	C	124	ALA	C-N-CA	-7.53	107.16	121.54
1	B	134	LEU	CB-CA-C	-7.33	95.83	110.42
1	B	192	HIS	N-CA-C	-7.17	102.85	113.61
1	C	325	GLN	CG-CD-NE2	7.16	127.15	116.40
1	C	294	ASP	N-CA-C	-7.10	103.54	111.71
1	B	262	ASN	N-CA-C	-6.55	105.33	113.38
1	D	294	ASP	N-CA-C	-6.50	103.43	111.75
1	B	294	ASP	N-CA-C	-6.43	103.52	111.75
1	C	125	HIS	CA-CB-CG	-6.41	107.39	113.80
1	A	122	GLN	N-CA-CB	-6.38	102.26	111.70
1	B	133	ALA	N-CA-C	-6.35	102.03	111.81
1	A	294	ASP	N-CA-C	-6.33	103.65	111.75
1	A	262	ASN	N-CA-C	-6.31	105.62	113.38
1	D	262	ASN	N-CA-C	-6.31	105.62	113.38
1	A	82	GLN	CA-C-N	-6.28	109.54	121.54
1	A	82	GLN	C-N-CA	-6.28	109.54	121.54
1	A	119	GLU	N-CA-C	-6.28	104.71	112.38
1	C	238	LYS	N-CA-C	6.27	118.39	110.24
1	C	262	ASN	N-CA-C	-6.26	105.65	113.28
1	A	143	ALA	N-CA-C	-6.23	104.40	111.07
1	A	89	HIS	N-CA-C	-6.11	105.78	113.18
1	B	238	LYS	N-CA-C	6.07	118.13	110.24
1	C	87	TYR	CA-C-N	6.07	125.95	119.28
1	C	87	TYR	C-N-CA	6.07	125.95	119.28
1	A	122	GLN	N-CA-C	5.95	119.60	111.39
1	B	81	PHE	N-CA-C	5.94	116.12	108.34
1	B	98	PHE	N-CA-C	5.91	118.23	111.02
1	A	92	VAL	N-CA-C	5.86	121.53	109.34
1	A	140	GLN	N-CA-C	-5.83	105.26	112.90
1	A	238	LYS	N-CA-C	5.81	117.79	110.24
1	B	97	SER	N-CA-C	-5.80	106.24	113.38
1	C	85	ALA	CA-C-N	-5.74	110.57	121.54
1	C	85	ALA	C-N-CA	-5.74	110.57	121.54
1	A	61	PHE	N-CA-CB	-5.69	101.52	110.79
1	A	117	VAL	N-CA-C	-5.67	107.22	112.43
1	D	61	PHE	N-CA-CB	-5.65	101.59	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LYS	CA-C-N	-5.62	113.39	121.98
1	A	106	LYS	C-N-CA	-5.62	113.39	121.98
1	C	200	LEU	N-CA-C	5.62	120.14	113.12
1	B	200	LEU	N-CA-C	5.60	120.12	113.12
1	A	14	GLY	N-CA-C	-5.46	106.64	111.67
1	B	61	PHE	N-CA-CB	-5.44	101.54	110.95
1	A	162	SER	N-CA-C	5.41	117.87	111.33
1	C	162	SER	N-CA-C	5.37	117.83	111.33
1	D	200	LEU	N-CA-C	5.37	119.83	113.12
1	C	133	ALA	N-CA-C	-5.36	106.41	113.17
1	A	200	LEU	N-CA-C	5.34	119.79	113.12
1	B	121	LEU	N-CA-C	-5.24	106.73	113.02
1	C	61	PHE	N-CA-CB	-5.24	102.24	110.79
1	B	162	SER	N-CA-C	5.21	117.64	111.33
1	D	336	LEU	N-CA-C	5.12	117.61	107.98
1	B	336	LEU	N-CA-C	5.11	117.59	107.98
1	A	336	LEU	N-CA-C	5.09	117.54	107.98
1	C	80	VAL	N-CA-C	-5.09	96.76	111.00
1	C	336	LEU	N-CA-C	5.03	117.43	107.98

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	GLN	Peptide
1	B	134	LEU	Peptide
1	B	325	GLN	Peptide
1	C	85	ALA	Peptide
1	D	325	GLN	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	2882	0	2946	251	2
1	B	2893	0	2956	221	3
1	C	2800	0	2869	251	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2318	0	2350	162	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
All	All	11005	0	11169	866	4

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 39.

All (866) 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:326:ASN:N	1:A:326:ASN:CA	1.89	1.36
1:D:326:ASN:N	1:D:326:ASN:CA	1.96	1.28
1:C:87:TYR:N	1:C:87:TYR:CA	1.98	1.26
1:B:326:ASN:N	1:B:326:ASN:CA	2.06	1.18
1:B:326:ASN:N	1:B:326:ASN:HB2	1.62	1.13
1:B:26:ILE:HD12	1:B:32:VAL:HG21	1.27	1.13
1:B:323:ILE:CG2	1:B:325:GLN:HE21	1.61	1.13
1:A:120:VAL:HG12	1:A:182:ARG:HH11	0.99	1.12
1:C:86:LEU:N	1:C:86:LEU:CA	2.13	1.11
1:D:26:ILE:HD12	1:D:32:VAL:HG21	1.26	1.11
1:C:120:VAL:HG13	1:C:182:ARG:NH2	1.66	1.09
1:B:286:ARG:HB2	1:B:289:HIS:HD2	1.18	1.09
1:B:326:ASN:N	1:B:326:ASN:CB	2.17	1.08
1:D:326:ASN:N	1:D:326:ASN:CB	2.17	1.07
1:D:326:ASN:N	1:D:326:ASN:HB2	1.69	1.07
1:A:120:VAL:HG12	1:A:182:ARG:NH1	1.69	1.07
1:C:86:LEU:C	1:C:87:TYR:CA	2.27	1.06
1:A:326:ASN:N	1:A:326:ASN:CB	2.19	1.06
1:B:260:MET:HA	1:B:322:SER:HB3	1.38	1.04
1:D:286:ARG:HB2	1:D:289:HIS:HD2	1.23	1.03
1:A:260:MET:HA	1:A:322:SER:HB3	1.38	1.03
1:A:286:ARG:HB2	1:A:289:HIS:HD2	1.18	1.03
1:B:135:SER:O	1:B:137:GLY:N	1.89	1.03
1:C:260:MET:HA	1:C:322:SER:HB3	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:MET:HA	1:D:322:SER:HB3	1.39	1.03
1:C:120:VAL:HG13	1:C:182:ARG:HH22	1.19	1.02
1:C:86:LEU:O	1:C:87:TYR:CA	2.08	1.02
1:C:286:ARG:HB2	1:C:289:HIS:HD2	1.19	1.01
1:B:323:ILE:HD12	1:B:324:ARG:NH1	1.78	0.99
1:B:323:ILE:HG22	1:B:325:GLN:HE21	1.25	0.97
1:A:240:ASN:HD21	1:A:328:VAL:H	1.12	0.96
1:A:326:ASN:N	1:A:326:ASN:HB2	1.76	0.96
1:A:236:SER:HB2	1:A:237:PRO:HD3	1.47	0.95
1:A:120:VAL:HA	1:C:324:ARG:HH21	1.27	0.95
1:B:236:SER:HB2	1:B:237:PRO:HD3	1.47	0.95
1:C:236:SER:HB2	1:C:237:PRO:HD3	1.49	0.94
1:D:240:ASN:HD21	1:D:328:VAL:H	1.14	0.94
1:D:236:SER:HB2	1:D:237:PRO:HD3	1.47	0.93
1:B:240:ASN:HD21	1:B:328:VAL:H	1.15	0.92
1:A:286:ARG:HB2	1:A:289:HIS:CD2	2.04	0.92
1:C:240:ASN:HD21	1:C:328:VAL:H	1.13	0.91
1:D:191:THR:HG22	1:D:193:ASP:H	1.35	0.91
1:C:286:ARG:HB2	1:C:289:HIS:CD2	2.05	0.91
1:B:80:VAL:HG21	1:B:144:ILE:HD13	1.52	0.90
1:B:286:ARG:HB2	1:B:289:HIS:CD2	2.05	0.90
1:A:90:LEU:HB3	1:A:131:PRO:HD2	1.53	0.90
1:C:259:PRO:HB2	1:C:323:ILE:HD12	1.53	0.89
1:D:48:MET:HB3	1:D:55:ILE:HD11	1.55	0.89
1:A:120:VAL:HG13	1:C:324:ARG:NH2	1.87	0.89
1:C:191:THR:HG22	1:C:193:ASP:H	1.38	0.88
1:A:325:GLN:C	1:A:326:ASN:CA	2.46	0.88
1:D:286:ARG:HB2	1:D:289:HIS:CD2	2.09	0.87
1:C:20:LYS:HE2	1:C:209:ALA:O	1.73	0.87
1:B:323:ILE:HD12	1:B:324:ARG:HH12	1.39	0.86
1:B:191:THR:HG22	1:B:193:ASP:H	1.40	0.86
1:A:138:GLN:HA	1:A:141:ARG:HE	1.39	0.86
1:B:134:LEU:C	1:B:136:GLY:H	1.71	0.86
1:D:325:GLN:C	1:D:326:ASN:CA	2.49	0.86
1:D:152:PRO:HG2	1:D:153:SER:H	1.39	0.85
1:C:79:MET:HE3	1:C:156:LEU:HB3	1.56	0.85
1:D:2:ALA:HB2	1:D:153:SER:HB2	1.58	0.85
1:A:197:ALA:HB1	1:A:204:ILE:HD12	1.59	0.85
1:C:197:ALA:HB1	1:C:204:ILE:HD12	1.60	0.84
1:D:48:MET:HB3	1:D:55:ILE:CD1	2.07	0.84
1:A:191:THR:HG22	1:A:193:ASP:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:SER:CB	1:C:237:PRO:HD3	2.08	0.84
1:A:236:SER:CB	1:A:237:PRO:HD3	2.07	0.83
1:B:236:SER:CB	1:B:237:PRO:HD3	2.07	0.83
1:D:151:GLU:HB2	1:D:185:ARG:NH2	1.94	0.83
1:D:236:SER:CB	1:D:237:PRO:HD3	2.09	0.82
1:D:301:GLU:O	1:D:320:ILE:HD13	1.79	0.82
1:D:260:MET:HA	1:D:322:SER:CB	2.10	0.81
1:A:260:MET:HA	1:A:322:SER:CB	2.10	0.81
1:B:323:ILE:CG2	1:B:325:GLN:NE2	2.43	0.81
1:C:324:ARG:H	1:C:324:ARG:HD3	1.46	0.81
1:A:138:GLN:HG2	1:A:141:ARG:HH21	1.43	0.81
1:B:260:MET:HA	1:B:322:SER:CB	2.11	0.81
1:B:325:GLN:C	1:B:326:ASN:CA	2.54	0.80
1:C:260:MET:HA	1:C:322:SER:CB	2.10	0.80
1:C:2:ALA:HB2	1:C:153:SER:HB3	1.63	0.80
1:D:292:PRO:O	1:D:293:SER:HB3	1.83	0.79
1:A:2:ALA:CB	1:A:153:SER:HB2	2.13	0.79
1:C:96:MET:HE3	1:C:145:GLY:HA3	1.65	0.79
1:C:46:LEU:HB3	1:C:79:MET:HE1	1.65	0.79
1:C:86:LEU:N	1:C:86:LEU:C	2.41	0.79
1:C:292:PRO:O	1:C:293:SER:HB3	1.83	0.78
1:B:292:PRO:O	1:B:293:SER:HB3	1.83	0.78
1:A:46:LEU:HB3	1:A:79:MET:HE1	1.65	0.78
1:A:155:PHE:HB3	1:A:187:MET:HG2	1.65	0.78
1:B:119:GLU:O	1:B:120:VAL:HG23	1.84	0.78
1:A:292:PRO:O	1:A:293:SER:HB3	1.81	0.78
1:B:374:ALA:O	1:B:375:SER:HB2	1.84	0.78
1:D:4:VAL:HG22	1:D:62:ILE:HD12	1.64	0.78
1:B:134:LEU:O	1:B:136:GLY:N	2.17	0.77
1:C:87:TYR:N	1:C:87:TYR:CG	2.53	0.77
1:B:87:TYR:H	1:B:95:ASN:HD21	1.28	0.77
1:D:42:LYS:HD2	1:D:190:VAL:HG13	1.66	0.77
1:D:2:ALA:N	1:D:186:THR:HG1	1.83	0.76
1:B:134:LEU:C	1:B:136:GLY:N	2.44	0.76
1:D:33:VAL:HG22	1:D:189:TYR:HB3	1.68	0.76
1:A:33:VAL:HB	1:A:204:ILE:HD13	1.68	0.76
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.50	0.76
1:D:6:LEU:HD23	1:D:22:ILE:HD11	1.67	0.75
1:C:33:VAL:HB	1:C:204:ILE:HD13	1.67	0.75
1:C:97:SER:HB3	1:C:110:ILE:HD11	1.67	0.75
1:A:6:LEU:HD23	1:A:22:ILE:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HB3	1:B:79:MET:HE1	1.68	0.75
1:D:46:LEU:HB3	1:D:79:MET:HE1	1.67	0.75
1:A:236:SER:HB2	1:A:237:PRO:CD	2.17	0.75
1:B:236:SER:HB2	1:B:237:PRO:CD	2.15	0.75
1:A:155:PHE:HD2	1:A:187:MET:HE3	1.51	0.75
1:D:80:VAL:HG23	1:D:157:LEU:HG	1.68	0.75
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.52	0.75
1:D:236:SER:HB2	1:D:237:PRO:CD	2.16	0.74
1:A:61:PHE:CZ	1:A:64:GLU:HA	2.22	0.74
1:C:34:PHE:HB2	1:C:190:VAL:HG22	1.69	0.74
1:B:80:VAL:HG21	1:B:144:ILE:CD1	2.16	0.74
1:D:61:PHE:CZ	1:D:64:GLU:HA	2.22	0.74
1:C:6:LEU:HD23	1:C:22:ILE:HD11	1.70	0.74
1:C:157:LEU:HD12	1:C:157:LEU:N	2.03	0.74
1:C:87:TYR:N	1:C:87:TYR:CD1	2.54	0.74
1:A:116:GLN:O	1:A:120:VAL:HB	1.87	0.73
1:B:135:SER:C	1:B:137:GLY:H	1.95	0.73
1:A:140:GLN:O	1:A:144:ILE:HG12	1.89	0.73
1:A:92:VAL:HG23	1:A:129:ARG:O	1.86	0.73
1:A:42:LYS:HD2	1:A:190:VAL:HG13	1.71	0.73
1:C:236:SER:HB2	1:C:237:PRO:CD	2.17	0.73
1:B:148:LEU:HD13	1:B:179:LEU:CD1	2.18	0.73
1:C:9:VAL:HB	1:C:22:ILE:HD13	1.71	0.72
1:A:33:VAL:HG22	1:A:189:TYR:HB3	1.71	0.72
1:D:4:VAL:HG22	1:D:62:ILE:CD1	2.19	0.72
1:A:62:ILE:HD12	1:A:67:MET:HG3	1.70	0.72
1:B:253:GLN:HG2	1:B:267:TRP:CE3	2.25	0.72
1:C:61:PHE:CZ	1:C:64:GLU:HA	2.24	0.72
1:C:120:VAL:CG1	1:C:182:ARG:HH22	2.02	0.72
1:C:137:GLY:HA2	1:C:172:MET:HE1	1.72	0.72
1:A:191:THR:HG22	1:A:192:HIS:H	1.55	0.71
1:B:61:PHE:CZ	1:B:64:GLU:HA	2.24	0.71
1:C:253:GLN:HG2	1:C:267:TRP:CE3	2.25	0.71
1:D:9:VAL:HB	1:D:22:ILE:HD13	1.72	0.71
1:C:120:VAL:HG22	1:C:182:ARG:HH12	1.56	0.71
1:A:119:GLU:N	1:A:124:ALA:HB2	2.06	0.71
1:C:33:VAL:HG22	1:C:189:TYR:HB3	1.72	0.71
1:A:120:VAL:O	1:A:121:LEU:HB2	1.91	0.71
1:C:228:ARG:HG3	1:C:228:ARG:HH11	1.55	0.71
1:D:228:ARG:HH11	1:D:228:ARG:HG3	1.54	0.71
1:D:191:THR:HG22	1:D:192:HIS:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:HG2	1:A:267:TRP:CE3	2.26	0.70
1:A:260:MET:C	1:A:262:ASN:H	1.97	0.70
1:B:26:ILE:HG21	1:B:188:ILE:HD11	1.71	0.70
1:A:155:PHE:CD2	1:A:187:MET:HE3	2.27	0.70
1:C:155:PHE:C	1:C:156:LEU:HD12	2.17	0.70
1:C:191:THR:HG22	1:C:192:HIS:H	1.56	0.70
1:C:86:LEU:O	1:C:87:TYR:HA	1.91	0.70
1:C:260:MET:C	1:C:262:ASN:H	1.98	0.70
1:A:9:VAL:HB	1:A:22:ILE:HD13	1.72	0.70
1:A:34:PHE:HB2	1:A:190:VAL:HG22	1.74	0.70
1:D:323:ILE:CG2	1:D:325:GLN:HE21	2.04	0.70
1:D:22:ILE:HD12	1:D:45:LEU:HD21	1.74	0.69
1:B:62:ILE:HD12	1:B:67:MET:HG3	1.73	0.69
1:D:260:MET:C	1:D:262:ASN:H	1.97	0.69
1:D:253:GLN:HG2	1:D:267:TRP:CE3	2.27	0.69
1:B:191:THR:HG22	1:B:192:HIS:H	1.56	0.69
1:B:260:MET:C	1:B:262:ASN:H	1.97	0.69
1:A:22:ILE:HD12	1:A:45:LEU:HD21	1.74	0.69
1:A:323:ILE:HG22	1:A:325:GLN:HG2	1.75	0.69
1:B:6:LEU:HD22	1:B:22:ILE:HD11	1.75	0.69
1:C:87:TYR:N	1:C:87:TYR:CB	2.56	0.69
1:C:6:LEU:HD21	1:C:49:ILE:HD11	1.74	0.69
1:C:323:ILE:HG22	1:C:325:GLN:HG2	1.75	0.68
1:A:2:ALA:HB3	1:A:153:SER:HB2	1.74	0.68
1:C:22:ILE:HD12	1:C:45:LEU:HD21	1.74	0.68
1:A:96:MET:O	1:A:149:VAL:HG21	1.94	0.68
1:C:101:LYS:HB2	1:C:101:LYS:HZ3	1.57	0.68
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.08	0.68
1:C:86:LEU:O	1:C:87:TYR:C	2.36	0.68
1:A:2:ALA:N	1:A:186:THR:HG1	1.92	0.67
1:A:125:HIS:O	1:A:126:LEU:HD23	1.95	0.67
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.09	0.67
1:B:12:ALA:H	1:B:56:THR:HG21	1.60	0.67
1:C:45:LEU:HD12	1:C:207:LEU:HD11	1.76	0.67
1:A:12:ALA:H	1:A:56:THR:HG21	1.60	0.67
1:D:12:ALA:H	1:D:56:THR:HG21	1.60	0.66
1:A:6:LEU:HD21	1:A:49:ILE:HD11	1.76	0.66
1:A:120:VAL:CG1	1:A:182:ARG:HH11	1.93	0.66
1:A:240:ASN:ND2	1:A:328:VAL:H	1.91	0.66
1:C:113:ARG:HB3	1:C:149:VAL:HG13	1.77	0.66
1:C:113:ARG:O	1:C:117:VAL:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ALA:N	1:B:186:THR:HG1	1.93	0.66
1:B:260:MET:HE2	1:B:300:LEU:HD22	1.76	0.66
1:C:9:VAL:HB	1:C:22:ILE:CD1	2.26	0.66
1:A:9:VAL:HB	1:A:22:ILE:CD1	2.26	0.66
1:A:324:ARG:H	1:A:324:ARG:HD3	1.60	0.66
1:C:260:MET:HE2	1:C:300:LEU:HD22	1.77	0.66
1:C:228:ARG:HG3	1:C:228:ARG:NH1	2.11	0.66
1:A:100:LEU:HD13	1:A:110:ILE:HA	1.78	0.66
1:B:183:LEU:HD12	1:B:183:LEU:O	1.96	0.66
1:B:43:SER:O	1:B:47:ARG:HG3	1.96	0.66
1:B:323:ILE:HG22	1:B:325:GLN:NE2	2.04	0.66
1:D:323:ILE:HG22	1:D:325:GLN:HE21	1.61	0.66
1:B:324:ARG:HD3	1:B:324:ARG:H	1.61	0.65
1:C:120:VAL:HG22	1:C:182:ARG:NH1	2.11	0.65
1:C:240:ASN:ND2	1:C:328:VAL:H	1.92	0.65
1:A:87:TYR:O	1:A:90:LEU:HD13	1.96	0.65
1:D:345:ILE:HD13	1:D:345:ILE:N	2.11	0.65
1:A:112:GLN:O	1:A:116:GLN:HB2	1.97	0.65
1:B:307:VAL:HG13	1:B:316:ILE:CD1	2.26	0.65
1:D:9:VAL:HB	1:D:22:ILE:CD1	2.27	0.65
1:B:345:ILE:HD13	1:B:345:ILE:N	2.12	0.65
1:B:6:LEU:HD21	1:B:49:ILE:HD11	1.77	0.65
1:C:2:ALA:CB	1:C:153:SER:HB3	2.26	0.65
1:D:251:ILE:HD12	1:D:251:ILE:H	1.61	0.65
1:A:292:PRO:O	1:A:293:SER:CB	2.45	0.65
1:A:260:MET:HE2	1:A:300:LEU:HD22	1.79	0.65
1:D:183:LEU:HD12	1:D:183:LEU:O	1.95	0.65
1:A:251:ILE:HD12	1:A:251:ILE:H	1.61	0.65
1:A:111:ASN:O	1:A:115:ASN:HB2	1.97	0.64
1:B:128:ASP:O	1:B:129:ARG:HB2	1.96	0.64
1:D:260:MET:HE2	1:D:300:LEU:HD22	1.77	0.64
1:C:43:SER:O	1:C:47:ARG:HG3	1.98	0.64
1:D:48:MET:SD	1:D:55:ILE:HD13	2.38	0.64
1:B:271:GLU:O	1:B:272:SER:HB3	1.96	0.64
1:C:2:ALA:HA	1:C:28:GLU:OE1	1.98	0.64
1:C:307:VAL:HG13	1:C:316:ILE:CD1	2.28	0.64
1:A:183:LEU:O	1:A:183:LEU:HD12	1.97	0.64
1:C:62:ILE:HD12	1:C:67:MET:HG3	1.77	0.64
1:C:98:PHE:O	1:C:99:GLY:O	2.16	0.64
1:C:137:GLY:HA2	1:C:172:MET:CE	2.27	0.64
1:C:271:GLU:O	1:C:272:SER:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:SER:O	1:D:47:ARG:HG3	1.97	0.64
1:B:260:MET:C	1:B:262:ASN:N	2.56	0.64
1:D:2:ALA:HA	1:D:28:GLU:OE1	1.98	0.64
1:D:228:ARG:HG3	1:D:228:ARG:NH1	2.11	0.63
1:A:90:LEU:HD12	1:A:131:PRO:CG	2.28	0.63
1:C:183:LEU:O	1:C:183:LEU:HD12	1.98	0.63
1:A:271:GLU:O	1:A:272:SER:HB3	1.97	0.63
1:A:43:SER:O	1:A:47:ARG:HG3	1.99	0.63
1:C:146:ARG:HH11	1:C:146:ARG:HG2	1.64	0.63
1:A:109:VAL:HG13	1:C:357:GLU:CD	2.24	0.63
1:A:288:GLU:HG2	1:B:312:ASN:HB2	1.81	0.63
1:B:147:THR:O	1:B:150:ALA:O	2.16	0.63
1:B:300:LEU:HB3	1:B:320:ILE:HD11	1.80	0.63
1:B:135:SER:C	1:B:137:GLY:N	2.52	0.63
1:C:130:LYS:O	1:C:132:LYS:N	2.26	0.63
1:A:147:THR:O	1:A:150:ALA:HB3	1.98	0.63
1:A:88:PRO:O	1:A:90:LEU:HD22	1.99	0.62
1:A:120:VAL:HG13	1:C:324:ARG:HH22	1.63	0.62
1:A:260:MET:C	1:A:262:ASN:N	2.56	0.62
1:D:260:MET:C	1:D:262:ASN:N	2.56	0.62
1:A:2:ALA:HA	1:A:28:GLU:OE1	1.99	0.62
1:D:292:PRO:O	1:D:293:SER:CB	2.47	0.62
1:D:307:VAL:HG13	1:D:316:ILE:CD1	2.29	0.62
1:D:323:ILE:HG22	1:D:325:GLN:HG2	1.79	0.62
1:A:26:ILE:HG21	1:A:188:ILE:HD11	1.82	0.62
1:A:138:GLN:HA	1:A:141:ARG:NE	2.13	0.61
1:A:300:LEU:HB2	1:A:345:ILE:HD11	1.82	0.61
1:D:271:GLU:O	1:D:272:SER:HB3	2.00	0.61
1:A:109:VAL:HG22	1:C:357:GLU:HG2	1.83	0.61
1:B:236:SER:CB	1:B:237:PRO:CD	2.77	0.61
1:C:103:ALA:C	1:C:105:ALA:H	2.08	0.61
1:D:273:ARG:O	1:D:275:VAL:HG12	1.99	0.61
1:A:240:ASN:HD21	1:A:328:VAL:N	1.93	0.61
1:A:118:ALA:HB1	1:A:124:ALA:HA	1.83	0.61
1:B:198:MET:HE1	1:B:218:PRO:HA	1.83	0.61
1:C:300:LEU:HB2	1:C:345:ILE:HD11	1.83	0.61
1:D:198:MET:HE1	1:D:218:PRO:HA	1.83	0.61
1:B:34:PHE:HB2	1:B:190:VAL:HG22	1.81	0.61
1:B:273:ARG:O	1:B:275:VAL:HG12	2.00	0.61
1:A:312:ASN:HB2	1:B:288:GLU:HG2	1.83	0.61
1:B:89:HIS:NE2	1:B:90:LEU:HD13	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ALA:HA	1:C:28:GLU:CD	2.26	0.60
1:C:97:SER:CB	1:C:110:ILE:HD11	2.31	0.60
1:D:44:THR:HG22	1:D:48:MET:HE2	1.83	0.60
1:A:119:GLU:H	1:A:124:ALA:HB2	1.66	0.60
1:C:260:MET:C	1:C:262:ASN:N	2.56	0.60
1:D:155:PHE:HE1	1:D:185:ARG:HD3	1.65	0.60
1:B:2:ALA:HA	1:B:28:GLU:OE1	2.02	0.60
1:C:40:CYS:SG	1:C:42:LYS:HG3	2.42	0.60
1:C:42:LYS:HD2	1:C:190:VAL:HG13	1.82	0.60
1:C:108:GLU:HG3	1:C:109:VAL:N	2.16	0.60
1:A:166:ALA:H	1:B:192:HIS:CD2	2.19	0.60
1:D:2:ALA:HA	1:D:28:GLU:CD	2.26	0.60
1:B:2:ALA:N	1:B:186:THR:HB	2.17	0.60
1:B:240:ASN:ND2	1:B:328:VAL:H	1.94	0.60
1:B:105:ALA:HB3	1:B:110:ILE:HD11	1.83	0.60
1:C:98:PHE:O	1:C:99:GLY:C	2.44	0.60
1:C:273:ARG:O	1:C:275:VAL:HG12	2.02	0.60
1:C:292:PRO:O	1:C:293:SER:CB	2.48	0.60
1:A:273:ARG:O	1:A:275:VAL:HG12	2.02	0.59
1:A:296:ALA:HA	1:A:299:ILE:HD11	1.84	0.59
1:C:108:GLU:HG3	1:C:109:VAL:H	1.66	0.59
1:A:300:LEU:HB2	1:A:345:ILE:CD1	2.32	0.59
1:A:2:ALA:HA	1:A:28:GLU:CD	2.27	0.59
1:C:123:LEU:O	1:C:124:ALA:HB3	2.02	0.59
1:D:191:THR:HG22	1:D:192:HIS:N	2.17	0.59
1:B:120:VAL:HG13	1:B:175:GLU:HG3	1.84	0.59
1:A:26:ILE:HD13	1:A:188:ILE:HD11	1.84	0.59
1:C:312:ASN:HB2	1:D:288:GLU:HG2	1.83	0.59
1:B:138:GLN:O	1:B:142:VAL:HG23	2.02	0.59
1:B:300:LEU:HB3	1:B:320:ILE:CD1	2.32	0.59
1:B:292:PRO:O	1:B:293:SER:CB	2.48	0.59
1:D:240:ASN:ND2	1:D:328:VAL:H	1.93	0.59
1:C:41:GLY:HA2	3:C:403:ADP:O2A	2.02	0.59
1:C:44:THR:HG22	1:C:48:MET:HE2	1.84	0.59
1:C:198:MET:HE1	1:C:218:PRO:HA	1.84	0.59
1:B:6:LEU:CD2	1:B:22:ILE:HD11	2.33	0.58
1:B:155:PHE:HB2	1:B:187:MET:HG2	1.84	0.58
1:B:44:THR:HG22	1:B:48:MET:HE2	1.85	0.58
1:C:291:LEU:HB3	1:C:292:PRO:HD2	1.84	0.58
1:C:300:LEU:HB2	1:C:345:ILE:CD1	2.32	0.58
1:A:44:THR:HG22	1:A:48:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:HG11	1:B:144:ILE:HD13	1.85	0.58
1:A:98:PHE:HB2	1:A:146:ARG:HD2	1.84	0.58
1:B:191:THR:HG22	1:B:192:HIS:N	2.17	0.58
1:D:316:ILE:CG2	1:D:318:ILE:HD11	2.33	0.58
1:A:119:GLU:HB2	1:A:124:ALA:CB	2.33	0.58
1:B:144:ILE:HD11	1:B:160:PRO:CB	2.33	0.58
1:B:2:ALA:HA	1:B:28:GLU:CD	2.29	0.58
1:A:26:ILE:HD13	1:A:188:ILE:CD1	2.33	0.58
1:C:101:LYS:HB2	1:C:101:LYS:NZ	2.19	0.58
1:B:40:CYS:SG	1:B:42:LYS:HG3	2.44	0.58
1:B:67:MET:O	1:B:68:ASN:C	2.46	0.58
1:D:283:LEU:C	1:D:283:LEU:HD23	2.29	0.58
1:A:198:MET:HE1	1:A:218:PRO:HA	1.84	0.58
1:B:273:ARG:O	1:B:275:VAL:N	2.37	0.58
1:C:273:ARG:O	1:C:275:VAL:N	2.37	0.58
1:D:40:CYS:SG	1:D:42:LYS:HG3	2.43	0.58
1:A:119:GLU:HB2	1:A:124:ALA:HB2	1.85	0.57
1:B:89:HIS:CD2	1:B:90:LEU:HD13	2.39	0.57
1:C:253:GLN:HG2	1:C:267:TRP:HE3	1.69	0.57
1:B:86:LEU:O	1:B:88:PRO:HD3	2.04	0.57
1:B:148:LEU:HD13	1:B:179:LEU:HD11	1.85	0.57
1:C:92:VAL:HG23	1:C:129:ARG:O	2.04	0.57
1:B:35:VAL:HG23	1:B:204:ILE:HG23	1.86	0.57
1:B:100:LEU:HD23	1:B:110:ILE:HD13	1.87	0.57
1:B:253:GLN:HG2	1:B:267:TRP:HE3	1.69	0.57
1:C:9:VAL:HG13	1:C:55:ILE:HG23	1.85	0.57
1:A:100:LEU:HB3	1:A:110:ILE:HG22	1.85	0.57
1:C:191:THR:HG22	1:C:192:HIS:N	2.18	0.57
1:C:296:ALA:HA	1:C:299:ILE:HD11	1.85	0.57
1:D:291:LEU:HB3	1:D:292:PRO:HD2	1.87	0.57
1:A:150:ALA:HB3	1:A:152:PRO:HD3	1.86	0.57
1:B:240:ASN:HD21	1:B:328:VAL:N	1.95	0.57
1:C:89:HIS:CD2	1:C:90:LEU:HD13	2.40	0.57
1:D:9:VAL:HG13	1:D:55:ILE:HG23	1.86	0.57
1:C:106:LYS:C	1:C:108:GLU:H	2.10	0.57
1:B:86:LEU:HD12	1:B:131:PRO:HB3	1.87	0.57
1:B:323:ILE:HG22	1:B:325:GLN:HG2	1.87	0.57
1:C:107:LYS:HA	1:C:110:ILE:CG2	2.35	0.57
1:D:67:MET:O	1:D:68:ASN:C	2.48	0.56
1:A:98:PHE:CB	1:A:146:ARG:HD2	2.35	0.56
1:A:105:ALA:O	1:A:109:VAL:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:HB2	1:B:260:MET:HG2	1.87	0.56
1:B:350:GLU:CD	1:B:350:GLU:H	2.13	0.56
1:C:350:GLU:CD	1:C:350:GLU:H	2.13	0.56
1:A:67:MET:O	1:A:68:ASN:C	2.48	0.56
1:A:110:ILE:O	1:A:114:VAL:HG23	2.05	0.56
1:B:80:VAL:CG2	1:B:144:ILE:HD13	2.29	0.56
1:B:90:LEU:HG	1:B:94:GLU:HB3	1.88	0.56
1:B:100:LEU:CD2	1:B:110:ILE:HD13	2.35	0.56
1:B:315:GLN:HG2	1:B:330:ARG:HG2	1.87	0.56
1:C:2:ALA:N	1:C:186:THR:HG1	2.02	0.56
1:C:42:LYS:HB3	1:C:190:VAL:CG1	2.35	0.56
1:D:34:PHE:CD2	1:D:205:VAL:CG1	2.88	0.56
1:B:316:ILE:CG2	1:B:318:ILE:HD11	2.36	0.56
1:C:92:VAL:O	1:C:96:MET:HG3	2.06	0.56
1:A:120:VAL:HA	1:C:324:ARG:NH2	2.10	0.56
1:B:9:VAL:HG13	1:B:55:ILE:HG23	1.87	0.56
1:C:197:ALA:HB1	1:C:204:ILE:CD1	2.34	0.56
1:C:236:SER:CB	1:C:237:PRO:CD	2.78	0.56
1:D:324:ARG:CG	1:D:325:GLN:H	2.18	0.56
1:D:350:GLU:CD	1:D:350:GLU:H	2.12	0.56
1:A:40:CYS:SG	1:A:42:LYS:HG3	2.46	0.56
1:C:140:GLN:HE21	1:C:144:ILE:HG12	1.69	0.56
1:C:283:LEU:HD23	1:C:283:LEU:C	2.31	0.56
1:A:9:VAL:HG13	1:A:55:ILE:HG23	1.87	0.56
1:A:273:ARG:O	1:A:275:VAL:N	2.39	0.56
1:C:258:LEU:HB2	1:C:260:MET:HG2	1.88	0.55
1:A:130:LYS:HE3	1:A:130:LYS:H	1.70	0.55
1:B:35:VAL:HG12	1:B:233:PHE:HE2	1.70	0.55
1:B:283:LEU:C	1:B:283:LEU:HD23	2.31	0.55
1:C:315:GLN:HG2	1:C:330:ARG:HG2	1.89	0.55
1:A:253:GLN:HG2	1:A:267:TRP:HE3	1.70	0.55
1:D:273:ARG:O	1:D:275:VAL:N	2.39	0.55
1:A:197:ALA:HB1	1:A:204:ILE:CD1	2.33	0.55
1:C:157:LEU:N	1:C:157:LEU:CD1	2.69	0.55
1:C:252:ASP:HB3	1:C:365:LEU:HD13	1.89	0.55
1:D:300:LEU:HB3	1:D:320:ILE:HD11	1.89	0.55
1:B:32:VAL:HB	1:B:188:ILE:HD13	1.88	0.55
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.87	0.55
1:A:120:VAL:O	1:A:182:ARG:NH1	2.40	0.55
1:A:283:LEU:C	1:A:283:LEU:HD23	2.32	0.55
1:B:258:LEU:CB	1:B:260:MET:HG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ILE:O	1:C:22:ILE:HG12	2.07	0.55
1:A:315:GLN:HG2	1:A:330:ARG:HG2	1.89	0.55
1:C:67:MET:O	1:C:68:ASN:C	2.48	0.54
1:D:152:PRO:HG2	1:D:153:SER:N	2.15	0.54
1:D:240:ASN:HD21	1:D:328:VAL:N	1.95	0.54
1:D:300:LEU:HB3	1:D:320:ILE:CD1	2.36	0.54
1:A:130:LYS:C	1:A:132:LYS:H	2.14	0.54
1:A:148:LEU:HD13	1:A:183:LEU:HD21	1.89	0.54
1:B:131:PRO:O	1:B:139:ARG:HD3	2.07	0.54
1:B:260:MET:CE	1:B:300:LEU:HD22	2.38	0.54
1:D:236:SER:CB	1:D:237:PRO:CD	2.79	0.54
1:A:191:THR:HG22	1:A:192:HIS:N	2.19	0.54
1:C:79:MET:HE3	1:C:156:LEU:CB	2.35	0.54
1:C:110:ILE:O	1:C:114:VAL:HG12	2.08	0.54
1:C:121:LEU:O	1:C:122:GLN:HB2	2.07	0.54
1:C:36:GLY:O	1:C:192:HIS:HA	2.07	0.54
1:C:112:GLN:O	1:C:116:GLN:HG3	2.07	0.54
1:A:46:LEU:HB3	1:A:79:MET:CE	2.38	0.54
1:A:91:SER:HB3	1:A:94:GLU:HB2	1.89	0.54
1:A:120:VAL:O	1:A:182:ARG:CZ	2.56	0.54
1:B:35:VAL:HG12	1:B:233:PHE:CE2	2.43	0.54
1:B:252:ASP:HB3	1:B:365:LEU:HD13	1.89	0.54
1:C:134:LEU:HB2	1:C:139:ARG:NH1	2.23	0.54
1:A:258:LEU:HB2	1:A:260:MET:HG2	1.89	0.54
1:D:155:PHE:HB2	1:D:187:MET:HG2	1.88	0.54
1:B:148:LEU:HD22	1:B:179:LEU:HD11	1.89	0.54
1:C:258:LEU:CB	1:C:260:MET:HG2	2.38	0.54
1:A:252:ASP:HB3	1:A:365:LEU:HD13	1.89	0.54
1:A:350:GLU:H	1:A:350:GLU:CD	2.14	0.54
1:A:90:LEU:O	1:A:91:SER:HB3	2.08	0.53
1:A:98:PHE:H	1:A:146:ARG:HD2	1.73	0.53
1:A:291:LEU:HB3	1:A:292:PRO:HD2	1.89	0.53
1:B:123:LEU:O	1:B:126:LEU:HD12	2.08	0.53
1:D:34:PHE:HD2	1:D:205:VAL:HG13	1.72	0.53
1:D:323:ILE:CG2	1:D:325:GLN:NE2	2.71	0.53
1:A:114:VAL:HG12	1:A:127:LEU:HD11	1.90	0.53
1:B:140:GLN:OE1	1:B:140:GLN:HA	2.08	0.53
1:D:252:ASP:HB3	1:D:365:LEU:HD13	1.89	0.53
1:C:86:LEU:CD1	1:C:131:PRO:HB3	2.38	0.53
1:C:33:VAL:HB	1:C:204:ILE:CD1	2.37	0.53
1:D:221:LEU:HB3	1:D:234:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.23	0.53
1:D:315:GLN:HG2	1:D:330:ARG:HG2	1.90	0.53
1:B:304:VAL:HG22	1:B:318:ILE:CD1	2.38	0.53
1:D:34:PHE:CD2	1:D:205:VAL:HG11	2.44	0.53
1:C:26:ILE:N	1:C:26:ILE:HD12	2.24	0.53
1:C:324:ARG:HD3	1:C:324:ARG:N	2.19	0.53
1:D:48:MET:HB3	1:D:55:ILE:HD13	1.87	0.53
1:A:55:ILE:N	1:A:55:ILE:HD12	2.23	0.53
1:B:22:ILE:HD13	1:B:45:LEU:HD21	1.90	0.53
1:B:33:VAL:HG22	1:B:189:TYR:HB3	1.91	0.53
1:B:150:ALA:O	1:B:152:PRO:HD3	2.08	0.53
1:C:246:VAL:HG12	1:C:279:ALA:O	2.07	0.53
1:B:323:ILE:HG21	1:B:325:GLN:HE21	1.65	0.53
1:B:157:LEU:HD13	1:B:189:TYR:HD1	1.74	0.52
1:A:258:LEU:CB	1:A:260:MET:HG2	2.38	0.52
1:D:258:LEU:HB2	1:D:260:MET:HG2	1.90	0.52
1:D:260:MET:CE	1:D:300:LEU:HD22	2.39	0.52
1:A:120:VAL:CG1	1:C:324:ARG:NH2	2.68	0.52
1:A:295:ILE:HD12	1:A:295:ILE:N	2.24	0.52
1:C:149:VAL:C	1:C:151:GLU:H	2.17	0.52
1:A:22:ILE:O	1:A:22:ILE:HG12	2.05	0.52
1:C:255:GLN:HB2	1:C:267:TRP:CD2	2.45	0.52
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.75	0.52
1:A:316:ILE:HD12	1:A:316:ILE:N	2.24	0.52
1:C:37:PRO:O	1:C:38:SER:C	2.52	0.52
1:A:55:ILE:HD12	1:A:55:ILE:H	1.74	0.52
1:A:292:PRO:HG2	1:A:295:ILE:HD13	1.90	0.52
1:D:251:ILE:HD12	1:D:251:ILE:N	2.25	0.52
1:D:258:LEU:CB	1:D:260:MET:HG2	2.39	0.52
1:A:113:ARG:NE	1:C:357:GLU:OE2	2.42	0.52
1:B:255:GLN:HB2	1:B:267:TRP:CD2	2.45	0.52
1:C:137:GLY:CA	1:C:172:MET:HE1	2.40	0.52
1:D:46:LEU:HB3	1:D:79:MET:CE	2.39	0.52
1:A:135:SER:O	1:A:137:GLY:N	2.43	0.52
1:C:46:LEU:HB3	1:C:79:MET:CE	2.36	0.52
1:C:260:MET:CE	1:C:300:LEU:HD22	2.39	0.52
1:D:301:GLU:N	1:D:320:ILE:HD11	2.25	0.52
1:A:260:MET:CE	1:A:300:LEU:HD22	2.40	0.52
1:A:65:LYS:HD3	1:A:65:LYS:N	2.25	0.51
1:D:304:VAL:HG22	1:D:318:ILE:CD1	2.40	0.51
1:A:33:VAL:HG12	1:A:35:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:HG12	1:C:35:VAL:HG22	1.92	0.51
1:D:299:ILE:N	1:D:299:ILE:HD12	2.25	0.51
1:A:255:GLN:HB2	1:A:267:TRP:CD2	2.46	0.51
1:A:37:PRO:O	1:A:38:SER:C	2.53	0.51
1:A:251:ILE:HD12	1:A:251:ILE:N	2.25	0.51
1:B:35:VAL:CG1	1:B:233:PHE:HE2	2.24	0.51
1:B:191:THR:CG2	1:B:193:ASP:H	2.17	0.51
1:D:272:SER:O	1:D:273:ARG:O	2.29	0.51
1:A:154:VAL:HG13	1:A:186:THR:HG22	1.93	0.51
1:A:11:LYS:HD2	1:A:56:THR:HG23	1.93	0.51
1:B:307:VAL:HG13	1:B:316:ILE:HD13	1.91	0.51
1:C:33:VAL:HA	1:C:189:TYR:O	2.11	0.51
1:D:33:VAL:HG12	1:D:35:VAL:HG22	1.92	0.51
1:A:86:LEU:N	1:A:86:LEU:HD12	2.26	0.51
1:C:110:ILE:HG23	1:C:111:ASN:ND2	2.25	0.51
1:C:65:LYS:HD3	1:C:65:LYS:N	2.26	0.51
1:C:307:VAL:HG13	1:C:316:ILE:HD13	1.92	0.51
1:D:37:PRO:O	1:D:38:SER:C	2.53	0.51
1:A:33:VAL:HB	1:A:204:ILE:CD1	2.39	0.51
1:A:148:LEU:C	1:A:150:ALA:N	2.68	0.51
1:A:288:GLU:HG3	1:A:330:ARG:HD3	1.93	0.50
1:C:91:SER:O	1:C:95:ASN:HB2	2.11	0.50
1:D:34:PHE:HB2	1:D:190:VAL:HG22	1.91	0.50
1:D:307:VAL:HG13	1:D:316:ILE:HD13	1.93	0.50
1:B:37:PRO:O	1:B:38:SER:C	2.54	0.50
1:B:233:PHE:HB3	1:B:234:ILE:HD12	1.93	0.50
1:D:34:PHE:HD2	1:D:205:VAL:CG1	2.24	0.50
1:A:123:LEU:HD11	1:A:141:ARG:HB3	1.93	0.50
1:A:151:GLU:N	1:A:152:PRO:CD	2.74	0.50
1:B:35:VAL:CG2	1:B:204:ILE:HG23	2.40	0.50
1:B:323:ILE:HG21	1:B:325:GLN:NE2	2.24	0.50
1:C:191:THR:CG2	1:C:193:ASP:H	2.17	0.50
1:C:325:GLN:O	1:C:326:ASN:O	2.29	0.50
1:D:316:ILE:HG22	1:D:318:ILE:HD11	1.93	0.50
1:A:151:GLU:HG3	1:A:185:ARG:NH2	2.27	0.50
1:B:96:MET:HE2	1:B:114:VAL:HG13	1.92	0.50
1:D:11:LYS:HD2	1:D:56:THR:HG23	1.94	0.50
1:B:246:VAL:HG12	1:B:279:ALA:O	2.12	0.50
1:C:42:LYS:HB3	1:C:190:VAL:HG13	1.93	0.50
1:D:253:GLN:HG2	1:D:267:TRP:HE3	1.72	0.50
1:D:151:GLU:HB2	1:D:185:ARG:HH21	1.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:PHE:HE1	1:D:185:ARG:CD	2.23	0.50
1:D:255:GLN:HB2	1:D:267:TRP:CD2	2.47	0.50
1:A:148:LEU:C	1:A:150:ALA:H	2.20	0.50
1:B:95:ASN:HD22	1:B:146:ARG:HH21	1.58	0.50
1:D:22:ILE:O	1:D:22:ILE:HG12	2.09	0.50
1:A:90:LEU:HD12	1:A:131:PRO:HG3	1.93	0.49
1:A:133:ALA:O	1:A:135:SER:OG	2.21	0.49
1:A:325:GLN:O	1:A:326:ASN:CA	2.60	0.49
1:C:134:LEU:HA	1:C:138:GLN:NE2	2.27	0.49
1:C:120:VAL:HG12	1:C:121:LEU:N	2.26	0.49
1:C:123:LEU:HD21	1:C:142:VAL:HG22	1.94	0.49
1:B:29:GLY:O	1:B:180:HIS:CE1	2.65	0.49
1:A:246:VAL:HG12	1:A:279:ALA:O	2.11	0.49
1:B:42:LYS:HB3	1:B:190:VAL:CG1	2.42	0.49
1:B:271:GLU:HG2	1:B:273:ARG:HB2	1.95	0.49
1:C:140:GLN:NE2	1:C:144:ILE:HG12	2.27	0.49
1:D:65:LYS:HD3	1:D:65:LYS:N	2.26	0.49
1:D:198:MET:HE2	1:D:204:ILE:CD1	2.42	0.49
1:B:272:SER:O	1:B:273:ARG:O	2.31	0.49
1:B:288:GLU:HG3	1:B:330:ARG:HD3	1.95	0.49
1:C:146:ARG:HG2	1:C:146:ARG:NH1	2.25	0.49
1:C:6:LEU:HD11	1:C:49:ILE:CD1	2.42	0.49
1:C:240:ASN:HD21	1:C:328:VAL:N	1.94	0.49
1:A:90:LEU:O	1:A:91:SER:CB	2.61	0.49
1:B:65:LYS:N	1:B:65:LYS:HD3	2.27	0.49
1:C:288:GLU:HG2	1:D:312:ASN:HB2	1.95	0.49
1:D:272:SER:HA	1:D:275:VAL:HG11	1.95	0.49
1:A:191:THR:CG2	1:A:193:ASP:H	2.19	0.49
1:A:96:MET:HE1	1:A:117:VAL:HG23	1.95	0.49
1:C:271:GLU:HG2	1:C:273:ARG:HB2	1.94	0.49
1:C:293:SER:C	1:C:295:ILE:N	2.68	0.49
1:B:11:LYS:HD2	1:B:56:THR:HG23	1.94	0.48
1:D:198:MET:HE2	1:D:204:ILE:HD12	1.95	0.48
1:A:133:ALA:O	1:A:135:SER:N	2.47	0.48
1:A:146:ARG:O	1:A:149:VAL:HG22	2.14	0.48
1:B:234:ILE:HD12	1:B:234:ILE:N	2.29	0.48
1:B:293:SER:C	1:B:295:ILE:N	2.68	0.48
1:D:271:GLU:HG2	1:D:273:ARG:HB2	1.95	0.48
1:C:107:LYS:HA	1:C:110:ILE:HG21	1.95	0.48
1:A:318:ILE:HD12	1:A:318:ILE:N	2.28	0.48
1:C:45:LEU:CD1	1:C:207:LEU:HD11	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLU:OE1	1:C:263:ARG:HB3	2.13	0.48
1:C:318:ILE:HD12	1:C:318:ILE:N	2.29	0.48
1:D:34:PHE:CE2	1:D:205:VAL:HG11	2.49	0.48
1:B:71:PRO:HG2	1:B:74:GLU:CD	2.39	0.48
1:B:374:ALA:O	1:B:375:SER:CB	2.60	0.48
1:C:370:GLY:HA2	1:D:336:LEU:HD21	1.96	0.48
1:D:34:PHE:CD2	1:D:205:VAL:HG13	2.48	0.48
1:A:6:LEU:HD11	1:A:49:ILE:CD1	2.43	0.48
1:A:293:SER:C	1:A:295:ILE:N	2.68	0.48
1:B:33:VAL:HG12	1:B:35:VAL:HG22	1.95	0.48
1:B:257:GLU:OE1	1:B:263:ARG:HB3	2.14	0.48
1:B:320:ILE:HD12	1:B:327:LEU:HD22	1.96	0.48
1:B:46:LEU:HB3	1:B:79:MET:CE	2.39	0.48
1:B:324:ARG:CG	1:B:325:GLN:H	2.27	0.48
1:C:97:SER:O	1:C:98:PHE:CB	2.60	0.48
1:A:82:GLN:O	1:A:82:GLN:HG2	2.14	0.48
1:A:257:GLU:OE1	1:A:263:ARG:HB3	2.13	0.48
1:B:260:MET:O	1:B:263:ARG:N	2.35	0.48
1:C:117:VAL:HG21	1:C:149:VAL:HG22	1.96	0.48
1:A:32:VAL:HB	1:A:188:ILE:CD1	2.44	0.47
1:C:106:LYS:C	1:C:108:GLU:N	2.70	0.47
1:D:288:GLU:HG3	1:D:330:ARG:HD3	1.96	0.47
1:A:272:SER:O	1:A:273:ARG:O	2.32	0.47
1:D:257:GLU:OE1	1:D:263:ARG:HB3	2.14	0.47
1:B:6:LEU:HD11	1:B:49:ILE:CD1	2.44	0.47
1:D:325:GLN:O	1:D:326:ASN:CA	2.61	0.47
1:A:134:LEU:O	1:A:139:ARG:NE	2.47	0.47
1:A:192:HIS:CD2	1:B:165:ASP:HA	2.49	0.47
1:A:324:ARG:CG	1:A:325:GLN:H	2.26	0.47
1:B:42:LYS:HB3	1:B:190:VAL:HG13	1.95	0.47
1:D:172:MET:O	1:D:176:ILE:HG12	2.15	0.47
1:A:92:VAL:HB	1:A:127:LEU:O	2.15	0.47
1:B:316:ILE:HG22	1:B:318:ILE:HD11	1.96	0.47
1:C:6:LEU:HD11	1:C:49:ILE:HD11	1.95	0.47
1:C:323:ILE:HG22	1:C:325:GLN:CG	2.45	0.47
1:D:79:MET:HE3	1:D:156:LEU:HB3	1.96	0.47
1:A:71:PRO:HG2	1:A:74:GLU:CD	2.40	0.47
1:B:232:GLY:O	1:B:238:LYS:HE2	2.13	0.47
1:C:95:ASN:O	1:C:146:ARG:HD2	2.15	0.47
1:C:135:SER:OG	1:C:138:GLN:HG3	2.15	0.47
1:C:232:GLY:O	1:C:238:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD11	1:A:49:ILE:HD11	1.96	0.47
1:A:109:VAL:HG13	1:C:357:GLU:HG2	1.95	0.47
1:B:22:ILE:HD12	1:B:24:LEU:HD22	1.97	0.47
1:B:42:LYS:HD2	1:B:190:VAL:HG13	1.96	0.47
1:B:235:GLY:O	1:B:236:SER:C	2.57	0.47
1:C:107:LYS:HA	1:C:110:ILE:HG22	1.97	0.47
1:C:114:VAL:HG22	1:C:127:LEU:HD21	1.97	0.47
1:C:141:ARG:HG3	1:C:141:ARG:HH11	1.80	0.47
1:C:272:SER:HA	1:C:275:VAL:HG11	1.97	0.47
1:C:272:SER:O	1:C:273:ARG:O	2.32	0.47
1:C:288:GLU:HG3	1:C:330:ARG:HD3	1.96	0.47
1:A:108:GLU:OE1	1:A:108:GLU:N	2.47	0.47
1:C:80:VAL:HG21	1:C:144:ILE:HD13	1.97	0.47
1:C:103:ALA:O	1:C:105:ALA:N	2.46	0.47
1:A:194:GLN:HB2	1:A:234:ILE:HD13	1.96	0.47
1:B:2:ALA:N	1:B:186:THR:CB	2.78	0.47
1:B:272:SER:HA	1:B:275:VAL:HG11	1.96	0.47
1:D:246:VAL:HG12	1:D:279:ALA:O	2.14	0.47
1:A:118:ALA:C	1:A:120:VAL:N	2.72	0.47
1:A:271:GLU:HG2	1:A:273:ARG:HB2	1.96	0.47
1:C:288:GLU:H	1:C:288:GLU:CD	2.22	0.47
1:C:367:LYS:HD2	1:C:373:SER:OG	2.15	0.47
1:B:79:MET:HE3	1:B:156:LEU:HB3	1.97	0.46
1:C:71:PRO:HG2	1:C:74:GLU:CD	2.40	0.46
1:C:134:LEU:HB2	1:C:139:ARG:HD3	1.96	0.46
1:C:172:MET:O	1:C:176:ILE:HG12	2.15	0.46
1:C:247:THR:O	1:C:248:ALA:HB2	2.15	0.46
1:B:288:GLU:CD	1:B:288:GLU:H	2.23	0.46
1:C:30:GLU:OE1	1:C:203:LYS:HE3	2.15	0.46
1:D:221:LEU:HB3	1:D:234:ILE:CD1	2.45	0.46
1:A:2:ALA:HB2	1:A:153:SER:HB2	1.93	0.46
1:C:86:LEU:HD13	1:C:131:PRO:HB3	1.97	0.46
1:D:293:SER:C	1:D:295:ILE:N	2.68	0.46
1:A:192:HIS:CD2	1:B:166:ALA:H	2.33	0.46
1:B:22:ILE:O	1:B:22:ILE:HG13	2.13	0.46
1:B:106:LYS:HB2	1:B:109:VAL:HG23	1.97	0.46
1:B:144:ILE:HD11	1:B:160:PRO:HB3	1.97	0.46
1:C:79:MET:HG3	1:C:156:LEU:O	2.15	0.46
1:A:172:MET:O	1:A:176:ILE:HG12	2.15	0.46
1:B:198:MET:HE2	1:B:204:ILE:CD1	2.45	0.46
1:D:71:PRO:HG2	1:D:74:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLY:O	1:A:236:SER:C	2.59	0.46
1:B:131:PRO:C	1:B:133:ALA:H	2.24	0.46
1:B:6:LEU:HD11	1:B:49:ILE:HD11	1.96	0.46
1:C:101:LYS:NZ	1:C:101:LYS:CB	2.79	0.46
1:A:241:PHE:C	1:A:242:LEU:HD23	2.41	0.46
1:A:272:SER:HA	1:A:275:VAL:HG11	1.97	0.46
1:B:45:LEU:HD12	1:B:207:LEU:HD11	1.98	0.46
1:B:88:PRO:HA	1:B:131:PRO:HG3	1.97	0.46
1:C:64:GLU:C	1:C:65:LYS:HD3	2.41	0.46
1:C:103:ALA:C	1:C:105:ALA:N	2.74	0.46
1:D:197:ALA:HB1	1:D:204:ILE:HD13	1.97	0.46
1:A:64:GLU:C	1:A:65:LYS:HD3	2.40	0.46
1:D:64:GLU:C	1:D:65:LYS:HD3	2.41	0.46
1:D:288:GLU:CD	1:D:288:GLU:H	2.24	0.46
1:A:96:MET:CE	1:A:117:VAL:HG23	2.46	0.45
1:A:258:LEU:C	1:A:260:MET:H	2.23	0.45
1:B:86:LEU:HB3	1:B:95:ASN:ND2	2.30	0.45
1:B:258:LEU:C	1:B:260:MET:H	2.25	0.45
1:D:155:PHE:N	1:D:186:THR:O	2.42	0.45
1:B:122:GLN:HB2	1:B:141:ARG:HH21	1.81	0.45
1:C:241:PHE:C	1:C:242:LEU:HD23	2.42	0.45
1:A:137:GLY:O	1:A:141:ARG:HD3	2.17	0.45
1:B:241:PHE:C	1:B:242:LEU:HD23	2.40	0.45
1:C:179:LEU:C	1:C:179:LEU:HD23	2.41	0.45
1:D:300:LEU:C	1:D:320:ILE:HD11	2.40	0.45
1:A:129:ARG:HH11	1:A:129:ARG:HG2	1.80	0.45
1:B:34:PHE:HD2	1:B:205:VAL:HG13	1.82	0.45
1:B:323:ILE:HD12	1:B:324:ARG:HH11	1.75	0.45
1:C:138:GLN:O	1:C:139:ARG:C	2.58	0.45
1:C:194:GLN:HB2	1:C:234:ILE:HD13	1.97	0.45
1:D:198:MET:CE	1:D:204:ILE:HD12	2.46	0.45
1:C:42:LYS:HB3	1:C:190:VAL:HG11	1.99	0.45
1:C:318:ILE:O	1:C:326:ASN:HA	2.16	0.45
1:B:100:LEU:HG	1:B:110:ILE:HD13	1.98	0.45
1:D:323:ILE:HG22	1:D:325:GLN:NE2	2.29	0.45
1:B:173:ARG:NE	1:B:196:GLU:HG2	2.32	0.45
1:B:320:ILE:CD1	1:B:327:LEU:HD22	2.47	0.45
1:D:179:LEU:C	1:D:179:LEU:HD23	2.42	0.45
1:A:288:GLU:CD	1:A:288:GLU:H	2.24	0.45
1:C:134:LEU:HB2	1:C:139:ARG:HH11	1.80	0.45
1:A:76:GLY:O	1:A:153:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLY:O	1:B:180:HIS:HE1	1.98	0.45
1:C:34:PHE:HD2	1:C:205:VAL:HG13	1.82	0.45
1:D:191:THR:CG2	1:D:193:ASP:H	2.16	0.45
1:D:258:LEU:C	1:D:260:MET:H	2.25	0.45
1:A:42:LYS:HB3	1:A:190:VAL:CG1	2.47	0.45
1:A:109:VAL:HG13	1:C:357:GLU:CG	2.47	0.45
1:A:333:ASP:CG	1:A:334:VAL:H	2.25	0.45
1:C:96:MET:HE3	1:C:145:GLY:CA	2.42	0.45
1:B:64:GLU:C	1:B:65:LYS:HD3	2.42	0.44
1:A:268:LEU:O	1:A:270:VAL:N	2.49	0.44
1:B:2:ALA:O	1:B:3:SER:HB3	2.17	0.44
1:B:179:LEU:C	1:B:179:LEU:HD23	2.41	0.44
1:C:173:ARG:NE	1:C:196:GLU:HG2	2.32	0.44
1:D:268:LEU:O	1:D:270:VAL:N	2.49	0.44
1:D:316:ILE:HG21	1:D:318:ILE:HD11	2.00	0.44
1:A:90:LEU:HD12	1:A:131:PRO:HG2	1.99	0.44
1:B:325:GLN:C	1:B:326:ASN:CB	2.87	0.44
1:C:135:SER:O	1:C:136:GLY:C	2.58	0.44
1:C:155:PHE:CD1	1:C:155:PHE:N	2.84	0.44
1:D:241:PHE:C	1:D:242:LEU:HD23	2.43	0.44
1:D:301:GLU:O	1:D:320:ILE:CD1	2.60	0.44
1:B:71:PRO:HA	1:B:72:PRO:HD3	1.87	0.44
1:C:141:ARG:O	1:C:145:GLY:N	2.48	0.44
1:C:258:LEU:C	1:C:260:MET:H	2.24	0.44
1:C:374:ALA:O	1:C:375:SER:CB	2.65	0.44
1:A:179:LEU:C	1:A:179:LEU:HD23	2.43	0.44
1:B:198:MET:HE2	1:B:198:MET:HA	1.99	0.44
1:B:247:THR:O	1:B:248:ALA:HB2	2.18	0.44
1:C:87:TYR:HA	1:C:88:PRO:HD3	1.61	0.44
1:C:140:GLN:HE21	1:C:144:ILE:CG1	2.31	0.44
1:C:237:PRO:HD2	1:C:330:ARG:HH11	1.83	0.44
1:D:25:ASP:O	1:D:203:LYS:NZ	2.50	0.44
1:D:333:ASP:CG	1:D:334:VAL:H	2.26	0.44
1:A:117:VAL:HG21	1:A:149:VAL:CG1	2.48	0.44
1:C:89:HIS:NE2	1:C:90:LEU:HD13	2.32	0.44
1:A:94:GLU:C	1:A:95:ASN:O	2.58	0.44
1:B:27:HIS:O	1:B:30:GLU:HB2	2.18	0.44
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.80	0.44
1:D:198:MET:HE2	1:D:198:MET:HA	2.00	0.44
1:B:12:ALA:H	1:B:56:THR:CG2	2.29	0.43
1:B:100:LEU:HG	1:B:110:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HD11	1:B:160:PRO:HB2	1.99	0.43
1:C:2:ALA:O	1:C:3:SER:HB3	2.18	0.43
1:C:135:SER:H	1:C:138:GLN:NE2	2.16	0.43
1:D:2:ALA:O	1:D:3:SER:HB3	2.18	0.43
1:D:345:ILE:N	1:D:345:ILE:CD1	2.78	0.43
1:A:95:ASN:C	1:A:97:SER:N	2.75	0.43
1:C:37:PRO:HD3	1:C:233:PHE:CE1	2.53	0.43
1:D:323:ILE:HD12	1:D:323:ILE:N	2.33	0.43
1:A:12:ALA:H	1:A:56:THR:CG2	2.31	0.43
1:A:46:LEU:HD13	1:A:79:MET:CE	2.48	0.43
1:A:154:VAL:HG12	1:A:155:PHE:N	2.33	0.43
1:C:20:LYS:O	1:C:21:ASP:C	2.62	0.43
1:C:333:ASP:CG	1:C:334:VAL:H	2.26	0.43
1:A:33:VAL:HA	1:A:189:TYR:O	2.18	0.43
1:A:79:MET:HG2	1:A:81:PHE:CE2	2.52	0.43
1:B:34:PHE:CD2	1:B:205:VAL:HG13	2.52	0.43
1:B:34:PHE:CD2	1:B:205:VAL:CG1	3.01	0.43
1:C:108:GLU:HG3	1:C:109:VAL:HG23	2.01	0.43
1:A:20:LYS:HE2	1:A:209:ALA:O	2.18	0.43
1:A:34:PHE:HD2	1:A:205:VAL:HG13	1.84	0.43
1:A:356:ARG:HB2	1:A:358:ASP:OD1	2.18	0.43
1:B:134:LEU:CA	1:B:139:ARG:HH12	2.31	0.43
1:A:32:VAL:HB	1:A:188:ILE:HD13	2.00	0.43
1:A:323:ILE:N	1:A:323:ILE:HD12	2.33	0.43
1:B:83:SER:HA	1:B:163:ASN:OD1	2.19	0.43
1:C:108:GLU:CG	1:C:109:VAL:H	2.31	0.43
1:A:11:LYS:HB2	1:A:48:MET:SD	2.59	0.43
1:A:39:GLY:HA2	3:A:401:ADP:O3B	2.19	0.43
1:C:112:GLN:HA	1:C:112:GLN:OE1	2.18	0.43
1:A:93:ALA:HB2	1:A:127:LEU:HG	2.00	0.42
1:A:106:LYS:O	1:A:110:ILE:HG23	2.19	0.42
1:A:163:ASN:N	1:A:163:ASN:ND2	2.66	0.42
1:B:62:ILE:CD1	1:B:67:MET:HG3	2.47	0.42
1:A:325:GLN:C	1:A:326:ASN:CB	2.87	0.42
1:B:100:LEU:CG	1:B:110:ILE:HD13	2.48	0.42
1:D:260:MET:O	1:D:263:ARG:N	2.35	0.42
1:A:173:ARG:NE	1:A:196:GLU:HG2	2.34	0.42
1:B:63:GLY:O	1:B:64:GLU:HG2	2.20	0.42
1:B:333:ASP:CG	1:B:334:VAL:H	2.26	0.42
1:C:85:ALA:C	1:C:86:LEU:CA	2.85	0.42
1:A:119:GLU:CA	1:A:124:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:O	1:A:248:ALA:HB2	2.18	0.42
1:C:27:HIS:O	1:C:30:GLU:HB2	2.20	0.42
1:D:12:ALA:H	1:D:56:THR:CG2	2.30	0.42
1:D:175:GLU:OE1	1:D:175:GLU:HA	2.20	0.42
1:A:130:LYS:C	1:A:132:LYS:N	2.78	0.42
1:C:120:VAL:HG12	1:C:121:LEU:HD23	2.00	0.42
1:D:27:HIS:O	1:D:30:GLU:HB2	2.19	0.42
1:D:173:ARG:NE	1:D:196:GLU:HG2	2.34	0.42
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.87	0.42
1:B:2:ALA:HB2	1:B:153:SER:HB2	2.02	0.42
1:B:157:LEU:HD13	1:B:189:TYR:CD1	2.53	0.42
1:C:227:ASP:HB2	1:C:359:GLY:O	2.20	0.42
1:A:148:LEU:O	1:A:150:ALA:N	2.53	0.42
1:A:288:GLU:HG2	1:B:312:ASN:CB	2.47	0.42
1:B:198:MET:CE	1:B:204:ILE:HD12	2.49	0.42
1:A:76:GLY:O	1:A:153:SER:OG	2.30	0.42
1:A:137:GLY:O	1:A:140:GLN:HB3	2.19	0.42
1:A:324:ARG:HG2	1:A:325:GLN:H	1.85	0.42
1:C:107:LYS:C	1:C:110:ILE:HG22	2.44	0.42
1:D:316:ILE:HG22	1:D:318:ILE:CD1	2.48	0.42
1:A:27:HIS:O	1:A:30:GLU:HB2	2.20	0.42
1:B:107:LYS:HG2	1:B:111:ASN:OD1	2.19	0.42
1:A:20:LYS:O	1:A:21:ASP:C	2.62	0.42
1:A:117:VAL:O	1:A:121:LEU:HB2	2.19	0.42
1:B:304:VAL:HA	1:B:318:ILE:HD13	2.01	0.42
1:C:108:GLU:CG	1:C:109:VAL:N	2.82	0.42
1:C:110:ILE:HG23	1:C:111:ASN:N	2.35	0.42
1:C:117:VAL:HG21	1:C:149:VAL:CG2	2.50	0.42
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.86	0.42
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.93	0.42
1:C:356:ARG:HB2	1:C:358:ASP:OD1	2.19	0.41
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.34	0.41
1:A:320:ILE:O	1:A:320:ILE:HG22	2.21	0.41
1:B:300:LEU:HD13	1:B:320:ILE:HD13	2.01	0.41
1:B:316:ILE:HG22	1:B:318:ILE:CD1	2.51	0.41
1:B:324:ARG:HG2	1:B:325:GLN:H	1.85	0.41
1:C:107:LYS:O	1:C:111:ASN:OD1	2.38	0.41
1:D:247:THR:O	1:D:248:ALA:HB2	2.19	0.41
1:A:2:ALA:O	1:A:3:SER:HB3	2.20	0.41
1:A:175:GLU:OE1	1:A:175:GLU:HA	2.20	0.41
1:B:20:LYS:O	1:B:21:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD13	1:B:79:MET:CE	2.49	0.41
1:B:325:GLN:O	1:B:326:ASN:CA	2.68	0.41
1:C:42:LYS:CD	1:C:191:THR:O	2.68	0.41
1:C:103:ALA:HB2	1:C:110:ILE:HD13	2.01	0.41
1:C:109:VAL:HG13	1:C:113:ARG:NH1	2.36	0.41
1:C:163:ASN:ND2	1:C:163:ASN:N	2.67	0.41
1:C:323:ILE:O	1:C:324:ARG:O	2.38	0.41
1:A:84:TYR:O	1:A:84:TYR:CD2	2.73	0.41
1:A:90:LEU:CB	1:A:131:PRO:HD2	2.37	0.41
1:B:356:ARG:HB2	1:B:358:ASP:OD1	2.20	0.41
1:C:46:LEU:HD13	1:C:79:MET:CE	2.50	0.41
1:C:92:VAL:HB	1:C:127:LEU:HA	2.02	0.41
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.86	0.41
1:B:198:MET:HE2	1:B:204:ILE:HD12	2.01	0.41
1:B:291:LEU:HD11	1:B:348:PRO:HB3	2.02	0.41
1:A:62:ILE:HB	1:A:67:MET:HG3	2.03	0.41
1:A:309:GLN:O	1:A:310:LEU:HD23	2.21	0.41
1:B:316:ILE:HG21	1:B:318:ILE:HD11	2.01	0.41
1:B:362:CYS:O	1:B:363:ARG:C	2.64	0.41
1:C:63:GLY:O	1:C:64:GLU:HG2	2.20	0.41
1:C:93:ALA:HB2	1:C:127:LEU:HB3	2.03	0.41
1:A:45:LEU:HD12	1:A:207:LEU:HD11	2.02	0.41
1:B:163:ASN:N	1:B:163:ASN:ND2	2.68	0.41
1:B:324:ARG:O	1:B:325:GLN:HB2	2.19	0.41
1:D:9:VAL:CB	1:D:22:ILE:HD13	2.47	0.41
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.87	0.41
1:A:155:PHE:CB	1:A:187:MET:HG2	2.44	0.41
1:A:237:PRO:HD2	1:A:330:ARG:HH11	1.86	0.41
1:C:34:PHE:CD2	1:C:205:VAL:HG13	2.56	0.41
1:C:109:VAL:O	1:C:110:ILE:C	2.64	0.41
1:C:362:CYS:O	1:C:363:ARG:C	2.64	0.41
1:D:46:LEU:HD13	1:D:79:MET:CE	2.51	0.41
1:D:291:LEU:HD11	1:D:348:PRO:HB3	2.02	0.41
1:A:34:PHE:CD2	1:A:205:VAL:CG1	3.03	0.41
1:C:198:MET:HE2	1:C:198:MET:HA	2.02	0.41
1:D:34:PHE:HA	1:D:205:VAL:HG13	2.04	0.41
1:D:304:VAL:HA	1:D:318:ILE:HD13	2.03	0.41
1:A:41:GLY:HA2	3:A:401:ADP:O2A	2.22	0.40
1:A:362:CYS:O	1:A:363:ARG:C	2.64	0.40
1:B:88:PRO:HA	1:B:131:PRO:CG	2.51	0.40
1:C:92:VAL:HG13	1:C:142:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LYS:O	1:D:21:ASP:C	2.64	0.40
1:A:62:ILE:CD1	1:A:67:MET:HG3	2.44	0.40
1:B:135:SER:CB	1:B:138:GLN:HE21	2.35	0.40
1:D:45:LEU:HD12	1:D:207:LEU:HD11	2.03	0.40
1:B:290:LEU:HD23	1:B:290:LEU:HA	1.92	0.40
1:C:36:GLY:HA3	1:C:40:CYS:SG	2.62	0.40
1:B:198:MET:HE1	1:B:218:PRO:CA	2.51	0.40
1:C:60:LEU:HD12	1:C:61:PHE:H	1.85	0.40
1:C:71:PRO:HA	1:C:72:PRO:HD3	1.87	0.40
1:A:34:PHE:CD2	1:A:205:VAL:HG13	2.57	0.40
1:A:130:LYS:N	1:A:130:LYS:CD	2.85	0.40
1:A:145:GLY:O	1:A:149:VAL:HG13	2.22	0.40
1:A:201:ALA:HB3	1:A:204:ILE:HD11	2.03	0.40
1:A:322:SER:O	1:A:323:ILE:HB	2.21	0.40
1:B:46:LEU:HD22	1:B:156:LEU:HB3	2.02	0.40
1:B:84:TYR:HB3	1:B:143:ALA:CB	2.51	0.40
1:C:86:LEU:HD12	1:C:131:PRO:HB3	2.03	0.40
1:C:104:GLY:O	1:C:105:ALA:HB2	2.22	0.40
1:C:175:GLU:OE1	1:C:175:GLU:HA	2.21	0.40
1:C:268:LEU:O	1:C:270:VAL:N	2.52	0.40
1:D:11:LYS:HB2	1:D:48:MET:SD	2.62	0.40
1:D:237:PRO:HD2	1:D:330:ARG:HH11	1.85	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CE2	1:B:374:ALA:CB[1_655]	1.76	0.44
1:A:61:PHE:CZ	1:B:374:ALA:CB[1_655]	1.86	0.34
1:B:102:LEU:CD2	1:D:367:LYS:NZ[1_545]	2.04	0.16
1:C:374:ALA:CB	1:D:61:PHE:CE2[1_655]	2.17	0.03

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	370/381 (97%)	309 (84%)	35 (10%)	26 (7%)	1	2
1	B	372/381 (98%)	319 (86%)	29 (8%)	24 (6%)	1	3
1	C	357/381 (94%)	297 (83%)	34 (10%)	26 (7%)	1	2
1	D	293/381 (77%)	256 (87%)	19 (6%)	18 (6%)	1	3
All	All	1392/1524 (91%)	1181 (85%)	117 (8%)	94 (7%)	1	2

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	121	LEU
1	A	134	LEU
1	A	136	GLY
1	A	273	ARG
1	A	274	ASP
1	A	296	ALA
1	A	324	ARG
1	A	326	ASN
1	B	38	SER
1	B	82	GLN
1	B	96	MET
1	B	120	VAL
1	B	236	SER
1	B	273	ARG
1	B	274	ASP
1	B	296	ALA
1	B	324	ARG
1	B	326	ASN
1	C	38	SER
1	C	86	LEU
1	C	98	PHE
1	C	99	GLY
1	C	236	SER
1	C	273	ARG
1	C	274	ASP
1	C	296	ALA
1	C	324	ARG
1	D	38	SER
1	D	152	PRO

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Mol	Chain	Res	Type
1	D	153	SER
1	D	273	ARG
1	D	274	ASP
1	D	296	ALA
1	D	324	ARG
1	D	326	ASN
1	A	82	GLN
1	A	135	SER
1	A	182	ARG
1	A	236	SER
1	A	293	SER
1	B	104	GLY
1	B	134	LEU
1	B	136	GLY
1	B	182	ARG
1	B	293	SER
1	C	150	ALA
1	C	182	ARG
1	C	293	SER
1	C	326	ASN
1	D	182	ARG
1	D	236	SER
1	D	293	SER
1	A	90	LEU
1	A	91	SER
1	A	95	ASN
1	A	104	GLY
1	A	271	GLU
1	A	322	SER
1	B	129	ARG
1	B	271	GLU
1	B	322	SER
1	C	105	ALA
1	C	131	PRO
1	C	271	GLU
1	C	297	ASP
1	C	322	SER
1	D	271	GLU
1	D	322	SER
1	A	297	ASP
1	A	323	ILE
1	B	297	ASP

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Mol	Chain	Res	Type
1	B	323	ILE
1	C	120	VAL
1	C	125	HIS
1	C	152	PRO
1	C	323	ILE
1	D	297	ASP
1	D	323	ILE
1	A	3	SER
1	A	151	GLU
1	B	3	SER
1	C	3	SER
1	C	101	LYS
1	C	298	VAL
1	D	3	SER
1	D	64	GLU
1	A	64	GLU
1	A	298	VAL
1	B	64	GLU
1	B	298	VAL
1	C	64	GLU
1	D	298	VAL
1	B	151	GLU

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	315/323 (98%)	289 (92%)	26 (8%)	10	32
1	B	316/323 (98%)	288 (91%)	28 (9%)	9	29
1	C	307/323 (95%)	283 (92%)	24 (8%)	11	35
1	D	256/323 (79%)	235 (92%)	21 (8%)	10	33
All	All	1194/1292 (92%)	1095 (92%)	99 (8%)	10	32

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	22	ILE
1	A	24	LEU
1	A	35	VAL
1	A	57	SER
1	A	65	LYS
1	A	84	TYR
1	A	90	LEU
1	A	107	LYS
1	A	115	ASN
1	A	130	LYS
1	A	151	GLU
1	A	157	LEU
1	A	168	LEU
1	A	175	GLU
1	A	205	VAL
1	A	228	ARG
1	A	246	VAL
1	A	275	VAL
1	A	288	GLU
1	A	320	ILE
1	A	324	ARG
1	A	326	ASN
1	A	347	LEU
1	A	350	GLU
1	A	351	ARG
1	B	16	VAL
1	B	22	ILE
1	B	24	LEU
1	B	35	VAL
1	B	57	SER
1	B	65	LYS
1	B	80	VAL
1	B	90	LEU
1	B	95	ASN
1	B	116	GLN
1	B	120	VAL
1	B	126	LEU
1	B	157	LEU
1	B	168	LEU
1	B	175	GLU
1	B	205	VAL
1	B	228	ARG

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Mol	Chain	Res	Type
1	B	246	VAL
1	B	275	VAL
1	B	288	GLU
1	B	320	ILE
1	B	323	ILE
1	B	324	ARG
1	B	326	ASN
1	B	345	ILE
1	B	347	LEU
1	B	350	GLU
1	B	351	ARG
1	C	22	ILE
1	C	24	LEU
1	C	35	VAL
1	C	57	SER
1	C	65	LYS
1	C	80	VAL
1	C	97	SER
1	C	98	PHE
1	C	101	LYS
1	C	120	VAL
1	C	123	LEU
1	C	132	LYS
1	C	168	LEU
1	C	175	GLU
1	C	205	VAL
1	C	228	ARG
1	C	246	VAL
1	C	275	VAL
1	C	288	GLU
1	C	320	ILE
1	C	324	ARG
1	C	347	LEU
1	C	350	GLU
1	C	351	ARG
1	D	16	VAL
1	D	22	ILE
1	D	24	LEU
1	D	35	VAL
1	D	57	SER
1	D	65	LYS
1	D	154	VAL

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Mol	Chain	Res	Type
1	D	168	LEU
1	D	175	GLU
1	D	205	VAL
1	D	228	ARG
1	D	246	VAL
1	D	275	VAL
1	D	288	GLU
1	D	320	ILE
1	D	324	ARG
1	D	326	ASN
1	D	345	ILE
1	D	347	LEU
1	D	350	GLU
1	D	351	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	111	ASN
1	A	112	GLN
1	A	115	ASN
1	A	116	GLN
1	A	122	GLN
1	A	140	GLN
1	A	163	ASN
1	A	171	GLN
1	A	192	HIS
1	A	240	ASN
1	A	255	GLN
1	A	264	GLN
1	A	265	GLN
1	A	305	GLN
1	A	319	GLN
1	A	325	GLN
1	A	331	GLN
1	A	353	HIS
1	B	82	GLN
1	B	95	ASN
1	B	115	ASN
1	B	116	GLN
1	B	138	GLN

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Mol	Chain	Res	Type
1	B	171	GLN
1	B	180	HIS
1	B	192	HIS
1	B	223	HIS
1	B	240	ASN
1	B	255	GLN
1	B	264	GLN
1	B	265	GLN
1	B	305	GLN
1	B	319	GLN
1	B	325	GLN
1	B	331	GLN
1	C	95	ASN
1	C	111	ASN
1	C	115	ASN
1	C	116	GLN
1	C	138	GLN
1	C	140	GLN
1	C	163	ASN
1	C	171	GLN
1	C	223	HIS
1	C	240	ASN
1	C	255	GLN
1	C	305	GLN
1	C	319	GLN
1	C	331	GLN
1	C	353	HIS
1	D	171	GLN
1	D	240	ASN
1	D	255	GLN
1	D	264	GLN
1	D	305	GLN
1	D	325	GLN
1	D	331	GLN
1	D	353	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ADP	B	402	2	28,29,29	1.34	6 (21%)	43,45,45	1.96	9 (20%)
3	ADP	C	403	-	28,29,29	1.23	3 (10%)	43,45,45	1.85	6 (13%)
3	ADP	A	401	2	28,29,29	1.30	2 (7%)	43,45,45	1.93	8 (18%)
3	ADP	D	404	2	28,29,29	1.22	3 (10%)	43,45,45	1.83	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	402	2	-	2/16/32/32	0/3/3/3
3	ADP	C	403	-	-	3/16/32/32	0/3/3/3
3	ADP	A	401	2	-	3/16/32/32	0/3/3/3
3	ADP	D	404	2	-	2/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C2-N1	3.37	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	ADP	C2-N1	3.30	1.39	1.33
3	D	404	ADP	C2-N1	3.12	1.39	1.33
3	B	402	ADP	C2-N1	2.98	1.39	1.33
3	A	401	ADP	PA-O3A	-2.76	1.56	1.59
3	B	402	ADP	PA-O3A	-2.71	1.56	1.59
3	D	404	ADP	C6-N6	-2.36	1.28	1.34
3	B	402	ADP	C1'-N9	2.32	1.52	1.46
3	B	402	ADP	C8-N7	2.26	1.36	1.31
3	C	403	ADP	C1'-N9	2.25	1.52	1.46
3	B	402	ADP	PB-O3B	-2.25	1.46	1.54
3	C	403	ADP	C6-N6	-2.11	1.28	1.34
3	B	402	ADP	C6-N6	-2.11	1.28	1.34
3	D	404	ADP	C1'-N9	2.00	1.51	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	O5'-PA-O1A	-8.37	75.78	108.94
3	C	403	ADP	O5'-PA-O1A	-8.25	76.22	108.94
3	B	402	ADP	O5'-PA-O1A	-8.04	77.05	108.94
3	D	404	ADP	O5'-PA-O1A	-7.78	78.09	108.94
3	B	402	ADP	O2A-PA-O5'	-4.16	88.71	107.57
3	B	402	ADP	O2A-PA-O1A	3.72	129.73	112.44
3	C	403	ADP	O2A-PA-O5'	-3.71	90.74	107.57
3	D	404	ADP	O2A-PA-O5'	-3.70	90.82	107.57
3	C	403	ADP	N3-C2-N1	-3.66	123.04	128.58
3	A	401	ADP	O2A-PA-O5'	-3.56	91.42	107.57
3	A	401	ADP	N3-C2-N1	-3.55	123.21	128.58
3	A	401	ADP	O2A-PA-O1A	3.51	128.77	112.44
3	D	404	ADP	N3-C2-N1	-3.41	123.43	128.58
3	B	402	ADP	N3-C2-N1	-3.33	123.55	128.58
3	C	403	ADP	O2A-PA-O1A	3.23	127.46	112.44
3	D	404	ADP	O2A-PA-O3A	3.10	115.66	107.27
3	C	403	ADP	C2-N1-C6	2.97	123.61	118.73
3	B	402	ADP	O2A-PA-O3A	2.94	115.23	107.27
3	A	401	ADP	C2-N1-C6	2.93	123.55	118.73
3	D	404	ADP	O2A-PA-O1A	2.92	126.05	112.44
3	D	404	ADP	C2-N1-C6	2.89	123.48	118.73
3	B	402	ADP	C2-N1-C6	2.84	123.39	118.73
3	B	402	ADP	O4'-C1'-N9	2.80	113.46	108.09
3	A	401	ADP	C3'-C2'-C1'	2.65	106.48	101.46
3	C	403	ADP	O2A-PA-O3A	2.59	114.27	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	O2A-PA-O3A	2.37	113.67	107.27
3	B	402	ADP	C3'-C2'-C1'	2.34	105.89	101.46
3	A	401	ADP	O5'-C5'-C4'	2.26	116.70	108.99
3	D	404	ADP	O5'-C5'-C4'	2.26	116.68	108.99
3	B	402	ADP	O5'-C5'-C4'	2.24	116.61	108.99
3	D	404	ADP	C3'-C2'-C1'	2.22	105.67	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

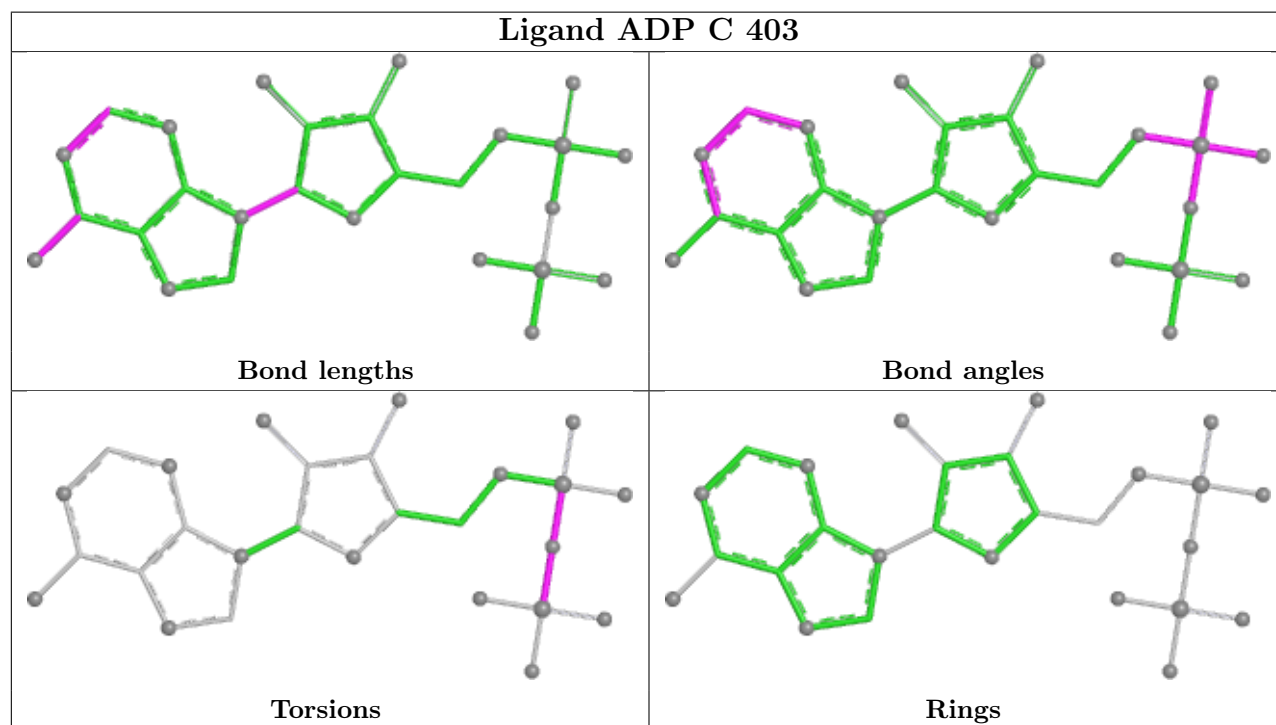
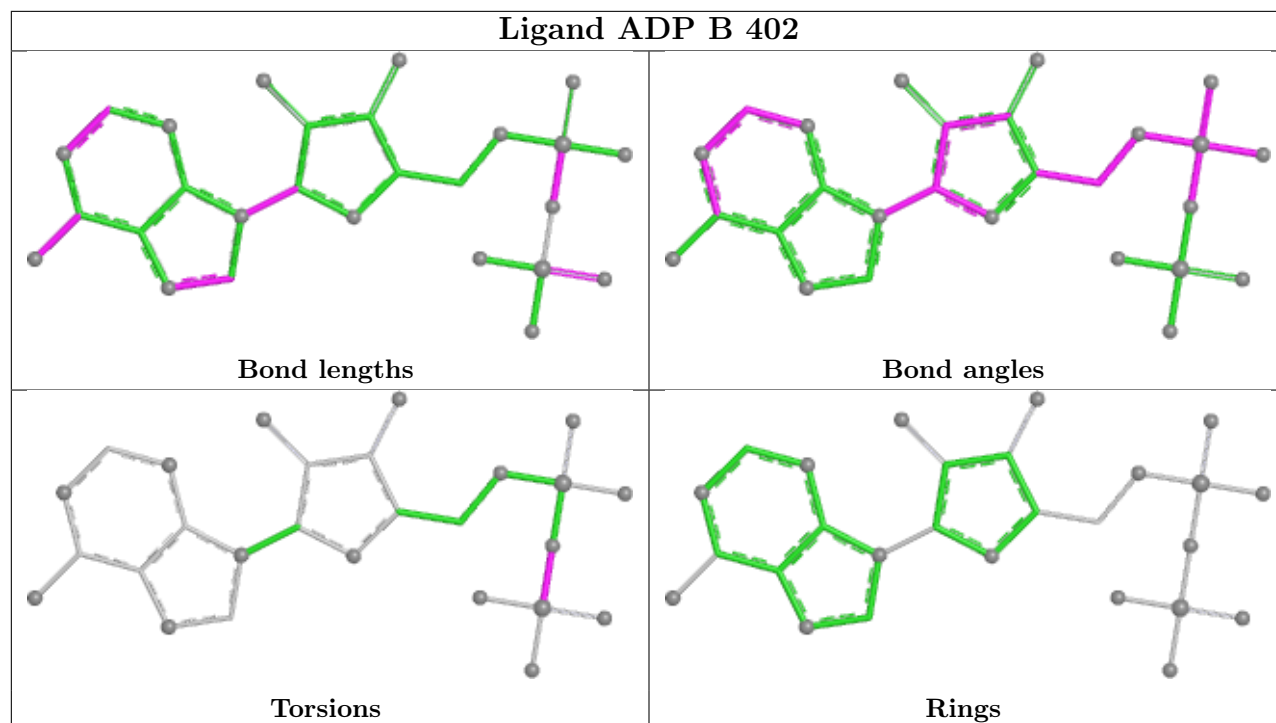
Mol	Chain	Res	Type	Atoms
3	A	401	ADP	PA-O3A-PB-O2B
3	B	402	ADP	PA-O3A-PB-O2B
3	C	403	ADP	PA-O3A-PB-O2B
3	D	404	ADP	PA-O3A-PB-O2B
3	A	401	ADP	PA-O3A-PB-O3B
3	B	402	ADP	PA-O3A-PB-O3B
3	C	403	ADP	PA-O3A-PB-O3B
3	D	404	ADP	PA-O3A-PB-O3B
3	A	401	ADP	PB-O3A-PA-O2A
3	C	403	ADP	PB-O3A-PA-O1A

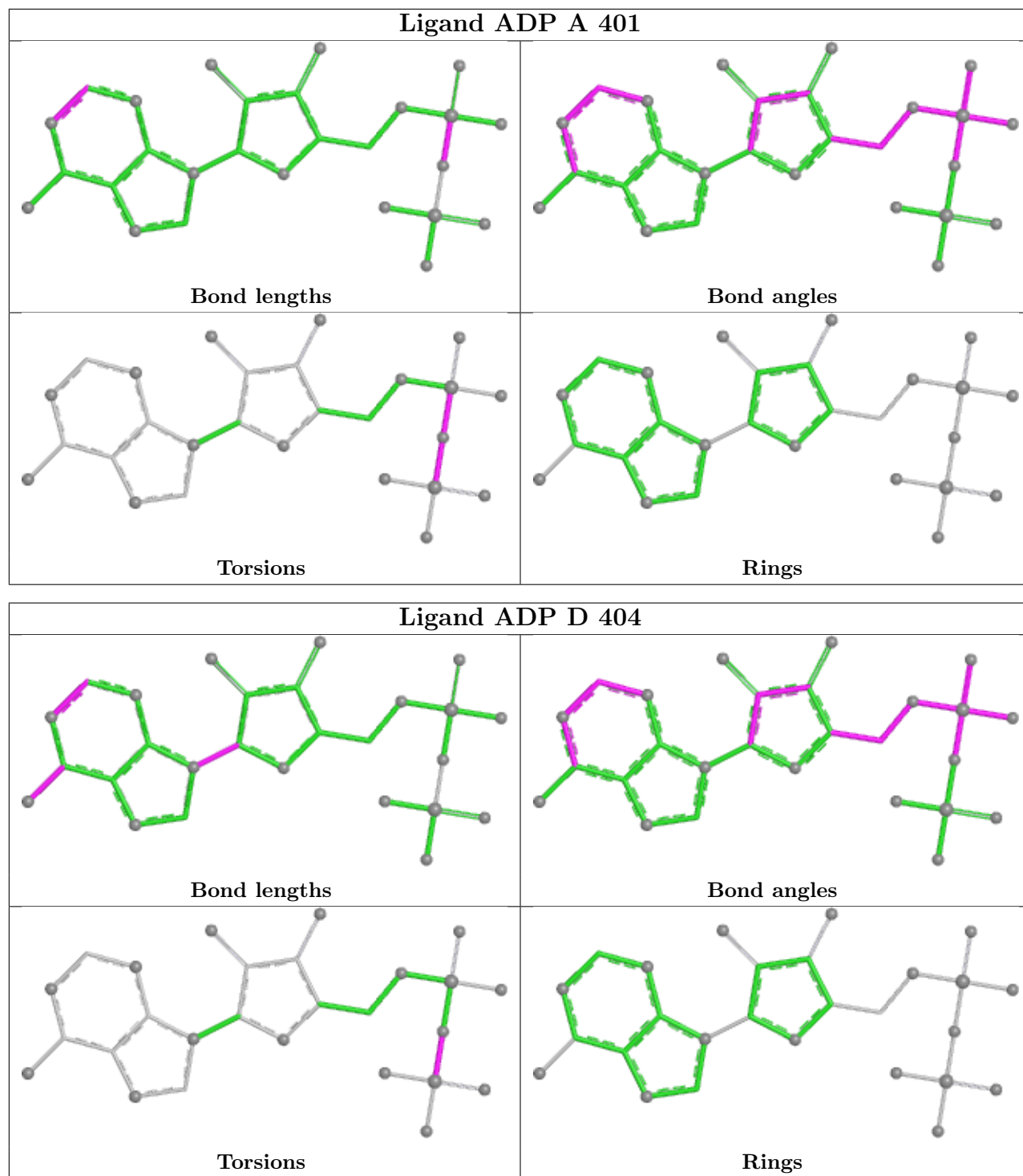
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	ADP	1	0
3	A	401	ADP	2	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	372/381 (97%)	0.79	55 (14%) 5 4	18, 57, 133, 168	0
1	B	374/381 (98%)	0.37	32 (8%) 16 12	16, 38, 91, 168	0
1	C	363/381 (95%)	1.07	77 (21%) 2 2	22, 71, 137, 172	0
1	D	299/381 (78%)	0.80	47 (15%) 5 4	18, 51, 129, 175	0
All	All	1408/1524 (92%)	0.75	211 (14%) 5 4	16, 52, 131, 175	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	GLN	6.2
1	D	61	PHE	6.1
1	A	65	LYS	5.7
1	C	60	LEU	5.4
1	A	38	SER	5.3
1	D	252	ASP	5.1
1	C	103	ALA	5.0
1	A	296	ALA	5.0
1	C	6	LEU	4.9
1	D	183	LEU	4.9
1	C	62	ILE	4.9
1	B	38	SER	4.8
1	A	61	PHE	4.5
1	C	26	ILE	4.5
1	B	134	LEU	4.5
1	C	102	LEU	4.5
1	C	19	SER	4.3
1	B	236	SER	4.3
1	B	326	ASN	4.3
1	C	22	ILE	4.2
1	C	260	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	260	MET	4.2
1	D	251	ILE	4.2
1	B	323	ILE	4.1
1	B	61	PHE	4.1
1	D	160	PRO	4.0
1	D	276	GLN	3.9
1	C	80	VAL	3.8
1	D	65	LYS	3.8
1	B	325	GLN	3.8
1	A	105	ALA	3.7
1	B	183	LEU	3.7
1	D	295	ILE	3.7
1	C	38	SER	3.7
1	A	325	GLN	3.6
1	B	295	ILE	3.6
1	C	18	VAL	3.6
1	B	135	SER	3.5
1	D	367	LYS	3.5
1	B	324	ARG	3.5
1	A	295	ILE	3.5
1	A	63	GLY	3.5
1	C	10	THR	3.5
1	C	24	LEU	3.4
1	A	252	ASP	3.4
1	C	295	ILE	3.4
1	C	72	PRO	3.4
1	C	4	VAL	3.3
1	C	316	ILE	3.3
1	C	56	THR	3.3
1	C	178	ARG	3.3
1	B	336	LEU	3.3
1	D	323	ILE	3.3
1	B	375	SER	3.3
1	A	119	GLU	3.2
1	B	297	ASP	3.2
1	C	263	ARG	3.2
1	C	71	PRO	3.2
1	A	98	PHE	3.2
1	A	134	LEU	3.2
1	C	236	SER	3.2
1	A	143	ALA	3.2
1	C	374	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	184	GLY	3.1
1	A	133	ALA	3.1
1	D	172	MET	3.1
1	A	299	ILE	3.1
1	D	324	ARG	3.1
1	A	2	ALA	3.1
1	D	182	ARG	3.1
1	C	86	LEU	3.1
1	B	271	GLU	3.0
1	C	261	PRO	3.0
1	C	5	GLN	3.0
1	A	102	LEU	3.0
1	A	88	PRO	3.0
1	D	171	GLN	2.9
1	D	325	GLN	2.9
1	A	96	MET	2.9
1	A	15	GLU	2.9
1	B	273	ARG	2.9
1	A	87	TYR	2.9
1	C	168	LEU	2.9
1	A	276	GLN	2.8
1	C	375	SER	2.8
1	A	121	LEU	2.8
1	A	297	ASP	2.8
1	C	182	ARG	2.8
1	D	185	ARG	2.8
1	C	69	ASP	2.8
1	A	260	MET	2.8
1	D	320	ILE	2.8
1	A	262	ASN	2.8
1	D	236	SER	2.8
1	B	374	ALA	2.7
1	D	366	HIS	2.7
1	A	163	ASN	2.7
1	D	321	PRO	2.7
1	C	127	LEU	2.7
1	C	2	ALA	2.7
1	C	23	ASN	2.7
1	C	68	ASN	2.7
1	C	46	LEU	2.7
1	D	176	ILE	2.6
1	B	133	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	187	MET	2.6
1	B	102	LEU	2.6
1	C	105	ALA	2.6
1	A	83	SER	2.6
1	A	173	ARG	2.6
1	D	174	ILE	2.6
1	D	5	GLN	2.6
1	C	85	ALA	2.6
1	A	373	SER	2.6
1	C	321	PRO	2.6
1	C	61	PHE	2.6
1	D	179	LEU	2.5
1	A	108	GLU	2.5
1	B	276	GLN	2.5
1	D	322	SER	2.5
1	A	84	TYR	2.5
1	C	322	SER	2.5
1	C	55	ILE	2.5
1	A	298	VAL	2.5
1	D	173	ARG	2.5
1	B	327	LEU	2.5
1	A	236	SER	2.5
1	B	261	PRO	2.5
1	C	271	GLU	2.5
1	A	319	GLN	2.5
1	D	169	ARG	2.5
1	A	274	ASP	2.4
1	C	59	ASP	2.4
1	D	168	LEU	2.4
1	C	104	GLY	2.4
1	D	373	SER	2.4
1	B	262	ASN	2.4
1	B	24	LEU	2.4
1	D	16	VAL	2.4
1	A	81	PHE	2.4
1	A	118	ALA	2.4
1	C	171	GLN	2.4
1	C	44	THR	2.4
1	D	80	VAL	2.4
1	D	180	HIS	2.4
1	B	296	ALA	2.4
1	C	147	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	262	ASN	2.3
1	A	131	PRO	2.3
1	C	100	LEU	2.3
1	C	148	LEU	2.3
1	D	57	SER	2.3
1	A	136	GLY	2.3
1	C	76	GLY	2.3
1	C	296	ALA	2.3
1	B	318	ILE	2.3
1	A	64	GLU	2.3
1	A	271	GLU	2.3
1	C	30	GLU	2.3
1	C	276	GLN	2.3
1	C	176	ILE	2.3
1	C	54	THR	2.3
1	C	343	PHE	2.2
1	D	167	ALA	2.2
1	A	90	LEU	2.2
1	B	320	ILE	2.2
1	B	83	SER	2.2
1	C	123	LEU	2.2
1	D	68	ASN	2.2
1	A	7	GLN	2.2
1	A	89	HIS	2.2
1	B	298	VAL	2.2
1	A	123	LEU	2.2
1	C	326	ASN	2.2
1	D	152	PRO	2.2
1	C	70	THR	2.2
1	C	67	MET	2.2
1	A	261	PRO	2.2
1	B	21	ASP	2.2
1	C	165	ASP	2.2
1	D	170	VAL	2.2
1	C	73	ALA	2.2
1	D	271	GLU	2.2
1	A	322	SER	2.1
1	A	372	ALA	2.1
1	C	150	ALA	2.1
1	D	73	ALA	2.1
1	C	66	ARG	2.1
1	D	27	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	340	GLY	2.1
1	D	13	TRP	2.1
1	C	34	PHE	2.1
1	D	294	ASP	2.1
1	C	53	GLU	2.1
1	C	108	GLU	2.1
1	A	367	LYS	2.1
1	D	164	LEU	2.1
1	A	182	ARG	2.1
1	D	178	ARG	2.1
1	C	57	SER	2.0
1	A	16	VAL	2.0
1	C	37	PRO	2.0
1	C	98	PHE	2.0
1	D	14	GLY	2.0
1	B	319	GLN	2.0
1	C	3	SER	2.0
1	A	369	PRO	2.0
1	A	14	GLY	2.0
1	C	299	ILE	2.0
1	C	191	THR	2.0
1	A	28	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

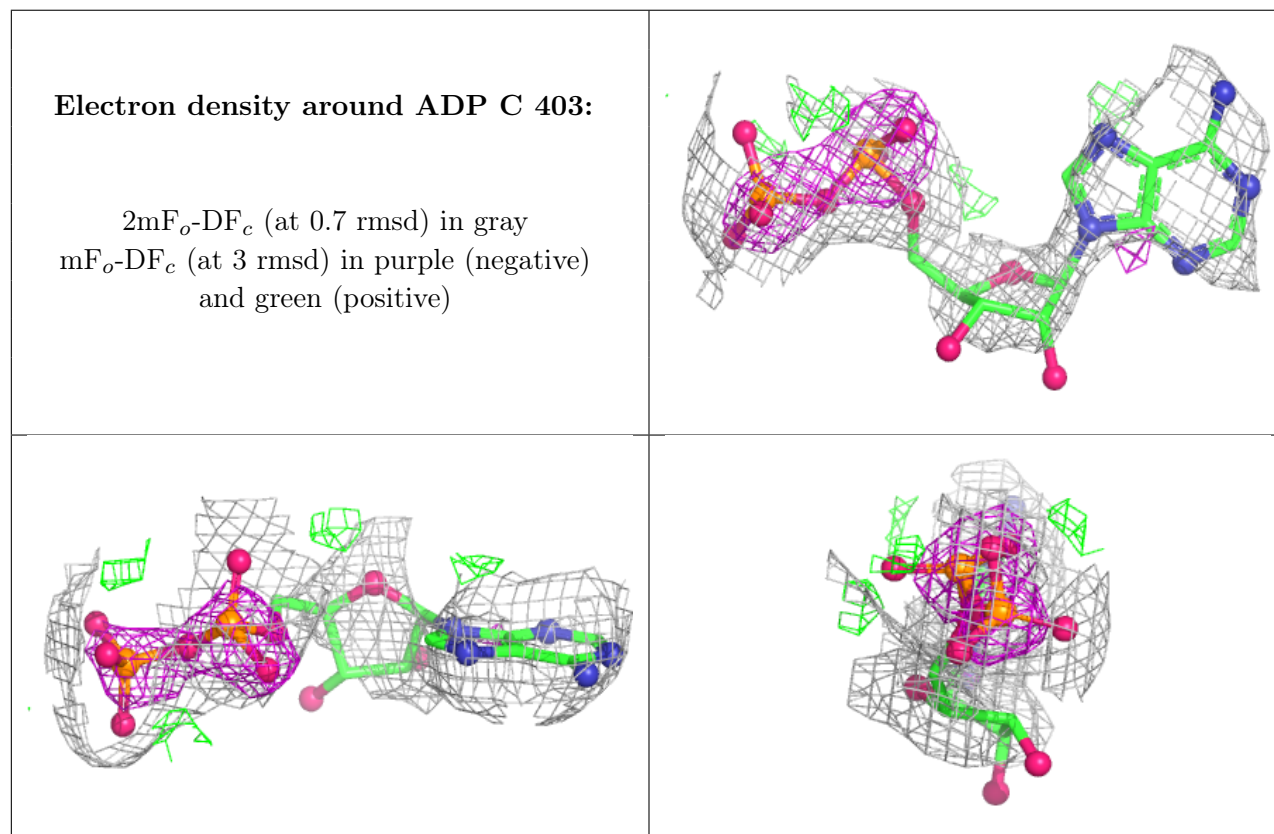
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	C	403	27/27	0.82	0.15	44,86,93,93	0

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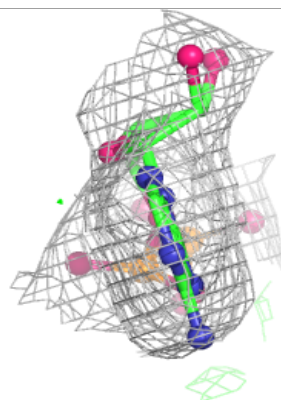
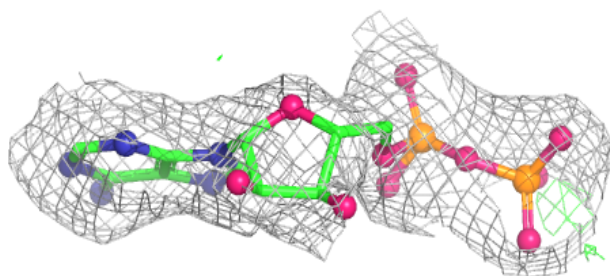
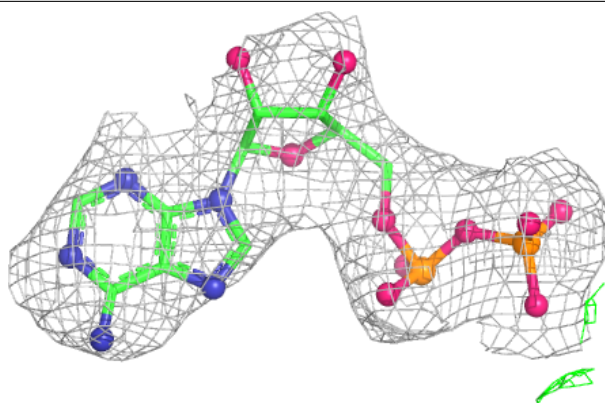
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	504	1/1	0.85	0.17	33,33,33,33	0
2	MG	B	501	1/1	0.90	0.24	29,29,29,29	0
3	ADP	D	404	27/27	0.90	0.12	44,79,83,84	0
3	ADP	A	401	27/27	0.92	0.14	38,77,83,84	0
2	MG	A	502	1/1	0.93	0.17	29,29,29,29	0
2	MG	C	503	1/1	0.94	0.05	28,28,28,28	0
3	ADP	B	402	27/27	0.95	0.14	33,70,79,80	0

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

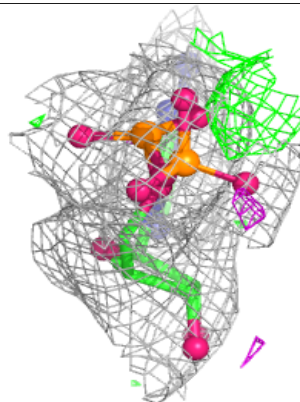
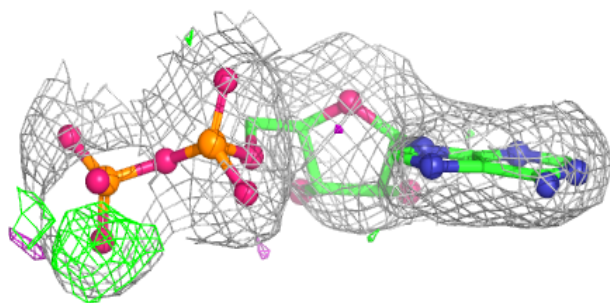
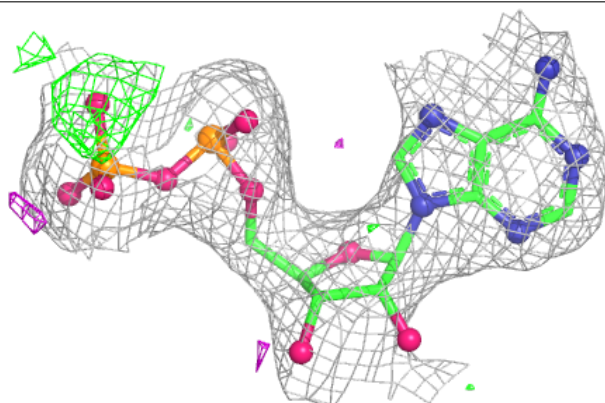


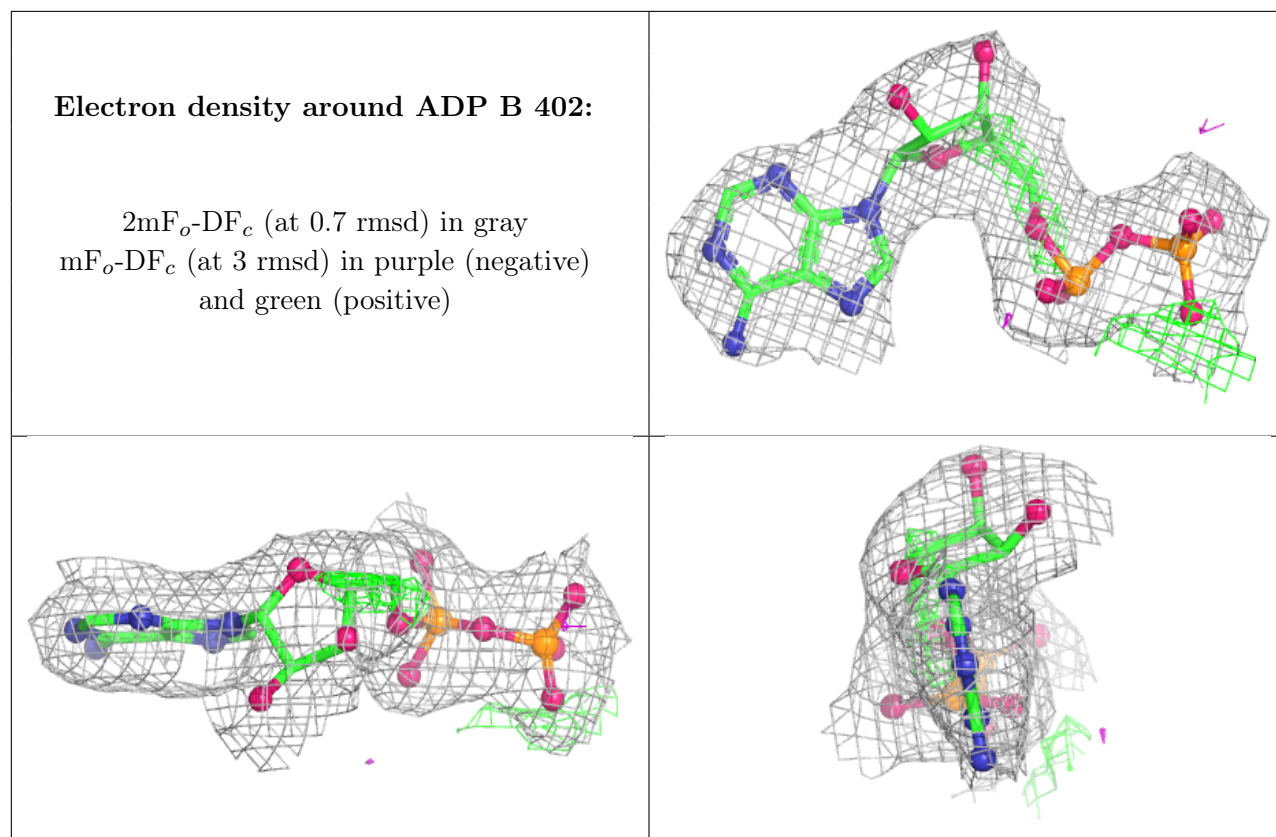
Electron density around ADP D 404:

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

**Electron density around ADP A 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.