



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2R65 / pdb_00002r65
Title : Crystal structure of Helicobacter pylori ATP dependent protease, FtsH ADP complex
Authors : Kim, S.H.; Kang, G.B.; Song, H.-E.; Park, S.J.; Bae, M.-H.; Eom, S.H.
Deposited on : 2007-09-05
Resolution : 3.30 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

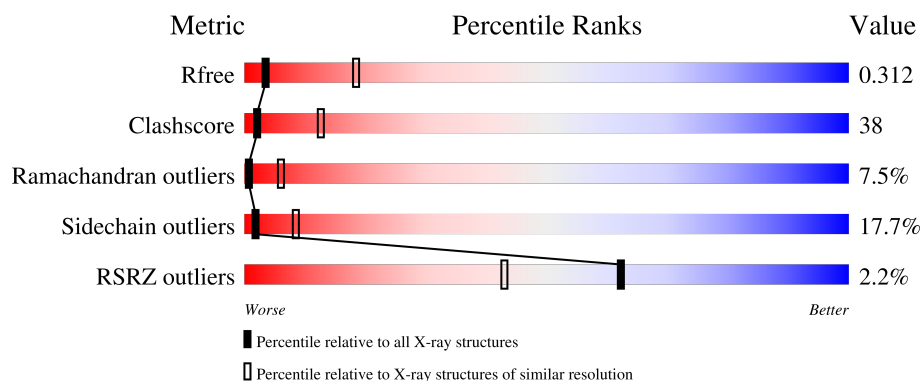
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	268	2% 38% 45% 9% 7%
1	B	268	2% 41% 43% 8% 7%
1	C	268	% 35% 40% 14% 7%
1	D	268	4% 30% 44% 16% 7%
1	E	268	% 38% 41% 13% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	D	4	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9645 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 Cell division protease ftsH homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1902	1203	336	358	5			
1	B	249	Total	C	N	O	S	0	0	0
			1902	1203	336	358	5			
1	C	249	Total	C	N	O	S	0	0	0
			1902	1203	336	358	5			
1	D	249	Total	C	N	O	S	0	0	0
			1902	1203	336	358	5			
1	E	249	Total	C	N	O	S	0	0	0
			1902	1203	336	358	5			

There are 45 discrepancies between the modelled and reference sequences:

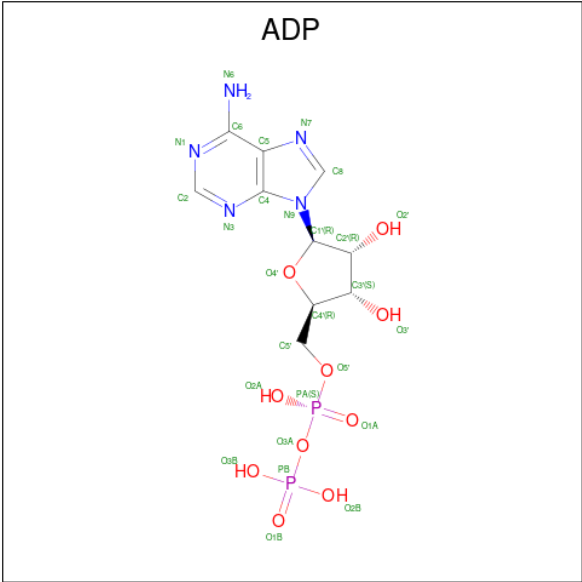
Chain	Residue	Modelled	Actual	Comment	Reference
A	170	LYS	ASN	engineered mutation	UNP P71408
A	420	LEU	-	expression tag	UNP P71408
A	421	GLU	-	expression tag	UNP P71408
A	422	HIS	-	expression tag	UNP P71408
A	423	HIS	-	expression tag	UNP P71408
A	424	HIS	-	expression tag	UNP P71408
A	425	HIS	-	expression tag	UNP P71408
A	426	HIS	-	expression tag	UNP P71408
A	427	HIS	-	expression tag	UNP P71408
B	170	LYS	ASN	engineered mutation	UNP P71408
B	420	LEU	-	expression tag	UNP P71408
B	421	GLU	-	expression tag	UNP P71408
B	422	HIS	-	expression tag	UNP P71408
B	423	HIS	-	expression tag	UNP P71408
B	424	HIS	-	expression tag	UNP P71408
B	425	HIS	-	expression tag	UNP P71408
B	426	HIS	-	expression tag	UNP P71408
B	427	HIS	-	expression tag	UNP P71408
C	170	LYS	ASN	engineered mutation	UNP P71408

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Chain	Residue	Modelled	Actual	Comment	Reference
C	420	LEU	-	expression tag	UNP P71408
C	421	GLU	-	expression tag	UNP P71408
C	422	HIS	-	expression tag	UNP P71408
C	423	HIS	-	expression tag	UNP P71408
C	424	HIS	-	expression tag	UNP P71408
C	425	HIS	-	expression tag	UNP P71408
C	426	HIS	-	expression tag	UNP P71408
C	427	HIS	-	expression tag	UNP P71408
D	170	LYS	ASN	engineered mutation	UNP P71408
D	420	LEU	-	expression tag	UNP P71408
D	421	GLU	-	expression tag	UNP P71408
D	422	HIS	-	expression tag	UNP P71408
D	423	HIS	-	expression tag	UNP P71408
D	424	HIS	-	expression tag	UNP P71408
D	425	HIS	-	expression tag	UNP P71408
D	426	HIS	-	expression tag	UNP P71408
D	427	HIS	-	expression tag	UNP P71408
E	170	LYS	ASN	engineered mutation	UNP P71408
E	420	LEU	-	expression tag	UNP P71408
E	421	GLU	-	expression tag	UNP P71408
E	422	HIS	-	expression tag	UNP P71408
E	423	HIS	-	expression tag	UNP P71408
E	424	HIS	-	expression tag	UNP P71408
E	425	HIS	-	expression tag	UNP P71408
E	426	HIS	-	expression tag	UNP P71408
E	427	HIS	-	expression tag	UNP P71408

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

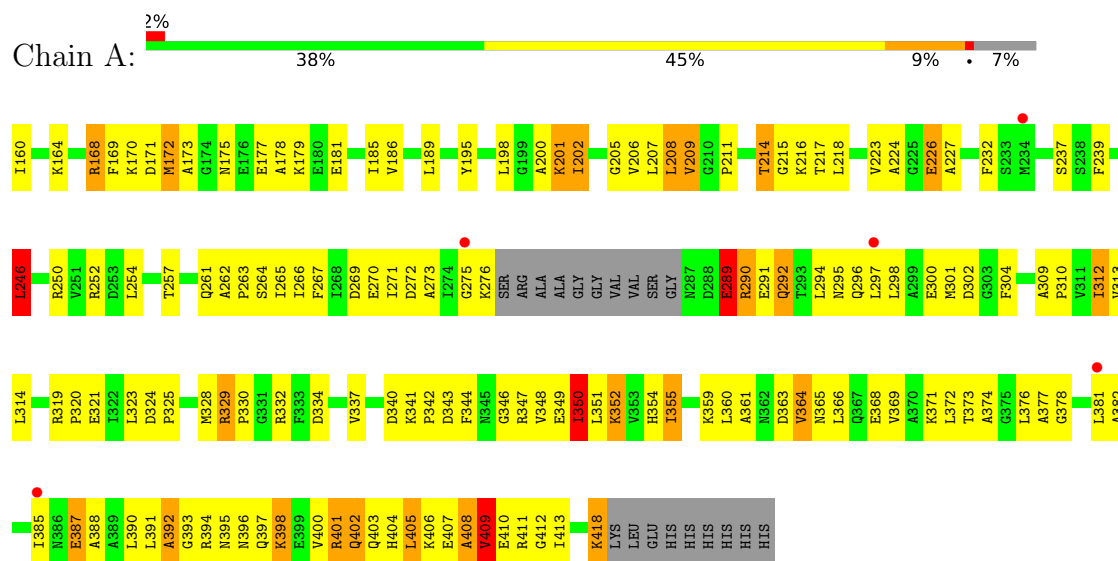


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

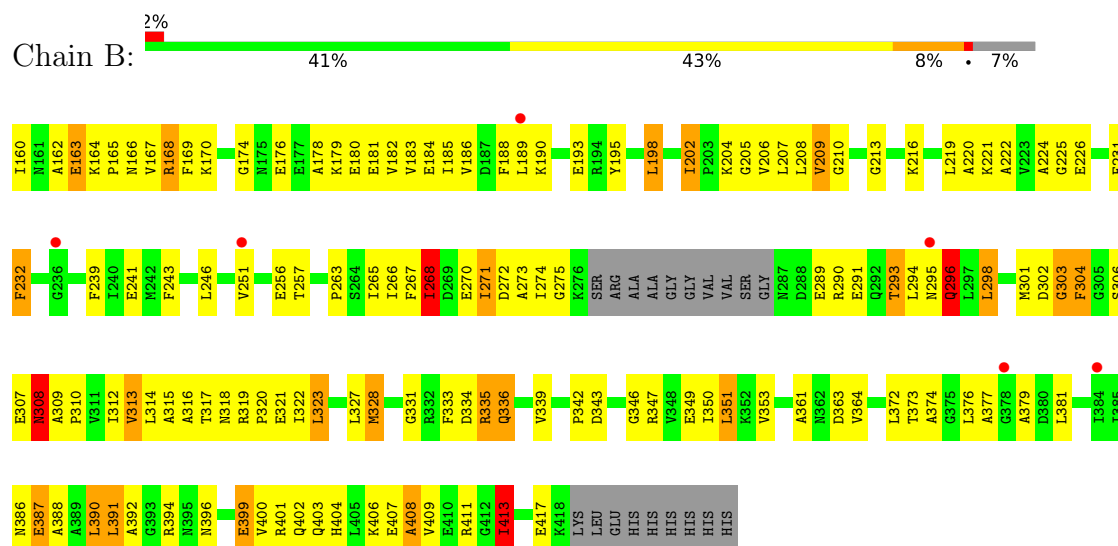
3 Residue-property plots

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: Cell division protease ftsH homolog



• Molecule 1: Cell division protease ftsH homolog



• Molecule 1: Cell division protease ftsH homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.47Å 219.49Å 146.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-3.30) 98.4 (50.00-3.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.288 , 0.331 0.269 , 0.312	Depositor DCC
R_{free} test set	1403 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	116.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 163.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9645	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

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	0.97	7/1928 (0.4%)	1.08	6/2598 (0.2%)
1	B	0.87	1/1928 (0.1%)	1.01	1/2598 (0.0%)
1	C	1.55	30/1928 (1.6%)	1.47	31/2598 (1.2%)
1	D	1.02	9/1928 (0.5%)	1.23	14/2598 (0.5%)
1	E	1.04	6/1928 (0.3%)	1.15	5/2598 (0.2%)
All	All	1.11	53/9640 (0.5%)	1.20	57/12990 (0.4%)

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	2
1	C	0	1
1	D	0	1
All	All	0	4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	ALA	C-N	22.28	1.62	1.33
1	C	400	VAL	C-N	15.53	1.54	1.33
1	D	406	LYS	CE-NZ	15.15	1.94	1.49
1	E	397	GLN	CD-OE1	13.39	1.49	1.23
1	A	352	LYS	CD-CE	12.69	1.90	1.52
1	C	394	ARG	C-O	12.62	1.38	1.24
1	A	289	GLU	CD-OE2	11.78	1.47	1.25
1	A	352	LYS	CG-CD	11.73	1.87	1.52
1	C	393	GLY	C-N	10.88	1.47	1.33
1	C	365	ASN	C-O	-10.27	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	390	LEU	CG-CD1	9.94	1.85	1.52
1	D	180	GLU	CD-OE1	9.80	1.44	1.25
1	C	388	ALA	CA-CB	9.06	1.68	1.53
1	C	402	GLN	C-O	-8.92	1.12	1.24
1	E	397	GLN	CD-NE2	8.83	1.51	1.33
1	C	304	PHE	C-O	8.33	1.34	1.24
1	D	406	LYS	CD-CE	8.21	1.77	1.52
1	A	289	GLU	CD-OE1	7.97	1.40	1.25
1	C	390	LEU	CB-CG	7.90	1.69	1.53
1	C	397	GLN	C-N	7.75	1.44	1.33
1	D	180	GLU	CD-OE2	7.74	1.40	1.25
1	C	387	GLU	CB-CG	7.58	1.75	1.52
1	C	386	ASN	C-O	-7.26	1.15	1.23
1	E	367	GLN	CD-NE2	7.05	1.48	1.33
1	C	388	ALA	N-CA	6.83	1.54	1.46
1	C	303	GLY	C-O	6.81	1.33	1.23
1	C	395	ASN	CG-OD1	6.68	1.36	1.23
1	C	384	ILE	C-O	6.56	1.31	1.24
1	C	401	ARG	N-CA	-6.47	1.37	1.46
1	C	390	LEU	N-CA	-6.42	1.38	1.46
1	C	392	ALA	CA-CB	-6.24	1.43	1.53
1	C	387	GLU	C-O	6.15	1.31	1.24
1	C	386	ASN	N-CA	6.07	1.53	1.46
1	C	397	GLN	CA-CB	6.01	1.62	1.53
1	D	361	ALA	CA-C	5.96	1.60	1.52
1	D	290	ARG	N-CA	5.93	1.53	1.46
1	C	394	ARG	CB-CG	5.73	1.69	1.52
1	E	229	VAL	C-O	5.72	1.28	1.24
1	C	401	ARG	CA-C	5.71	1.60	1.52
1	B	387	GLU	CD-OE1	5.69	1.36	1.25
1	C	389	ALA	C-O	5.61	1.31	1.24
1	E	244	VAL	CA-CB	5.58	1.62	1.54
1	E	387	GLU	CD-OE2	5.57	1.35	1.25
1	D	244	VAL	CA-CB	5.43	1.60	1.54
1	A	329	ARG	CZ-NH1	5.41	1.40	1.32
1	D	184	GLU	CD-OE2	5.40	1.35	1.25
1	A	352	LYS	CE-NZ	5.35	1.65	1.49
1	D	289	GLU	C-N	5.34	1.41	1.33
1	C	390	LEU	CA-CB	-5.27	1.45	1.53
1	C	406	LYS	CE-NZ	5.24	1.65	1.49
1	C	391	LEU	N-CA	-5.19	1.40	1.46
1	C	400	VAL	C-O	5.15	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	MET	SD-CE	5.12	1.92	1.79

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361	ALA	N-CA-C	13.32	131.04	113.72
1	D	210	GLY	CA-C-N	13.21	129.30	119.66
1	D	210	GLY	C-N-CA	13.21	129.30	119.66
1	C	379	ALA	N-CA-C	-13.12	96.60	111.82
1	D	273	ALA	N-CA-C	-12.46	98.73	114.56
1	A	352	LYS	CG-CD-CE	-11.70	84.39	111.30
1	C	397	GLN	N-CA-CB	10.72	126.86	109.28
1	C	410	GLU	N-CA-C	-10.53	97.98	112.30
1	E	397	GLN	OE1-CD-NE2	10.39	132.99	122.60
1	C	397	GLN	N-CA-C	-10.16	95.05	110.30
1	C	389	ALA	O-C-N	-9.04	110.57	122.59
1	D	410	GLU	N-CA-C	-9.04	101.22	112.88
1	C	390	LEU	CA-C-O	8.85	130.09	120.80
1	C	395	ASN	CA-CB-CG	-8.80	103.80	112.60
1	C	389	ALA	N-CA-CB	8.74	125.26	110.49
1	C	388	ALA	N-CA-CB	8.34	124.59	110.49
1	C	384	ILE	CA-C-O	-8.12	112.56	121.17
1	C	391	LEU	CD1-CG-CD2	-8.06	93.06	110.80
1	D	406	LYS	CD-CE-NZ	-7.51	87.85	111.90
1	C	390	LEU	CD1-CG-CD2	-7.04	95.31	110.80
1	A	352	LYS	CD-CE-NZ	-6.91	89.77	111.90
1	D	311	VAL	CB-CA-C	-6.86	104.30	111.23
1	A	377	ALA	N-CA-C	6.83	119.31	111.11
1	C	365	ASN	CA-C-O	6.62	127.54	120.46
1	D	368	GLU	N-CA-C	-6.54	98.55	109.07
1	C	163	GLU	N-CA-C	6.43	118.80	107.61
1	E	209	VAL	N-CA-C	6.13	116.76	108.17
1	C	393	GLY	CA-C-N	6.09	128.69	120.65
1	C	393	GLY	C-N-CA	6.09	128.69	120.65
1	A	350	ILE	CB-CA-C	-5.94	104.10	111.70
1	C	395	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	C	388	ALA	CA-C-N	5.81	132.63	121.54
1	C	388	ALA	C-N-CA	5.81	132.63	121.54
1	A	352	LYS	CB-CG-CD	-5.80	97.96	111.30
1	D	266	ILE	CB-CA-C	-5.80	102.80	110.98
1	C	394	ARG	N-CA-CB	5.79	118.37	109.91
1	C	387	GLU	CA-C-N	5.63	132.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	GLU	C-N-CA	5.63	132.29	121.54
1	C	391	LEU	CB-CG-CD2	-5.58	93.95	110.70
1	D	202	ILE	CA-C-N	5.51	125.52	119.90
1	D	202	ILE	C-N-CA	5.51	125.52	119.90
1	E	239	PHE	N-CA-C	-5.46	106.79	113.50
1	C	388	ALA	O-C-N	-5.44	115.36	122.59
1	C	411	ARG	N-CA-C	-5.42	106.25	112.92
1	D	368	GLU	CA-C-N	5.33	131.29	121.70
1	D	368	GLU	C-N-CA	5.33	131.29	121.70
1	C	246	LEU	N-CA-C	5.30	117.74	109.52
1	C	397	GLN	CA-CB-CG	-5.25	103.61	114.10
1	A	390	LEU	N-CA-C	-5.18	104.58	112.04
1	C	171	ASP	N-CA-C	-5.17	106.66	113.17
1	C	404	HIS	N-CA-C	5.15	116.58	111.07
1	B	296	GLN	N-CA-C	-5.14	107.08	113.55
1	E	397	GLN	CG-CD-OE1	-5.12	110.56	120.80
1	E	232	PHE	N-CA-C	5.08	116.77	108.63
1	C	324	ASP	CA-C-N	5.05	126.16	119.84
1	C	324	ASP	C-N-CA	5.05	126.16	119.84
1	D	211	PRO	N-CA-C	5.04	115.31	110.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	GLU	Peptide,Sidechain
1	C	387	GLU	Mainchain
1	D	360	LEU	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	1902	0	1948	125	0
1	B	1902	0	1948	118	0
1	C	1902	0	1948	193	0
1	D	1902	0	1948	182	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1902	0	1948	126	0
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	3	0
2	D	27	0	12	10	0
2	E	27	0	12	0	0
All	All	9645	0	9800	732	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 38.

All (732) 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:D:406:LYS:CE	1:D:406:LYS:CD	1.77	1.57
1:C:387:GLU:CB	1:C:387:GLU:CG	1.75	1.55
1:C:390:LEU:CG	1:C:390:LEU:CD1	1.85	1.52
1:A:352:LYS:CD	1:A:352:LYS:CG	1.87	1.50
1:A:352:LYS:CD	1:A:352:LYS:CE	1.90	1.50
1:D:406:LYS:CE	1:D:406:LYS:NZ	1.94	1.30
1:D:303:GLY:HA3	1:D:307:GLU:HG3	1.25	1.17
1:E:296:GLN:HE21	1:E:296:GLN:HA	1.03	1.14
1:C:373:THR:HG21	1:C:381:LEU:HD21	1.23	1.12
1:D:373:THR:HG21	1:D:381:LEU:HD21	1.29	1.11
1:C:365:ASN:H	1:C:402:GLN:NE2	1.48	1.09
1:C:401:ARG:HH11	1:C:401:ARG:HB3	1.13	1.06
1:B:208:LEU:HD21	1:B:219:LEU:HD23	1.33	1.04
1:C:383:ASN:HB3	1:C:411:ARG:HH12	0.88	1.04
1:C:383:ASN:HB3	1:C:411:ARG:NH1	1.74	1.03
1:E:246:LEU:HD12	1:E:247:GLY:H	1.25	1.00
1:E:296:GLN:HA	1:E:296:GLN:NE2	1.72	0.99
1:D:242:MET:HB3	1:D:247:GLY:HA2	1.43	0.99
1:C:383:ASN:CB	1:C:411:ARG:HH12	1.76	0.98
1:D:276:LYS:HG3	1:D:290:ARG:NH2	1.78	0.98
1:E:258:ALA:HB2	1:E:266:ILE:HD11	1.42	0.97
1:C:294:LEU:HD23	1:C:295:ASN:H	1.26	0.97
1:A:239:PHE:HZ	1:A:250:ARG:HB2	1.30	0.95
1:D:173:ALA:H	2:D:4:ADP:N6	1.65	0.94
1:D:242:MET:CB	1:D:247:GLY:HA2	1.99	0.93
1:B:188:PHE:HB3	1:B:202:ILE:HD13	1.48	0.92
1:D:184:GLU:HG2	1:D:188:PHE:HE2	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:HG3	1:A:403:GLN:HB3	1.50	0.90
1:D:373:THR:HG22	1:D:373:THR:O	1.72	0.90
1:C:173:ALA:HB2	1:C:353:VAL:HG21	1.54	0.90
1:C:214:THR:HG23	1:C:339:VAL:HG22	1.54	0.89
1:B:351:LEU:HD11	1:B:381:LEU:HD22	1.53	0.89
1:C:355:ILE:HD12	1:C:385:ILE:HD13	1.55	0.89
1:C:373:THR:HG22	1:C:373:THR:O	1.70	0.88
1:D:236:GLY:HA3	1:D:270:GLU:HB3	1.56	0.88
1:C:294:LEU:HD21	1:C:298:LEU:HD11	1.54	0.87
1:E:258:ALA:CB	1:E:266:ILE:HD11	2.03	0.87
1:C:406:LYS:NZ	1:C:406:LYS:HB2	1.88	0.86
1:A:355:ILE:HG12	1:A:360:LEU:HD11	1.57	0.86
1:E:210:GLY:O	1:E:216:LYS:NZ	2.09	0.86
1:D:258:ALA:CB	1:D:266:ILE:HD11	2.06	0.86
1:C:410:GLU:O	1:C:410:GLU:HG2	1.75	0.85
1:A:352:LYS:CG	1:A:352:LYS:CE	2.53	0.85
1:B:185:ILE:HA	1:B:188:PHE:CD2	2.10	0.85
1:E:296:GLN:HE21	1:E:296:GLN:CA	1.74	0.85
1:C:365:ASN:H	1:C:402:GLN:HE22	1.19	0.84
1:A:266:ILE:HB	1:A:313:VAL:HG23	1.57	0.83
1:D:351:LEU:HB3	1:D:366:LEU:HD23	1.61	0.83
1:C:401:ARG:HH11	1:C:401:ARG:CB	1.90	0.83
1:D:184:GLU:HG2	1:D:188:PHE:CE2	2.12	0.83
1:C:346:GLY:O	1:C:349:GLU:HG2	1.78	0.82
1:B:224:ALA:HB2	1:B:265:ILE:HD12	1.60	0.82
1:C:365:ASN:N	1:C:402:GLN:NE2	2.26	0.82
1:A:239:PHE:CZ	1:A:250:ARG:HB2	2.15	0.81
1:D:182:VAL:HG21	1:D:219:LEU:HD11	1.61	0.81
1:D:289:GLU:HG3	1:D:290:ARG:H	1.42	0.81
1:D:373:THR:CG2	1:D:381:LEU:HD21	2.10	0.81
1:C:365:ASN:N	1:C:402:GLN:HE22	1.79	0.81
1:E:246:LEU:HD12	1:E:247:GLY:N	1.96	0.81
1:B:160:ILE:N	1:B:257:THR:HG1	1.80	0.80
1:C:276:LYS:HZ1	1:C:290:ARG:HH11	1.27	0.80
1:C:351:LEU:HD11	1:C:381:LEU:HD22	1.61	0.80
1:C:294:LEU:CD2	1:C:298:LEU:HD11	2.11	0.80
1:C:390:LEU:CD1	1:C:390:LEU:CD2	2.60	0.79
1:D:401:ARG:HB2	1:D:401:ARG:HH11	1.48	0.79
1:C:182:VAL:HG21	1:C:219:LEU:HD11	1.64	0.79
1:A:352:LYS:CD	1:A:352:LYS:CB	2.61	0.79
1:C:240:ILE:HG23	1:C:290:ARG:NH2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:VAL:HG21	1:B:320:PRO:HB3	1.65	0.78
1:C:373:THR:CG2	1:C:381:LEU:HD21	2.11	0.78
1:D:406:LYS:CE	1:D:406:LYS:CG	2.61	0.77
1:C:173:ALA:HB3	1:C:350:ILE:HD13	1.64	0.77
1:A:209:VAL:HG21	1:A:320:PRO:HG3	1.67	0.77
1:D:215:GLY:HA3	2:D:4:ADP:C2	2.20	0.77
1:B:169:PHE:HB3	1:B:179:LYS:HE3	1.67	0.76
1:E:186:VAL:HG11	1:E:226:GLU:HB3	1.66	0.76
1:D:401:ARG:HH11	1:D:401:ARG:CB	1.99	0.76
1:D:402:GLN:CG	1:D:406:LYS:HE3	2.15	0.76
1:D:408:ALA:C	1:D:410:GLU:H	1.91	0.76
1:B:206:VAL:HB	1:B:314:LEU:HD23	1.68	0.76
1:C:355:ILE:CD1	1:C:385:ILE:HD13	2.16	0.76
1:C:412:GLY:O	1:C:413:ILE:HD12	1.86	0.75
1:D:173:ALA:N	2:D:4:ADP:N6	2.34	0.75
1:B:207:LEU:HB3	1:B:336:GLN:HG3	1.68	0.75
1:A:217:THR:HG23	1:A:267:PHE:CE2	2.22	0.75
1:B:188:PHE:HB3	1:B:202:ILE:CD1	2.17	0.75
1:E:172:MET:HE3	1:E:219:LEU:HD13	1.69	0.75
1:D:189:LEU:HD22	1:D:229:VAL:HG21	1.69	0.75
1:D:185:ILE:HD11	1:D:206:VAL:HG21	1.67	0.75
1:D:243:PHE:HB2	1:D:246:LEU:HB2	1.67	0.74
1:D:347:ARG:O	1:D:351:LEU:HD13	1.87	0.74
1:C:294:LEU:HD23	1:C:295:ASN:N	2.02	0.74
1:B:188:PHE:CG	1:B:202:ILE:HG21	2.23	0.74
1:B:208:LEU:CD2	1:B:219:LEU:HD23	2.16	0.74
1:E:289:GLU:O	1:E:292:GLN:N	2.15	0.74
1:C:297:LEU:HD23	1:C:327:LEU:HD21	1.70	0.74
1:E:354:HIS:HB2	1:E:385:ILE:HD12	1.69	0.73
1:A:352:LYS:CD	1:A:352:LYS:NZ	2.51	0.73
1:C:401:ARG:HB3	1:C:401:ARG:NH1	1.98	0.73
1:E:327:LEU:O	1:E:332:ARG:HB2	1.89	0.73
1:D:288:ASP:O	1:D:289:GLU:O	2.06	0.73
1:A:319:ARG:HB3	1:A:321:GLU:HG2	1.71	0.72
1:A:373:THR:HG21	1:A:381:LEU:HD22	1.71	0.72
1:C:390:LEU:CD1	1:C:390:LEU:CB	2.66	0.72
1:D:215:GLY:HA3	2:D:4:ADP:H2	1.54	0.72
1:A:368:GLU:O	1:A:372:LEU:HD12	1.88	0.72
1:C:364:VAL:HA	1:C:402:GLN:HE21	1.52	0.72
1:D:172:MET:HE3	1:D:175:ASN:HB2	1.71	0.71
1:A:173:ALA:HB1	1:A:349:GLU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:ARG:H	1:D:404:HIS:HD2	1.38	0.71
1:D:289:GLU:CG	1:D:290:ARG:H	2.02	0.71
1:A:205:GLY:HA2	1:A:313:VAL:O	1.91	0.71
1:C:354:HIS:CD2	1:C:382:ALA:HB2	2.25	0.71
1:D:401:ARG:N	1:D:404:HIS:HD2	1.89	0.71
1:D:354:HIS:NE2	2:D:4:ADP:H8	1.89	0.70
1:D:365:ASN:O	1:D:368:GLU:O	2.09	0.70
1:C:400:VAL:HG12	1:C:400:VAL:O	1.91	0.70
1:C:387:GLU:CG	1:C:387:GLU:CA	2.66	0.70
1:C:397:GLN:HG3	1:C:401:ARG:NH2	2.07	0.70
1:C:189:LEU:HD11	1:C:265:ILE:HD11	1.74	0.70
1:E:296:GLN:NE2	1:E:296:GLN:CA	2.40	0.70
1:B:391:LEU:HA	1:B:394:ARG:HG3	1.74	0.69
1:D:271:ILE:HG22	1:D:316:ALA:O	1.93	0.69
1:D:408:ALA:C	1:D:410:GLU:N	2.46	0.69
1:C:163:GLU:O	1:C:231:PHE:N	2.18	0.69
1:C:343:ASP:O	1:C:347:ARG:HD3	1.93	0.69
1:D:276:LYS:HD2	1:D:276:LYS:C	2.16	0.69
1:A:401:ARG:HH11	1:A:401:ARG:HB3	1.58	0.69
1:C:396:ASN:O	1:C:398:LYS:HD3	1.93	0.69
1:D:168:ARG:HG3	1:D:226:GLU:OE2	1.92	0.69
1:D:373:THR:HG23	1:D:376:LEU:HB2	1.75	0.69
1:D:293:THR:C	1:D:294:LEU:O	2.29	0.68
1:D:318:ASN:N	1:D:318:ASN:HD22	1.91	0.68
1:E:258:ALA:HB2	1:E:266:ILE:CD1	2.21	0.67
1:D:276:LYS:HE3	1:D:276:LYS:H	1.59	0.67
1:C:351:LEU:HD21	1:C:369:VAL:CG2	2.24	0.67
1:C:402:GLN:HG3	1:C:406:LYS:NZ	2.09	0.67
1:D:406:LYS:CD	1:D:406:LYS:NZ	2.58	0.67
1:E:172:MET:HG2	1:E:218:LEU:HG	1.75	0.67
1:C:179:LYS:O	1:C:183:VAL:HG23	1.95	0.67
1:C:200:ALA:HB2	1:D:389:ALA:HB1	1.76	0.67
1:D:354:HIS:NE2	2:D:4:ADP:C8	2.63	0.67
1:E:185:ILE:HG23	1:E:312:ILE:HD12	1.75	0.67
1:A:408:ALA:C	1:A:410:GLU:H	2.03	0.67
1:E:293:THR:C	1:E:294:LEU:O	2.36	0.67
1:C:234:MET:HE2	1:C:254:LEU:HD13	1.76	0.66
1:D:184:GLU:HB2	1:E:394:ARG:HH21	1.60	0.66
1:B:186:VAL:HG11	1:B:226:GLU:HB3	1.78	0.66
1:E:293:THR:O	1:E:294:LEU:O	2.13	0.66
1:D:276:LYS:HG3	1:D:290:ARG:CZ	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:ARG:H	1:D:404:HIS:CD2	2.13	0.66
1:E:195:TYR:HB3	1:E:200:ALA:HB3	1.76	0.66
1:B:185:ILE:HA	1:B:188:PHE:HD2	1.61	0.66
1:C:360:LEU:HD23	1:C:364:VAL:HG11	1.79	0.65
1:D:175:ASN:HB3	1:D:178:ALA:HB3	1.78	0.65
1:D:169:PHE:HD1	1:D:226:GLU:HG2	1.61	0.65
1:C:182:VAL:CG2	1:C:219:LEU:HD11	2.27	0.65
1:D:234:MET:HB3	1:D:268:ILE:HA	1.78	0.65
1:C:177:GLU:H	1:C:177:GLU:CD	2.05	0.65
1:E:216:LYS:HD2	1:E:316:ALA:HB1	1.79	0.64
1:C:274:ILE:HA	1:C:290:ARG:HD3	1.78	0.64
1:B:204:LYS:HD2	1:B:331:GLY:O	1.97	0.64
1:C:410:GLU:O	1:C:410:GLU:CG	2.45	0.64
1:D:300:GLU:OE1	1:D:300:GLU:HA	1.97	0.64
1:C:373:THR:O	1:C:373:THR:CG2	2.41	0.64
1:A:172:MET:HG3	1:A:218:LEU:HD23	1.80	0.64
1:A:401:ARG:H	1:A:404:HIS:HD2	1.45	0.63
1:D:237:SER:O	1:D:240:ILE:HG12	1.98	0.63
1:C:240:ILE:HG23	1:C:290:ARG:HH22	1.64	0.63
1:B:373:THR:HG23	1:B:376:LEU:HD13	1.81	0.63
1:C:402:GLN:HG3	1:C:406:LYS:HZ3	1.62	0.63
1:D:289:GLU:O	1:D:291:GLU:N	2.29	0.63
1:D:397:GLN:HG2	1:D:401:ARG:HE	1.63	0.63
1:D:408:ALA:O	1:D:410:GLU:N	2.30	0.63
1:A:373:THR:HG23	1:A:376:LEU:HG	1.80	0.63
1:B:302:ASP:O	1:B:304:PHE:N	2.29	0.63
1:A:363:ASP:O	1:A:402:GLN:HB2	1.99	0.63
1:D:373:THR:O	1:D:373:THR:CG2	2.46	0.63
1:A:347:ARG:O	1:A:351:LEU:HB2	1.99	0.63
1:C:173:ALA:HB3	1:C:350:ILE:CD1	2.29	0.63
1:C:359:LYS:O	1:C:400:VAL:HB	1.99	0.62
1:C:406:LYS:HB2	1:C:406:LYS:HZ3	1.64	0.62
1:D:402:GLN:HG2	1:D:406:LYS:HE3	1.81	0.62
1:E:169:PHE:CD1	1:E:226:GLU:HG2	2.35	0.62
1:E:274:ILE:O	1:E:294:LEU:HD13	1.99	0.62
1:D:185:ILE:CD1	1:D:206:VAL:HG21	2.29	0.62
1:E:363:ASP:OD1	1:E:401:ARG:HB3	2.00	0.62
1:A:185:ILE:HG23	1:A:312:ILE:HD12	1.80	0.62
1:D:401:ARG:HB2	1:D:401:ARG:NH1	2.15	0.61
1:C:406:LYS:HB2	1:C:406:LYS:HZ2	1.65	0.61
1:A:346:GLY:O	1:A:350:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:C	1:A:273:ALA:H	2.09	0.61
1:A:401:ARG:H	1:A:404:HIS:CD2	2.19	0.61
1:D:289:GLU:HG3	1:D:290:ARG:N	2.13	0.61
1:C:397:GLN:HG3	1:C:401:ARG:HH21	1.64	0.61
1:E:162:ALA:O	1:E:163:GLU:HB2	1.98	0.61
1:E:347:ARG:HG3	1:E:381:LEU:HD11	1.83	0.61
1:B:239:PHE:CE2	1:B:251:VAL:HG23	2.36	0.60
1:C:408:ALA:O	1:C:409:VAL:C	2.41	0.60
1:D:289:GLU:C	1:D:291:GLU:H	2.08	0.60
1:D:381:LEU:HD23	1:D:384:ILE:HD12	1.83	0.60
1:C:257:THR:HA	1:C:260:LYS:HB3	1.84	0.60
1:C:351:LEU:O	1:C:355:ILE:HB	2.01	0.60
1:D:169:PHE:CD1	1:D:226:GLU:HG2	2.37	0.60
1:D:323:LEU:HD22	1:D:327:LEU:CD1	2.32	0.60
1:B:411:ARG:C	1:B:413:ILE:H	2.09	0.60
1:D:383:ASN:O	1:D:384:ILE:C	2.43	0.60
1:C:274:ILE:O	1:C:294:LEU:HD12	2.02	0.60
1:C:276:LYS:HZ1	1:C:290:ARG:NH1	1.99	0.60
1:D:214:THR:OG1	1:D:339:VAL:HG22	2.02	0.60
1:E:234:MET:HE2	1:E:254:LEU:HD13	1.83	0.60
1:B:189:LEU:HG	1:B:312:ILE:HD12	1.84	0.59
1:D:205:GLY:HA2	1:D:313:VAL:O	2.02	0.59
1:A:355:ILE:CG1	1:A:360:LEU:HD11	2.30	0.59
1:C:352:LYS:HE2	1:C:352:LYS:O	2.03	0.59
1:B:401:ARG:H	1:B:404:HIS:HD2	1.49	0.59
1:C:259:LYS:HA	1:C:311:VAL:HG21	1.85	0.59
1:C:320:PRO:O	1:C:323:LEU:HB2	2.01	0.59
1:A:378:GLY:HA2	1:A:381:LEU:HG	1.84	0.59
1:C:203:PRO:HG3	1:C:335:ARG:NH1	2.18	0.59
1:C:348:VAL:HG23	1:C:370:ALA:HB2	1.83	0.59
1:A:407:GLU:O	1:A:410:GLU:HB2	2.03	0.59
1:C:355:ILE:CG1	1:C:360:LEU:HD21	2.32	0.59
1:B:364:VAL:HA	1:B:402:GLN:HB2	1.85	0.58
1:C:214:THR:HG23	1:C:339:VAL:CG2	2.32	0.58
1:C:349:GLU:O	1:C:353:VAL:HG23	2.03	0.58
1:A:392:ALA:O	1:A:394:ARG:N	2.37	0.58
1:E:294:LEU:C	1:E:296:GLN:H	2.12	0.58
1:B:294:LEU:O	1:B:295:ASN:CB	2.51	0.58
1:D:318:ASN:N	1:D:318:ASN:ND2	2.51	0.58
1:A:408:ALA:C	1:A:410:GLU:N	2.57	0.58
1:A:405:LEU:O	1:A:409:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:O	1:A:408:ALA:O	2.22	0.58
1:C:364:VAL:HA	1:C:402:GLN:NE2	2.17	0.58
1:D:161:ASN:O	1:D:232:PHE:CE2	2.57	0.58
1:D:355:ILE:HG13	1:D:360:LEU:HD11	1.85	0.57
1:E:187:ASP:HB3	1:E:195:TYR:OH	2.05	0.57
1:A:172:MET:CE	1:A:175:ASN:HB2	2.35	0.57
1:E:289:GLU:HA	1:E:292:GLN:CD	2.28	0.57
1:B:216:LYS:HE3	1:B:316:ALA:HB1	1.86	0.57
1:B:165:PRO:HD3	1:B:231:PHE:HB3	1.87	0.57
1:C:361:ALA:HB3	1:C:401:ARG:HA	1.84	0.57
1:C:379:ALA:HA	2:C:3:ADP:O4'	2.04	0.57
1:B:193:GLU:HA	1:B:193:GLU:OE2	2.04	0.57
1:D:276:LYS:HG3	1:D:290:ARG:HH22	1.69	0.57
1:D:408:ALA:O	1:D:409:VAL:C	2.48	0.57
1:B:163:GLU:O	1:B:231:PHE:HB3	2.05	0.57
1:C:194:ARG:O	1:C:198:LEU:HB2	2.05	0.57
1:A:347:ARG:HG3	1:A:381:LEU:HD11	1.86	0.57
1:C:207:LEU:HD21	1:C:323:LEU:HD11	1.86	0.57
1:C:347:ARG:CG	1:C:381:LEU:HD11	2.35	0.57
1:D:242:MET:HB2	1:D:247:GLY:HA2	1.85	0.57
1:C:207:LEU:HD11	1:C:271:ILE:HG21	1.87	0.56
1:E:271:ILE:HB	1:E:315:ALA:HB1	1.86	0.56
1:A:250:ARG:O	1:A:254:LEU:HB2	2.05	0.56
1:A:289:GLU:HB3	1:A:290:ARG:HA	1.87	0.56
1:D:298:LEU:HD21	1:D:327:LEU:HD23	1.87	0.56
1:A:211:PRO:O	1:A:214:THR:CG2	2.53	0.56
1:C:361:ALA:O	1:C:363:ASP:N	2.38	0.56
1:E:239:PHE:HB3	1:E:293:THR:CG2	2.36	0.56
1:E:248:ALA:O	1:E:251:VAL:N	2.38	0.56
1:B:184:GLU:C	1:B:188:PHE:CE2	2.83	0.56
1:C:405:LEU:O	1:C:409:VAL:HG23	2.06	0.56
1:D:390:LEU:O	1:D:394:ARG:HG3	2.06	0.56
1:D:289:GLU:CG	1:D:290:ARG:N	2.67	0.56
1:A:266:ILE:CB	1:A:313:VAL:HG23	2.34	0.56
1:D:271:ILE:CG2	1:D:317:THR:HB	2.36	0.56
1:B:296:GLN:HE21	1:B:296:GLN:HA	1.71	0.56
1:A:195:TYR:HB3	1:A:200:ALA:HB3	1.87	0.56
1:B:174:GLY:HA3	1:B:349:GLU:OE2	2.06	0.56
1:D:289:GLU:C	1:D:291:GLU:N	2.64	0.56
1:E:178:ALA:C	1:E:180:GLU:H	2.13	0.56
1:A:294:LEU:C	1:A:296:GLN:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HD12	1:A:366:LEU:HD11	1.86	0.55
1:A:185:ILE:HD11	1:A:206:VAL:HG21	1.86	0.55
1:E:294:LEU:O	1:E:296:GLN:N	2.36	0.55
1:B:219:LEU:O	1:B:221:LYS:N	2.40	0.55
1:B:239:PHE:CD2	1:B:293:THR:HG21	2.42	0.55
1:C:348:VAL:HG23	1:C:370:ALA:CB	2.36	0.55
1:B:182:VAL:HG11	1:B:219:LEU:HD21	1.88	0.55
1:C:342:PRO:O	1:C:347:ARG:HD2	2.06	0.55
1:D:402:GLN:HG3	1:D:406:LYS:HE3	1.89	0.55
1:C:343:ASP:N	1:C:343:ASP:OD1	2.34	0.55
1:D:172:MET:HG3	2:D:4:ADP:N1	2.21	0.55
1:E:240:ILE:C	1:E:242:MET:H	2.13	0.55
1:E:262:ALA:HA	1:E:263:PRO:C	2.32	0.55
1:A:267:PHE:CE2	1:A:269:ASP:HB2	2.42	0.55
1:C:214:THR:CG2	1:C:339:VAL:HG22	2.32	0.55
1:D:347:ARG:NH1	1:D:373:THR:O	2.40	0.55
1:D:373:THR:HG23	1:D:376:LEU:HD12	1.88	0.55
1:E:213:GLY:O	1:E:377:ALA:HB1	2.06	0.55
1:B:210:GLY:HA3	1:B:339:VAL:O	2.07	0.54
1:D:227:ALA:HB3	1:D:229:VAL:HG22	1.89	0.54
1:D:173:ALA:H	2:D:4:ADP:HN61	1.52	0.54
1:E:239:PHE:HB3	1:E:293:THR:HG21	1.88	0.54
1:B:195:TYR:OH	1:C:394:ARG:HA	2.07	0.54
1:D:160:ILE:O	1:D:161:ASN:ND2	2.41	0.54
1:C:407:GLU:C	1:C:408:ALA:O	2.50	0.54
1:D:209:VAL:HG21	1:D:320:PRO:HG3	1.90	0.54
1:D:271:ILE:HG23	1:D:272:ASP:N	2.22	0.54
1:B:213:GLY:O	1:B:377:ALA:HB1	2.07	0.54
1:C:188:PHE:HB3	1:C:202:ILE:HD12	1.90	0.54
1:A:364:VAL:HA	1:A:402:GLN:OE1	2.07	0.54
1:A:354:HIS:CD2	1:A:382:ALA:HB2	2.42	0.54
1:C:374:ALA:C	1:C:376:LEU:H	2.15	0.54
1:D:346:GLY:O	1:D:347:ARG:C	2.51	0.54
1:A:211:PRO:HG3	1:A:341:LYS:HG3	1.90	0.54
1:A:215:GLY:N	2:A:1:ADP:O2A	2.41	0.54
1:E:302:ASP:C	1:E:304:PHE:H	2.16	0.54
1:D:276:LYS:H	1:D:276:LYS:CE	2.20	0.54
1:B:182:VAL:O	1:B:185:ILE:N	2.41	0.53
1:D:259:LYS:O	1:D:261:GLN:N	2.40	0.53
1:E:289:GLU:O	1:E:290:ARG:C	2.51	0.53
1:B:408:ALA:O	1:B:409:VAL:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ALA:HB2	1:E:353:VAL:HG21	1.89	0.53
1:A:401:ARG:N	1:A:404:HIS:HD2	2.05	0.53
1:B:178:ALA:O	1:B:182:VAL:HG22	2.08	0.53
1:C:360:LEU:HB3	1:C:364:VAL:HG21	1.89	0.53
1:B:184:GLU:O	1:B:188:PHE:CE2	2.61	0.53
1:B:266:ILE:HB	1:B:313:VAL:HB	1.90	0.53
1:C:294:LEU:HD23	1:C:298:LEU:CD1	2.38	0.53
1:D:184:GLU:O	1:D:187:ASP:HB2	2.09	0.53
1:E:173:ALA:HB2	1:E:353:VAL:CG2	2.39	0.53
1:B:167:VAL:O	1:B:222:ALA:HA	2.08	0.53
1:A:239:PHE:HZ	1:A:250:ARG:CB	2.13	0.53
1:E:248:ALA:O	1:E:250:ARG:N	2.41	0.53
1:D:255:PHE:CD1	1:D:300:GLU:HG3	2.43	0.53
1:D:272:ASP:O	1:D:272:ASP:OD2	2.27	0.53
1:D:330:PRO:HA	1:D:334:ASP:OD1	2.09	0.53
1:D:367:GLN:O	1:D:370:ALA:HB3	2.09	0.53
1:B:274:ILE:O	1:B:294:LEU:HD22	2.08	0.53
1:C:342:PRO:HG2	1:C:347:ARG:HG3	1.89	0.53
1:E:248:ALA:O	1:E:249:SER:C	2.52	0.53
1:B:183:VAL:HA	1:B:186:VAL:HG23	1.90	0.52
1:B:188:PHE:CD1	1:B:202:ILE:HG21	2.44	0.52
1:C:167:VAL:O	1:C:168:ARG:HD2	2.09	0.52
1:E:305:GLY:O	1:E:307:GLU:HG3	2.09	0.52
1:A:330:PRO:HA	1:A:334:ASP:HB3	1.91	0.52
1:B:347:ARG:HD3	1:B:381:LEU:HD11	1.91	0.52
1:D:354:HIS:CD2	2:D:4:ADP:H8	2.28	0.52
1:C:214:THR:HG23	1:C:214:THR:O	2.08	0.52
1:A:207:LEU:HG	1:A:208:LEU:N	2.24	0.52
1:D:387:GLU:HB2	1:D:411:ARG:HH21	1.74	0.52
1:E:411:ARG:HD3	1:E:413:ILE:HD12	1.91	0.52
1:A:276:LYS:HE3	1:A:291:GLU:HG3	1.91	0.52
1:C:205:GLY:HA2	1:C:313:VAL:O	2.10	0.52
1:B:263:PRO:HG3	1:B:310:PRO:HG2	1.91	0.52
1:C:184:GLU:HB3	1:D:394:ARG:HE	1.75	0.52
1:B:216:LYS:CE	1:B:316:ALA:HB1	2.40	0.52
1:C:262:ALA:HB2	1:C:311:VAL:HG23	1.92	0.52
1:D:302:ASP:C	1:D:304:PHE:H	2.18	0.52
1:D:401:ARG:HH11	1:D:401:ARG:CG	2.22	0.52
1:A:211:PRO:O	1:A:214:THR:HG21	2.11	0.51
1:B:224:ALA:HB2	1:B:265:ILE:CD1	2.38	0.51
1:B:319:ARG:HD3	1:B:322:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ASN:OD1	1:B:396:ASN:O	2.28	0.51
1:E:378:GLY:HA2	1:E:381:LEU:HD12	1.90	0.51
1:B:301:MET:SD	1:B:333:PHE:CE1	3.03	0.51
1:C:405:LEU:HD22	1:C:405:LEU:N	2.25	0.51
1:A:361:ALA:CB	1:A:401:ARG:HA	2.40	0.51
1:D:204:LYS:HZ2	1:D:331:GLY:HA2	1.75	0.51
1:A:290:ARG:C	1:A:292:GLN:H	2.18	0.51
1:A:342:PRO:HB2	1:A:346:GLY:HA3	1.92	0.51
1:C:397:GLN:CG	1:C:401:ARG:NH2	2.74	0.51
1:D:397:GLN:HE21	1:D:401:ARG:HH21	1.58	0.51
1:E:163:GLU:O	1:E:230:PRO:HA	2.11	0.51
1:E:222:ALA:O	1:E:225:GLY:N	2.43	0.51
1:C:194:ARG:CZ	1:D:396:ASN:ND2	2.73	0.51
1:E:323:LEU:HD22	1:E:327:LEU:CD1	2.41	0.51
1:A:365:ASN:C	1:A:365:ASN:HD22	2.19	0.51
1:C:207:LEU:CD2	1:C:323:LEU:HD11	2.40	0.51
1:C:294:LEU:CD2	1:C:298:LEU:CD1	2.85	0.51
1:B:323:LEU:HB3	1:B:328:MET:HE1	1.93	0.51
1:C:274:ILE:HD11	1:C:297:LEU:HD22	1.92	0.51
1:C:405:LEU:N	1:C:405:LEU:CD2	2.74	0.50
1:D:294:LEU:HG	1:D:295:ASN:H	1.76	0.50
1:C:165:PRO:HG3	1:C:224:ALA:HB3	1.94	0.50
1:A:344:PHE:O	1:A:348:VAL:HG23	2.10	0.50
1:C:411:ARG:O	1:C:413:ILE:N	2.43	0.50
1:D:163:GLU:HB3	1:D:231:PHE:HB3	1.94	0.50
1:D:184:GLU:O	1:D:188:PHE:HD2	1.94	0.50
1:D:262:ALA:HA	1:D:263:PRO:C	2.36	0.50
1:E:266:ILE:HB	1:E:313:VAL:HB	1.94	0.50
1:A:270:GLU:O	1:A:273:ALA:HB3	2.12	0.50
1:B:180:GLU:OE1	1:B:180:GLU:HA	2.11	0.50
1:E:240:ILE:C	1:E:242:MET:N	2.67	0.50
1:B:379:ALA:HA	2:B:2:ADP:H1'	1.94	0.50
1:D:321:GLU:CD	1:D:321:GLU:H	2.20	0.50
1:E:169:PHE:HD1	1:E:226:GLU:HG2	1.77	0.50
1:E:269:ASP:OD1	1:E:270:GLU:N	2.45	0.50
1:B:204:LYS:HE2	1:B:303:GLY:H	1.75	0.49
1:A:347:ARG:HG3	1:A:381:LEU:CD1	2.42	0.49
1:A:374:ALA:H	1:A:376:LEU:HD23	1.77	0.49
1:B:176:GLU:O	1:B:180:GLU:HG2	2.11	0.49
1:C:397:GLN:HE21	1:C:397:GLN:HA	1.77	0.49
1:D:184:GLU:HB2	1:E:394:ARG:NH2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ASN:HA	1:E:177:GLU:OE1	2.12	0.49
1:C:177:GLU:O	1:C:180:GLU:N	2.45	0.49
1:D:258:ALA:HB3	1:D:266:ILE:HD11	1.93	0.49
1:C:405:LEU:CD2	1:C:405:LEU:H	2.25	0.49
1:B:372:LEU:HD13	1:B:406:LYS:HD3	1.95	0.49
1:D:169:PHE:HD1	1:D:226:GLU:CG	2.24	0.49
1:D:274:ILE:HD11	1:D:297:LEU:HD12	1.94	0.49
1:A:301:MET:SD	1:A:313:VAL:HG11	2.52	0.49
1:C:347:ARG:NE	1:C:373:THR:O	2.41	0.49
1:C:402:GLN:O	1:C:403:GLN:C	2.53	0.49
1:D:172:MET:HE1	1:D:219:LEU:HD22	1.95	0.49
1:E:254:LEU:HD21	1:E:266:ILE:HG23	1.95	0.49
1:A:186:VAL:HG13	1:A:227:ALA:HB2	1.94	0.49
1:A:262:ALA:HA	1:A:263:PRO:C	2.37	0.49
1:A:387:GLU:OE1	1:A:387:GLU:HA	2.13	0.49
1:B:185:ILE:HG23	1:B:312:ILE:HD13	1.94	0.49
1:C:234:MET:HG2	1:C:254:LEU:HD22	1.95	0.49
1:A:411:ARG:C	1:A:413:ILE:H	2.20	0.48
1:D:347:ARG:H	1:D:347:ARG:HD3	1.77	0.48
1:D:355:ILE:CG1	1:D:360:LEU:HD11	2.43	0.48
1:E:252:ARG:HG3	1:E:296:GLN:OE1	2.12	0.48
1:C:200:ALA:HB2	1:D:389:ALA:CB	2.43	0.48
1:C:347:ARG:NH2	1:C:374:ALA:HB2	2.28	0.48
1:D:380:ASP:O	1:D:383:ASN:HB2	2.13	0.48
1:C:396:ASN:O	1:C:396:ASN:OD1	2.31	0.48
1:A:175:ASN:HB3	1:A:178:ALA:HB3	1.95	0.48
1:B:347:ARG:CZ	1:B:374:ALA:HA	2.43	0.48
1:C:201:LYS:HE3	1:C:204:LYS:NZ	2.28	0.48
1:D:276:LYS:C	1:D:276:LYS:CD	2.85	0.48
1:E:247:GLY:O	1:E:248:ALA:C	2.57	0.48
1:A:215:GLY:O	1:A:216:LYS:C	2.56	0.48
1:A:352:LYS:O	1:A:355:ILE:HG22	2.13	0.48
1:E:227:ALA:HB3	1:E:229:VAL:HG22	1.95	0.48
1:E:257:THR:O	1:E:258:ALA:C	2.56	0.48
1:B:164:LYS:HG3	1:B:164:LYS:O	2.13	0.48
1:E:161:ASN:HB2	1:E:257:THR:HG21	1.94	0.48
1:E:240:ILE:HG13	1:E:241:GLU:N	2.27	0.48
1:E:289:GLU:O	1:E:291:GLU:N	2.47	0.48
1:C:274:ILE:O	1:C:294:LEU:CD1	2.62	0.48
1:D:214:THR:HG22	1:D:216:LYS:HZ2	1.79	0.48
1:D:248:ALA:O	1:D:250:ARG:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:ALA:C	1:C:410:GLU:N	2.71	0.47
1:D:291:GLU:O	1:D:292:GLN:C	2.57	0.47
1:B:219:LEU:C	1:B:221:LYS:N	2.72	0.47
1:D:184:GLU:O	1:D:188:PHE:CD2	2.67	0.47
1:D:418:LYS:H	1:D:418:LYS:HD3	1.79	0.47
1:E:240:ILE:O	1:E:242:MET:N	2.47	0.47
1:B:350:ILE:HD12	2:B:2:ADP:N6	2.29	0.47
1:C:401:ARG:NH1	1:C:401:ARG:CG	2.77	0.47
1:A:169:PHE:H	1:A:226:GLU:CD	2.21	0.47
1:D:271:ILE:HG23	1:D:272:ASP:H	1.80	0.47
1:A:359:LYS:O	1:A:360:LEU:HD23	2.14	0.47
1:A:374:ALA:N	1:A:376:LEU:HD23	2.30	0.47
1:B:185:ILE:HA	1:B:188:PHE:CE2	2.49	0.47
1:B:268:ILE:CG2	1:B:271:ILE:HB	2.45	0.47
1:B:391:LEU:HA	1:B:394:ARG:CG	2.44	0.47
1:C:273:ALA:O	1:C:290:ARG:CZ	2.62	0.47
1:D:384:ILE:HD13	1:D:409:VAL:HG22	1.95	0.47
1:E:290:ARG:H	1:E:290:ARG:HD3	1.79	0.47
1:E:298:LEU:H	1:E:298:LEU:CD1	2.26	0.47
1:E:329:ARG:HG2	1:E:330:PRO:HD2	1.97	0.47
1:A:271:ILE:C	1:A:273:ALA:N	2.72	0.47
1:C:184:GLU:OE1	1:C:335:ARG:NH2	2.48	0.47
1:D:402:GLN:HE21	1:D:406:LYS:HE3	1.79	0.47
1:A:232:PHE:HE1	1:A:264:SER:HB2	1.80	0.47
1:A:365:ASN:N	1:A:402:GLN:OE1	2.46	0.47
1:B:306:SER:C	1:B:308:ASN:H	2.22	0.47
1:B:388:ALA:O	1:B:392:ALA:HB2	2.14	0.47
1:C:397:GLN:HA	1:C:397:GLN:NE2	2.29	0.47
1:C:401:ARG:HH11	1:C:401:ARG:CG	2.26	0.47
1:D:186:VAL:HG11	1:D:226:GLU:HB3	1.97	0.47
1:A:294:LEU:HG	1:A:295:ASN:H	1.79	0.47
1:C:298:LEU:HD23	1:C:332:ARG:NH1	2.29	0.47
1:D:344:PHE:HA	1:D:347:ARG:NH2	2.30	0.47
1:D:328:MET:O	1:D:329:ARG:HB2	2.14	0.47
1:E:185:ILE:O	1:E:188:PHE:HB2	2.14	0.47
1:E:349:GLU:HA	1:E:352:LYS:HB2	1.96	0.47
1:D:239:PHE:O	1:D:241:GLU:N	2.45	0.47
1:D:255:PHE:HD1	1:D:300:GLU:HG3	1.79	0.47
1:D:373:THR:HG21	1:D:381:LEU:CD2	2.21	0.47
1:D:204:LYS:HD2	1:D:301:MET:O	2.15	0.46
1:D:259:LYS:C	1:D:261:GLN:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:VAL:C	1:C:168:ARG:HD2	2.40	0.46
1:C:254:LEU:HG	1:C:266:ILE:HD12	1.97	0.46
1:D:180:GLU:O	1:D:183:VAL:HG12	2.15	0.46
1:D:276:LYS:HE2	1:D:290:ARG:NE	2.30	0.46
1:E:290:ARG:HD3	1:E:290:ARG:N	2.31	0.46
1:B:165:PRO:HD3	1:B:231:PHE:CB	2.44	0.46
1:C:298:LEU:HB3	1:C:332:ARG:NE	2.30	0.46
1:C:328:MET:HE2	1:C:328:MET:HB3	1.75	0.46
1:E:332:ARG:HG3	1:E:332:ARG:HH11	1.80	0.46
1:A:172:MET:HE1	1:A:175:ASN:HB2	1.96	0.46
1:A:202:ILE:CD1	1:A:310:PRO:HB3	2.46	0.46
1:B:219:LEU:C	1:B:221:LYS:H	2.23	0.46
1:B:231:PHE:CG	1:B:231:PHE:O	2.67	0.46
1:A:257:THR:O	1:A:261:GLN:HG2	2.15	0.46
1:C:254:LEU:HG	1:C:266:ILE:CD1	2.45	0.46
1:E:301:MET:SD	1:E:333:PHE:CE1	3.09	0.46
1:D:206:VAL:HG13	1:D:335:ARG:HG3	1.96	0.46
1:B:205:GLY:O	1:B:333:PHE:HA	2.16	0.46
1:C:210:GLY:O	1:C:216:LYS:NZ	2.48	0.46
1:D:186:VAL:HG12	1:D:227:ALA:HB2	1.96	0.46
1:E:254:LEU:HD21	1:E:266:ILE:CG2	2.46	0.46
1:E:355:ILE:HD12	1:E:385:ILE:HD13	1.98	0.46
1:B:184:GLU:O	1:B:188:PHE:CD2	2.69	0.46
1:C:201:LYS:HE3	1:C:204:LYS:HZ1	1.81	0.46
1:C:209:VAL:O	1:C:338:LEU:HA	2.16	0.46
1:D:184:GLU:CB	1:E:394:ARG:HH21	2.29	0.46
1:A:289:GLU:HA	1:A:292:GLN:HB3	1.98	0.46
1:C:347:ARG:HG2	1:C:381:LEU:HD11	1.98	0.46
1:E:301:MET:HE2	1:E:301:MET:HB3	1.58	0.46
1:B:167:VAL:C	1:B:168:ARG:HE	2.24	0.45
1:B:401:ARG:HG3	1:B:403:GLN:HB3	1.97	0.45
1:C:394:ARG:HG2	1:C:394:ARG:HH11	1.81	0.45
1:D:235:GLY:HA3	1:D:238:SER:HB3	1.98	0.45
1:E:295:ASN:O	1:E:299:ALA:HB2	2.16	0.45
1:B:167:VAL:O	1:B:225:GLY:HA3	2.15	0.45
1:B:386:ASN:O	1:B:390:LEU:HB2	2.16	0.45
1:B:168:ARG:HG3	1:B:226:GLU:OE1	2.16	0.45
1:B:178:ALA:C	1:B:180:GLU:H	2.24	0.45
1:B:210:GLY:O	1:B:318:ASN:ND2	2.41	0.45
1:B:213:GLY:HA2	2:B:2:ADP:O5'	2.16	0.45
1:C:227:ALA:C	1:C:228:HIS:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ASN:C	1:C:364:VAL:N	2.75	0.45
1:D:391:LEU:HD21	1:D:407:GLU:HG2	1.97	0.45
1:E:189:LEU:HD21	1:E:312:ILE:HG13	1.96	0.45
1:E:293:THR:O	1:E:294:LEU:C	2.59	0.45
1:A:223:VAL:O	1:A:224:ALA:C	2.59	0.45
1:D:383:ASN:HB3	1:D:411:ARG:CZ	2.46	0.45
1:A:246:LEU:HD22	1:A:246:LEU:H	1.82	0.45
1:B:301:MET:SD	1:B:333:PHE:HE1	2.40	0.45
1:C:248:ALA:HB2	1:C:292:GLN:HE21	1.81	0.45
1:D:293:THR:O	1:D:294:LEU:O	2.35	0.45
1:E:294:LEU:HG	1:E:295:ASN:H	1.81	0.45
1:E:395:ASN:O	1:E:396:ASN:C	2.58	0.45
1:A:309:ALA:HA	1:A:310:PRO:HD3	1.83	0.45
1:A:334:ASP:OD2	1:A:334:ASP:N	2.45	0.45
1:C:351:LEU:CD2	1:C:369:VAL:CG2	2.94	0.45
1:D:288:ASP:HB3	1:D:289:GLU:H	1.50	0.45
1:D:378:GLY:C	1:D:380:ASP:N	2.72	0.45
1:E:209:VAL:HG21	1:E:320:PRO:HG3	1.97	0.45
1:A:418:LYS:HD3	1:A:418:LYS:H	1.82	0.45
1:C:263:PRO:HA	1:C:310:PRO:O	2.16	0.45
1:D:214:THR:HG22	1:D:216:LYS:NZ	2.31	0.45
1:E:258:ALA:O	1:E:259:LYS:C	2.60	0.45
1:A:211:PRO:O	1:A:214:THR:HG22	2.17	0.45
1:E:222:ALA:O	1:E:224:ALA:N	2.50	0.45
1:E:232:PHE:CE1	1:E:258:ALA:HA	2.51	0.45
1:A:186:VAL:HG22	1:A:223:VAL:HG13	1.99	0.44
1:C:177:GLU:C	1:C:179:LYS:H	2.25	0.44
1:E:182:VAL:HA	1:E:185:ILE:HD12	1.99	0.44
1:E:294:LEU:C	1:E:296:GLN:N	2.75	0.44
1:A:252:ARG:HG2	1:A:300:GLU:OE1	2.17	0.44
1:A:373:THR:HG21	1:A:381:LEU:CD2	2.42	0.44
1:C:173:ALA:HB1	1:C:349:GLU:HG3	1.99	0.44
1:D:173:ALA:N	2:D:4:ADP:HN62	2.12	0.44
1:E:323:LEU:HD22	1:E:327:LEU:HD11	1.99	0.44
1:E:381:LEU:O	1:E:382:ALA:C	2.60	0.44
1:B:162:ALA:HA	1:B:232:PHE:HD2	1.83	0.44
1:A:217:THR:HB	2:A:1:ADP:O1A	2.17	0.44
1:B:182:VAL:HG21	1:B:219:LEU:HD11	1.99	0.44
1:B:263:PRO:HA	1:B:310:PRO:O	2.18	0.44
1:B:206:VAL:HG12	1:B:207:LEU:N	2.33	0.44
1:B:342:PRO:HB2	1:B:346:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLU:O	1:B:353:VAL:HG23	2.18	0.44
1:C:387:GLU:CB	1:C:387:GLU:CD	2.80	0.44
1:C:408:ALA:O	1:C:410:GLU:N	2.50	0.44
1:D:262:ALA:HB1	1:D:263:PRO:HA	1.98	0.44
1:E:206:VAL:HB	1:E:314:LEU:HD23	1.99	0.44
1:A:171:ASP:OD2	1:A:171:ASP:N	2.50	0.44
1:A:351:LEU:HD21	1:A:369:VAL:HB	1.99	0.44
1:C:271:ILE:HB	1:C:315:ALA:HB1	2.00	0.44
1:A:172:MET:HE2	1:A:179:LYS:HE2	1.98	0.44
1:A:347:ARG:CZ	1:A:374:ALA:HA	2.47	0.44
1:C:177:GLU:HG2	1:C:178:ALA:H	1.83	0.44
1:D:298:LEU:CD2	1:D:327:LEU:HD23	2.48	0.44
1:D:348:VAL:O	1:D:351:LEU:HB2	2.18	0.44
1:C:167:VAL:HG12	1:C:222:ALA:HA	2.00	0.43
1:C:177:GLU:C	1:C:179:LYS:N	2.76	0.43
1:C:388:ALA:C	1:C:390:LEU:N	2.76	0.43
1:D:289:GLU:HA	1:D:292:GLN:HB2	1.99	0.43
1:E:402:GLN:HE21	1:E:402:GLN:HB3	1.51	0.43
1:B:216:LYS:HZ1	1:B:317:THR:N	2.15	0.43
1:E:267:PHE:HA	1:E:314:LEU:O	2.18	0.43
1:E:335:ARG:HH11	1:E:335:ARG:HB2	1.83	0.43
1:E:363:ASP:HB2	1:E:402:GLN:H	1.82	0.43
1:C:309:ALA:HA	1:C:310:PRO:HD3	1.82	0.43
1:A:181:GLU:HB3	1:A:337:VAL:HG22	2.01	0.43
1:A:324:ASP:HA	1:A:325:PRO:HD2	1.89	0.43
1:B:186:VAL:HG11	1:B:226:GLU:CB	2.46	0.43
1:B:275:GLY:HA3	1:B:327:LEU:HD11	2.00	0.43
1:C:297:LEU:HD23	1:C:327:LEU:CD2	2.46	0.43
1:D:169:PHE:HD2	1:D:179:LYS:HE2	1.83	0.43
1:D:240:ILE:O	1:D:240:ILE:HG13	2.18	0.43
1:A:211:PRO:HD2	1:A:340:ASP:HA	2.00	0.43
1:A:265:ILE:HG21	1:A:314:LEU:HD12	2.01	0.43
1:C:354:HIS:O	1:C:385:ILE:HG21	2.18	0.43
1:D:364:VAL:HA	1:D:402:GLN:OE1	2.18	0.43
1:A:298:LEU:HD23	1:A:332:ARG:CZ	2.49	0.43
1:B:198:LEU:HG	1:C:400:VAL:HG23	2.00	0.43
1:B:289:GLU:HG2	1:B:290:ARG:H	1.83	0.43
1:B:298:LEU:HD21	1:B:327:LEU:HD23	2.01	0.43
1:B:411:ARG:C	1:B:413:ILE:N	2.74	0.43
1:C:218:LEU:HD22	2:C:3:ADP:H2'	1.99	0.43
1:B:216:LYS:HE3	1:B:216:LYS:HB3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PHE:O	1:B:268:ILE:HG13	2.18	0.43
1:C:258:ALA:HB2	1:C:266:ILE:HD11	2.00	0.43
1:C:376:LEU:HD23	1:C:376:LEU:HA	1.75	0.43
1:D:291:GLU:OE2	1:E:241:GLU:OE2	2.37	0.43
1:C:172:MET:HE2	1:C:219:LEU:HD13	2.01	0.43
1:C:240:ILE:HG12	1:C:290:ARG:HH22	1.83	0.43
1:C:267:PHE:CE2	1:C:269:ASP:HB2	2.53	0.43
1:E:274:ILE:HD11	1:E:297:LEU:HD22	2.01	0.43
1:A:185:ILE:CD1	1:A:206:VAL:HG21	2.49	0.43
1:A:201:LYS:HB3	1:B:386:ASN:OD1	2.19	0.43
1:A:398:LYS:HA	1:A:398:LYS:HD3	1.74	0.43
1:D:230:PRO:HG2	1:D:264:SER:HB3	2.00	0.43
1:A:387:GLU:OE1	1:A:387:GLU:CA	2.67	0.43
1:C:381:LEU:HD23	1:C:381:LEU:HA	1.45	0.43
1:D:210:GLY:O	1:D:216:LYS:NZ	2.52	0.43
1:E:381:LEU:C	1:E:383:ASN:N	2.76	0.43
1:C:207:LEU:HD12	1:C:207:LEU:HA	1.81	0.42
1:D:270:GLU:O	1:D:272:ASP:N	2.52	0.42
1:A:173:ALA:H	2:A:1:ADP:HN62	1.67	0.42
1:A:177:GLU:CD	1:A:178:ALA:H	2.27	0.42
1:D:180:GLU:C	1:D:182:VAL:H	2.27	0.42
1:D:227:ALA:O	1:D:228:HIS:C	2.62	0.42
1:E:222:ALA:C	1:E:224:ALA:N	2.76	0.42
1:B:309:ALA:HA	1:B:310:PRO:HD3	1.91	0.42
1:C:191:TYR:CD1	1:C:194:ARG:NH1	2.88	0.42
1:D:232:PHE:HB2	1:D:266:ILE:HA	2.02	0.42
1:D:294:LEU:O	1:D:296:GLN:N	2.52	0.42
1:E:271:ILE:O	1:E:271:ILE:HG13	2.18	0.42
1:E:172:MET:CE	1:E:219:LEU:HD13	2.46	0.42
1:B:268:ILE:HG22	1:B:271:ILE:HB	2.01	0.42
1:C:294:LEU:C	1:C:296:GLN:H	2.28	0.42
1:C:354:HIS:HB2	1:C:385:ILE:HD12	2.01	0.42
1:C:376:LEU:HD13	1:C:380:ASP:HB3	2.01	0.42
1:C:388:ALA:O	1:C:390:LEU:N	2.53	0.42
1:A:266:ILE:CG2	1:A:313:VAL:HG23	2.50	0.42
1:C:392:ALA:O	1:C:395:ASN:N	2.52	0.42
1:D:309:ALA:HA	1:D:310:PRO:HD3	1.91	0.42
1:D:343:ASP:O	1:D:344:PHE:C	2.63	0.42
1:D:344:PHE:HA	1:D:347:ARG:HH21	1.83	0.42
1:E:209:VAL:HB	1:E:317:THR:HG23	2.02	0.42
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASP:H	1:B:346:GLY:HA3	1.85	0.42
1:D:207:LEU:HB3	1:D:336:GLN:HA	2.02	0.42
1:D:208:LEU:O	1:D:316:ALA:HA	2.20	0.42
1:E:275:GLY:O	1:E:276:LYS:C	2.63	0.42
1:A:289:GLU:CB	1:A:290:ARG:HA	2.49	0.42
1:B:291:GLU:HG2	1:B:294:LEU:HD23	2.01	0.42
1:D:276:LYS:HE2	1:D:290:ARG:CZ	2.50	0.42
1:E:297:LEU:O	1:E:298:LEU:C	2.62	0.42
1:A:369:VAL:C	1:A:371:LYS:N	2.78	0.42
1:C:402:GLN:HE21	1:C:402:GLN:HB2	1.56	0.42
1:D:258:ALA:HB2	1:D:266:ILE:HD11	1.98	0.42
1:C:234:MET:HE2	1:C:254:LEU:HB2	2.02	0.41
1:C:394:ARG:HG2	1:C:394:ARG:NH1	2.35	0.41
1:A:172:MET:HE3	1:A:175:ASN:HB2	2.03	0.41
1:B:386:ASN:O	1:B:390:LEU:N	2.35	0.41
1:C:173:ALA:HB2	1:C:353:VAL:CG2	2.36	0.41
1:C:362:ASN:C	1:C:364:VAL:H	2.28	0.41
1:E:161:ASN:O	1:E:162:ALA:HB2	2.20	0.41
1:E:260:LYS:HE3	1:E:261:GLN:HE21	1.85	0.41
1:E:345:ASN:OD1	1:E:345:ASN:N	2.51	0.41
1:A:351:LEU:O	1:A:355:ILE:HB	2.21	0.41
1:C:175:ASN:O	1:C:179:LYS:HG2	2.21	0.41
1:C:231:PHE:CZ	1:C:267:PHE:HB2	2.55	0.41
1:C:240:ILE:HG23	1:C:290:ARG:CZ	2.50	0.41
1:C:253:ASP:O	1:C:256:GLU:HB3	2.20	0.41
1:D:180:GLU:O	1:D:182:VAL:N	2.53	0.41
1:E:187:ASP:C	1:E:189:LEU:H	2.28	0.41
1:E:289:GLU:HA	1:E:292:GLN:HG3	2.03	0.41
1:A:407:GLU:C	1:A:408:ALA:O	2.61	0.41
1:B:407:GLU:O	1:B:408:ALA:O	2.38	0.41
1:B:411:ARG:HB3	1:B:413:ILE:HG13	2.02	0.41
1:C:172:MET:HE1	1:C:219:LEU:HB2	2.01	0.41
1:D:358:VAL:HG12	1:D:359:LYS:N	2.36	0.41
1:D:410:GLU:O	1:D:413:ILE:HD11	2.20	0.41
1:A:275:GLY:HA2	1:A:294:LEU:HD22	2.02	0.41
1:B:181:GLU:HB3	1:B:335:ARG:NH2	2.35	0.41
1:B:361:ALA:C	1:B:363:ASP:H	2.28	0.41
1:E:223:VAL:O	1:E:223:VAL:HG12	2.20	0.41
1:A:276:LYS:HD3	1:A:290:ARG:HD3	2.01	0.41
1:A:388:ALA:O	1:A:391:LEU:HB3	2.20	0.41
1:B:168:ARG:NH2	1:B:225:GLY:CA	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:PRO:HG3	1:C:335:ARG:HH11	1.86	0.41
1:E:231:PHE:CE1	1:E:267:PHE:CB	3.03	0.41
1:E:361:ALA:HB2	1:E:399:GLU:HB3	2.03	0.41
1:A:350:ILE:HG22	1:A:354:HIS:HD2	1.86	0.41
1:C:392:ALA:HB3	1:C:393:GLY:H	1.46	0.41
1:C:397:GLN:NE2	1:C:397:GLN:CA	2.83	0.41
1:D:270:GLU:O	1:D:271:ILE:C	2.63	0.41
1:E:244:VAL:C	1:E:246:LEU:H	2.29	0.41
1:B:231:PHE:O	1:B:231:PHE:CD2	2.74	0.41
1:C:249:SER:O	1:C:252:ARG:N	2.53	0.41
1:D:295:ASN:O	1:D:296:GLN:C	2.64	0.41
1:E:392:ALA:C	1:E:394:ARG:H	2.29	0.41
1:A:172:MET:HE2	1:A:172:MET:HB3	1.83	0.41
1:A:276:LYS:CE	1:A:291:GLU:HG3	2.50	0.41
1:A:361:ALA:C	1:A:363:ASP:H	2.28	0.41
1:B:188:PHE:CE1	1:C:390:LEU:HD22	2.55	0.41
1:B:271:ILE:HG23	1:B:317:THR:HB	2.02	0.41
1:B:296:GLN:HA	1:B:296:GLN:NE2	2.33	0.41
1:B:306:SER:O	1:B:308:ASN:N	2.54	0.41
1:C:186:VAL:HG22	1:C:223:VAL:HG13	2.03	0.41
1:C:402:GLN:CG	1:C:406:LYS:NZ	2.83	0.41
1:D:173:ALA:HB3	1:D:350:ILE:HA	2.02	0.41
1:D:175:ASN:O	1:D:179:LYS:N	2.54	0.41
1:D:342:PRO:HB2	1:D:347:ARG:HD3	2.03	0.41
1:B:268:ILE:HG22	1:B:268:ILE:O	2.19	0.41
1:C:216:LYS:HB2	2:C:3:ADP:O3B	2.21	0.41
1:C:388:ALA:HB1	1:C:405:LEU:HD22	2.02	0.41
1:D:173:ALA:HB2	1:D:353:VAL:HG21	2.03	0.41
1:C:187:ASP:OD1	1:C:195:TYR:OH	2.33	0.40
1:A:396:ASN:O	1:A:397:GLN:C	2.64	0.40
1:C:177:GLU:O	1:C:179:LYS:N	2.55	0.40
1:E:215:GLY:O	1:E:216:LYS:C	2.65	0.40
1:E:234:MET:HG2	1:E:239:PHE:CZ	2.57	0.40
1:E:268:ILE:O	1:E:315:ALA:HA	2.21	0.40
1:A:189:LEU:HD11	1:A:265:ILE:HD11	2.02	0.40
1:C:172:MET:CE	1:C:219:LEU:HB2	2.52	0.40
1:C:406:LYS:NZ	1:C:406:LYS:CB	2.71	0.40
1:D:241:GLU:O	1:D:241:GLU:HG3	2.21	0.40
1:E:172:MET:HE2	1:E:219:LEU:HB2	2.02	0.40
1:E:234:MET:CE	1:E:254:LEU:HB2	2.51	0.40
1:E:346:GLY:O	1:E:350:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:O	1:A:169:PHE:C	2.65	0.40
1:A:275:GLY:O	1:A:276:LYS:C	2.64	0.40
1:E:231:PHE:CE1	1:E:267:PHE:HB2	2.57	0.40
1:E:289:GLU:HA	1:E:292:GLN:CG	2.52	0.40
1:B:208:LEU:N	1:B:315:ALA:O	2.53	0.40
1:C:405:LEU:H	1:C:405:LEU:HD23	1.87	0.40
1:E:222:ALA:O	1:E:223:VAL:C	2.64	0.40
1:E:271:ILE:CB	1:E:315:ALA:HB1	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	245/268 (91%)	191 (78%)	41 (17%)	13 (5%)	1	10
1	B	245/268 (91%)	173 (71%)	55 (22%)	17 (7%)	1	7
1	C	245/268 (91%)	174 (71%)	56 (23%)	15 (6%)	1	9
1	D	245/268 (91%)	176 (72%)	43 (18%)	26 (11%)	0	2
1	E	245/268 (91%)	163 (66%)	61 (25%)	21 (9%)	0	4
All	All	1225/1340 (91%)	877 (72%)	256 (21%)	92 (8%)	1	6

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	ALA
1	A	393	GLY
1	B	308	ASN
1	B	400	VAL
1	B	408	ALA
1	C	388	ALA

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Mol	Chain	Res	Type
1	C	389	ALA
1	C	408	ALA
1	D	248	ALA
1	D	249	SER
1	D	260	LYS
1	D	271	ILE
1	D	289	GLU
1	D	294	LEU
1	D	329	ARG
1	E	244	VAL
1	E	248	ALA
1	E	249	SER
1	E	289	GLU
1	E	290	ARG
1	E	294	LEU
1	E	364	VAL
1	E	396	ASN
1	E	397	GLN
1	A	198	LEU
1	A	289	GLU
1	A	402	GLN
1	B	220	ALA
1	B	243	PHE
1	B	303	GLY
1	B	307	GLU
1	B	413	ILE
1	C	170	LYS
1	C	178	ALA
1	C	290	ARG
1	C	362	ASN
1	C	392	ALA
1	C	412	GLY
1	C	415	GLY
1	D	240	ILE
1	D	241	GLU
1	D	272	ASP
1	D	408	ALA
1	E	163	GLU
1	E	179	LYS
1	E	198	LEU
1	E	271	ILE
1	E	400	VAL

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Mol	Chain	Res	Type
1	E	409	VAL
1	A	246	LEU
1	A	343	ASP
1	A	408	ALA
1	B	272	ASP
1	B	334	ASP
1	B	391	LEU
1	C	327	LEU
1	C	402	GLN
1	D	228	HIS
1	D	295	ASN
1	D	377	ALA
1	D	413	ILE
1	D	414	ALA
1	E	241	GLU
1	E	293	THR
1	E	343	ASP
1	A	272	ASP
1	A	409	VAL
1	B	232	PHE
1	B	399	GLU
1	B	417	GLU
1	D	378	GLY
1	E	334	ASP
1	A	201	LYS
1	B	273	ALA
1	B	335	ARG
1	C	304	PHE
1	C	321	GLU
1	D	194	ARG
1	D	290	ARG
1	D	384	ILE
1	E	273	ALA
1	D	412	GLY
1	E	393	GLY
1	D	346	GLY
1	D	348	VAL
1	D	409	VAL
1	A	400	VAL
1	B	268	ILE
1	D	400	VAL
1	A	412	GLY

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Mol	Chain	Res	Type
1	C	240	ILE
1	D	303	GLY

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	198/212 (93%)	167 (84%)	31 (16%)	2	12
1	B	198/212 (93%)	169 (85%)	29 (15%)	3	14
1	C	198/212 (93%)	160 (81%)	38 (19%)	1	7
1	D	198/212 (93%)	159 (80%)	39 (20%)	1	6
1	E	198/212 (93%)	160 (81%)	38 (19%)	1	7
All	All	990/1060 (93%)	815 (82%)	175 (18%)	2	8

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ILE
1	A	164	LYS
1	A	168	ARG
1	A	170	LYS
1	A	172	MET
1	A	202	ILE
1	A	208	LEU
1	A	209	VAL
1	A	214	THR
1	A	226	GLU
1	A	237	SER
1	A	246	LEU
1	A	290	ARG
1	A	292	GLN
1	A	297	LEU
1	A	302	ASP
1	A	304	PHE

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Mol	Chain	Res	Type
1	A	312	ILE
1	A	323	LEU
1	A	329	ARG
1	A	350	ILE
1	A	355	ILE
1	A	364	VAL
1	A	385	ILE
1	A	387	GLU
1	A	395	ASN
1	A	398	LYS
1	A	401	ARG
1	A	405	LEU
1	A	409	VAL
1	A	418	LYS
1	B	163	GLU
1	B	166	ASN
1	B	168	ARG
1	B	170	LYS
1	B	190	LYS
1	B	198	LEU
1	B	202	ILE
1	B	209	VAL
1	B	241	GLU
1	B	246	LEU
1	B	256	GLU
1	B	268	ILE
1	B	270	GLU
1	B	271	ILE
1	B	293	THR
1	B	296	GLN
1	B	298	LEU
1	B	304	PHE
1	B	308	ASN
1	B	313	VAL
1	B	321	GLU
1	B	323	LEU
1	B	328	MET
1	B	336	GLN
1	B	351	LEU
1	B	387	GLU
1	B	390	LEU
1	B	399	GLU

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Mol	Chain	Res	Type
1	B	413	ILE
1	C	163	GLU
1	C	164	LYS
1	C	170	LYS
1	C	172	MET
1	C	184	GLU
1	C	208	LEU
1	C	209	VAL
1	C	214	THR
1	C	228	HIS
1	C	233	SER
1	C	234	MET
1	C	237	SER
1	C	240	ILE
1	C	256	GLU
1	C	265	ILE
1	C	296	GLN
1	C	313	VAL
1	C	321	GLU
1	C	323	LEU
1	C	338	LEU
1	C	339	VAL
1	C	352	LYS
1	C	359	LYS
1	C	366	LEU
1	C	369	VAL
1	C	371	LYS
1	C	373	THR
1	C	376	LEU
1	C	390	LEU
1	C	397	GLN
1	C	399	GLU
1	C	401	ARG
1	C	402	GLN
1	C	405	LEU
1	C	406	LYS
1	C	407	GLU
1	C	410	GLU
1	C	413	ILE
1	D	164	LYS
1	D	168	ARG
1	D	177	GLU

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Mol	Chain	Res	Type
1	D	186	VAL
1	D	206	VAL
1	D	208	LEU
1	D	209	VAL
1	D	237	SER
1	D	241	GLU
1	D	249	SER
1	D	256	GLU
1	D	259	LYS
1	D	270	GLU
1	D	274	ILE
1	D	276	LYS
1	D	289	GLU
1	D	297	LEU
1	D	304	PHE
1	D	313	VAL
1	D	318	ASN
1	D	332	ARG
1	D	334	ASP
1	D	336	GLN
1	D	338	LEU
1	D	351	LEU
1	D	363	ASP
1	D	368	GLU
1	D	369	VAL
1	D	380	ASP
1	D	391	LEU
1	D	397	GLN
1	D	398	LYS
1	D	399	GLU
1	D	401	ARG
1	D	405	LEU
1	D	409	VAL
1	D	413	ILE
1	D	417	GLU
1	D	418	LYS
1	E	167	VAL
1	E	168	ARG
1	E	169	PHE
1	E	170	LYS
1	E	172	MET
1	E	187	ASP

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Mol	Chain	Res	Type
1	E	188	PHE
1	E	204	LYS
1	E	209	VAL
1	E	217	THR
1	E	226	GLU
1	E	242	MET
1	E	244	VAL
1	E	246	LEU
1	E	261	GLN
1	E	264	SER
1	E	270	GLU
1	E	295	ASN
1	E	296	GLN
1	E	301	MET
1	E	312	ILE
1	E	313	VAL
1	E	317	THR
1	E	327	LEU
1	E	336	GLN
1	E	339	VAL
1	E	345	ASN
1	E	347	ARG
1	E	353	VAL
1	E	355	ILE
1	E	364	VAL
1	E	372	LEU
1	E	373	THR
1	E	396	ASN
1	E	398	LYS
1	E	402	GLN
1	E	406	LYS
1	E	418	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	295	ASN
1	A	354	HIS
1	A	365	ASN
1	A	395	ASN
1	A	396	ASN

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Mol	Chain	Res	Type
1	A	404	HIS
1	B	296	GLN
1	B	336	GLN
1	B	362	ASN
1	B	383	ASN
1	B	404	HIS
1	C	228	HIS
1	C	292	GLN
1	C	308	ASN
1	C	397	GLN
1	C	402	GLN
1	C	403	GLN
1	D	161	ASN
1	D	166	ASN
1	D	292	GLN
1	D	318	ASN
1	D	397	GLN
1	D	404	HIS
1	E	197	ASN
1	E	261	GLN
1	E	292	GLN
1	E	296	GLN
1	E	365	ASN
1	E	402	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	B	2	-	28,29,29	1.53	5 (17%)	43,45,45	1.79	8 (18%)
2	ADP	A	1	-	28,29,29	1.50	6 (21%)	43,45,45	2.05	11 (25%)
2	ADP	E	5	-	28,29,29	1.50	5 (17%)	43,45,45	1.88	9 (20%)
2	ADP	D	4	-	28,29,29	1.58	5 (17%)	43,45,45	2.15	13 (30%)
2	ADP	C	3	-	28,29,29	1.42	5 (17%)	43,45,45	2.20	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	2	-	-	1/16/32/32	0/3/3/3
2	ADP	A	1	-	-	4/16/32/32	0/3/3/3
2	ADP	E	5	-	-	6/16/32/32	0/3/3/3
2	ADP	D	4	-	-	4/16/32/32	0/3/3/3
2	ADP	C	3	-	-	1/16/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	ADP	C5-C4	5.21	1.48	1.39
2	B	2	ADP	C5-C4	5.11	1.48	1.39
2	E	5	ADP	C5-C4	5.04	1.48	1.39
2	A	1	ADP	C5-C4	4.61	1.47	1.39
2	C	3	ADP	C5-C4	3.88	1.46	1.39
2	D	4	ADP	C5-N7	-3.78	1.32	1.39
2	C	3	ADP	C5-N7	-2.97	1.33	1.39
2	A	1	ADP	C5-N7	-2.88	1.33	1.39
2	E	5	ADP	C5-C6	2.79	1.48	1.41
2	A	1	ADP	C8-N7	2.70	1.36	1.31
2	B	2	ADP	C5-N7	-2.63	1.34	1.39
2	B	2	ADP	C5-C6	2.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	ADP	C4-N9	-2.49	1.32	1.37
2	E	5	ADP	PA-O3A	2.44	1.62	1.59
2	B	2	ADP	C8-N7	2.39	1.36	1.31
2	E	5	ADP	C5-N7	-2.35	1.34	1.39
2	A	1	ADP	PA-O3A	2.29	1.62	1.59
2	B	2	ADP	PA-O3A	2.26	1.61	1.59
2	D	4	ADP	C4-N9	-2.21	1.33	1.37
2	A	1	ADP	C5-C6	2.16	1.47	1.41
2	C	3	ADP	PA-O3A	2.16	1.61	1.59
2	A	1	ADP	C4-N9	-2.11	1.33	1.37
2	C	3	ADP	C5-C6	2.10	1.46	1.41
2	E	5	ADP	C8-N7	2.08	1.35	1.31
2	D	4	ADP	C8-N7	2.04	1.35	1.31
2	D	4	ADP	C5-C6	2.02	1.46	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	ADP	C5-C4-N3	-6.36	117.97	126.72
2	C	3	ADP	C5-C4-N3	-6.35	117.97	126.72
2	A	1	ADP	C5-C4-N3	-6.18	118.20	126.72
2	E	5	ADP	C5-C4-N3	-6.01	118.44	126.72
2	B	2	ADP	C5-C4-N3	-5.61	118.99	126.72
2	C	3	ADP	C5'-C4'-C3'	-5.32	96.08	115.21
2	E	5	ADP	N3-C4-N9	5.13	135.90	127.17
2	D	4	ADP	O4'-C1'-N9	4.94	117.58	108.09
2	D	4	ADP	N3-C4-N9	4.82	135.36	127.17
2	D	4	ADP	C2'-C1'-N9	-4.78	101.44	113.30
2	C	3	ADP	N3-C4-N9	4.70	135.17	127.17
2	A	1	ADP	N3-C4-N9	4.57	134.94	127.17
2	B	2	ADP	N3-C4-N9	4.46	134.75	127.17
2	C	3	ADP	C2-N3-C4	3.98	121.55	111.83
2	A	1	ADP	C5'-C4'-C3'	-3.85	101.35	115.21
2	C	3	ADP	C2'-C1'-N9	-3.72	104.05	113.30
2	E	5	ADP	C2-N3-C4	3.72	120.91	111.83
2	A	1	ADP	C2'-C1'-N9	-3.69	104.14	113.30
2	B	2	ADP	C2-N3-C4	3.58	120.58	111.83
2	C	3	ADP	N3-C2-N1	-3.57	123.18	128.58
2	A	1	ADP	C2-N3-C4	3.54	120.48	111.83
2	C	3	ADP	C4-C5-N7	-3.39	106.71	110.58
2	D	4	ADP	C2-N3-C4	3.32	119.93	111.83
2	E	5	ADP	N3-C2-N1	-3.26	123.65	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	ADP	C5'-C4'-C3'	-3.25	103.52	115.21
2	B	2	ADP	N3-C2-N1	-3.18	123.77	128.58
2	A	1	ADP	C4-C5-N7	-3.00	107.15	110.58
2	E	5	ADP	C4-C5-N7	-2.91	107.25	110.58
2	A	1	ADP	N3-C2-N1	-2.89	124.20	128.58
2	D	4	ADP	C3'-C2'-C1'	2.80	106.76	101.46
2	B	2	ADP	C4-C5-N7	-2.68	107.52	110.58
2	A	1	ADP	C3'-C2'-C1'	2.63	106.44	101.46
2	D	4	ADP	N3-C2-N1	-2.61	124.63	128.58
2	E	5	ADP	C3'-C2'-C1'	2.57	106.32	101.46
2	C	3	ADP	C3'-C2'-C1'	2.55	106.28	101.46
2	E	5	ADP	C4-N9-C8	2.50	108.36	105.74
2	A	1	ADP	O4'-C4'-C5'	2.48	117.27	109.33
2	B	2	ADP	O2A-PA-O1A	2.45	123.86	112.44
2	A	1	ADP	O2A-PA-O1A	2.42	123.72	112.44
2	E	5	ADP	O3B-PB-O2B	2.37	116.67	107.80
2	C	3	ADP	C5-N7-C8	2.32	107.09	103.45
2	D	4	ADP	C4-N9-C1'	2.28	131.96	126.63
2	E	5	ADP	C5-N7-C8	2.24	106.97	103.45
2	D	4	ADP	C4-C5-N7	-2.24	108.02	110.58
2	C	3	ADP	O5'-C5'-C4'	2.22	116.55	108.99
2	D	4	ADP	C1'-N9-C8	-2.20	122.21	127.09
2	D	4	ADP	O3B-PB-O2B	2.17	115.94	107.80
2	A	1	ADP	O4'-C1'-N9	2.16	112.25	108.09
2	B	2	ADP	C3'-C2'-C1'	2.09	105.41	101.46
2	C	3	ADP	C4-N9-C8	2.06	107.91	105.74
2	D	4	ADP	N6-C6-N1	2.05	122.93	118.38
2	B	2	ADP	O3A-PA-O1A	-2.02	104.63	110.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ADP	C5'-O5'-PA-O2A
2	A	1	ADP	C5'-O5'-PA-O3A
2	B	2	ADP	C5'-O5'-PA-O1A
2	D	4	ADP	C5'-O5'-PA-O3A
2	E	5	ADP	PA-O3A-PB-O2B
2	E	5	ADP	C5'-O5'-PA-O1A
2	E	5	ADP	C5'-O5'-PA-O2A
2	E	5	ADP	C5'-O5'-PA-O3A
2	E	5	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	1	ADP	O4'-C4'-C5'-O5'
2	A	1	ADP	C3'-C4'-C5'-O5'
2	D	4	ADP	O4'-C1'-N9-C8
2	D	4	ADP	O4'-C1'-N9-C4
2	E	5	ADP	C3'-C4'-C5'-O5'
2	C	3	ADP	C5'-O5'-PA-O1A
2	D	4	ADP	C5'-O5'-PA-O1A

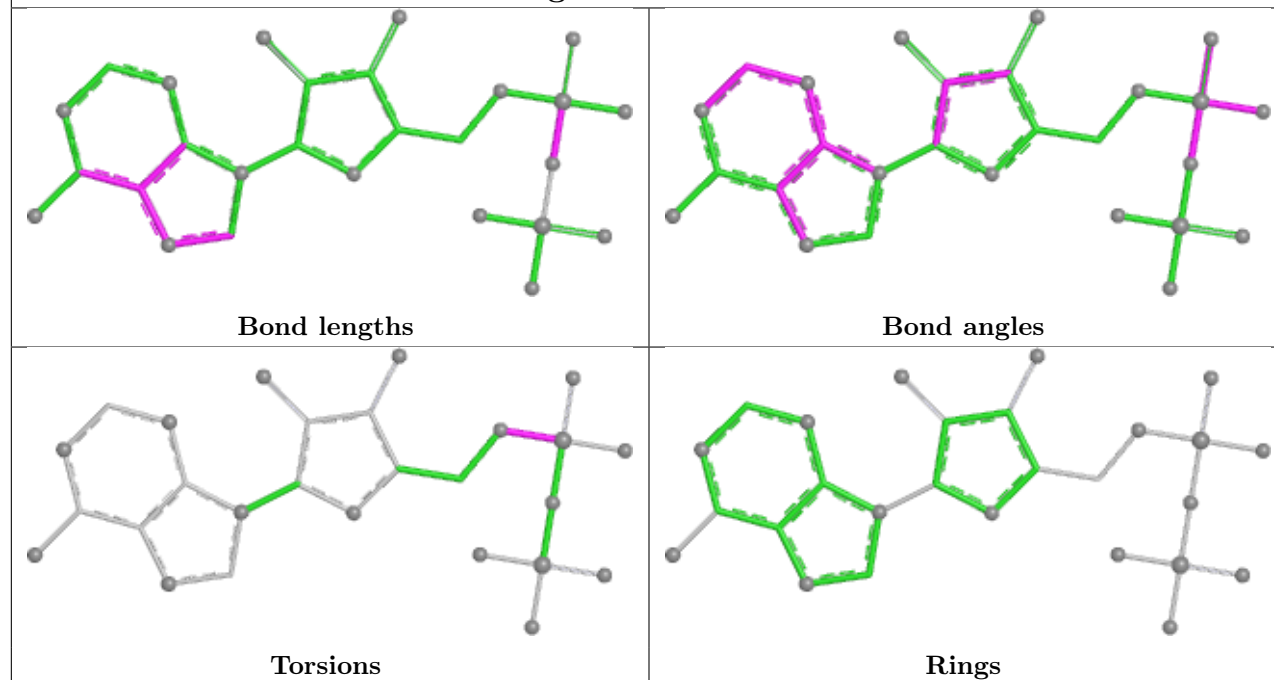
There are no ring outliers.

4 monomers are involved in 19 short contacts:

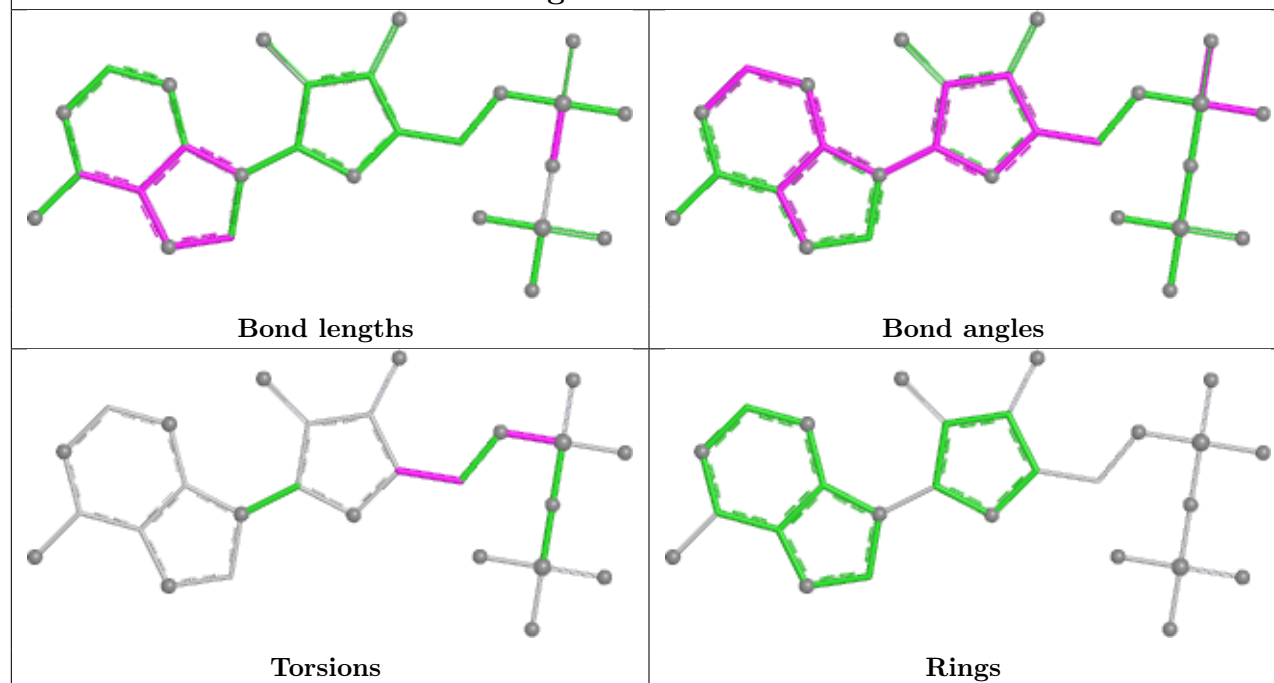
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	ADP	3	0
2	A	1	ADP	3	0
2	D	4	ADP	10	0
2	C	3	ADP	3	0

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

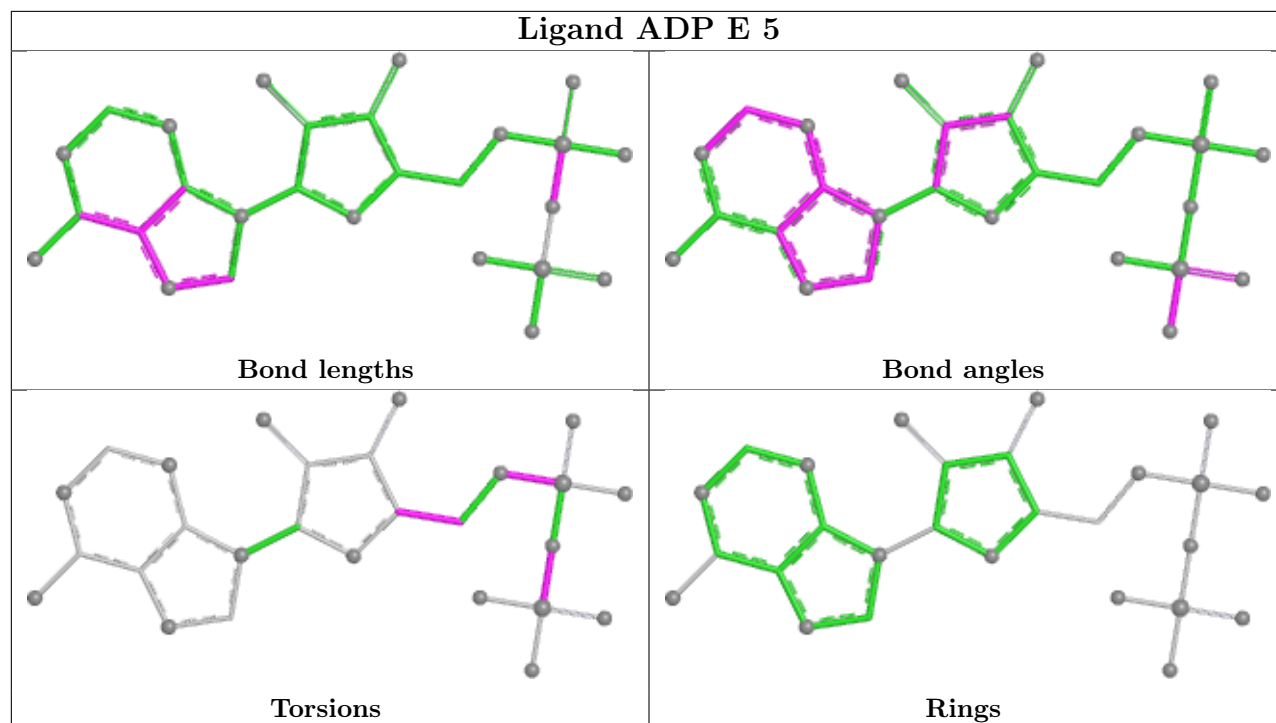
Ligand ADP B 2



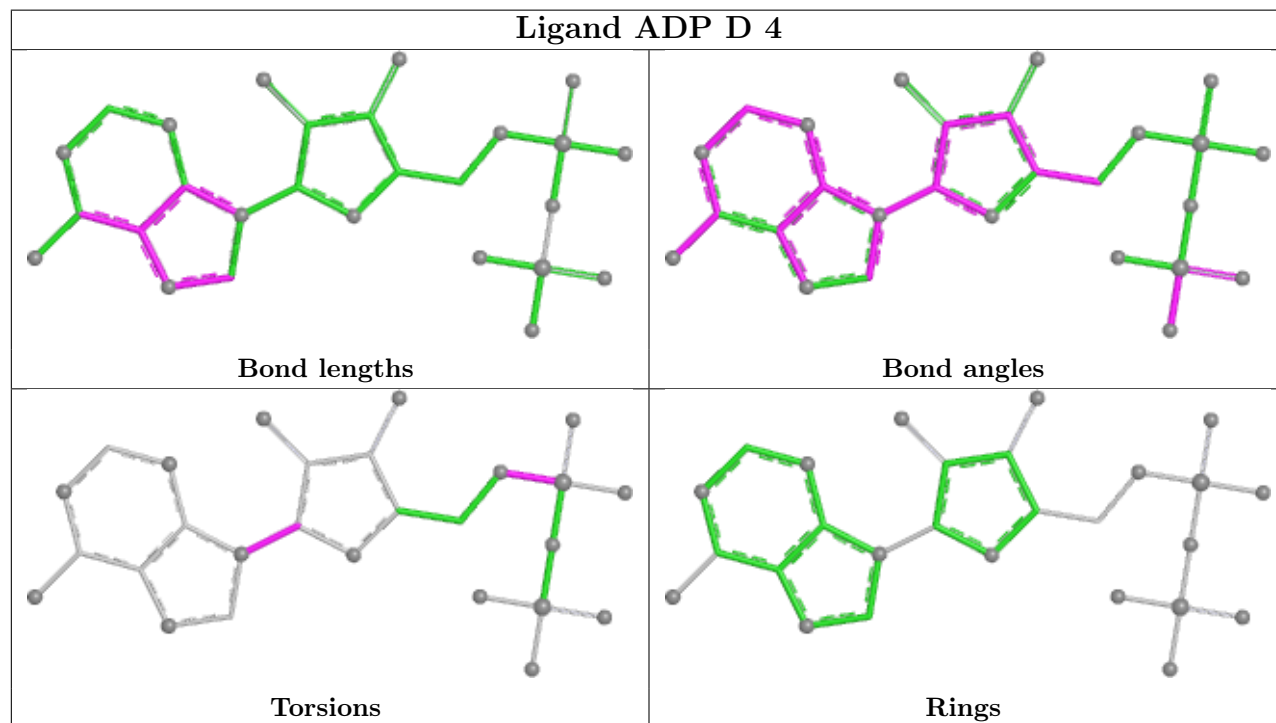
Ligand ADP A 1

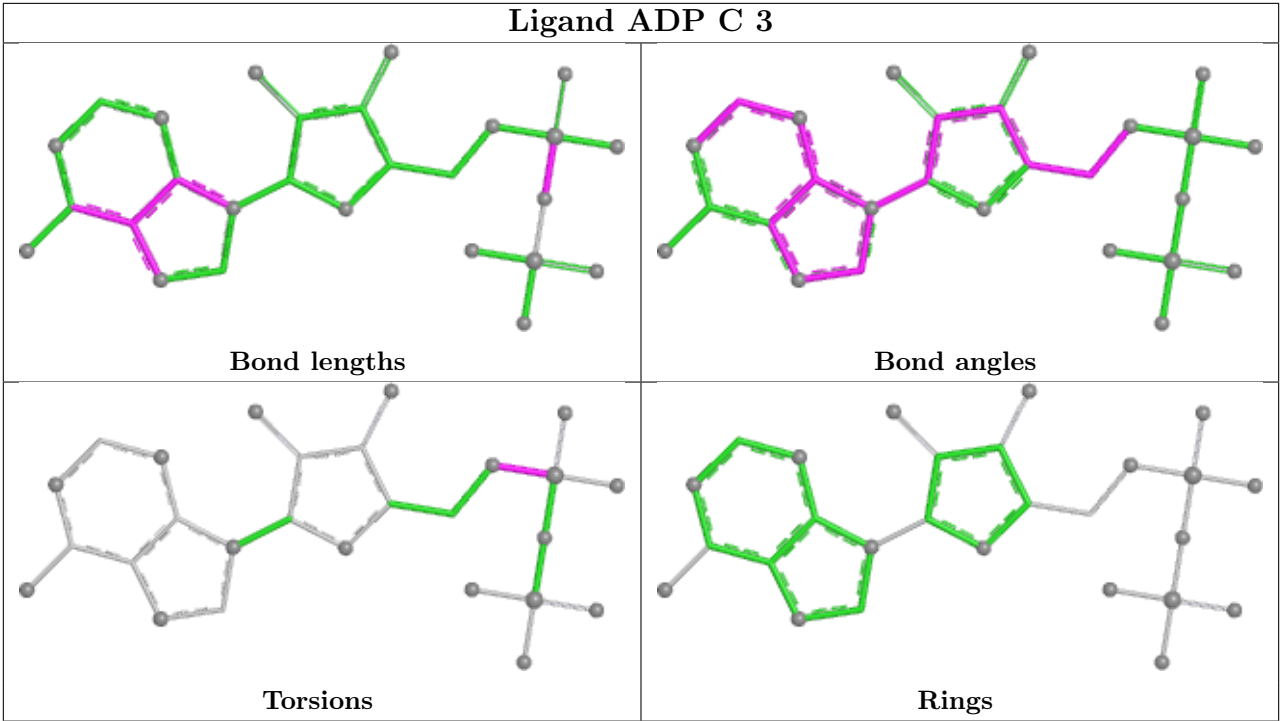


Ligand ADP E 5



Ligand ADP D 4





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	389:ALA	C	390:LEU	N	1.62

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	249/268 (92%)	0.02	5 (2%) 65 46	88, 129, 166, 185	0
1	B	249/268 (92%)	0.18	6 (2%) 59 40	83, 151, 172, 175	0
1	C	249/268 (92%)	-0.02	3 (1%) 76 58	70, 103, 157, 167	0
1	D	249/268 (92%)	0.12	11 (4%) 39 25	98, 126, 158, 171	0
1	E	249/268 (92%)	0.07	3 (1%) 76 58	85, 122, 161, 185	0
All	All	1245/1340 (92%)	0.07	28 (2%) 62 43	70, 127, 166, 185	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	311	VAL	3.7
1	B	236	GLY	3.1
1	D	290	ARG	3.1
1	D	414	ALA	2.7
1	D	310	PRO	2.6
1	B	295	ASN	2.6
1	A	297	LEU	2.6
1	A	385	ILE	2.6
1	D	255	PHE	2.6
1	A	275	GLY	2.5
1	B	384	ILE	2.4
1	A	381	LEU	2.4
1	D	214	THR	2.4
1	C	251	VAL	2.4
1	D	312	ILE	2.4
1	C	375	GLY	2.4
1	D	246	LEU	2.3
1	C	409	VAL	2.3
1	B	251	VAL	2.3
1	E	416	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	GLY	2.2
1	D	244	VAL	2.2
1	D	329	ARG	2.2
1	E	373	THR	2.1
1	B	189	LEU	2.1
1	A	234	MET	2.1
1	E	244	VAL	2.1
1	D	314	LEU	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](#)

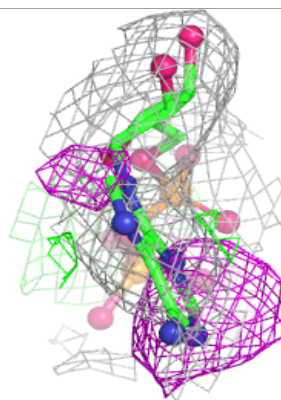
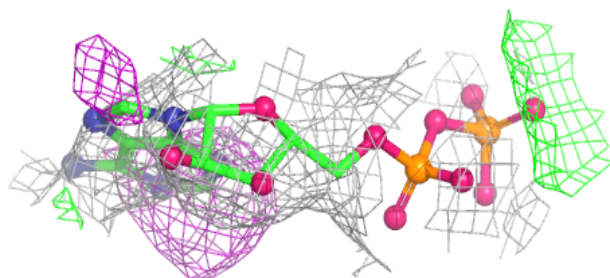
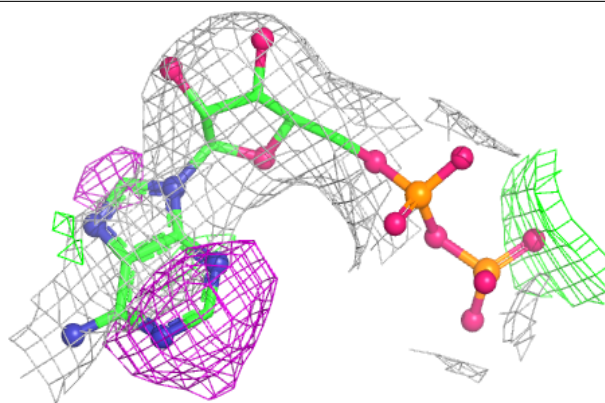
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	D	4	27/27	0.78	0.13	115,120,129,129	0
2	ADP	B	2	27/27	0.86	0.10	129,134,137,138	0
2	ADP	A	1	27/27	0.86	0.11	96,101,113,115	0
2	ADP	C	3	27/27	0.87	0.10	91,98,115,116	0
2	ADP	E	5	27/27	0.87	0.10	122,123,128,128	0

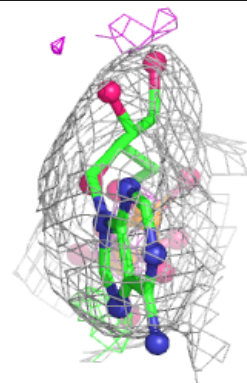
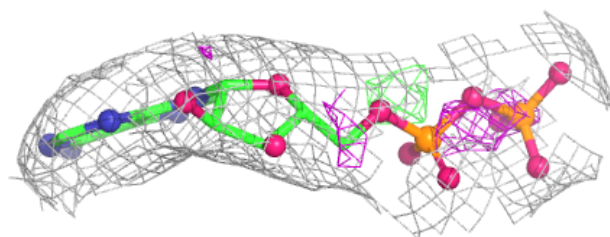
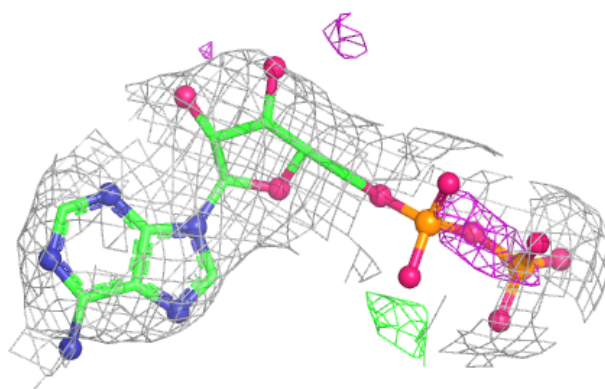
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 4:

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

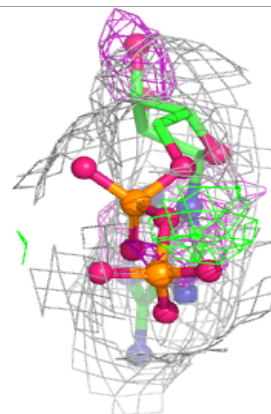
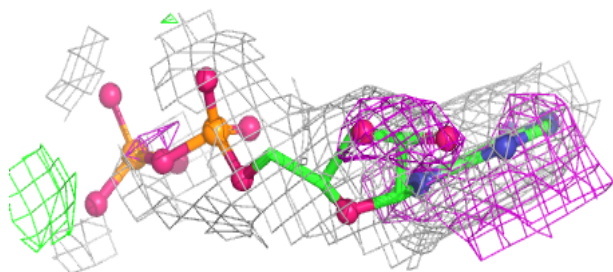
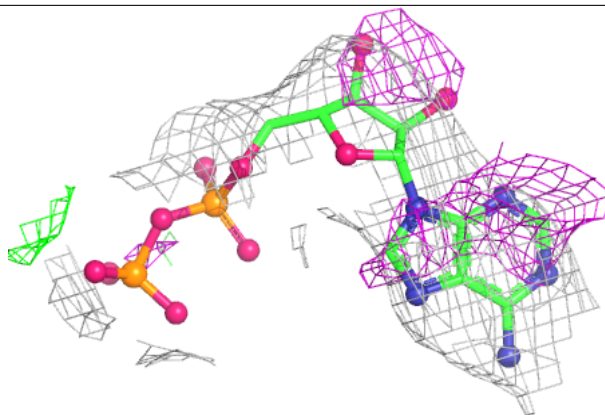
**Electron density around ADP B 2:**

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

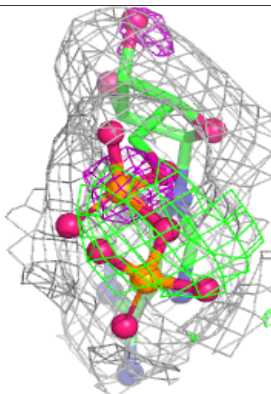
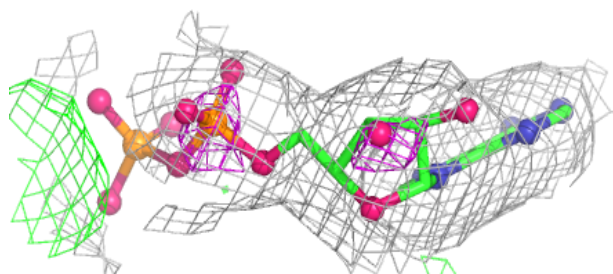
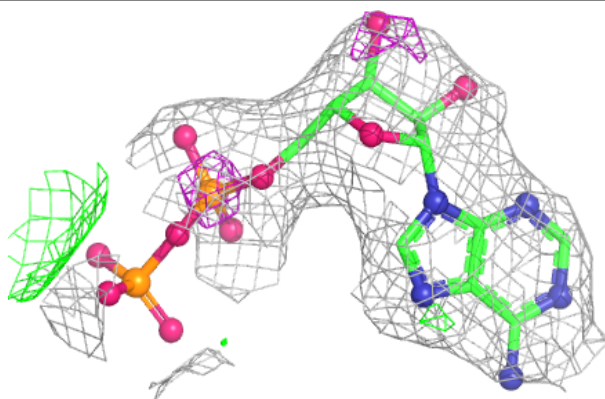


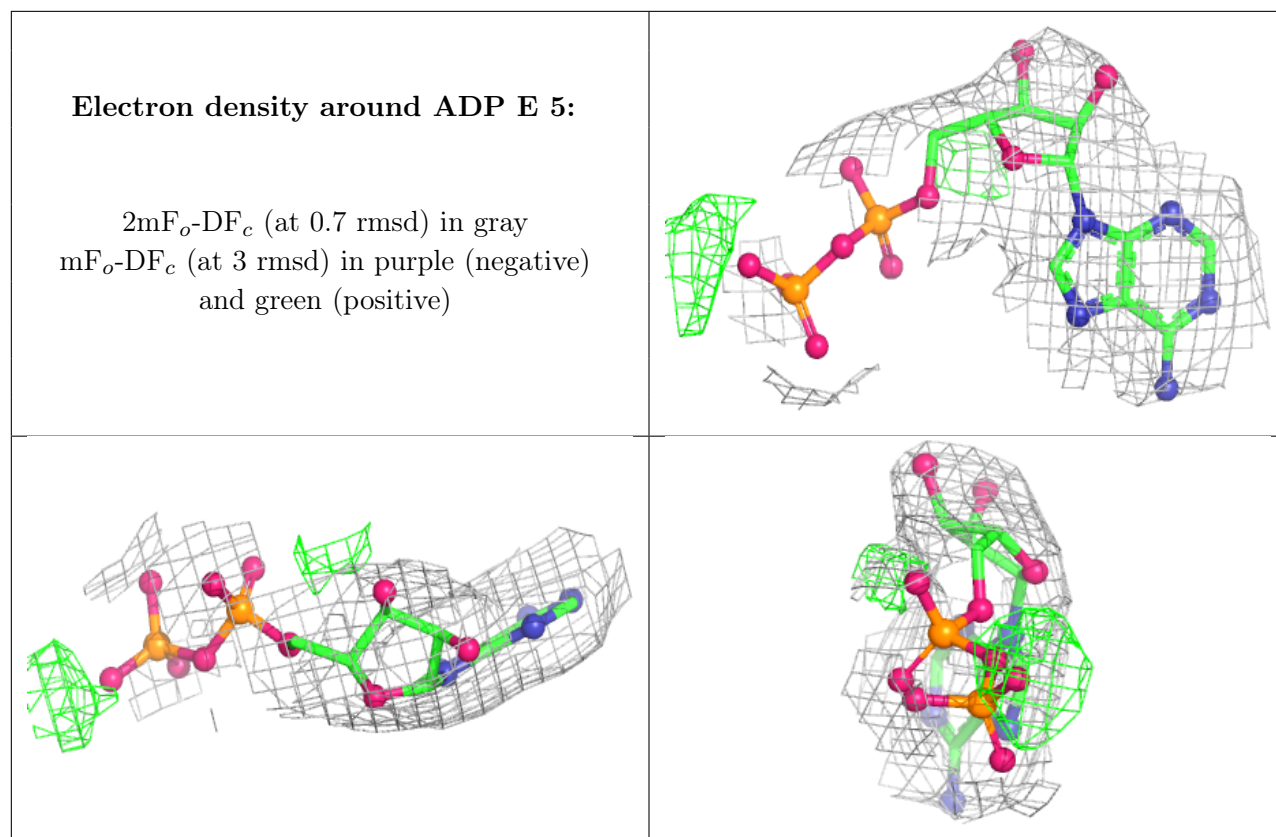
Electron density around ADP A 1:

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

**Electron density around ADP C 3:**

$2mF_o-DF_c$ (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.