



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 3I12 / pdb_00003i12
Title : The crystal structure of the D-alanyl-alanine synthetase A from *Salmonella enterica* subsp. *enterica* serovar Typhimurium str. LT2
Authors : Zhang, R.; Maltseva, N.; Papazisi, L.; Anderson, W.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2009-06-25
Resolution : 2.20 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

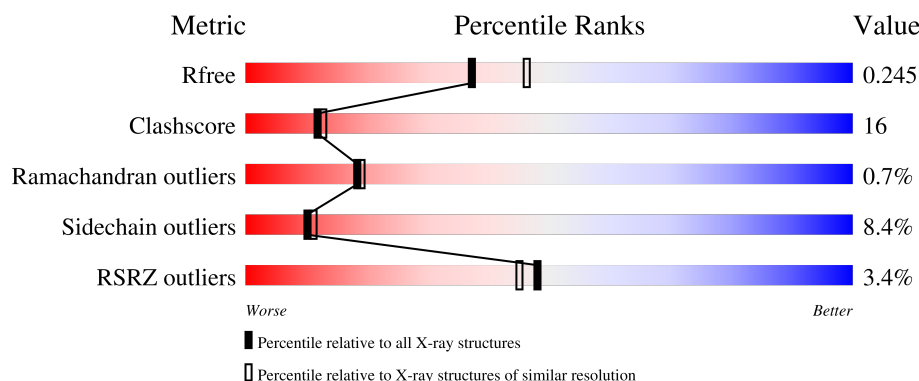
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	364	 4% 71% 22% 6% •
1	B	364	 2% 75% 15% • 5%
1	C	364	 5% 67% 23% 5% •
1	D	364	 2% 73% 18% 5% •

2 Entry composition [i](#)

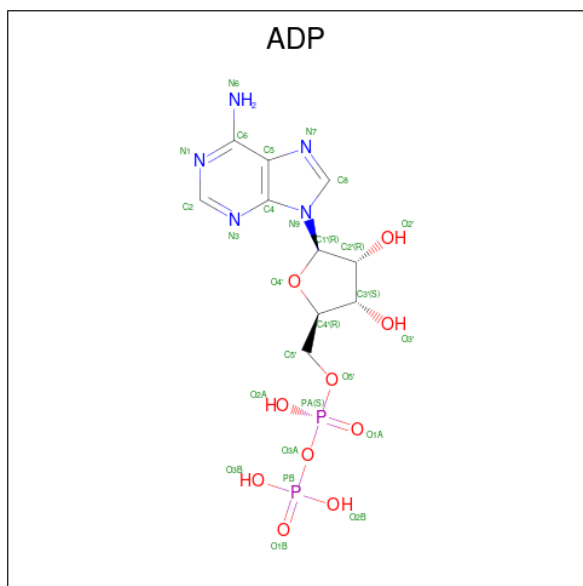
There are 3 unique types of molecules in this entry. The entry contains 11104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanine-D-alanine ligase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2735	1723	480	524	8			
1	B	346	Total	C	N	O	S	0	0	0
			2621	1652	463	497	9			
1	C	348	Total	C	N	O	S	0	0	0
			2630	1657	465	499	9			
1	D	355	Total	C	N	O	S	0	0	0
			2695	1697	474	516	8			

- 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		

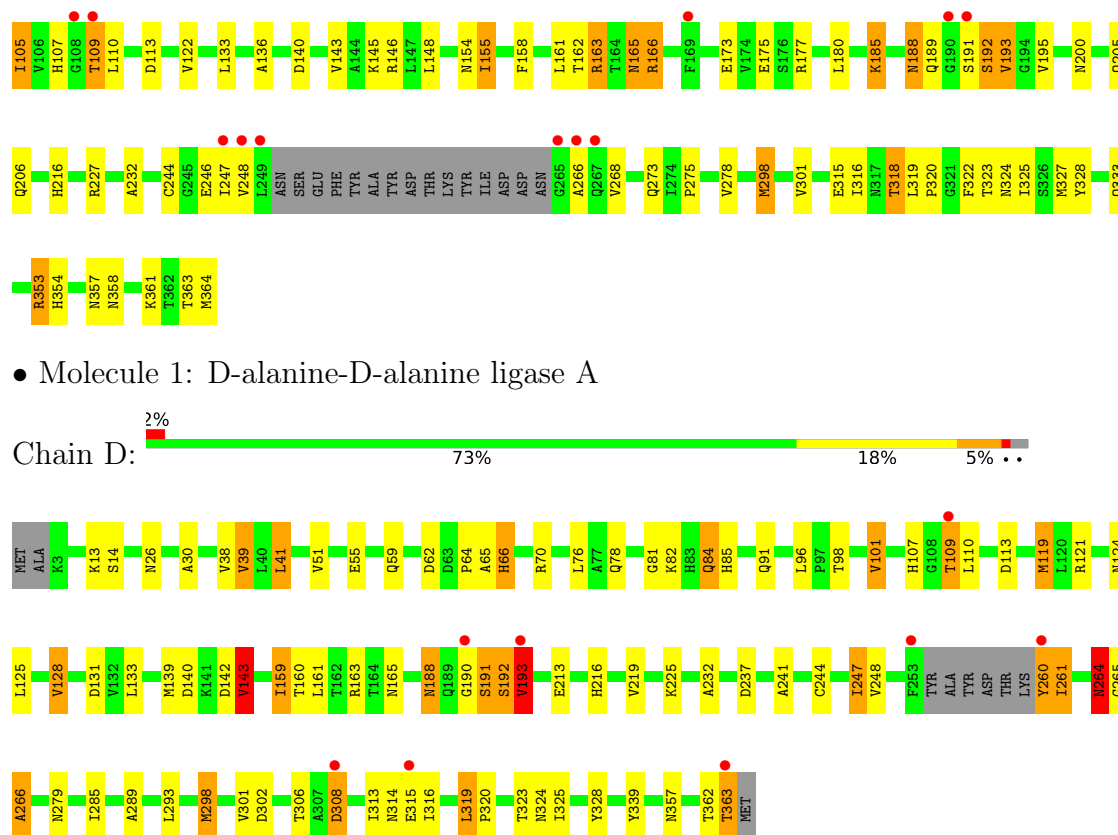
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total	O	0	0
			96	96		
3	B	79	Total	O	0	0
			79	79		
3	C	60	Total	O	0	0
			60	60		
3	D	80	Total	O	0	0
			80	80		



● Molecule 1: D-alanine-D-alanine ligase A

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.15Å 85.81Å 230.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 2.20 47.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.54-2.20) 99.9 (47.54-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.197 , 0.249 0.198 , 0.245	Depositor DCC
R_{free} test set	4332 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11104	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.28	8/2781 (0.3%)	1.19	12/3780 (0.3%)
1	B	1.23	6/2664 (0.2%)	1.18	15/3620 (0.4%)
1	C	1.16	2/2673 (0.1%)	1.22	15/3632 (0.4%)
1	D	1.26	4/2740 (0.1%)	1.15	11/3724 (0.3%)
All	All	1.23	20/10858 (0.2%)	1.19	53/14756 (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	C	0	1
1	D	0	3
All	All	0	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	ASP	CB-CG	-7.90	1.32	1.52
1	D	128	VAL	CA-CB	6.54	1.61	1.54
1	A	44	ASP	CB-CG	-6.16	1.36	1.52
1	C	298	MET	SD-CE	-6.12	1.64	1.79
1	A	218	VAL	CA-CB	-6.09	1.46	1.54
1	A	270	VAL	N-CA	-5.69	1.41	1.45
1	D	188	ASN	CA-C	-5.56	1.45	1.53
1	B	188	ASN	C-O	5.54	1.30	1.24
1	B	236	ASN	CA-C	5.50	1.55	1.52
1	A	44	ASP	CA-C	-5.46	1.45	1.52
1	D	289	ALA	CA-CB	5.43	1.61	1.53
1	A	79	VAL	CA-CB	5.31	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	GLY	N-CA	5.26	1.52	1.45
1	B	238	ASN	C-O	-5.26	1.18	1.24
1	A	129	GLY	C-O	5.22	1.31	1.24
1	B	158	PHE	C-O	-5.15	1.17	1.23
1	A	111	GLY	C-O	-5.12	1.18	1.24
1	B	111	GLY	C-O	-5.10	1.18	1.24
1	D	241	ALA	CA-CB	-5.10	1.45	1.53
1	A	307	ALA	CA-CB	5.01	1.61	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	GLU	N-CA-CB	-17.35	84.81	110.49
1	C	54	ALA	N-CA-C	10.15	132.42	110.80
1	A	109	THR	N-CA-C	9.11	122.05	111.11
1	C	55	GLU	N-CA-C	-8.98	101.85	113.17
1	A	44	ASP	CB-CA-C	-8.56	93.38	110.42
1	A	109	THR	CA-C-N	-8.54	108.10	122.11
1	A	109	THR	C-N-CA	-8.54	108.10	122.11
1	B	51	VAL	CB-CA-C	-8.40	100.79	110.96
1	A	353	ARG	CG-CD-NE	-7.73	94.99	112.00
1	B	139	MET	CG-SD-CE	-7.49	84.41	100.90
1	D	298	MET	CG-SD-CE	-7.24	84.96	100.90
1	A	353	ARG	NE-CZ-NH2	-7.16	112.76	119.20
1	C	44	ASP	CB-CG-OD1	-7.11	102.06	118.40
1	D	125	LEU	CA-C-N	-7.05	112.52	119.78
1	D	125	LEU	C-N-CA	-7.05	112.52	119.78
1	B	101	VAL	CB-CA-C	-6.98	98.62	111.18
1	D	101	VAL	CB-CA-C	-6.91	98.75	111.18
1	B	237	ASP	CA-C-N	-6.85	114.21	123.46
1	B	237	ASP	C-N-CA	-6.85	114.21	123.46
1	D	237	ASP	CA-C-N	-6.85	114.50	123.34
1	D	237	ASP	C-N-CA	-6.85	114.50	123.34
1	C	107	HIS	N-CA-C	-6.66	101.94	110.53
1	C	101	VAL	CB-CA-C	-6.55	99.39	111.18
1	A	279	ASN	N-CA-C	-6.40	104.22	111.07
1	C	353	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	B	143	VAL	N-CA-C	6.31	117.09	110.72
1	B	237	ASP	N-CA-C	6.27	118.20	111.36
1	B	109	THR	CA-C-N	-6.25	111.86	122.11
1	B	109	THR	C-N-CA	-6.25	111.86	122.11
1	B	109	THR	N-CA-C	6.23	121.59	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	VAL	N-CA-CB	5.87	117.69	111.00
1	D	109	THR	CA-C-N	-5.77	111.45	122.53
1	D	109	THR	C-N-CA	-5.77	111.45	122.53
1	C	44	ASP	CB-CA-C	-5.76	98.95	110.42
1	D	81	GLY	N-CA-C	-5.75	107.16	115.27
1	A	109	THR	O-C-N	-5.68	116.18	122.09
1	B	191	SER	N-CA-C	5.61	122.74	110.80
1	A	96	LEU	CA-C-N	-5.55	114.06	119.78
1	A	96	LEU	C-N-CA	-5.55	114.06	119.78
1	B	63	ASP	CA-C-N	5.54	125.38	119.28
1	B	63	ASP	C-N-CA	5.54	125.38	119.28
1	C	65	ALA	N-CA-C	-5.52	99.52	108.52
1	C	200	ASN	N-CA-C	5.46	116.45	108.14
1	C	163	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	C	318	THR	CA-C-N	-5.36	116.95	122.85
1	C	318	THR	C-N-CA	-5.36	116.95	122.85
1	A	244	CYS	CA-C-N	5.24	125.65	121.61
1	A	244	CYS	C-N-CA	5.24	125.65	121.61
1	D	143	VAL	N-CA-C	5.20	115.92	110.62
1	D	264	ASN	N-CA-C	5.16	121.79	110.80
1	B	248	VAL	CB-CA-C	-5.12	102.98	110.62
1	C	244	CYS	CA-C-N	5.10	125.96	121.58
1	C	244	CYS	C-N-CA	5.10	125.96	121.58

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	188	ASN	Peptide
1	D	191	SER	Peptide
1	D	193	VAL	Peptide
1	D	264	ASN	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	2735	0	2731	115	0
1	B	2621	0	2645	59	0
1	C	2630	0	2650	98	0
1	D	2695	0	2696	93	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	3	0
3	A	96	0	0	4	0
3	B	79	0	0	1	0
3	C	60	0	0	9	0
3	D	80	0	0	6	0
All	All	11104	0	10770	341	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 16.

All (341) 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:57:TYR:CE1	1:A:58:LEU:HG	1.79	1.16
1:C:268:VAL:HG13	1:C:327:MET:HE1	1.22	1.16
1:A:57:TYR:CD1	1:A:58:LEU:HG	1.81	1.15
1:A:59:GLN:NE2	1:A:70:ARG:HD2	1.62	1.11
1:A:298:MET:CE	1:A:328:TYR:CE2	2.34	1.11
1:A:122:VAL:HG21	1:B:119:MET:CE	1.81	1.09
1:A:57:TYR:CE1	1:A:58:LEU:CD1	2.37	1.08
1:A:57:TYR:CE1	1:A:58:LEU:CG	2.40	1.04
1:A:122:VAL:HG21	1:B:119:MET:HE1	1.41	1.02
1:A:298:MET:HE2	1:A:328:TYR:CE2	1.95	1.01
1:A:298:MET:HE2	1:A:328:TYR:CZ	1.95	1.01
1:A:59:GLN:HE21	1:A:70:ARG:HD2	0.82	0.99
1:C:163:ARG:HD3	3:C:407:HOH:O	1.67	0.95
1:A:59:GLN:HE21	1:A:70:ARG:CD	1.78	0.95
1:C:165:ASN:C	1:C:165:ASN:HD22	1.76	0.94
1:A:57:TYR:CE1	1:A:58:LEU:HD11	2.00	0.93
1:D:84:GLN:HB2	1:D:98:THR:HG21	1.51	0.92
1:D:85:HIS:H	1:D:98:THR:HG22	1.33	0.91
1:C:298:MET:HE3	1:C:328:TYR:CE2	2.06	0.91
1:D:247:ILE:HD13	1:D:248:VAL:N	1.88	0.89
1:B:142:ASP:OD1	1:B:160:THR:HG21	1.73	0.89
1:D:244:CYS:H	1:D:279:ASN:HD21	1.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:HIS:HD2	3:C:380:HOH:O	1.58	0.85
1:A:57:TYR:CZ	1:A:58:LEU:CD1	2.59	0.85
1:B:301:VAL:HG22	1:B:316:ILE:HD12	1.57	0.85
1:A:122:VAL:HG11	1:B:119:MET:HE1	1.57	0.84
1:C:268:VAL:CG1	1:C:327:MET:HE1	2.06	0.83
1:C:325:ILE:HD12	1:C:325:ILE:O	1.79	0.83
1:A:57:TYR:CZ	1:A:58:LEU:HD12	2.15	0.82
1:C:12:GLY:O	1:C:17:HIS:HD2	1.63	0.82
1:A:57:TYR:HE1	1:A:58:LEU:HD11	1.45	0.81
1:C:78:GLN:HE21	1:D:78:GLN:HE21	1.31	0.78
1:D:315:GLU:OE1	2:D:365:ADP:O1A	2.02	0.76
1:D:26:ASN:ND2	1:D:324:ASN:H	1.83	0.75
1:A:122:VAL:CG2	1:B:119:MET:HE1	2.14	0.75
1:D:160:THR:HG22	1:D:219:VAL:HG22	1.67	0.75
1:C:165:ASN:C	1:C:165:ASN:ND2	2.45	0.74
1:A:163:ARG:NH1	1:A:216:HIS:HD2	1.85	0.73
1:C:165:ASN:HD22	1:C:166:ARG:N	1.85	0.73
1:D:159:ILE:HD12	1:D:160:THR:N	2.03	0.73
1:A:185:LYS:HB3	1:A:195:VAL:HG22	1.71	0.72
1:C:298:MET:HE3	1:C:328:TYR:CZ	2.24	0.71
1:A:298:MET:HE1	1:A:328:TYR:CE2	2.22	0.71
1:C:59:GLN:HE22	1:C:70:ARG:HA	1.56	0.70
1:A:162:THR:H	1:A:165:ASN:ND2	1.90	0.70
1:C:44:ASP:HB3	1:C:46:ALA:H	1.57	0.69
1:C:191:SER:O	1:C:193:VAL:N	2.26	0.69
1:C:273:GLN:NE2	3:C:381:HOH:O	2.09	0.69
1:D:159:ILE:HD11	1:D:161:LEU:HD23	1.73	0.69
1:D:142:ASP:OD1	1:D:160:THR:HG21	1.92	0.69
1:A:298:MET:HE1	1:A:322:PHE:HE2	1.57	0.69
1:C:43:ILE:HD13	1:C:43:ILE:N	2.08	0.68
1:A:260:TYR:CE1	1:A:261:ILE:HD11	2.28	0.68
1:A:78:GLN:HE21	1:A:119:MET:HG2	1.58	0.68
1:B:298:MET:HE2	1:B:320:PRO:CD	2.23	0.67
1:A:122:VAL:CG1	1:B:119:MET:HE1	2.24	0.67
1:A:44:ASP:HB3	1:A:46:ALA:H	1.59	0.66
1:C:163:ARG:HH12	1:C:216:HIS:HD2	1.44	0.66
1:A:163:ARG:HH12	1:A:216:HIS:HD2	1.42	0.66
1:B:301:VAL:HG22	1:B:316:ILE:CD1	2.23	0.66
1:C:78:GLN:HE21	1:D:78:GLN:NE2	1.93	0.66
1:B:278:VAL:O	1:B:282:ILE:HD13	1.95	0.66
1:C:163:ARG:HG3	1:C:163:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLN:HG2	1:D:70:ARG:NH2	2.11	0.65
1:A:310:GLU:CG	3:A:431:HOH:O	2.44	0.65
1:A:330:LYS:NZ	1:A:333:GLN:HE22	1.94	0.65
1:A:56:ASN:HD21	1:A:70:ARG:HE	1.44	0.64
1:D:298:MET:HE1	1:D:320:PRO:CG	2.28	0.64
1:B:163:ARG:HH11	1:B:216:HIS:HD2	1.46	0.64
1:A:310:GLU:HG2	3:A:431:HOH:O	1.96	0.64
1:C:26:ASN:ND2	1:C:324:ASN:H	1.97	0.63
1:A:363:THR:C	3:A:454:HOH:O	2.41	0.63
1:D:298:MET:HE2	1:D:320:PRO:HD2	1.79	0.63
1:A:57:TYR:CD1	1:A:58:LEU:CG	2.70	0.63
1:D:285:ILE:CG2	1:D:313:ILE:HD11	2.29	0.62
1:A:26:ASN:ND2	1:A:324:ASN:H	1.97	0.62
1:D:85:HIS:N	1:D:98:THR:HG22	2.11	0.62
1:A:74:ILE:O	1:A:74:ILE:HG23	1.99	0.62
1:B:298:MET:HE2	1:B:320:PRO:HD2	1.82	0.62
1:C:298:MET:HE2	1:C:320:PRO:CG	2.29	0.62
1:B:298:MET:HE2	1:B:320:PRO:CG	2.30	0.61
1:A:330:LYS:HZ2	1:A:333:GLN:HE22	1.47	0.61
1:A:298:MET:CE	1:A:328:TYR:CZ	2.71	0.61
1:C:325:ILE:O	1:C:325:ILE:CD1	2.48	0.61
1:A:57:TYR:OH	1:A:58:LEU:HD12	2.00	0.61
1:D:84:GLN:HB2	1:D:98:THR:CG2	2.28	0.61
1:A:51:VAL:HG23	1:A:76:LEU:HD21	1.82	0.61
1:A:43:ILE:HD12	1:A:49:TRP:CD1	2.37	0.60
1:B:282:ILE:HD12	1:B:311:VAL:HG21	1.82	0.60
1:C:177:ARG:CD	3:C:400:HOH:O	2.49	0.60
1:A:51:VAL:HG21	1:A:96:LEU:HD21	1.83	0.60
1:D:247:ILE:HD13	1:D:248:VAL:H	1.63	0.60
1:A:74:ILE:O	1:A:74:ILE:CG2	2.50	0.59
1:D:298:MET:HE2	1:D:320:PRO:CD	2.32	0.59
1:D:121:ARG:NH2	1:D:131:ASP:OD2	2.35	0.59
1:D:306:THR:OG1	1:D:308:ASP:OD1	2.15	0.59
1:A:170:SER:OG	1:A:173:GLU:HB2	2.03	0.59
1:D:244:CYS:HB2	1:D:279:ASN:ND2	2.17	0.59
1:C:140:ASP:HB2	1:C:188:ASN:HD21	1.69	0.58
1:B:51:VAL:HG23	1:B:74:ILE:HG21	1.85	0.58
1:B:191:SER:O	1:B:192:SER:HB2	2.02	0.58
1:D:26:ASN:HD22	1:D:324:ASN:H	1.49	0.58
1:A:59:GLN:HG3	1:A:70:ARG:HG2	1.86	0.57
1:A:122:VAL:HG21	1:B:119:MET:HE2	1.79	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HA	1:A:165:ASN:HD21	1.68	0.57
1:B:43:ILE:N	1:B:43:ILE:HD13	2.17	0.57
1:A:165:ASN:C	1:A:165:ASN:HD22	2.12	0.57
1:A:59:GLN:HG3	1:A:70:ARG:CD	2.35	0.57
1:C:59:GLN:HE22	1:C:70:ARG:CA	2.15	0.57
1:B:171:PHE:CB	1:B:201:GLU:HG3	2.35	0.57
1:C:148:LEU:HD13	1:C:155:ILE:HD11	1.85	0.57
1:A:162:THR:H	1:A:165:ASN:HD21	1.53	0.57
1:A:12:GLY:O	1:A:17:HIS:HD2	1.88	0.56
1:D:247:ILE:HD11	1:D:266:ALA:CB	2.35	0.56
1:A:74:ILE:HD12	1:A:76:LEU:CD2	2.35	0.56
1:D:314:ASN:ND2	1:D:315:GLU:HG2	2.20	0.56
1:B:103:PHE:HA	1:B:128:VAL:HG13	1.88	0.56
1:D:139:MET:HG3	1:D:188:ASN:HD22	1.70	0.56
1:A:315:GLU:OE2	2:A:365:ADP:O1A	2.23	0.56
1:C:315:GLU:C	1:C:316:ILE:HD13	2.31	0.56
1:A:260:TYR:CE1	1:A:261:ILE:CD1	2.89	0.56
1:D:247:ILE:HD11	1:D:266:ALA:HB3	1.88	0.56
1:B:315:GLU:OE1	2:B:365:ADP:O1A	2.24	0.55
1:C:325:ILE:HD12	1:C:325:ILE:C	2.30	0.55
1:D:51:VAL:HG23	1:D:76:LEU:HD21	1.88	0.55
1:B:276:SER:H	1:C:94:GLN:HE22	1.53	0.55
1:C:14:SER:OG	1:C:16:GLU:OE1	2.20	0.55
1:D:301:VAL:HG22	1:D:316:ILE:HD12	1.88	0.55
1:A:51:VAL:CG2	1:A:96:LEU:HD21	2.37	0.55
1:C:56:ASN:C	1:C:70:ARG:NH1	2.65	0.55
1:B:171:PHE:HB3	1:B:201:GLU:HG3	1.89	0.54
1:A:26:ASN:HD22	1:A:323:THR:HA	1.72	0.54
1:C:12:GLY:O	1:C:17:HIS:CD2	2.53	0.54
1:D:30:ALA:CB	1:D:339:TYR:CD2	2.91	0.54
1:C:122:VAL:HG11	1:D:119:MET:HE1	1.90	0.54
1:C:275:PRO:HB2	1:C:278:VAL:HG23	1.88	0.54
1:C:315:GLU:O	1:C:316:ILE:HD13	2.06	0.54
1:D:165:ASN:C	1:D:165:ASN:OD1	2.51	0.54
1:A:163:ARG:HH12	1:A:216:HIS:CD2	2.24	0.54
1:D:65:ALA:HB1	1:D:66:HIS:CD2	2.42	0.54
1:C:143:VAL:HG21	1:D:133:LEU:HD21	1.90	0.54
1:C:298:MET:HE1	1:C:322:PHE:CE2	2.43	0.53
1:A:122:VAL:CG2	1:B:119:MET:CE	2.71	0.53
1:B:282:ILE:CD1	1:B:282:ILE:N	2.71	0.53
1:D:140:ASP:OD1	1:D:140:ASP:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:MET:HE1	1:D:320:PRO:HG2	1.90	0.53
1:C:163:ARG:HG3	1:C:163:ARG:NH1	2.22	0.53
1:C:185:LYS:HB3	1:C:195:VAL:HG22	1.90	0.53
1:B:85:HIS:H	1:B:98:THR:CG2	2.21	0.53
1:B:163:ARG:HG3	3:B:385:HOH:O	2.09	0.53
1:C:298:MET:HE1	1:C:322:PHE:HE2	1.73	0.53
1:C:28:VAL:O	1:C:33:LYS:NZ	2.42	0.53
1:B:298:MET:CE	1:B:320:PRO:CG	2.88	0.52
1:D:285:ILE:HG22	1:D:313:ILE:HD11	1.91	0.52
1:A:74:ILE:HD12	1:A:76:LEU:HD21	1.91	0.52
1:A:315:GLU:OE2	2:A:365:ADP:O1B	2.27	0.52
1:C:191:SER:C	1:C:193:VAL:H	2.17	0.52
1:B:244:CYS:H	1:B:279:ASN:HD21	1.55	0.52
1:C:357:ASN:OD1	1:D:216:HIS:HE1	1.93	0.52
1:D:163:ARG:HH12	1:D:216:HIS:HD2	1.56	0.52
1:A:330:LYS:HD3	1:A:339:TYR:OH	2.10	0.52
1:D:107:HIS:HD2	1:D:319:LEU:O	1.92	0.52
1:B:24:ALA:O	1:B:28:VAL:HG23	2.10	0.51
1:D:26:ASN:HD22	1:D:323:THR:HA	1.74	0.51
1:A:118:GLY:O	1:A:122:VAL:HG23	2.10	0.51
1:A:249:LEU:HD23	1:A:266:ALA:HB2	1.91	0.51
1:D:261:ILE:HG22	1:D:261:ILE:O	2.09	0.51
1:D:85:HIS:CE1	3:D:426:HOH:O	2.64	0.51
1:C:163:ARG:NH1	1:C:216:HIS:HD2	2.07	0.51
1:C:248:VAL:O	1:C:266:ALA:HB3	2.11	0.51
1:C:268:VAL:HG13	1:C:327:MET:CE	2.16	0.51
1:A:310:GLU:HG3	3:A:431:HOH:O	2.09	0.51
1:C:163:ARG:CD	3:C:407:HOH:O	2.40	0.51
1:A:109:THR:O	1:A:113:ASP:OD2	2.28	0.51
1:C:67:ILE:HG23	1:C:67:ILE:O	2.09	0.51
1:D:362:THR:O	1:D:363:THR:OG1	2.26	0.51
1:D:302:ASP:HB3	3:D:384:HOH:O	2.11	0.51
1:C:216:HIS:HE1	1:D:357:ASN:OD1	1.94	0.50
1:A:51:VAL:CG2	1:A:76:LEU:HD11	2.41	0.50
1:A:101:VAL:HG13	1:A:351:LEU:HD21	1.92	0.50
1:A:122:VAL:CB	1:B:119:MET:HE1	2.41	0.50
1:D:247:ILE:HD13	1:D:247:ILE:C	2.37	0.50
1:B:109:THR:O	1:B:113:ASP:OD2	2.29	0.50
1:C:42:GLY:C	1:C:43:ILE:HD13	2.36	0.50
1:C:298:MET:CE	1:C:328:TYR:CD2	2.94	0.50
1:D:192:SER:N	2:D:365:ADP:O2B	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLU:OE2	1:B:317:ASN:ND2	2.45	0.50
1:D:109:THR:O	1:D:113:ASP:OD2	2.30	0.49
1:C:109:THR:HG22	1:C:110:LEU:N	2.27	0.49
1:A:330:LYS:NZ	1:A:333:GLN:NE2	2.60	0.49
1:B:51:VAL:CG2	1:B:74:ILE:HG21	2.43	0.49
1:C:44:ASP:OD2	1:C:48:GLN:HG3	2.12	0.49
1:C:113:ASP:OD2	1:D:121:ARG:NH1	2.46	0.49
1:B:328:TYR:HB3	1:B:329:PRO:HD3	1.95	0.49
1:A:56:ASN:HD21	1:A:70:ARG:NE	2.09	0.49
1:A:74:ILE:CD1	1:A:76:LEU:HD23	2.42	0.49
1:C:26:ASN:HD22	1:C:323:THR:HA	1.77	0.49
1:D:26:ASN:HD22	1:D:323:THR:CA	2.26	0.49
1:A:77:ALA:HB2	1:B:79:VAL:HG22	1.95	0.49
1:D:298:MET:CE	1:D:320:PRO:HD2	2.42	0.49
1:A:193:VAL:HA	1:A:256:TYR:CD1	2.48	0.49
1:A:298:MET:HE1	1:A:328:TYR:CD2	2.48	0.49
1:A:59:GLN:HG3	1:A:70:ARG:CG	2.42	0.48
1:B:3:LYS:HE2	1:B:34:THR:O	2.13	0.48
1:D:232:ALA:HB1	1:D:328:TYR:CE1	2.47	0.48
1:C:44:ASP:HB2	1:C:48:GLN:H	1.77	0.48
1:D:244:CYS:HB2	1:D:279:ASN:HD22	1.78	0.48
1:C:298:MET:CE	1:C:328:TYR:CE2	2.88	0.48
1:D:84:GLN:CB	1:D:98:THR:HG21	2.32	0.48
1:A:260:TYR:CD1	1:A:261:ILE:HD12	2.48	0.48
1:A:165:ASN:ND2	1:A:165:ASN:C	2.71	0.48
1:B:298:MET:HE3	1:B:328:TYR:CZ	2.49	0.48
1:D:26:ASN:HD22	1:D:324:ASN:N	2.11	0.48
1:A:191:SER:O	1:A:191:SER:OG	2.29	0.48
1:A:190:GLY:O	1:A:193:VAL:CG1	2.62	0.48
1:A:357:ASN:OD1	1:B:216:HIS:HE1	1.97	0.48
1:B:190:GLY:O	1:B:193:VAL:HG23	2.14	0.48
1:C:66:HIS:N	3:C:410:HOH:O	2.44	0.48
1:C:298:MET:HE3	1:C:328:TYR:CD2	2.48	0.48
1:C:163:ARG:HH12	1:C:216:HIS:CD2	2.27	0.47
1:A:12:GLY:O	1:A:17:HIS:CD2	2.68	0.47
1:A:184:VAL:HG22	1:A:220:VAL:HG22	1.96	0.47
1:C:177:ARG:HD2	3:C:400:HOH:O	2.11	0.47
1:D:298:MET:CE	1:D:320:PRO:CG	2.92	0.47
1:A:107:HIS:HD2	1:A:319:LEU:O	1.98	0.47
1:C:163:ARG:HH11	1:C:163:ARG:CG	2.23	0.47
1:D:82:LYS:NZ	1:D:85:HIS:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HB	1:A:267:GLN:HB3	1.97	0.47
1:B:298:MET:HE1	1:B:320:PRO:HG2	1.96	0.47
1:D:302:ASP:HB2	1:D:315:GLU:HG3	1.96	0.47
1:A:101:VAL:HG12	1:A:126:PRO:HB2	1.96	0.47
1:C:44:ASP:HB3	1:C:46:ALA:N	2.28	0.47
1:A:192:SER:N	2:A:365:ADP:O2B	2.39	0.47
1:D:261:ILE:O	1:D:261:ILE:CG2	2.61	0.46
1:B:109:THR:O	1:B:113:ASP:CG	2.59	0.46
1:C:363:THR:HG22	3:C:421:HOH:O	2.15	0.46
1:A:57:TYR:OH	1:A:58:LEU:CD1	2.61	0.46
1:B:276:SER:H	1:C:94:GLN:NE2	2.13	0.46
1:A:180:LEU:HD22	1:A:199:ALA:HA	1.98	0.46
1:C:145:LYS:HE3	1:C:158:PHE:CD2	2.50	0.46
1:C:301:VAL:HG22	1:C:316:ILE:HD12	1.96	0.46
1:D:39:VAL:HG23	1:D:41:LEU:HD13	1.98	0.46
1:B:51:VAL:HG23	1:B:74:ILE:CG2	2.44	0.46
1:C:105:ILE:HD12	1:C:105:ILE:HA	1.80	0.46
1:B:305:LEU:HD11	1:B:309:ASN:HA	1.98	0.46
1:C:227:ARG:HB3	1:C:246:GLU:OE2	2.16	0.46
1:A:22:GLN:HB2	1:A:323:THR:HG22	1.97	0.46
1:C:56:ASN:C	1:C:70:ARG:HH11	2.24	0.46
1:D:38:VAL:HG23	1:D:38:VAL:O	2.16	0.46
1:D:163:ARG:NH1	1:D:216:HIS:HD2	2.14	0.46
1:D:124:ASN:HB3	3:D:377:HOH:O	2.15	0.45
1:B:78:GLN:NE2	1:B:119:MET:HG3	2.32	0.45
1:C:122:VAL:CG1	1:D:119:MET:HE1	2.46	0.45
1:C:154:ASN:O	1:C:155:ILE:HD12	2.16	0.45
1:C:175:GLU:OE1	1:C:180:LEU:HD11	2.16	0.45
1:C:43:ILE:N	1:C:43:ILE:CD1	2.78	0.45
1:D:159:ILE:HD11	1:D:161:LEU:CD2	2.44	0.45
1:A:324:ASN:O	1:A:339:TYR:OH	2.29	0.45
1:B:107:HIS:HD2	1:B:319:LEU:O	1.98	0.45
1:A:249:LEU:CD2	1:A:266:ALA:HB2	2.47	0.45
1:C:56:ASN:OD1	1:C:70:ARG:CZ	2.65	0.45
1:D:140:ASP:CG	1:D:143:VAL:HG13	2.42	0.45
1:A:119:MET:HE2	1:A:119:MET:HB3	1.87	0.45
1:B:32:ASP:OD1	1:B:32:ASP:C	2.59	0.45
1:B:298:MET:HE3	1:B:328:TYR:CE1	2.52	0.45
1:C:163:ARG:NH1	1:C:163:ARG:CG	2.78	0.45
1:C:354:HIS:CD2	1:C:358:ASN:HD21	2.35	0.45
1:D:298:MET:CE	1:D:320:PRO:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD22	1:B:100:ASP:CB	2.46	0.44
1:B:189:GLN:NE2	1:B:190:GLY:H	2.15	0.44
1:B:325:ILE:HG23	1:B:325:ILE:O	2.16	0.44
1:C:191:SER:C	1:C:193:VAL:N	2.74	0.44
1:D:66:HIS:CD2	1:D:66:HIS:N	2.85	0.44
1:A:163:ARG:NH1	1:A:216:HIS:CD2	2.75	0.44
1:D:293:LEU:HD12	1:D:316:ILE:HG13	2.00	0.44
1:B:298:MET:CE	1:B:320:PRO:HG2	2.47	0.44
1:C:65:ALA:O	1:C:66:HIS:HB2	2.17	0.44
1:D:261:ILE:HG21	1:D:265:GLY:N	2.32	0.44
1:D:298:MET:HB2	1:D:298:MET:HE3	1.59	0.44
1:D:362:THR:C	1:D:363:THR:OG1	2.60	0.44
1:A:94:GLN:HA	1:A:95:PRO:HD3	1.86	0.44
1:A:326:SER:O	1:A:330:LYS:HG2	2.18	0.44
1:C:26:ASN:HD22	1:C:323:THR:CA	2.31	0.44
1:A:105:ILE:HD12	1:A:105:ILE:HA	1.84	0.44
1:C:50:HIS:CD2	3:C:380:HOH:O	2.46	0.44
1:B:145:LYS:HB3	1:B:155:ILE:HD13	1.99	0.43
1:C:161:LEU:HA	1:C:165:ASN:HD21	1.82	0.43
1:D:65:ALA:C	1:D:66:HIS:CD2	2.96	0.43
1:D:301:VAL:HG13	1:D:316:ILE:CD1	2.48	0.43
1:A:59:GLN:NE2	1:A:70:ARG:CD	2.56	0.43
1:C:32:ASP:C	1:C:32:ASP:OD1	2.62	0.43
1:D:51:VAL:CG2	1:D:96:LEU:HD21	2.48	0.43
1:D:163:ARG:HH12	1:D:216:HIS:CD2	2.36	0.43
2:D:365:ADP:H5'2	3:D:443:HOH:O	2.18	0.43
1:A:112:GLU:HG3	1:A:319:LEU:HB2	1.99	0.43
1:D:85:HIS:H	1:D:98:THR:CG2	2.18	0.43
1:C:65:ALA:O	1:C:66:HIS:CB	2.66	0.43
1:C:162:THR:H	1:C:165:ASN:ND2	2.17	0.43
1:A:109:THR:HG22	1:A:110:LEU:HG	2.01	0.43
1:C:140:ASP:C	1:C:140:ASP:OD1	2.61	0.43
1:A:131:ASP:OD1	1:A:353:ARG:NH2	2.36	0.43
1:B:282:ILE:HD13	1:B:282:ILE:H	1.84	0.43
1:C:133:LEU:HD21	1:D:143:VAL:HG11	2.01	0.43
1:A:26:ASN:HD22	1:A:323:THR:CA	2.30	0.42
1:A:260:TYR:CD1	1:A:261:ILE:CD1	3.01	0.42
1:D:62:ASP:O	1:D:64:PRO:HD3	2.19	0.42
1:D:163:ARG:HH11	1:D:163:ARG:HG3	1.83	0.42
1:A:298:MET:CE	1:A:328:TYR:CD2	2.96	0.42
1:C:268:VAL:CG1	1:C:327:MET:CE	2.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ALA:CB	1:D:339:TYR:HD2	2.32	0.42
1:A:51:VAL:HG23	1:A:76:LEU:HD11	2.01	0.42
1:C:298:MET:HE2	1:C:320:PRO:HG3	2.00	0.42
1:A:190:GLY:O	1:A:193:VAL:HG12	2.19	0.42
1:C:146:ARG:HD2	3:D:399:HOH:O	2.18	0.42
1:D:98:THR:HG23	3:D:426:HOH:O	2.18	0.42
1:A:282:ILE:HD11	1:A:305:LEU:HD13	2.01	0.41
1:B:57:TYR:CD1	1:B:58:LEU:HG	2.55	0.41
1:A:51:VAL:HG22	1:A:76:LEU:HD11	2.02	0.41
1:A:244:CYS:HB2	1:A:279:ASN:OD1	2.21	0.41
1:C:232:ALA:HB1	1:C:328:TYR:CE1	2.55	0.41
1:C:318:THR:O	1:C:319:LEU:HG	2.20	0.41
1:D:65:ALA:HA	1:D:260:TYR:HD1	1.85	0.41
1:D:65:ALA:CA	1:D:260:TYR:HD1	2.33	0.41
1:A:189:GLN:HB3	1:A:190:GLY:H	1.42	0.41
1:A:256:TYR:O	1:A:259:LYS:HG3	2.21	0.41
1:C:26:ASN:HD22	1:C:324:ASN:H	1.66	0.41
1:D:261:ILE:HG22	1:D:264:ASN:HA	2.03	0.41
1:A:59:GLN:HE22	1:A:71:PRO:HD2	1.86	0.41
1:A:86:GLN:HG2	1:A:123:ALA:O	2.21	0.41
1:B:282:ILE:HD12	1:B:282:ILE:N	2.36	0.41
1:C:57:TYR:CD1	1:C:58:LEU:HG	2.55	0.41
1:A:79:VAL:HG22	1:B:77:ALA:HB2	2.02	0.41
1:D:191:SER:H	1:D:193:VAL:CG1	2.34	0.41
1:B:85:HIS:H	1:B:98:THR:HG22	1.86	0.40
1:C:78:GLN:NE2	1:D:78:GLN:HE21	2.09	0.40
1:C:361:LYS:HD2	1:D:213:GLU:HB3	2.03	0.40
1:A:154:ASN:O	1:A:155:ILE:HD12	2.21	0.40
1:C:136:ALA:HB1	1:D:133:LEU:HB2	2.03	0.40
1:D:244:CYS:CB	1:D:279:ASN:ND2	2.82	0.40
1:D:260:TYR:CE2	1:D:261:ILE:HD13	2.55	0.40
1:A:139:MET:HG3	1:A:188:ASN:HD22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/364 (98%)	342 (96%)	12 (3%)	2 (1%)	21	23
1	B	342/364 (94%)	329 (96%)	12 (4%)	1 (0%)	36	42
1	C	344/364 (94%)	325 (94%)	16 (5%)	3 (1%)	14	14
1	D	351/364 (96%)	337 (96%)	10 (3%)	4 (1%)	11	10
All	All	1393/1456 (96%)	1333 (96%)	50 (4%)	10 (1%)	18	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	191	SER
1	C	192	SER
1	D	192	SER
1	A	32	ASP
1	A	192	SER
1	D	14	SER
1	C	66	HIS
1	D	266	ALA
1	D	190	GLY
1	C	63	ASP

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	293/297 (99%)	269 (92%)	24 (8%)	10	12
1	B	282/297 (95%)	259 (92%)	23 (8%)	10	12
1	C	282/297 (95%)	255 (90%)	27 (10%)	8	8
1	D	290/297 (98%)	268 (92%)	22 (8%)	12	14
All	All	1147/1188 (96%)	1051 (92%)	96 (8%)	10	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	22	GLN
1	A	38	VAL
1	A	39	VAL
1	A	41	LEU
1	A	53	ASP
1	A	74	ILE
1	A	78	GLN
1	A	94	GLN
1	A	101	VAL
1	A	119	MET
1	A	142	ASP
1	A	155	ILE
1	A	165	ASN
1	A	177	ARG
1	A	193	VAL
1	A	197	LYS
1	A	225	LYS
1	A	256	TYR
1	A	259	LYS
1	A	298	MET
1	A	310	GLU
1	A	358	ASN
1	A	363	THR
1	B	38	VAL
1	B	39	VAL
1	B	43	ILE
1	B	51	VAL
1	B	53	ASP
1	B	78	GLN
1	B	98	THR
1	B	101	VAL
1	B	119	MET
1	B	128	VAL
1	B	143	VAL
1	B	160	THR
1	B	163	ARG
1	B	173	GLU
1	B	189	GLN
1	B	191	SER
1	B	225	LYS
1	B	277	GLU

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Mol	Chain	Res	Type
1	B	282	ILE
1	B	293	LEU
1	B	317	ASN
1	B	319	LEU
1	B	325	ILE
1	C	38	VAL
1	C	39	VAL
1	C	41	LEU
1	C	43	ILE
1	C	48	GLN
1	C	53	ASP
1	C	59	GLN
1	C	62	ASP
1	C	79	VAL
1	C	84	GLN
1	C	101	VAL
1	C	105	ILE
1	C	109	THR
1	C	155	ILE
1	C	165	ASN
1	C	166	ARG
1	C	173	GLU
1	C	185	LYS
1	C	189	GLN
1	C	192	SER
1	C	193	VAL
1	C	205	GLN
1	C	206	GLN
1	C	247	ILE
1	C	333	GLN
1	C	353	ARG
1	C	364	MET
1	D	13	LYS
1	D	39	VAL
1	D	41	LEU
1	D	55	GLU
1	D	66	HIS
1	D	84	GLN
1	D	91	GLN
1	D	101	VAL
1	D	110	LEU
1	D	119	MET

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Mol	Chain	Res	Type
1	D	128	VAL
1	D	143	VAL
1	D	159	ILE
1	D	193	VAL
1	D	225	LYS
1	D	247	ILE
1	D	260	TYR
1	D	261	ILE
1	D	308	ASP
1	D	319	LEU
1	D	325	ILE
1	D	363	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	GLN
1	A	26	ASN
1	A	56	ASN
1	A	59	GLN
1	A	60	ASN
1	A	66	HIS
1	A	78	GLN
1	A	107	HIS
1	A	124	ASN
1	A	154	ASN
1	A	165	ASN
1	A	188	ASN
1	A	216	HIS
1	A	222	GLN
1	A	240	GLN
1	A	291	GLN
1	A	324	ASN
1	A	333	GLN
1	A	354	HIS
1	A	358	ASN
1	B	78	GLN
1	B	84	GLN
1	B	107	HIS
1	B	124	ASN
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	216	HIS
1	B	222	GLN
1	B	236	ASN
1	B	240	GLN
1	B	267	GLN
1	B	279	ASN
1	B	317	ASN
1	C	17	HIS
1	C	26	ASN
1	C	48	GLN
1	C	50	HIS
1	C	59	GLN
1	C	66	HIS
1	C	94	GLN
1	C	107	HIS
1	C	154	ASN
1	C	165	ASN
1	C	188	ASN
1	C	206	GLN
1	C	216	HIS
1	C	240	GLN
1	C	267	GLN
1	C	288	GLN
1	C	314	ASN
1	C	354	HIS
1	C	358	ASN
1	D	26	ASN
1	D	66	HIS
1	D	78	GLN
1	D	85	HIS
1	D	107	HIS
1	D	188	ASN
1	D	206	GLN
1	D	216	HIS
1	D	236	ASN
1	D	273	GLN
1	D	279	ASN
1	D	324	ASN
1	D	354	HIS
1	D	358	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	C	365	-	28,29,29	1.42	4 (14%)	43,45,45	2.04	12 (27%)
2	ADP	A	365	-	28,29,29	1.49	4 (14%)	43,45,45	1.91	11 (25%)
2	ADP	B	365	-	28,29,29	1.46	5 (17%)	43,45,45	1.87	10 (23%)
2	ADP	D	365	-	28,29,29	1.88	4 (14%)	43,45,45	1.89	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	C	365	-	-	3/16/32/32	0/3/3/3
2	ADP	A	365	-	-	1/16/32/32	0/3/3/3
2	ADP	B	365	-	-	1/16/32/32	0/3/3/3
2	ADP	D	365	-	-	1/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	365	ADP	C5-C4	5.68	1.49	1.39
2	D	365	ADP	PA-O3A	4.95	1.64	1.59
2	A	365	ADP	C5-C4	4.65	1.47	1.39
2	C	365	ADP	C5-C4	3.91	1.46	1.39
2	D	365	ADP	C8-N7	3.67	1.38	1.31
2	B	365	ADP	C5-C4	3.44	1.45	1.39
2	B	365	ADP	C4-N9	-3.06	1.31	1.37
2	C	365	ADP	C4-N9	-3.04	1.31	1.37
2	B	365	ADP	C5-N7	-2.92	1.33	1.39
2	A	365	ADP	PA-O3A	2.81	1.62	1.59
2	D	365	ADP	C5-C6	2.58	1.48	1.41
2	B	365	ADP	C8-N7	2.46	1.36	1.31
2	C	365	ADP	PA-O3A	2.26	1.61	1.59
2	B	365	ADP	PA-O3A	2.24	1.61	1.59
2	A	365	ADP	C5-N7	-2.20	1.35	1.39
2	A	365	ADP	C8-N7	2.18	1.35	1.31
2	C	365	ADP	C5-C6	2.11	1.46	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	ADP	C5-C4-N3	-5.83	118.69	126.72
2	D	365	ADP	C5-C4-N3	-5.65	118.93	126.72
2	C	365	ADP	C5-C4-N3	-5.63	118.97	126.72
2	A	365	ADP	C5-C4-N3	-5.21	119.54	126.72
2	B	365	ADP	N3-C4-N9	4.88	135.47	127.17
2	A	365	ADP	N3-C4-N9	4.61	135.00	127.17
2	C	365	ADP	N3-C4-N9	4.59	134.97	127.17
2	C	365	ADP	C4-N9-C8	4.16	110.11	105.74
2	B	365	ADP	N3-C2-N1	-4.14	122.31	128.58
2	C	365	ADP	C2-N3-C4	4.04	121.69	111.83
2	A	365	ADP	N3-C2-N1	-4.00	122.53	128.58
2	C	365	ADP	N3-C2-N1	-3.93	122.63	128.58
2	D	365	ADP	O2B-PB-O1B	3.92	126.13	110.83
2	A	365	ADP	C2-N3-C4	3.88	121.32	111.83
2	D	365	ADP	N3-C4-N9	3.81	133.64	127.17
2	B	365	ADP	C2-N3-C4	3.76	121.01	111.83
2	D	365	ADP	C2-N3-C4	3.63	120.69	111.83
2	D	365	ADP	N3-C2-N1	-3.63	123.09	128.58
2	C	365	ADP	C4-C5-N7	-3.58	106.48	110.58
2	D	365	ADP	C4-C5-N7	-3.51	106.57	110.58
2	C	365	ADP	N9-C8-N7	-3.17	109.44	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	365	ADP	C4-N9-C8	3.11	109.00	105.74
2	B	365	ADP	N6-C6-N1	3.04	125.15	118.38
2	C	365	ADP	C5-N7-C8	2.82	107.88	103.45
2	D	365	ADP	O2A-PA-O1A	2.77	125.35	112.44
2	A	365	ADP	C4-C5-N7	-2.66	107.54	110.58
2	B	365	ADP	O2B-PB-O1B	2.60	120.98	110.83
2	A	365	ADP	N6-C6-N1	2.57	124.09	118.38
2	A	365	ADP	O2A-PA-O1A	2.55	124.32	112.44
2	B	365	ADP	C4-N9-C8	2.54	108.40	105.74
2	B	365	ADP	C5-C6-N6	-2.52	117.04	123.29
2	C	365	ADP	O2'-C2'-C1'	-2.46	101.62	110.10
2	C	365	ADP	C3'-C2'-C1'	2.38	105.97	101.46
2	D	365	ADP	C5-N7-C8	2.35	107.14	103.45
2	C	365	ADP	C6-C5-N7	2.34	136.60	132.09
2	A	365	ADP	C5-N7-C8	2.18	106.88	103.45
2	A	365	ADP	O2B-PB-O1B	2.16	119.25	110.83
2	D	365	ADP	C2-N1-C6	2.15	122.27	118.73
2	B	365	ADP	C2-N1-C6	2.14	122.25	118.73
2	D	365	ADP	C6-C5-N7	2.13	136.20	132.09
2	B	365	ADP	O2B-PB-O3A	-2.13	97.49	104.64
2	C	365	ADP	O3B-PB-O2B	2.11	115.71	107.80
2	D	365	ADP	O2B-PB-O3A	-2.09	97.64	104.64
2	A	365	ADP	C2-N1-C6	2.03	122.06	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	365	ADP	PA-O3A-PB-O3B
2	C	365	ADP	PB-O3A-PA-O1A
2	C	365	ADP	C4'-C5'-O5'-PA
2	B	365	ADP	C4'-C5'-O5'-PA
2	A	365	ADP	PB-O3A-PA-O2A
2	D	365	ADP	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 7 short contacts:

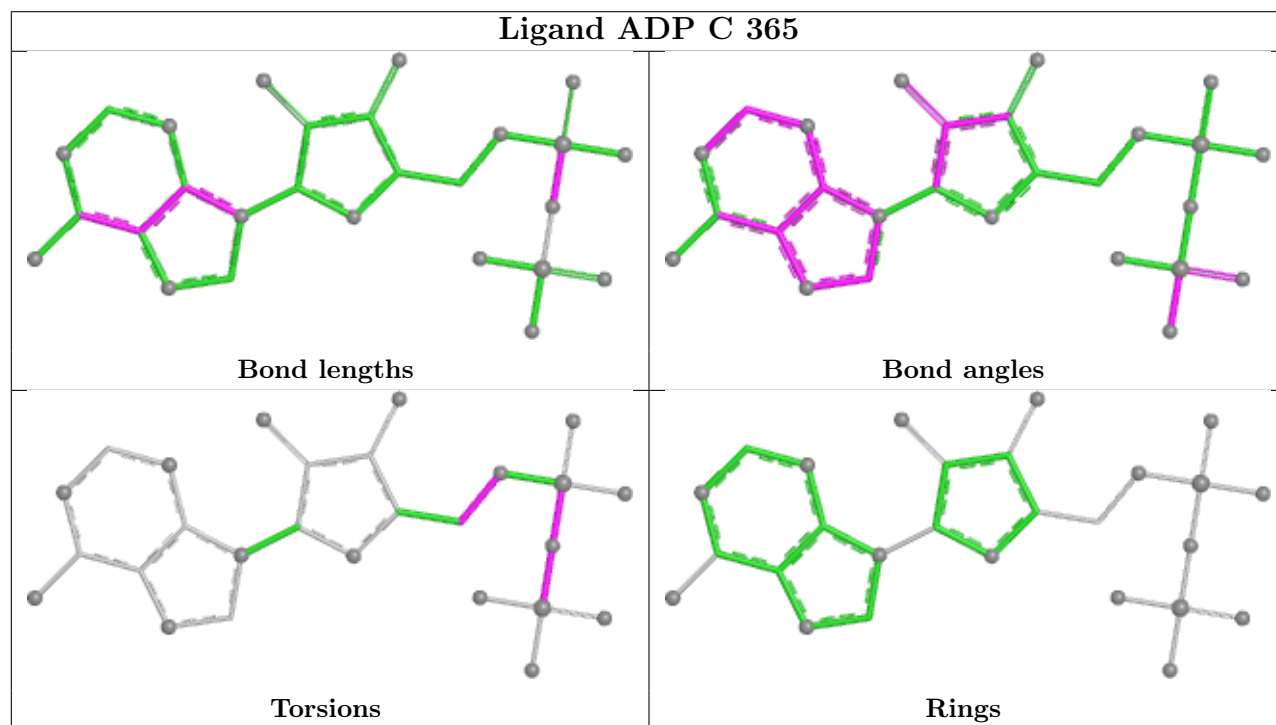
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	365	ADP	3	0
2	B	365	ADP	1	0

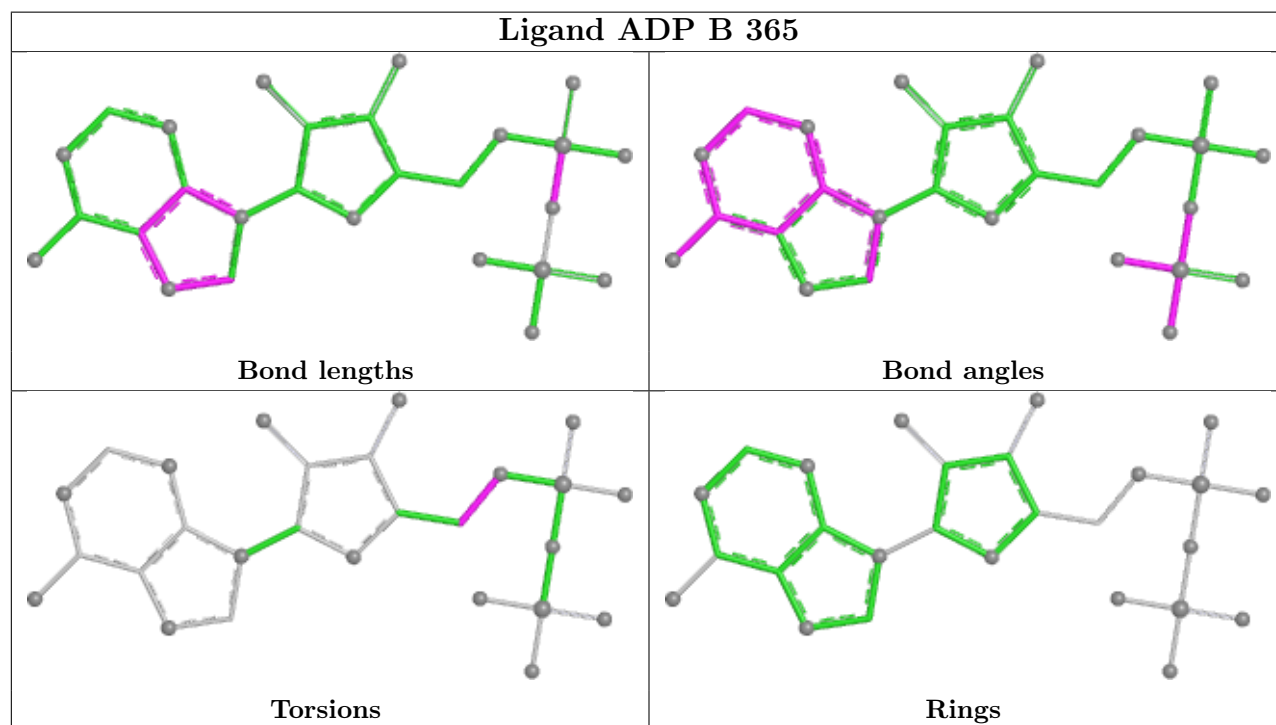
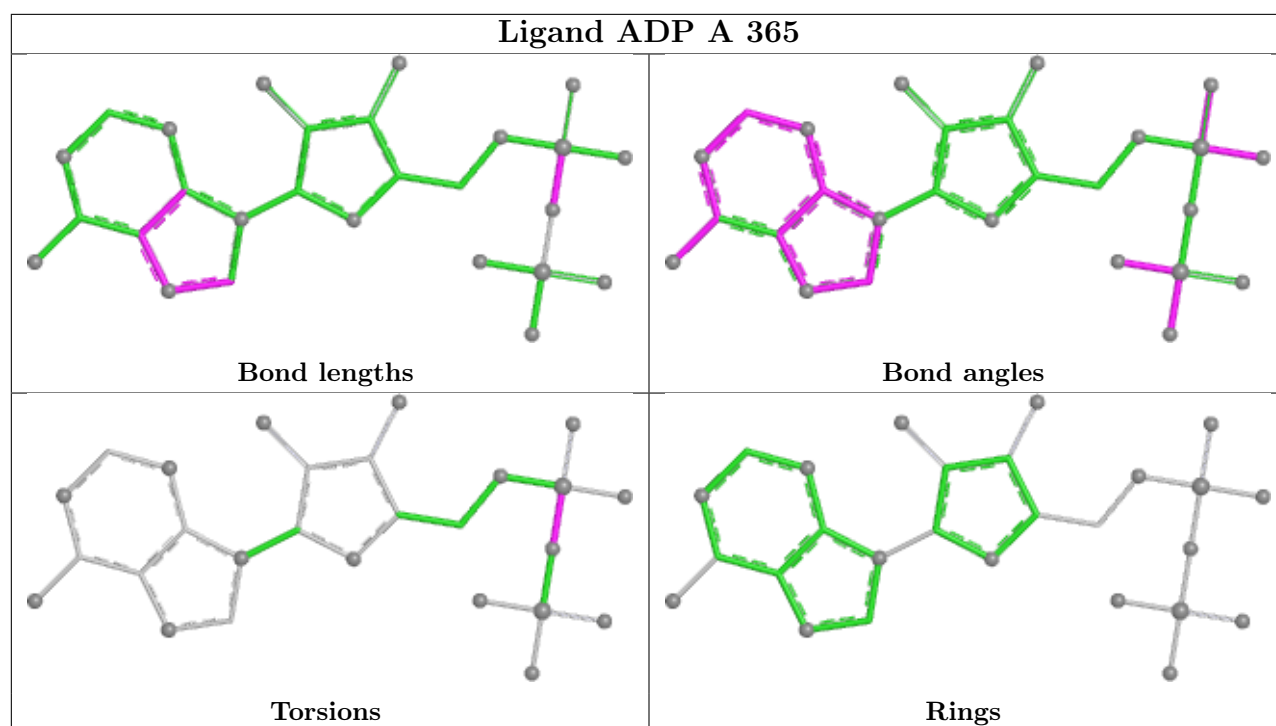
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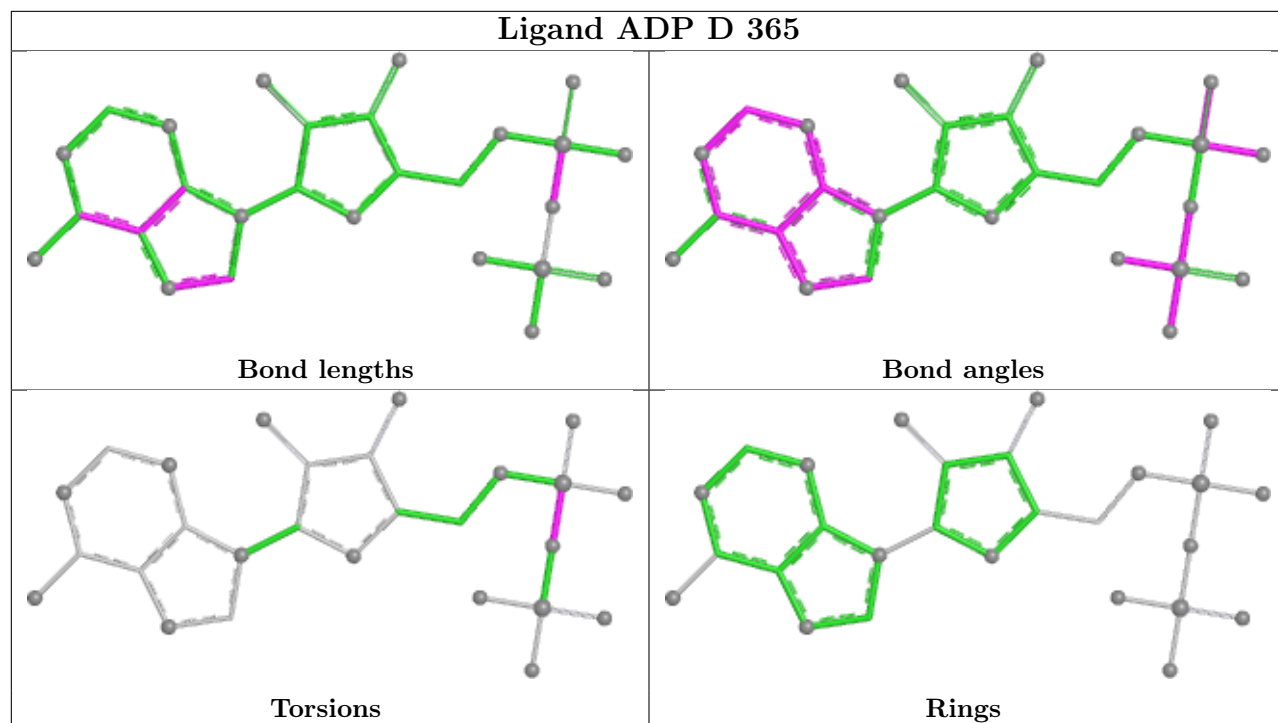
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	365	ADP	3	0

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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	360/364 (98%)	-0.05	15 (4%) 40 37	20, 31, 55, 77	0
1	B	346/364 (95%)	-0.15	7 (2%) 65 62	20, 30, 49, 67	0
1	C	348/364 (95%)	0.21	18 (5%) 33 29	24, 36, 59, 73	0
1	D	355/364 (97%)	-0.08	8 (2%) 61 58	19, 29, 52, 70	0
All	All	1409/1456 (96%)	-0.02	48 (3%) 48 45	19, 32, 54, 77	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	TYR	5.5
1	C	249	LEU	5.4
1	C	266	ALA	5.1
1	A	256	TYR	4.8
1	C	265	GLY	4.5
1	D	260	TYR	4.0
1	B	267	GLN	3.7
1	D	363	THR	3.4
1	D	193	VAL	3.2
1	A	258	THR	3.0
1	A	193	VAL	3.0
1	A	2	ALA	2.9
1	C	191	SER	2.9
1	C	108	GLY	2.9
1	C	190	GLY	2.9
1	B	2	ALA	2.9
1	A	260	TYR	2.8
1	C	2	ALA	2.8
1	B	1	MET	2.8
1	C	61	ALA	2.7
1	A	74	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	169	PHE	2.7
1	A	56	ASN	2.7
1	A	191	SER	2.6
1	D	109	THR	2.6
1	C	248	VAL	2.6
1	A	253	PHE	2.5
1	C	109	THR	2.5
1	D	253	PHE	2.5
1	A	109	THR	2.4
1	A	339	TYR	2.4
1	B	363	THR	2.4
1	D	315	GLU	2.4
1	D	190	GLY	2.3
1	C	65	ALA	2.3
1	C	55	GLU	2.3
1	B	249	LEU	2.3
1	B	109	THR	2.2
1	C	16	GLU	2.2
1	C	22	GLN	2.2
1	A	257	ASP	2.1
1	C	247	ILE	2.1
1	D	308	ASP	2.1
1	C	267	GLN	2.1
1	A	190	GLY	2.1
1	C	66	HIS	2.0
1	A	72	SER	2.0
1	B	74	ILE	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.

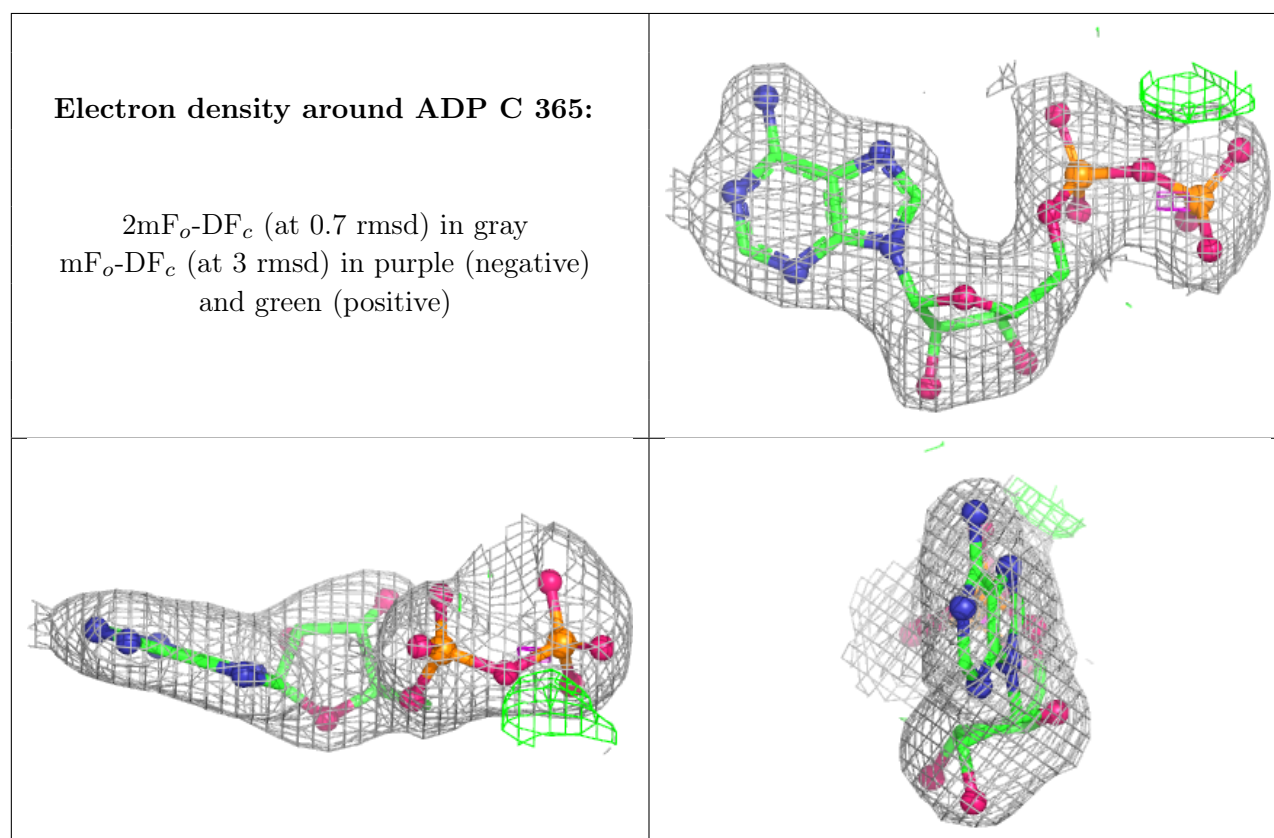
6.4 Ligands [i](#)

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.

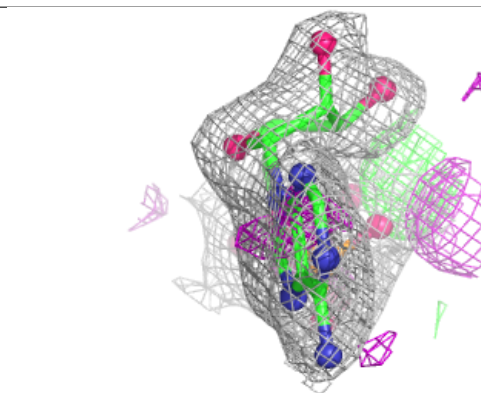
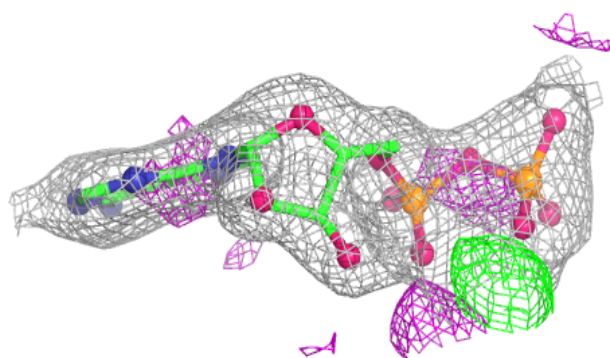
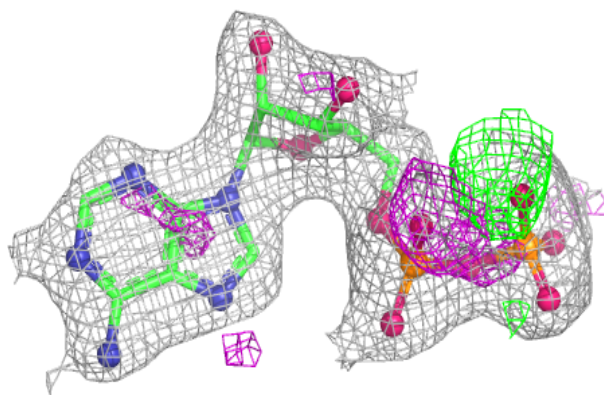
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	C	365	27/27	0.87	0.10	46,62,87,88	0
2	ADP	D	365	27/27	0.90	0.08	38,42,47,52	0
2	ADP	B	365	27/27	0.92	0.09	35,48,69,71	0
2	ADP	A	365	27/27	0.94	0.07	37,44,47,50	0

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.

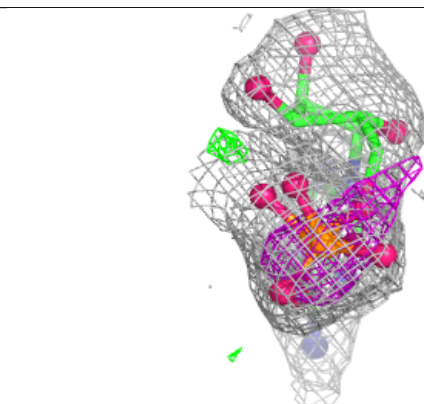
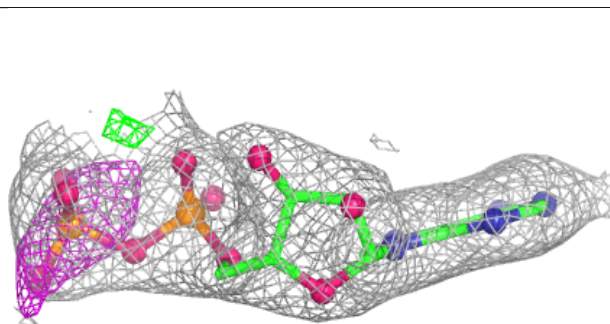
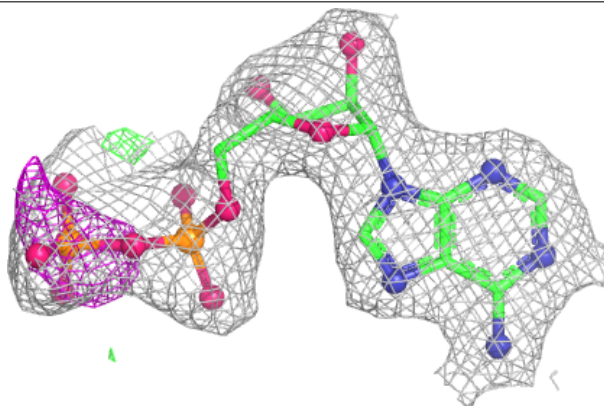


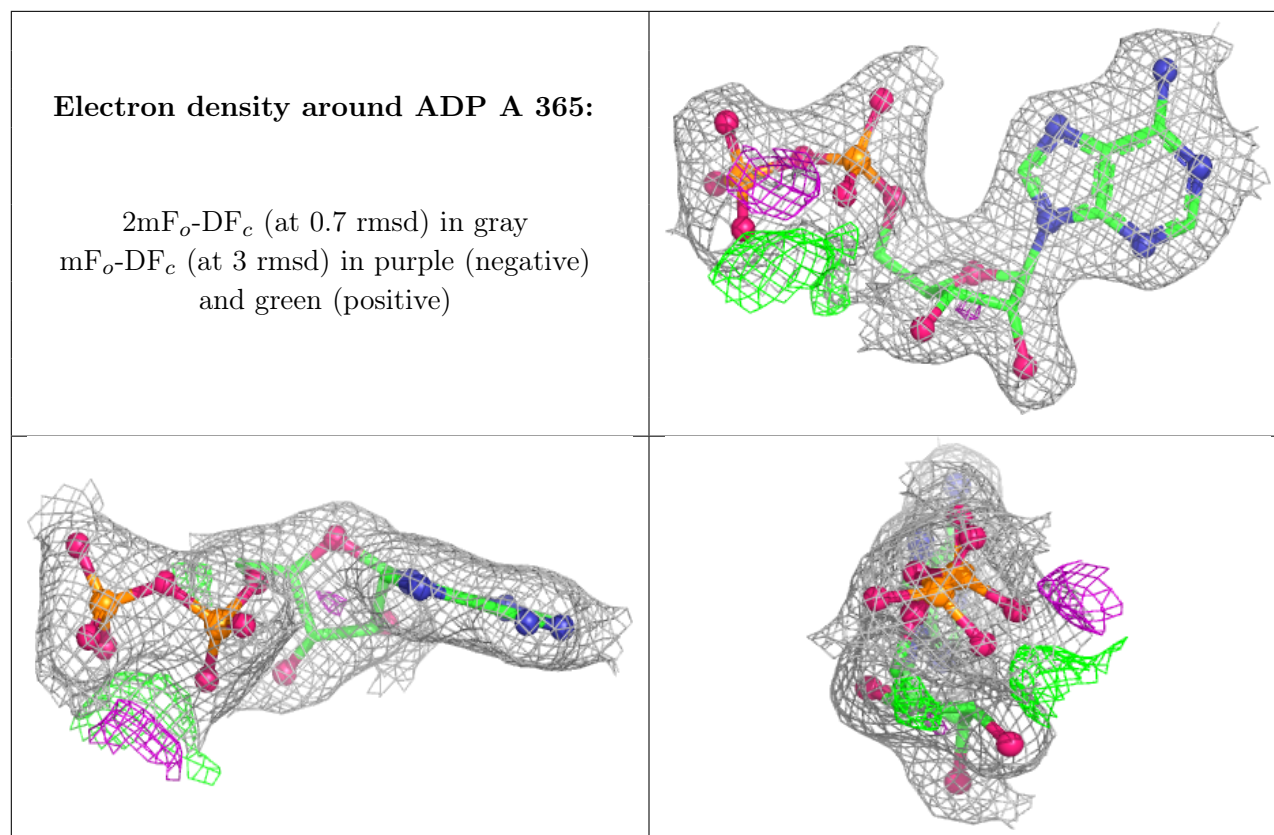
Electron density around ADP D 365:

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

**Electron density around ADP B 365:**

$2mF_o-DF_c$ (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.