



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:07 AM UTC

PDB ID : 1ZXN / pdb_00001zxn
Title : Human DNA topoisomerase IIa ATPase/ADP
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Deposited on : 2005-06-08
Resolution : 2.51 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

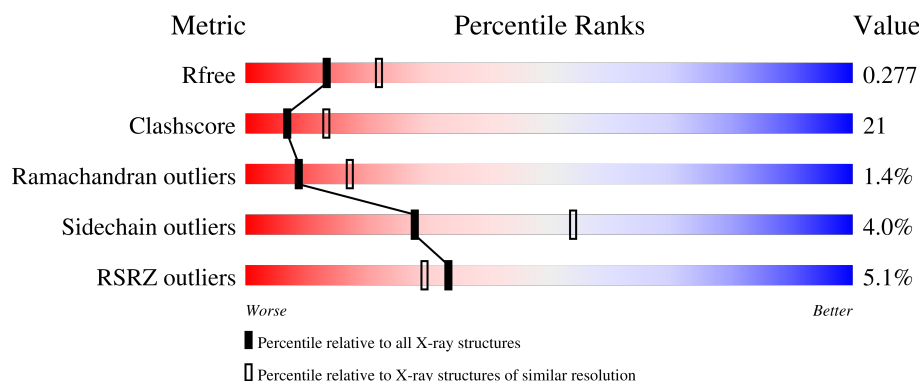
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	400	9% 55% 32% 8%
1	B	400	3% 58% 33% 5%
1	C	400	% 64% 28% %
1	D	400	6% 57% 34% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11646 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 DNA topoisomerase II, alpha isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2736	1748	455	515	18			
1	B	379	Total	C	N	O	S	0	0	0
			2886	1844	481	543	18			
1	C	384	Total	C	N	O	S	0	0	0
			2897	1850	485	543	19			
1	D	371	Total	C	N	O	S	0	0	0
			2761	1766	458	518	19			

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

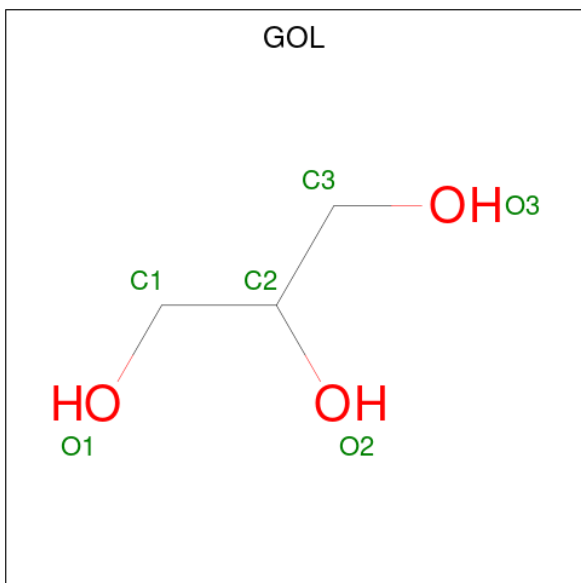
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

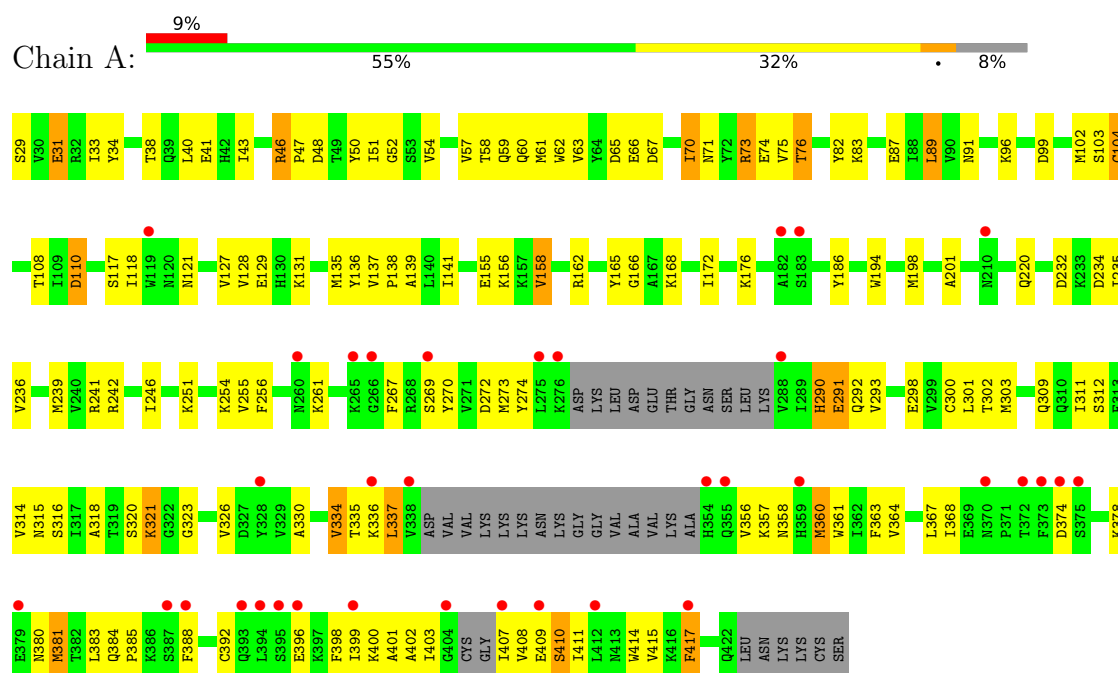
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		
6	B	72	Total	O	0	0
			72	72		
6	C	72	Total	O	0	0
			72	72		
6	D	35	Total	O	0	0
			35	35		

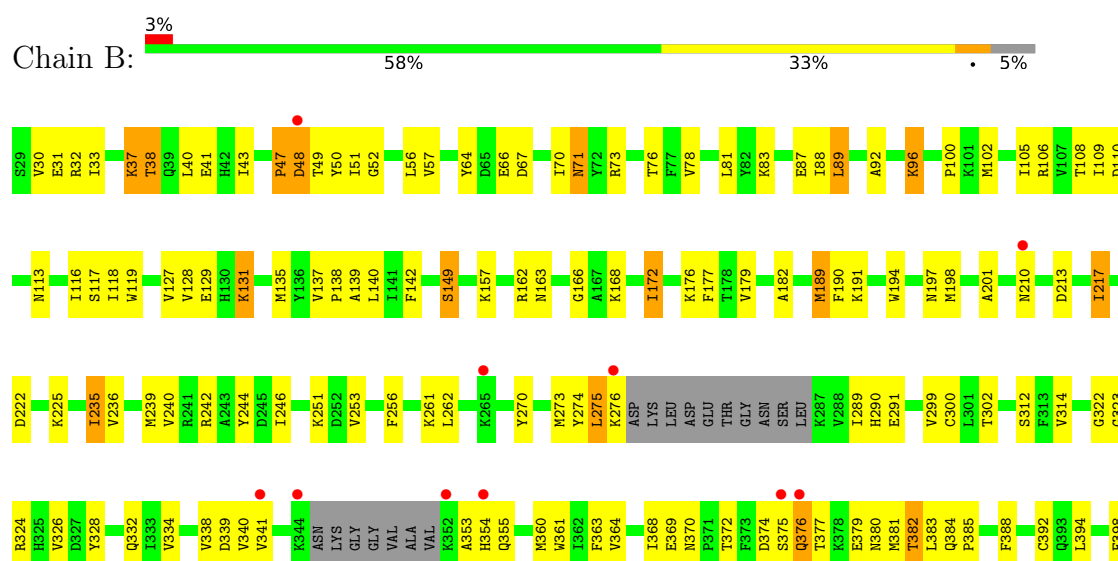
3 Residue-property plots [i](#)

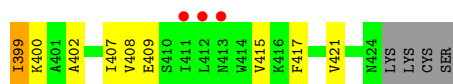
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

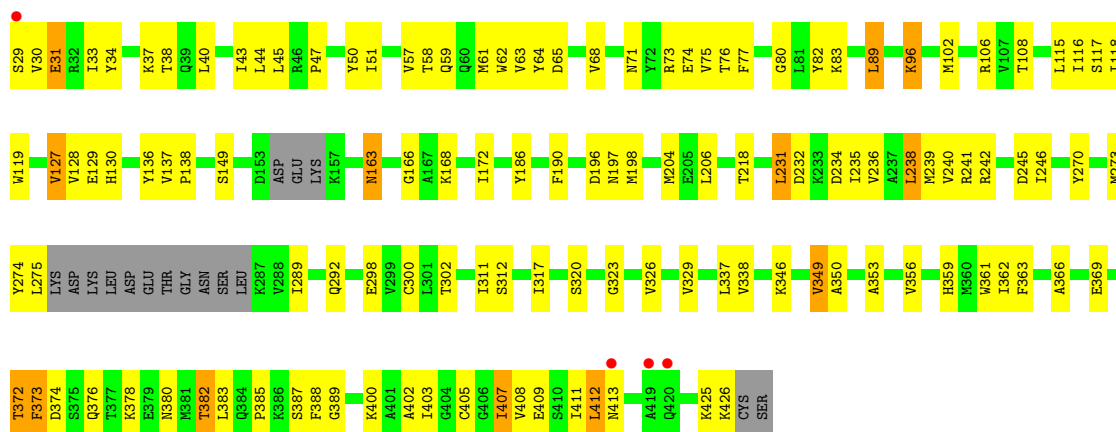


- Molecule 1: DNA topoisomerase II, alpha isozyme

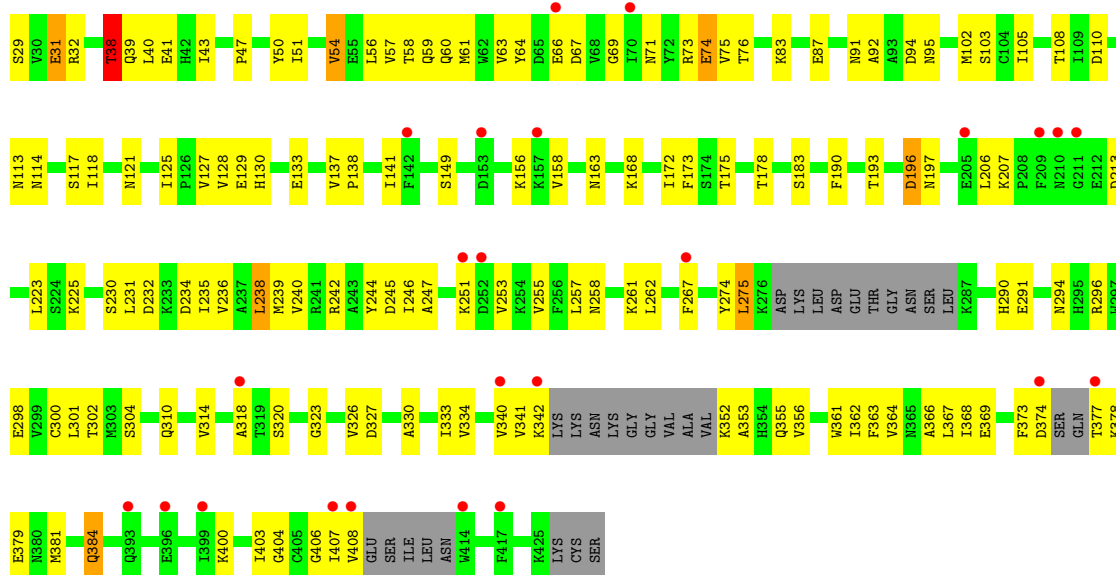




• Molecule 1: DNA topoisomerase II, alpha isozyme



• Molecule 1: DNA topoisomerase II, alpha isozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.02Å 90.49Å 148.29Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 50.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.51) 94.9 (50.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.281 0.231 , 0.277	Depositor DCC
R_{free} test set	4648 reflections (7.29%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: GOL, SO4, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/2790	0.98	14/3793 (0.4%)
1	B	0.50	0/2944	1.02	16/4003 (0.4%)
1	C	0.48	0/2956	0.97	14/4025 (0.3%)
1	D	0.40	0/2816	0.91	6/3832 (0.2%)
All	All	0.46	0/11506	0.97	50/15653 (0.3%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	SER	N-CA-C	-8.18	103.30	113.20
1	C	373	PHE	N-CA-C	7.57	121.26	109.52
1	C	413	ASN	N-CA-C	-7.44	103.25	111.36
1	A	74	GLU	N-CA-C	-6.68	98.50	109.40
1	B	382	THR	N-CA-C	6.67	121.02	113.02
1	B	131	LYS	N-CA-C	6.60	119.30	111.71
1	B	376	GLN	N-CA-C	-6.60	105.98	112.97
1	B	360	MET	N-CA-C	6.58	121.02	109.96
1	B	375	SER	N-CA-C	6.47	118.37	109.18
1	C	320	SER	N-CA-C	6.26	118.90	111.33
1	C	389	GLY	N-CA-C	-6.10	106.54	115.63
1	B	149	SER	N-CA-C	-6.09	105.02	112.88
1	C	232	ASP	N-CA-C	6.08	117.88	110.41
1	C	149	SER	N-CA-C	-5.91	105.26	112.88
1	D	74	GLU	N-CA-C	-5.88	99.41	109.24
1	C	37	LYS	N-CA-C	5.88	118.64	109.52
1	B	312	SER	N-CA-C	5.79	117.59	108.96
1	B	78	VAL	CA-C-N	5.71	125.17	119.24
1	B	78	VAL	C-N-CA	5.71	125.17	119.24
1	C	349	VAL	N-CA-C	-5.66	103.88	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	SER	N-CA-C	5.66	119.80	113.01
1	A	360	MET	N-CA-C	5.64	119.25	110.17
1	A	54	VAL	N-CA-C	-5.64	106.89	111.91
1	B	299	VAL	N-CA-C	5.63	116.59	108.48
1	A	396	GLU	N-CA-C	-5.58	104.58	111.33
1	A	46	ARG	CA-C-N	5.53	126.76	119.84
1	A	46	ARG	C-N-CA	5.53	126.76	119.84
1	D	54	VAL	N-CA-C	-5.50	106.05	111.77
1	A	255	VAL	N-CA-C	5.48	115.75	107.80
1	C	411	ILE	N-CA-C	5.45	116.18	110.62
1	D	38	THR	N-CA-C	-5.45	103.20	110.55
1	B	270	TYR	N-CA-C	-5.43	105.27	111.14
1	A	73	ARG	CB-CA-C	-5.39	104.69	113.37
1	B	33	ILE	N-CA-C	5.38	115.47	110.42
1	A	110	ASP	CA-C-N	5.35	125.42	119.32
1	A	110	ASP	C-N-CA	5.35	125.42	119.32
1	D	320	SER	N-CA-C	5.33	117.09	111.28
1	B	354	HIS	N-CA-C	-5.32	106.49	112.87
1	B	415	VAL	N-CA-C	-5.25	105.27	110.62
1	C	376	GLN	N-CA-C	-5.25	106.83	113.18
1	D	39	GLN	N-CA-C	-5.19	105.63	111.28
1	D	327	ASP	N-CA-C	-5.17	104.60	112.04
1	C	366	ALA	N-CA-C	5.14	117.20	109.23
1	A	104	CYS	N-CA-C	5.12	116.07	108.60
1	C	382	THR	N-CA-C	5.04	120.05	113.30
1	B	364	VAL	N-CA-C	5.04	115.22	107.77
1	B	172	ILE	CB-CA-C	-5.02	104.72	112.05
1	C	312	SER	N-CA-C	5.02	116.83	109.24
1	A	131	LYS	N-CA-C	5.02	117.48	111.71
1	C	74	GLU	N-CA-C	-5.02	101.13	109.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2736	0	2520	142	0
1	B	2886	0	2715	112	0
1	C	2897	0	2706	101	0
1	D	2761	0	2531	116	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	2	0
4	A	6	0	8	1	0
5	B	5	0	0	1	0
5	D	5	0	0	1	0
6	A	59	0	0	0	0
6	B	72	0	0	3	0
6	C	72	0	0	1	0
6	D	35	0	0	0	0
All	All	11646	0	10528	467	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 21.

All (467) 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:108:THR:HB	1:D:117:SER:HB3	1.32	1.07
1:B:38:THR:HG22	1:B:41:GLU:H	1.27	1.00
1:B:407:ILE:HG23	1:B:408:VAL:H	1.31	0.95
1:B:182:ALA:O	1:B:213:ASP:HB2	1.74	0.88
1:C:235:ILE:HG13	1:C:239:MET:HE2	1.55	0.88
1:D:38:THR:HG22	1:D:40:LEU:H	1.43	0.84
1:A:89:LEU:HD22	1:A:246:ILE:HG13	1.61	0.82
1:D:168:LYS:O	1:D:172:ILE:HG12	1.80	0.81
1:B:48:ASP:HA	1:B:52:GLY:O	1.80	0.81
1:A:321:LYS:HZ2	1:A:380:ASN:HB2	1.46	0.80
1:D:400:LYS:O	1:D:403:ILE:HG12	1.81	0.80
1:A:71:ASN:OD1	1:A:73:ARG:HG3	1.82	0.80
1:A:293:VAL:HG21	1:A:392:CYS:SG	2.22	0.79
1:D:38:THR:HB	1:D:41:GLU:HG3	1.64	0.77
1:C:289:ILE:HD11	1:C:405:CYS:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:ND1	1:A:291:GLU:N	2.32	0.77
1:D:231:LEU:HD23	1:D:239:MET:HE1	1.68	0.76
1:D:206:LEU:O	1:D:207:LYS:HG3	1.86	0.75
1:C:89:LEU:CD2	1:C:246:ILE:HG13	2.17	0.75
1:B:40:LEU:HD13	1:B:172:ILE:HD12	1.68	0.75
1:C:346:LYS:HE2	1:C:346:LYS:HA	1.70	0.74
1:A:235:ILE:HG13	1:A:239:MET:HE3	1.69	0.74
1:B:407:ILE:HG23	1:B:408:VAL:N	2.01	0.74
1:D:314:VAL:HG21	1:D:381:MET:HG3	1.68	0.73
1:D:173:PHE:HE1	1:D:225:LYS:HE2	1.52	0.73
1:A:168:LYS:O	1:A:172:ILE:HG12	1.88	0.73
1:D:38:THR:HG22	1:D:40:LEU:N	2.04	0.72
1:B:168:LYS:O	1:B:172:ILE:HG12	1.90	0.72
1:D:56:LEU:HD22	1:D:76:THR:HG22	1.70	0.72
1:D:314:VAL:HG13	1:D:368:ILE:HD13	1.70	0.72
1:A:104:CYS:HB2	1:A:254:LYS:O	1.89	0.72
1:D:173:PHE:CE1	1:D:225:LYS:HE2	2.26	0.71
1:A:62:TRP:CE3	1:A:70:ILE:HD11	2.27	0.70
1:A:400:LYS:C	1:A:402:ALA:H	2.00	0.69
1:A:29:SER:O	1:A:33:ILE:HG22	1.93	0.69
1:A:38:THR:HG23	1:A:41:GLU:H	1.57	0.69
1:C:127:VAL:HG12	1:C:127:VAL:O	1.93	0.69
1:C:289:ILE:CD1	1:C:402:ALA:HA	2.22	0.69
1:D:231:LEU:HD12	1:D:231:LEU:N	2.08	0.69
1:D:75:VAL:HG13	1:D:234:ASP:HB3	1.75	0.68
1:A:70:ILE:CG2	1:A:273:MET:HE2	2.23	0.68
1:B:289:ILE:HD13	1:B:402:ALA:HA	1.75	0.68
1:A:269:SER:O	1:A:272:ASP:HB2	1.94	0.67
1:C:33:ILE:HG23	1:C:34:TYR:CD2	2.30	0.67
1:C:89:LEU:HD21	1:C:246:ILE:HG13	1.76	0.67
1:A:321:LYS:NZ	1:A:380:ASN:HB2	2.09	0.67
1:B:64:TYR:HE2	1:B:273:MET:HE1	1.58	0.66
1:B:40:LEU:CD1	1:B:172:ILE:HD12	2.25	0.66
1:B:377:THR:HB	1:B:379:GLU:HG3	1.78	0.66
1:D:236:VAL:O	1:D:240:VAL:HG23	1.95	0.66
1:C:61:MET:SD	1:C:238:LEU:HD21	2.35	0.66
1:D:235:ILE:O	1:D:239:MET:HG3	1.95	0.66
1:B:81:LEU:HD23	1:B:235:ILE:HG13	1.78	0.66
1:D:301:LEU:HD22	1:D:333:ILE:HD13	1.78	0.66
1:A:172:ILE:HD11	1:A:198:MET:HE2	1.76	0.65
1:A:104:CYS:H	1:A:121:ASN:HD21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ILE:O	1:D:197:ASN:HA	1.96	0.65
1:D:368:ILE:HD12	1:D:368:ILE:N	2.11	0.65
1:A:108:THR:HB	1:A:117:SER:OG	1.96	0.65
1:B:289:ILE:CD1	1:B:402:ALA:HA	2.26	0.65
1:C:204:MET:HE3	1:C:206:LEU:HD11	1.79	0.65
1:B:251:LYS:O	1:B:253:VAL:HG23	1.98	0.64
1:A:314:VAL:HG13	1:A:368:ILE:HD13	1.80	0.64
1:D:384:GLN:H	1:D:384:GLN:NE2	1.94	0.64
1:A:38:THR:HG22	1:A:41:GLU:CG	2.28	0.63
1:A:62:TRP:HE3	1:A:70:ILE:HD11	1.63	0.63
1:C:168:LYS:O	1:C:172:ILE:HG12	1.98	0.63
1:A:403:ILE:O	1:A:408:VAL:HG22	1.99	0.63
1:C:302:THR:CG2	1:C:361:TRP:HB3	2.29	0.63
1:D:323:GLY:O	1:D:326:VAL:HG12	1.99	0.63
1:B:38:THR:CG2	1:B:41:GLU:H	2.09	0.63
1:A:70:ILE:HG21	1:A:273:MET:HE2	1.79	0.63
1:B:51:ILE:HA	1:B:83:LYS:HD3	1.81	0.63
1:B:189:MET:HE3	1:B:190:PHE:C	2.23	0.63
1:C:63:VAL:HG12	1:C:238:LEU:HD22	1.81	0.63
1:A:40:LEU:CD1	1:A:172:ILE:HD12	2.29	0.62
1:C:235:ILE:CG1	1:C:239:MET:HE2	2.28	0.62
1:D:58:THR:HA	1:D:75:VAL:O	1.98	0.62
1:D:137:VAL:HB	1:D:138:PRO:HD3	1.80	0.62
1:D:274:TYR:O	1:D:275:LEU:HD13	1.99	0.62
1:C:57:VAL:O	1:C:76:THR:HA	1.99	0.62
1:C:300:CYS:HB2	1:C:363:PHE:HB2	1.82	0.62
1:D:156:LYS:HB3	1:D:369:GLU:OE1	2.00	0.61
1:D:275:LEU:N	1:D:275:LEU:HD22	2.15	0.61
1:C:29:SER:O	1:C:33:ILE:HG22	2.00	0.61
1:B:314:VAL:HG13	1:B:368:ILE:HD13	1.82	0.61
1:D:117:SER:C	1:D:118:ILE:HD12	2.26	0.61
1:B:106:ARG:HG3	1:B:119:TRP:CE3	2.35	0.60
1:C:71:ASN:OD1	1:C:73:ARG:HG3	2.01	0.60
1:B:71:ASN:OD1	1:B:73:ARG:HG2	2.01	0.60
1:A:383:LEU:HD12	1:A:384:GLN:H	1.67	0.60
1:D:114:ASN:OD1	1:D:231:LEU:HD11	2.02	0.60
1:D:127:VAL:HG13	1:D:190:PHE:HB2	1.83	0.60
1:B:302:THR:HG22	1:B:361:TRP:HB3	1.84	0.60
1:D:300:CYS:HB2	1:D:363:PHE:HB2	1.83	0.60
1:C:236:VAL:O	1:C:240:VAL:HG23	2.02	0.59
1:B:372:THR:HG22	1:B:383:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:LEU:H	1:C:412:LEU:CD2	2.16	0.59
1:A:256:PHE:CZ	1:A:261:LYS:HB2	2.37	0.59
1:B:83:LYS:O	1:B:87:GLU:HG2	2.03	0.59
1:B:338:VAL:O	1:B:341:VAL:HB	2.03	0.59
1:D:47:PRO:HB2	1:D:54:VAL:HG11	1.85	0.58
1:D:92:ALA:HB1	1:D:105:ILE:HD12	1.85	0.58
1:A:38:THR:CG2	1:A:41:GLU:H	2.14	0.58
1:A:66:GLU:O	1:A:67:ASP:HB2	2.04	0.58
1:A:117:SER:C	1:A:118:ILE:HD12	2.29	0.58
1:A:274:TYR:CE1	1:A:311:ILE:HD13	2.39	0.58
1:B:89:LEU:HD22	1:B:246:ILE:HG13	1.86	0.58
1:A:135:MET:HE2	1:A:139:ALA:CB	2.33	0.58
1:A:368:ILE:HD12	1:A:368:ILE:N	2.18	0.58
1:D:232:ASP:O	1:D:236:VAL:HG23	2.04	0.58
1:A:51:ILE:HA	1:A:83:LYS:HD3	1.84	0.58
1:C:65:ASP:OD1	1:C:73:ARG:NH1	2.37	0.58
1:C:89:LEU:HD22	1:C:246:ILE:HG13	1.86	0.58
1:A:51:ILE:CA	1:A:83:LYS:HD3	2.34	0.57
1:A:368:ILE:HG12	1:A:381:MET:HE1	1.86	0.57
1:B:106:ARG:HB2	1:B:119:TRP:HB3	1.86	0.57
1:A:59:GLN:HG3	1:A:61:MET:HE3	1.86	0.57
1:A:242:ARG:NH1	1:A:318:ALA:HB2	2.19	0.57
1:A:323:GLY:O	1:A:326:VAL:HG12	2.04	0.57
1:D:367:LEU:C	1:D:368:ILE:HD12	2.28	0.57
1:C:292:GLN:HG3	1:C:298:GLU:HG3	1.86	0.57
1:B:289:ILE:HG22	1:B:398:PHE:CE2	2.39	0.57
1:B:256:PHE:CE2	1:B:261:LYS:HB2	2.40	0.57
1:A:71:ASN:OD1	1:A:73:ARG:CG	2.53	0.56
1:A:172:ILE:HD13	1:A:198:MET:HB3	1.86	0.56
1:B:182:ALA:O	1:B:213:ASP:CB	2.50	0.56
1:A:300:CYS:HB2	1:A:363:PHE:HB2	1.87	0.56
1:C:235:ILE:O	1:C:239:MET:HG3	2.06	0.56
1:B:302:THR:CG2	1:B:361:TRP:HB3	2.35	0.56
1:C:82:TYR:CD1	1:C:238:LEU:HD12	2.41	0.56
1:B:66:GLU:O	1:B:67:ASP:HB2	2.04	0.56
1:A:33:ILE:HG23	1:A:34:TYR:CD2	2.41	0.56
1:A:172:ILE:HD11	1:A:198:MET:CE	2.35	0.56
1:C:408:VAL:O	1:C:412:LEU:HD22	2.06	0.56
1:A:302:THR:HG23	1:A:361:TRP:HB3	1.88	0.56
1:B:407:ILE:CG2	1:B:408:VAL:H	2.12	0.56
1:A:302:THR:CG2	1:A:361:TRP:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PRO:HA	1:A:388:PHE:CE2	2.42	0.55
1:C:323:GLY:O	1:C:326:VAL:HG22	2.05	0.55
1:A:407:ILE:N	1:A:407:ILE:HD12	2.21	0.55
1:B:47:PRO:O	1:B:49:THR:N	2.39	0.55
1:B:88:ILE:HB	1:B:118:ILE:HD12	1.89	0.55
1:D:373:PHE:CD2	1:D:378:LYS:HG2	2.41	0.55
1:B:376:GLN:HE21	1:B:376:GLN:HA	1.71	0.55
1:A:83:LYS:O	1:A:87:GLU:HG2	2.07	0.55
1:B:96:LYS:HE2	1:B:100:PRO:O	2.07	0.55
1:D:29:SER:HB3	1:D:32:ARG:HB3	1.89	0.55
1:D:231:LEU:HD12	1:D:231:LEU:H	1.70	0.55
1:A:104:CYS:H	1:A:121:ASN:ND2	2.04	0.55
1:A:409:GLU:C	1:A:411:ILE:H	2.14	0.55
1:A:172:ILE:HD13	1:A:198:MET:CB	2.37	0.54
1:A:337:LEU:CD1	1:A:356:VAL:HG11	2.37	0.54
1:D:91:ASN:O	1:D:94:ASP:HB2	2.05	0.54
1:A:59:GLN:HE21	1:A:61:MET:CE	2.20	0.54
1:A:176:LYS:HD3	1:A:220:GLN:HE21	1.71	0.54
1:B:89:LEU:CD2	1:B:246:ILE:HG13	2.37	0.54
1:A:400:LYS:O	1:A:403:ILE:HG22	2.08	0.54
1:A:367:LEU:C	1:A:368:ILE:HD12	2.32	0.54
1:C:59:GLN:HG3	1:C:61:MET:HE3	1.90	0.54
1:C:302:THR:HG23	1:C:361:TRP:HB3	1.90	0.54
1:A:104:CYS:N	1:A:121:ASN:HD21	2.04	0.54
1:C:59:GLN:CG	1:C:61:MET:HE3	2.37	0.54
1:A:267:PHE:HB3	1:A:298:GLU:OE2	2.08	0.54
1:B:172:ILE:O	1:B:197:ASN:HB3	2.08	0.53
1:A:400:LYS:C	1:A:402:ALA:N	2.66	0.53
1:B:96:LYS:NZ	1:B:251:LYS:O	2.40	0.53
1:D:290:HIS:ND1	1:D:291:GLU:N	2.56	0.53
1:D:128:VAL:HG22	1:D:129:GLU:N	2.22	0.53
1:B:244:TYR:CZ	1:B:262:LEU:HD22	2.44	0.53
1:D:141:ILE:HD12	3:D:907:ADP:HI'	1.91	0.53
1:D:59:GLN:HE21	1:D:61:MET:CE	2.20	0.53
1:B:417:PHE:O	1:B:421:VAL:HG23	2.09	0.53
1:A:118:ILE:HD12	1:A:118:ILE:N	2.23	0.53
1:A:337:LEU:HD12	1:A:337:LEU:O	2.09	0.52
1:B:323:GLY:O	1:B:326:VAL:HG12	2.08	0.52
1:D:406:GLY:C	1:D:408:VAL:H	2.17	0.52
1:C:372:THR:HG23	1:C:382:THR:OG1	2.09	0.52
1:C:163:ASN:ND2	1:C:163:ASN:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LYS:O	1:D:356:VAL:HG23	2.09	0.52
1:D:302:THR:HG23	1:D:361:TRP:HB3	1.91	0.52
1:D:102:MET:HE3	1:D:105:ILE:HD11	1.91	0.52
1:D:183:SER:HA	1:D:213:ASP:OD1	2.10	0.52
1:D:257:LEU:HG	1:D:258:ASN:HD22	1.75	0.52
1:A:417:PHE:HD1	1:A:417:PHE:H	1.56	0.52
1:B:108:THR:HB	1:B:117:SER:OG	2.09	0.52
1:C:172:ILE:HD11	1:C:198:MET:HE2	1.92	0.52
1:B:64:TYR:CE2	1:B:273:MET:HE1	2.44	0.51
1:B:137:VAL:HB	1:B:138:PRO:HD3	1.92	0.51
1:B:399:ILE:HG23	1:B:400:LYS:N	2.26	0.51
1:C:385:PRO:HA	1:C:388:PHE:CZ	2.46	0.51
1:C:163:ASN:ND2	6:C:977:HOH:O	2.43	0.51
1:A:38:THR:HG22	1:A:41:GLU:HB2	1.93	0.51
1:A:70:ILE:O	1:A:70:ILE:HG13	2.10	0.51
1:C:40:LEU:HD13	1:C:172:ILE:HD12	1.91	0.51
1:A:176:LYS:HD3	1:A:220:GLN:NE2	2.26	0.51
1:C:302:THR:HG22	1:C:361:TRP:HB3	1.92	0.51
1:D:290:HIS:CG	1:D:291:GLU:N	2.79	0.50
1:B:38:THR:HG22	1:B:41:GLU:N	2.11	0.50
1:A:59:GLN:HE21	1:A:61:MET:HE3	1.75	0.50
1:A:128:VAL:HB	1:A:186:TYR:CD2	2.45	0.50
1:A:400:LYS:O	1:A:402:ALA:N	2.45	0.50
1:B:56:LEU:HD22	1:B:76:THR:HG22	1.93	0.50
1:C:412:LEU:H	1:C:412:LEU:HD23	1.76	0.50
1:A:96:LYS:HB2	1:A:102:MET:HE2	1.93	0.50
1:D:66:GLU:O	1:D:67:ASP:HB2	2.11	0.50
1:B:300:CYS:HB2	1:B:363:PHE:HB2	1.93	0.50
1:C:64:TYR:HE2	1:C:273:MET:HE1	1.75	0.50
1:C:374:ASP:HB2	1:C:380:ASN:HB3	1.94	0.50
1:D:274:TYR:C	1:D:275:LEU:HD13	2.37	0.50
1:D:342:LYS:N	1:D:342:LYS:HD2	2.26	0.50
1:A:63:VAL:HG11	1:A:75:VAL:HG21	1.93	0.50
1:A:303:MET:HG3	1:A:407:ILE:HG13	1.94	0.50
1:B:328:TYR:HE2	1:B:392:CYS:HB3	1.76	0.50
1:C:338:VAL:HG21	1:C:353:ALA:HA	1.93	0.50
1:B:135:MET:HE2	1:B:140:LEU:N	2.27	0.50
1:B:110:ASP:CG	1:B:113:ASN:HD22	2.19	0.50
1:B:163:ASN:HB2	5:B:909:SO4:O2	2.11	0.50
1:B:274:TYR:C	1:B:275:LEU:HD12	2.37	0.50
1:C:40:LEU:CD1	1:C:172:ILE:HD12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:OD2	1:A:110:ASP:C	2.55	0.49
1:C:128:VAL:HB	1:C:186:TYR:CD2	2.47	0.49
1:A:357:LYS:HA	1:A:360:MET:SD	2.52	0.49
1:C:65:ASP:CG	1:C:73:ARG:HH11	2.20	0.49
1:C:289:ILE:HD13	1:C:402:ALA:HA	1.92	0.49
1:C:108:THR:HB	1:C:117:SER:OG	2.13	0.49
1:A:165:TYR:HB2	4:A:599:GOL:H11	1.95	0.49
1:C:82:TYR:CE1	1:C:238:LEU:HD12	2.48	0.49
1:C:235:ILE:HG13	1:C:239:MET:CE	2.34	0.49
1:C:337:LEU:HD23	1:C:403:ILE:HG22	1.94	0.49
1:A:38:THR:HG22	1:A:41:GLU:CB	2.43	0.49
1:C:329:VAL:HG12	1:C:362:ILE:HD11	1.93	0.49
1:B:394:LEU:HD23	1:B:398:PHE:CD1	2.48	0.49
1:A:321:LYS:NZ	1:A:380:ASN:HD22	2.10	0.49
1:B:88:ILE:HG21	1:B:217:ILE:CG1	2.43	0.49
1:A:128:VAL:O	1:A:137:VAL:HG23	2.13	0.49
1:A:135:MET:HE2	1:A:139:ALA:HB1	1.94	0.48
1:D:60:GLN:HA	1:D:73:ARG:O	2.12	0.48
1:D:206:LEU:C	1:D:207:LYS:HG3	2.38	0.48
1:D:247:ALA:HA	1:D:255:VAL:HG21	1.94	0.48
1:D:130:HIS:HB3	1:D:133:GLU:HB2	1.96	0.48
1:B:275:LEU:N	1:B:275:LEU:CD1	2.75	0.48
1:C:129:GLU:HA	1:C:136:TYR:HA	1.95	0.48
1:D:51:ILE:HA	1:D:83:LYS:HD3	1.96	0.48
1:D:102:MET:CE	1:D:105:ILE:HD11	2.44	0.48
1:A:91:ASN:HB3	3:A:901:ADP:N7	2.28	0.48
1:D:59:GLN:HB2	1:D:61:MET:HE3	1.96	0.48
1:A:158:VAL:C	1:A:315:ASN:ND2	2.71	0.48
1:C:274:TYR:CE1	1:C:311:ILE:HD13	2.48	0.48
1:A:383:LEU:HD12	1:A:384:GLN:N	2.29	0.48
1:A:62:TRP:O	1:A:241:ARG:HD3	2.14	0.47
1:A:129:GLU:HA	1:A:136:TYR:HA	1.96	0.47
1:B:334:VAL:O	1:B:338:VAL:HG23	2.13	0.47
1:B:374:ASP:HB3	1:B:382:THR:HG21	1.96	0.47
1:C:373:PHE:CG	1:C:378:LYS:HG2	2.48	0.47
1:C:38:THR:HG22	1:C:40:LEU:H	1.79	0.47
1:C:130:HIS:NE2	1:D:31:GLU:HA	2.29	0.47
1:B:408:VAL:HG23	1:B:409:GLU:N	2.29	0.47
1:A:137:VAL:HB	1:A:138:PRO:HD3	1.96	0.47
1:C:383:LEU:HD11	1:C:387:SER:HB2	1.97	0.47
1:D:43:ILE:HA	1:D:50:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:OD1	1:D:113:ASN:ND2	2.45	0.47
1:A:292:GLN:HA	1:A:298:GLU:HG3	1.95	0.47
1:C:44:LEU:HD21	1:C:172:ILE:HG22	1.97	0.47
1:D:294:ASN:OD1	1:D:296:ARG:N	2.45	0.47
1:D:406:GLY:C	1:D:408:VAL:N	2.71	0.47
1:B:57:VAL:O	1:B:76:THR:HA	2.15	0.47
1:C:115:LEU:HD13	1:C:116:ILE:N	2.30	0.47
1:D:330:ALA:O	1:D:334:VAL:HG23	2.15	0.47
1:B:372:THR:HG23	1:B:382:THR:OG1	2.15	0.47
1:A:70:ILE:HG21	1:A:273:MET:HB3	1.97	0.47
1:B:47:PRO:O	1:B:48:ASP:C	2.58	0.47
1:C:359:HIS:HB2	1:C:407:ILE:HD13	1.96	0.47
1:A:57:VAL:O	1:A:76:THR:HA	2.15	0.46
1:A:415:VAL:C	1:A:417:PHE:H	2.22	0.46
1:C:116:ILE:HD11	1:C:231:LEU:HD21	1.96	0.46
1:D:261:LYS:HG2	1:D:262:LEU:N	2.30	0.46
1:D:362:ILE:HG12	1:D:364:VAL:HG23	1.96	0.46
1:A:48:ASP:HA	1:A:52:GLY:O	2.15	0.46
1:D:377:THR:OG1	1:D:379:GLU:HG3	2.16	0.46
1:A:60:GLN:HA	1:A:73:ARG:O	2.16	0.46
1:B:149:SER:O	1:B:157:LYS:NZ	2.48	0.46
1:B:322:GLY:O	1:B:380:ASN:HA	2.16	0.46
1:D:267:PHE:HB3	1:D:298:GLU:OE2	2.15	0.46
1:A:58:THR:HA	1:A:75:VAL:O	2.16	0.46
1:A:290:HIS:ND1	1:A:290:HIS:C	2.74	0.46
1:C:75:VAL:HG13	1:C:234:ASP:HB3	1.98	0.46
1:D:223:LEU:HD13	1:D:230:SER:HA	1.97	0.46
1:A:43:ILE:HA	1:A:50:TYR:CE2	2.51	0.46
1:B:70:ILE:O	1:B:70:ILE:HG23	2.16	0.46
1:D:63:VAL:HG12	1:D:238:LEU:HD22	1.97	0.46
1:D:163:ASN:HB2	5:D:908:SO4:O1	2.16	0.46
1:A:65:ASP:CG	1:A:73:ARG:HH11	2.24	0.46
1:B:88:ILE:CG2	1:B:217:ILE:HG12	2.47	0.46
1:A:334:VAL:O	1:A:335:THR:C	2.58	0.45
1:C:292:GLN:HA	1:C:298:GLU:HG3	1.98	0.45
1:A:40:LEU:HD13	1:A:172:ILE:HD12	1.99	0.45
1:A:141:ILE:HD12	3:A:901:ADP:HI'	1.97	0.45
1:A:409:GLU:C	1:A:411:ILE:N	2.73	0.45
1:B:177:PHE:CE1	1:B:217:ILE:HD13	2.51	0.45
1:C:349:VAL:CG1	1:C:350:ALA:N	2.78	0.45
1:A:256:PHE:CE2	1:A:261:LYS:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD12	1:A:302:THR:H	1.82	0.45
1:B:368:ILE:N	1:B:368:ILE:HD12	2.31	0.45
1:C:31:GLU:HA	1:D:130:HIS:CE1	2.52	0.45
1:D:103:SER:H	1:D:121:ASN:HD21	1.64	0.45
1:A:290:HIS:CG	1:A:291:GLU:N	2.85	0.45
1:B:194:TRP:CD1	1:B:201:ALA:HB2	2.52	0.45
1:B:353:ALA:C	1:B:355:GLN:N	2.71	0.45
1:B:394:LEU:HD23	1:B:398:PHE:CE1	2.52	0.45
1:C:190:PHE:CD2	1:C:190:PHE:C	2.95	0.45
1:A:82:TYR:CD2	1:A:82:TYR:C	2.93	0.45
1:A:232:ASP:O	1:A:236:VAL:HG23	2.17	0.45
1:A:415:VAL:HA	1:A:417:PHE:CE1	2.51	0.45
1:B:92:ALA:HB1	1:B:105:ILE:HD12	1.97	0.45
1:B:353:ALA:C	1:B:355:GLN:H	2.24	0.45
1:C:45:LEU:C	1:C:47:PRO:HD3	2.41	0.45
1:C:96:LYS:NZ	1:C:102:MET:O	2.50	0.45
1:A:51:ILE:HA	1:A:83:LYS:CD	2.47	0.45
1:C:59:GLN:NE2	1:C:61:MET:CE	2.80	0.45
1:D:57:VAL:O	1:D:76:THR:HA	2.17	0.45
1:B:225:LYS:HB3	1:B:225:LYS:HE3	1.80	0.44
1:C:338:VAL:HG22	1:C:356:VAL:HG21	1.99	0.44
1:D:73:ARG:HB3	1:D:74:GLU:H	1.52	0.44
1:A:337:LEU:HD13	1:A:356:VAL:HG11	1.99	0.44
1:B:135:MET:HE2	1:B:139:ALA:C	2.42	0.44
1:A:70:ILE:HG22	1:A:273:MET:HE2	1.97	0.44
1:A:311:ILE:HD12	1:A:363:PHE:CE2	2.52	0.44
1:D:304:SER:HB2	1:D:361:TRP:HB2	2.00	0.44
1:A:62:TRP:HE3	1:A:70:ILE:CD1	2.30	0.44
1:D:235:ILE:HG13	1:D:239:MET:HE2	1.98	0.44
1:A:312:SER:HA	1:A:364:VAL:O	2.17	0.44
1:C:58:THR:HA	1:C:75:VAL:O	2.17	0.44
1:C:59:GLN:HE21	1:C:61:MET:HE2	1.82	0.44
1:B:52:GLY:HA3	6:B:937:HOH:O	2.18	0.44
1:B:190:PHE:C	1:B:190:PHE:CD2	2.96	0.44
1:B:417:PHE:CD1	1:B:417:PHE:C	2.94	0.44
1:D:223:LEU:CD1	1:D:230:SER:HA	2.48	0.44
1:D:251:LYS:O	1:D:253:VAL:HG23	2.17	0.44
1:A:46:ARG:N	1:A:47:PRO:HD3	2.33	0.44
1:C:62:TRP:O	1:C:241:ARG:HD3	2.18	0.44
1:C:117:SER:C	1:C:118:ILE:HD12	2.43	0.44
1:A:267:PHE:O	1:A:270:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:GLU:HB2	1:C:388:PHE:O	2.18	0.44
1:B:235:ILE:O	1:B:239:MET:HG3	2.18	0.43
1:A:33:ILE:O	1:B:149:SER:HA	2.19	0.43
1:A:158:VAL:HG12	1:A:368:ILE:C	2.43	0.43
1:B:236:VAL:O	1:B:240:VAL:HG23	2.17	0.43
1:C:33:ILE:HG23	1:C:34:TYR:HD2	1.83	0.43
1:A:31:GLU:OE1	1:B:131:LYS:N	2.50	0.43
1:A:103:SER:OG	1:A:121:ASN:ND2	2.51	0.43
1:B:290:HIS:ND1	1:B:291:GLU:N	2.66	0.43
1:A:194:TRP:CD1	1:A:201:ALA:HB2	2.53	0.43
1:B:385:PRO:HA	1:B:388:PHE:CD2	2.53	0.43
1:C:33:ILE:O	1:D:149:SER:HA	2.19	0.43
1:C:51:ILE:HA	1:C:83:LYS:HD3	1.99	0.43
1:C:57:VAL:HG22	1:C:77:PHE:O	2.18	0.43
1:C:409:GLU:O	1:C:412:LEU:HD23	2.18	0.43
1:D:66:GLU:O	1:D:67:ASP:CB	2.66	0.43
1:D:242:ARG:O	1:D:245:ASP:HB2	2.18	0.43
3:D:907:ADP:H5'1	3:D:907:ADP:PB	2.59	0.43
1:D:47:PRO:CB	1:D:54:VAL:HG11	2.47	0.43
1:B:109:ILE:HG23	1:B:116:ILE:CD1	2.49	0.43
1:B:168:LYS:HD3	1:B:168:LYS:N	2.33	0.43
1:A:51:ILE:HA	1:A:83:LYS:HE2	2.01	0.43
1:C:409:GLU:HA	1:C:412:LEU:HD21	2.00	0.43
1:D:83:LYS:O	1:D:87:GLU:HG2	2.18	0.43
1:B:172:ILE:HD11	1:B:198:MET:HE2	2.00	0.43
1:C:65:ASP:HB2	1:C:68:VAL:HB	2.00	0.43
1:D:244:TYR:HA	1:D:247:ALA:HB3	2.01	0.43
1:A:96:LYS:HE3	1:A:251:LYS:O	2.19	0.43
1:C:115:LEU:HD11	1:C:218:THR:HG23	2.00	0.43
1:C:137:VAL:HB	1:C:138:PRO:HD3	2.01	0.43
1:D:368:ILE:N	1:D:368:ILE:CD1	2.80	0.43
1:B:128:VAL:HG22	1:B:129:GLU:N	2.32	0.42
1:B:328:TYR:CE2	1:B:392:CYS:HB3	2.54	0.42
1:C:106:ARG:HB2	1:C:119:TRP:HB3	2.00	0.42
1:A:38:THR:HG22	1:A:41:GLU:CD	2.44	0.42
1:A:75:VAL:HG13	1:A:234:ASP:HB3	2.00	0.42
1:A:335:THR:O	1:A:336:LYS:C	2.62	0.42
1:C:30:VAL:HA	1:C:33:ILE:HG22	2.01	0.42
1:D:178:THR:HG23	1:D:193:THR:OG1	2.19	0.42
1:A:155:GLU:O	1:A:156:LYS:C	2.62	0.42
1:A:315:ASN:O	1:A:316:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:HG3	1:A:409:GLU:O	2.19	0.42
1:B:385:PRO:HA	1:B:388:PHE:CG	2.54	0.42
1:D:242:ARG:HD2	1:D:245:ASP:OD1	2.19	0.42
1:D:340:VAL:C	1:D:342:LYS:H	2.28	0.42
1:D:403:ILE:HG13	1:D:404:GLY:N	2.35	0.42
1:B:376:GLN:HE21	1:B:376:GLN:CA	2.31	0.42
1:D:175:THR:O	1:D:196:ASP:N	2.36	0.42
1:D:242:ARG:NH1	1:D:318:ALA:HB2	2.35	0.42
1:D:274:TYR:C	1:D:275:LEU:HD22	2.45	0.42
1:B:222:ASP:OD1	1:B:225:LYS:HG2	2.20	0.42
1:C:242:ARG:O	1:C:246:ILE:HG12	2.20	0.42
1:D:56:LEU:HD22	1:D:76:THR:CG2	2.45	0.42
1:A:40:LEU:HD11	1:A:172:ILE:HD12	2.02	0.42
1:B:43:ILE:HA	1:B:50:TYR:CE2	2.54	0.42
1:D:384:GLN:H	1:D:384:GLN:CD	2.27	0.42
1:B:189:MET:HG2	1:B:190:PHE:N	2.34	0.42
1:B:242:ARG:HA	1:B:242:ARG:HD2	1.84	0.42
1:C:38:THR:HG22	1:C:40:LEU:N	2.34	0.42
1:D:240:VAL:HG13	1:D:257:LEU:CD2	2.50	0.42
1:B:369:GLU:O	1:B:370:ASN:C	2.62	0.42
1:A:33:ILE:HG23	1:A:34:TYR:N	2.34	0.41
1:A:51:ILE:HA	1:A:83:LYS:CE	2.50	0.41
1:A:99:ASP:OD1	1:A:99:ASP:C	2.61	0.41
1:A:141:ILE:HD12	3:A:901:ADP:CI'	2.50	0.41
1:B:135:MET:HE1	6:B:941:HOH:O	2.20	0.41
1:C:96:LYS:HB2	1:C:102:MET:HE2	2.02	0.41
1:C:317:ILE:HD13	1:C:378:LYS:HD2	2.02	0.41
1:C:349:VAL:HG12	1:C:350:ALA:N	2.35	0.41
1:D:310:GLN:C	1:D:310:GLN:CD	2.88	0.41
1:D:373:PHE:CG	1:D:378:LYS:HG2	2.55	0.41
1:B:102:MET:CE	1:B:105:ILE:HD11	2.50	0.41
1:B:381:MET:HE3	1:B:381:MET:HB3	1.92	0.41
1:D:373:PHE:HB3	1:D:378:LYS:HA	2.02	0.41
1:B:135:MET:HE2	1:B:140:LEU:HA	2.01	0.41
1:C:43:ILE:HA	1:C:50:TYR:CE2	2.55	0.41
1:A:303:MET:HE2	1:A:407:ILE:N	2.35	0.41
1:D:64:TYR:CE1	1:D:69:GLY:HA2	2.56	0.41
1:B:51:ILE:CA	1:B:83:LYS:HD3	2.49	0.41
1:B:324:ARG:NH1	6:B:946:HOH:O	2.53	0.41
1:C:128:VAL:HG22	1:C:129:GLU:N	2.35	0.41
1:D:231:LEU:N	1:D:231:LEU:CD1	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ARG:O	1:D:366:ALA:HA	2.21	0.41
1:A:38:THR:HG22	1:A:41:GLU:HG3	2.00	0.41
1:A:73:ARG:NH2	1:A:234:ASP:OD2	2.45	0.41
1:A:414:TRP:O	1:A:417:PHE:CD1	2.73	0.41
1:A:321:LYS:HZ2	1:A:380:ASN:HD22	1.69	0.41
1:D:95:ASN:HB3	1:D:102:MET:SD	2.61	0.41
1:D:118:ILE:HD12	1:D:118:ILE:N	2.35	0.41
1:D:125:ILE:HG21	1:D:141:ILE:HD11	2.03	0.41
1:A:61:MET:HE2	1:A:61:MET:HB3	1.91	0.41
1:A:309:GLN:O	1:A:361:TRP:HA	2.20	0.41
1:A:385:PRO:HA	1:A:388:PHE:CD2	2.56	0.41
1:B:332:GLN:OE1	1:B:394:LEU:HD13	2.20	0.41
1:C:51:ILE:O	1:C:80:GLY:HA2	2.21	0.41
1:C:204:MET:HE3	1:C:206:LEU:CD1	2.48	0.41
1:C:385:PRO:HA	1:C:388:PHE:CE1	2.55	0.41
1:C:425:LYS:O	1:C:426:LYS:CB	2.67	0.41
1:D:137:VAL:O	1:D:141:ILE:HG12	2.20	0.41
1:B:37:LYS:HD2	1:B:37:LYS:HA	1.89	0.41
1:B:64:TYR:HE2	1:B:273:MET:CE	2.28	0.41
1:B:323:GLY:O	1:B:326:VAL:CG1	2.69	0.41
1:D:69:GLY:O	1:D:71:ASN:ND2	2.54	0.41
1:D:242:ARG:HD2	1:D:242:ARG:HA	1.86	0.41
1:B:142:PHE:CG	1:B:179:VAL:HG21	2.56	0.40
1:C:245:ASP:OD2	1:C:270:TYR:OH	2.37	0.40
1:D:75:VAL:HG12	1:D:76:THR:N	2.35	0.40
1:D:128:VAL:CG2	1:D:129:GLU:N	2.84	0.40
1:D:406:GLY:O	1:D:408:VAL:N	2.54	0.40
1:A:410:SER:O	1:A:414:TRP:N	2.41	0.40
1:B:127:VAL:O	1:B:127:VAL:HG12	2.22	0.40
1:D:231:LEU:H	1:D:231:LEU:CD1	2.33	0.40
1:B:190:PHE:CD2	1:B:191:LYS:N	2.89	0.40
1:C:64:TYR:HE2	1:C:273:MET:CE	2.35	0.40
1:B:106:ARG:HG3	1:B:119:TRP:HE3	1.82	0.40
1:C:127:VAL:O	1:C:127:VAL:CG1	2.64	0.40
1:D:353:ALA:C	1:D:355:GLN:N	2.80	0.40
1:A:75:VAL:HG13	1:A:234:ASP:CG	2.47	0.40
1:A:127:VAL:O	1:A:127:VAL:HG12	2.20	0.40
1:A:398:PHE:O	1:A:399:ILE:C	2.64	0.40
1:B:369:GLU:HG3	1:B:388:PHE:O	2.21	0.40
1:C:172:ILE:O	1:C:197:ASN:HB3	2.21	0.40
1:C:400:LYS:O	1:C:403:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ARG:O	1:D:246:ILE:HG12	2.22	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	358/400 (90%)	316 (88%)	34 (10%)	8 (2%)	5	9
1	B	373/400 (93%)	343 (92%)	25 (7%)	5 (1%)	9	18
1	C	378/400 (94%)	361 (96%)	14 (4%)	3 (1%)	16	31
1	D	361/400 (90%)	325 (90%)	32 (9%)	4 (1%)	11	22
All	All	1470/1600 (92%)	1345 (92%)	105 (7%)	20 (1%)	9	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	GLY
1	A	334	VAL
1	A	401	ALA
1	B	48	ASP
1	B	162	ARG
1	B	166	GLY
1	C	166	GLY
1	A	374	ASP
1	A	378	LYS
1	D	196	ASP
1	A	162	ARG
1	B	210	ASN
1	C	196	ASP
1	D	341	VAL

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Mol	Chain	Res	Type
1	A	291	GLU
1	A	330	ALA
1	D	158	VAL
1	B	47	PRO
1	C	127	VAL
1	D	407	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/358 (76%)	260 (96%)	11 (4%)	27	53
1	B	297/358 (83%)	279 (94%)	18 (6%)	17	35
1	C	295/358 (82%)	285 (97%)	10 (3%)	32	60
1	D	272/358 (76%)	266 (98%)	6 (2%)	45	73
All	All	1135/1432 (79%)	1090 (96%)	45 (4%)	28	54

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	70	ILE
1	A	76	THR
1	A	89	LEU
1	A	158	VAL
1	A	290	HIS
1	A	321	LYS
1	A	337	LEU
1	A	358	ASN
1	A	381	MET
1	A	417	PHE
1	B	30	VAL
1	B	31	GLU
1	B	32	ARG
1	B	37	LYS

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Mol	Chain	Res	Type
1	B	38	THR
1	B	71	ASN
1	B	89	LEU
1	B	96	LYS
1	B	176	LYS
1	B	189	MET
1	B	217	ILE
1	B	235	ILE
1	B	275	LEU
1	B	276	LYS
1	B	339	ASP
1	B	340	VAL
1	B	384	GLN
1	B	399	ILE
1	C	31	GLU
1	C	89	LEU
1	C	96	LYS
1	C	163	ASN
1	C	231	LEU
1	C	238	LEU
1	C	275	LEU
1	C	372	THR
1	C	407	ILE
1	C	412	LEU
1	D	31	GLU
1	D	38	THR
1	D	238	LEU
1	D	275	LEU
1	D	374	ASP
1	D	384	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	59	GLN
1	A	97	GLN
1	A	144	GLN
1	A	150	ASN
1	A	192	GLN
1	A	220	GLN
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	380	ASN
1	B	59	GLN
1	B	97	GLN
1	B	113	ASN
1	B	144	GLN
1	B	376	GLN
1	B	380	ASN
1	C	59	GLN
1	C	60	GLN
1	C	97	GLN
1	C	144	GLN
1	C	197	ASN
1	C	260	ASN
1	C	358	ASN
1	C	380	ASN
1	C	413	ASN
1	C	424	ASN
1	D	35	GLN
1	D	39	GLN
1	D	59	GLN
1	D	144	GLN
1	D	258	ASN
1	D	384	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	C	905	2	28,29,29	1.51	5 (17%)	43,45,45	1.21	5 (11%)
3	ADP	B	903	2	28,29,29	1.44	5 (17%)	43,45,45	1.24	3 (6%)
3	ADP	A	901	2	28,29,29	1.46	4 (14%)	43,45,45	1.22	4 (9%)
5	SO4	D	908	-	4,4,4	0.35	0	6,6,6	0.09	0
3	ADP	D	907	2	28,29,29	1.55	4 (14%)	43,45,45	1.21	4 (9%)
5	SO4	B	909	-	4,4,4	0.38	0	6,6,6	0.16	0
4	GOL	A	599	-	5,5,5	1.35	1 (20%)	5,5,5	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	905	2	-	4/16/32/32	0/3/3/3
3	ADP	B	903	2	-	6/16/32/32	0/3/3/3
3	ADP	A	901	2	-	5/16/32/32	0/3/3/3
3	ADP	D	907	2	-	5/16/32/32	0/3/3/3
4	GOL	A	599	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ADP	C2-N1	4.35	1.41	1.33
3	D	907	ADP	PA-O3A	-4.27	1.54	1.59
3	C	905	ADP	C2-N1	4.10	1.41	1.33
3	D	907	ADP	C2-N1	3.90	1.40	1.33
3	B	903	ADP	C2-N1	3.78	1.40	1.33
3	C	905	ADP	C1'-N9	3.06	1.54	1.46
3	C	905	ADP	PA-O3A	-3.03	1.56	1.59
3	D	907	ADP	C1'-N9	2.86	1.54	1.46
3	A	901	ADP	C1'-N9	2.85	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	ADP	C5-N7	-2.67	1.34	1.39
3	B	903	ADP	PA-O3A	-2.57	1.56	1.59
3	A	901	ADP	C5-C6	2.50	1.48	1.41
3	C	905	ADP	C5-C6	2.43	1.47	1.41
3	B	903	ADP	C1'-N9	2.37	1.52	1.46
3	D	907	ADP	C5-C6	2.27	1.47	1.41
3	C	905	ADP	C6-N6	-2.15	1.28	1.34
3	B	903	ADP	C6-N6	-2.07	1.28	1.34
4	A	599	GOL	C1-C2	2.03	1.59	1.51
3	A	901	ADP	C6-N6	-2.03	1.29	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	907	ADP	N3-C2-N1	-3.93	122.63	128.58
3	B	903	ADP	N3-C2-N1	-3.91	122.67	128.58
3	A	901	ADP	N3-C2-N1	-3.90	122.68	128.58
3	C	905	ADP	N3-C2-N1	-3.74	122.92	128.58
3	B	903	ADP	C2-N1-C6	3.38	124.28	118.73
3	C	905	ADP	C2-N1-C6	3.13	123.87	118.73
3	D	907	ADP	C2-N1-C6	3.11	123.83	118.73
3	A	901	ADP	C2-N1-C6	3.08	123.78	118.73
3	A	901	ADP	C3'-C2'-C1'	2.44	106.08	101.46
3	D	907	ADP	O2A-PA-O5'	2.34	118.15	107.57
3	D	907	ADP	C3'-C2'-C1'	2.25	105.72	101.46
3	C	905	ADP	O5'-C5'-C4'	2.15	116.30	108.99
3	C	905	ADP	C3'-C2'-C1'	2.13	105.49	101.46
3	B	903	ADP	C3'-C2'-C1'	2.12	105.48	101.46
3	C	905	ADP	O2A-PA-O5'	2.09	117.02	107.57
3	A	901	ADP	O2A-PA-O5'	2.05	116.87	107.57

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ADP	PA-O3A-PB-O3B
3	B	903	ADP	PA-O3A-PB-O3B
3	C	905	ADP	PA-O3A-PB-O3B
3	D	907	ADP	PA-O3A-PB-O3B
3	A	901	ADP	C3'-C4'-C5'-O5'
3	B	903	ADP	C3'-C4'-C5'-O5'
3	C	905	ADP	C3'-C4'-C5'-O5'

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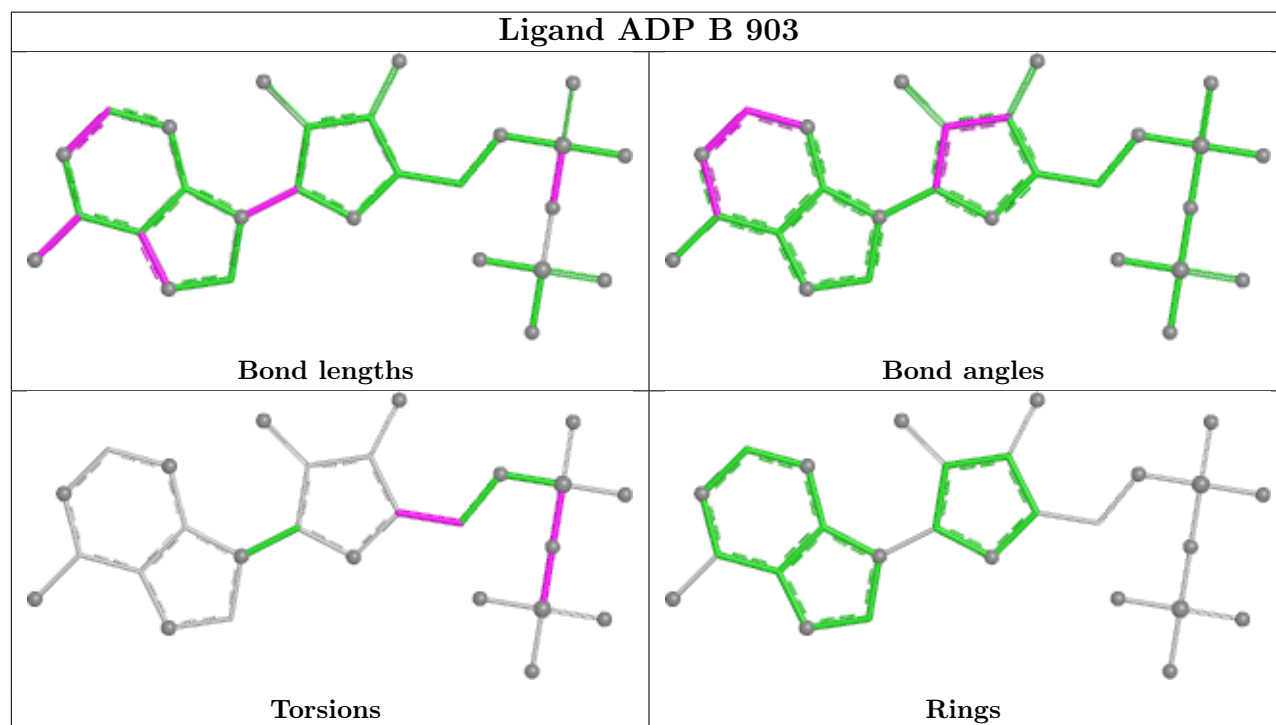
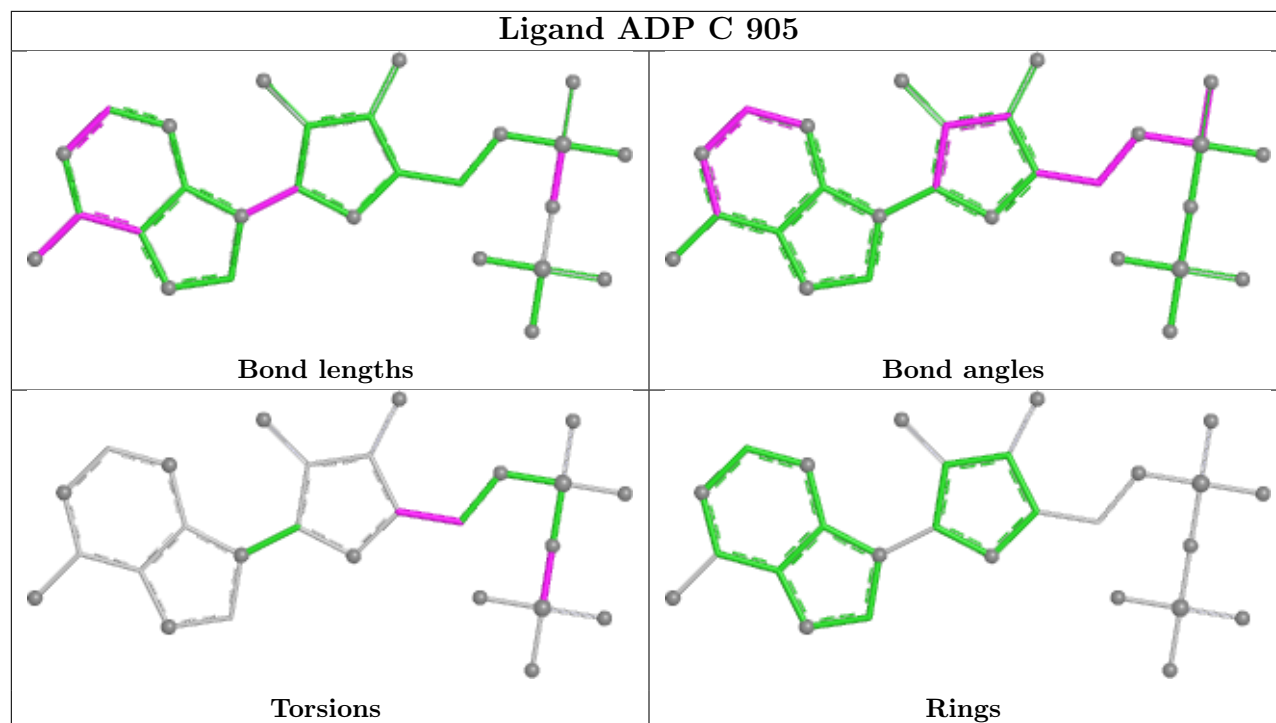
Mol	Chain	Res	Type	Atoms
4	A	599	GOL	O1-C1-C2-C3
3	A	901	ADP	O4'-C4'-C5'-O5'
3	B	903	ADP	O4'-C4'-C5'-O5'
3	C	905	ADP	O4'-C4'-C5'-O5'
4	A	599	GOL	O1-C1-C2-O2
3	D	907	ADP	C3'-C4'-C5'-O5'
3	B	903	ADP	PB-O3A-PA-O1A
3	A	901	ADP	PA-O3A-PB-O2B
3	B	903	ADP	PA-O3A-PB-O2B
3	C	905	ADP	PA-O3A-PB-O2B
3	D	907	ADP	PA-O3A-PB-O2B
3	B	903	ADP	PB-O3A-PA-O2A
3	A	901	ADP	PA-O3A-PB-O1B
3	D	907	ADP	PA-O3A-PB-O1B
3	D	907	ADP	O4'-C4'-C5'-O5'

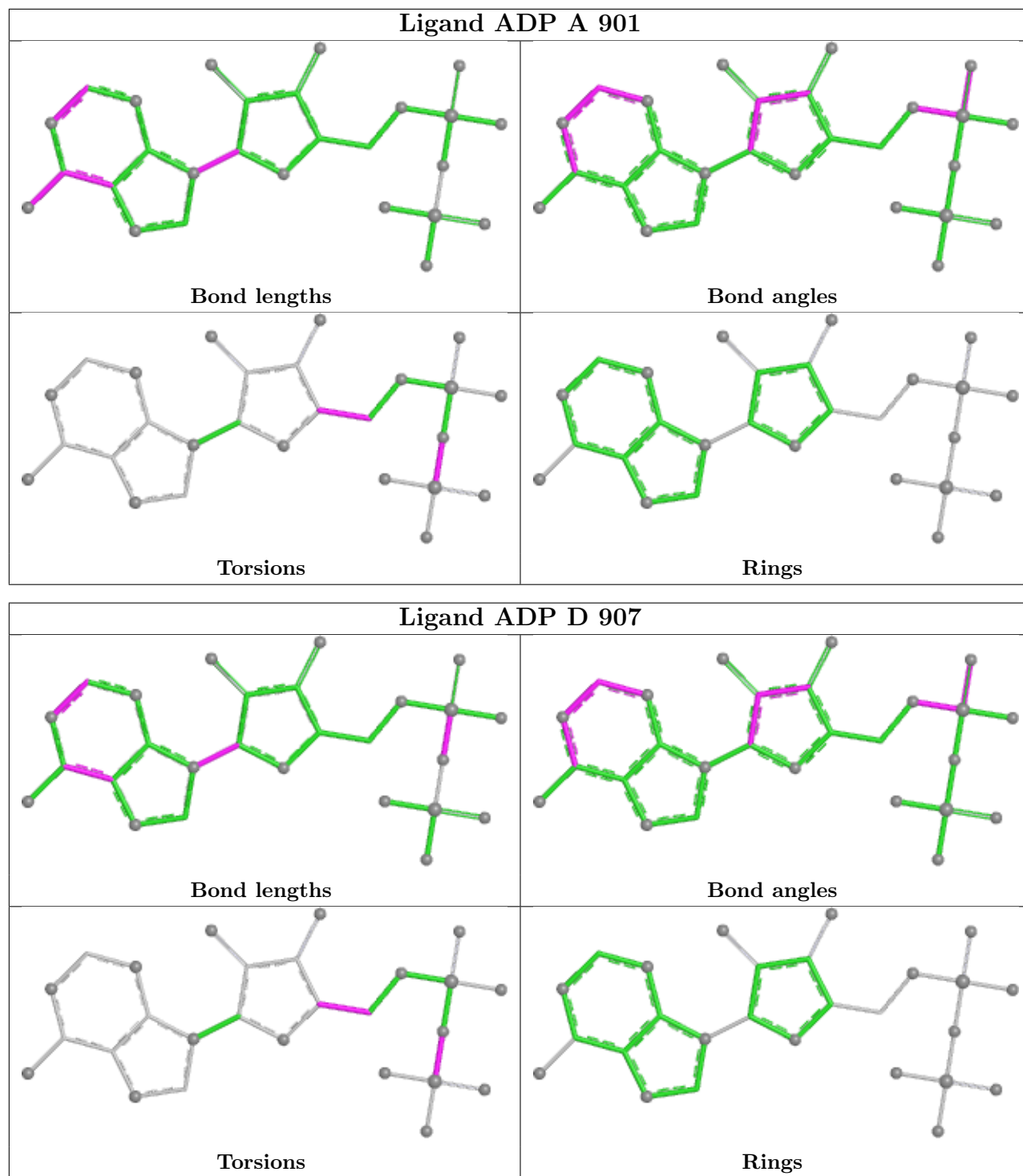
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ADP	3	0
5	D	908	SO4	1	0
3	D	907	ADP	2	0
5	B	909	SO4	1	0
4	A	599	GOL	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	366/400 (91%)	0.55	35 (9%)	13 11	20, 57, 84, 95	0
1	B	379/400 (94%)	0.24	13 (3%)	48 43	26, 51, 76, 94	0
1	C	384/400 (96%)	0.10	4 (1%)	79 76	32, 52, 67, 83	0
1	D	371/400 (92%)	0.62	24 (6%)	25 22	46, 68, 89, 103	0
All	All	1500/1600 (93%)	0.37	76 (5%)	33 29	20, 57, 83, 103	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	LEU	4.5
1	A	210	ASN	4.1
1	A	266	GLY	4.0
1	A	404	GLY	3.8
1	D	205	GLU	3.7
1	A	395	SER	3.7
1	D	408	VAL	3.6
1	D	318	ALA	3.5
1	B	352	LYS	3.4
1	C	29	SER	3.4
1	B	276	LYS	3.4
1	A	354	HIS	3.4
1	A	355	GLN	3.1
1	B	375	SER	3.1
1	B	354	HIS	3.1
1	A	393	GLN	3.0
1	A	387	SER	3.0
1	A	372	THR	2.9
1	D	407	ILE	2.9
1	D	342	LYS	2.9
1	B	344	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	276	LYS	2.7
1	B	265	LYS	2.7
1	A	379	GLU	2.7
1	D	252	ASP	2.7
1	D	414	TRP	2.7
1	B	376	GLN	2.7
1	A	407	ILE	2.7
1	A	373	PHE	2.6
1	B	210	ASN	2.6
1	B	413	ASN	2.6
1	D	142	PHE	2.5
1	A	359	HIS	2.5
1	D	210	ASN	2.5
1	A	288	VAL	2.5
1	D	340	VAL	2.5
1	A	399	ILE	2.4
1	A	183	SER	2.4
1	D	374	ASP	2.4
1	B	412	LEU	2.4
1	D	417	PHE	2.4
1	C	413	ASN	2.4
1	A	119	TRP	2.4
1	A	409	GLU	2.4
1	D	393	GLN	2.3
1	D	377	THR	2.3
1	B	48	ASP	2.3
1	D	251	LYS	2.3
1	A	260	ASN	2.3
1	D	211	GLY	2.3
1	D	399	ILE	2.3
1	A	338	VAL	2.3
1	A	412	LEU	2.2
1	A	265	LYS	2.2
1	A	275	LEU	2.2
1	D	396	GLU	2.2
1	A	370	ASN	2.2
1	A	336	LYS	2.2
1	D	157	LYS	2.2
1	A	396	GLU	2.2
1	D	153	ASP	2.2
1	A	417	PHE	2.2
1	D	209	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	341	VAL	2.1
1	B	411	ILE	2.1
1	C	420	GLN	2.1
1	A	182	ALA	2.1
1	D	66	GLU	2.1
1	A	388	PHE	2.1
1	D	70	ILE	2.1
1	A	374	ASP	2.1
1	A	269	SER	2.1
1	D	267	PHE	2.0
1	C	419	ALA	2.0
1	A	328	TYR	2.0
1	A	375	SER	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.

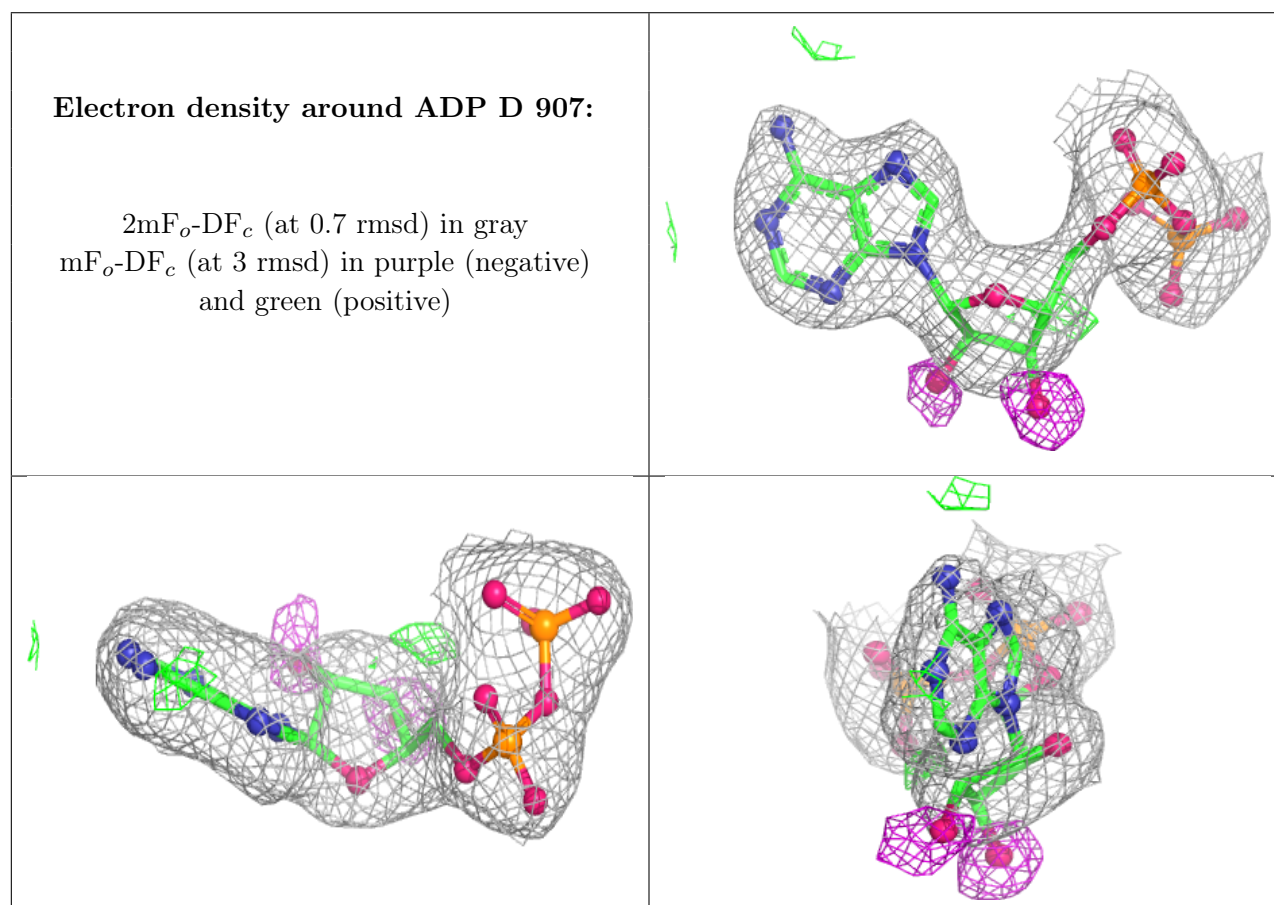
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	599	6/6	0.81	0.17	56,59,60,61	0
5	SO4	D	908	5/5	0.87	0.10	103,103,103,104	0
5	SO4	B	909	5/5	0.91	0.22	85,86,87,89	0
3	ADP	D	907	27/27	0.92	0.11	52,57,62,63	0
3	ADP	A	901	27/27	0.92	0.13	37,52,57,57	0
3	ADP	B	903	27/27	0.93	0.11	28,32,57,57	0
3	ADP	C	905	27/27	0.94	0.12	42,52,57,57	0
2	MG	C	904	1/1	0.98	0.05	36,36,36,36	0
2	MG	A	900	1/1	0.98	0.07	33,33,33,33	0
2	MG	D	906	1/1	0.99	0.05	42,42,42,42	0

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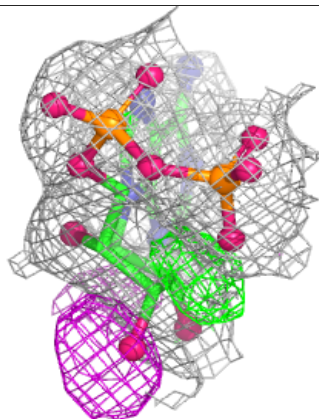
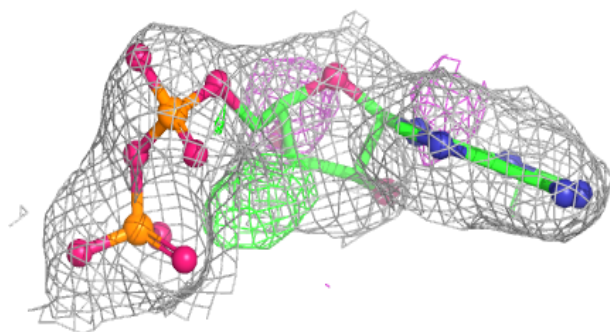
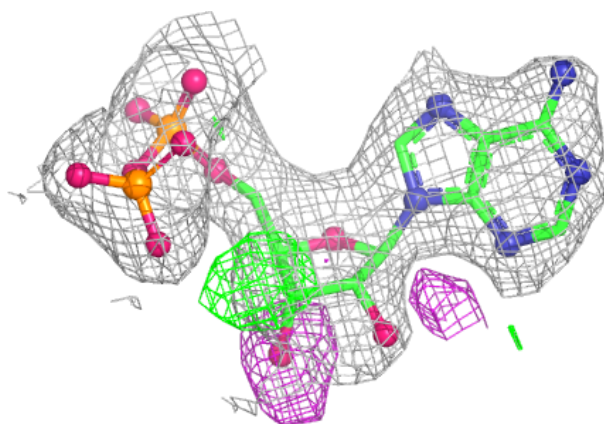
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	902	1/1	0.99	0.03	36,36,36,36	0

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.

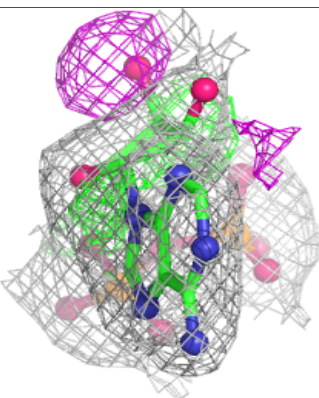
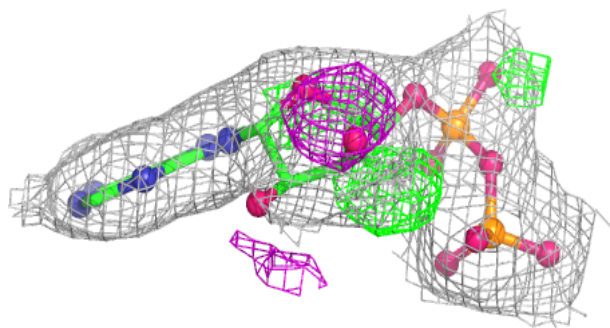
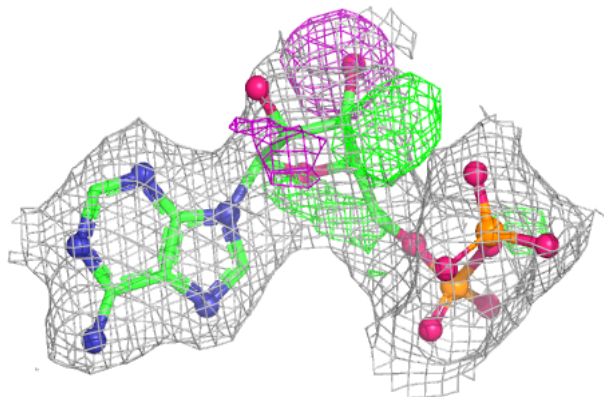


Electron density around ADP A 901:

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

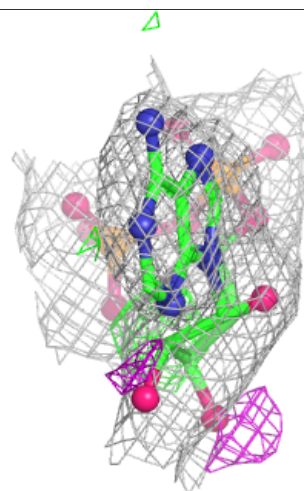
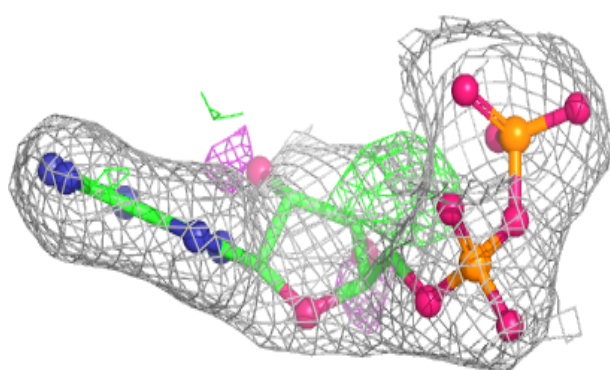
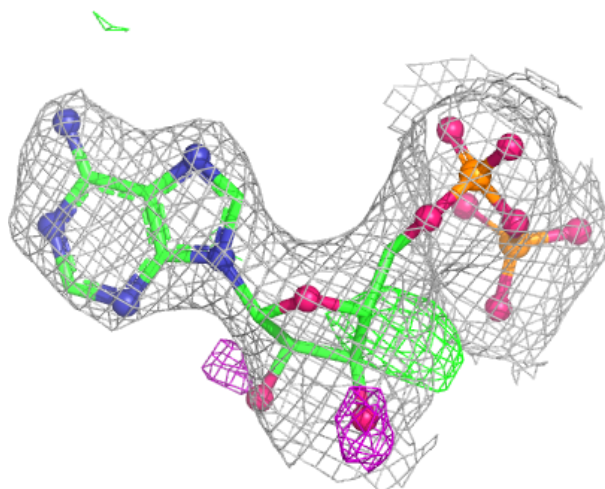
**Electron density around ADP B 903:**

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



Electron density around ADP C 905:

$2mF_o-DF_c$ (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.