



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:09 AM UTC

PDB ID : 7CPR / pdb_00007cpr
Title : glutamine synthetase from Drosophila
Authors : Yin, H.S.; Chen, W.T.
Deposited on : 2020-08-07
Resolution : 2.12 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

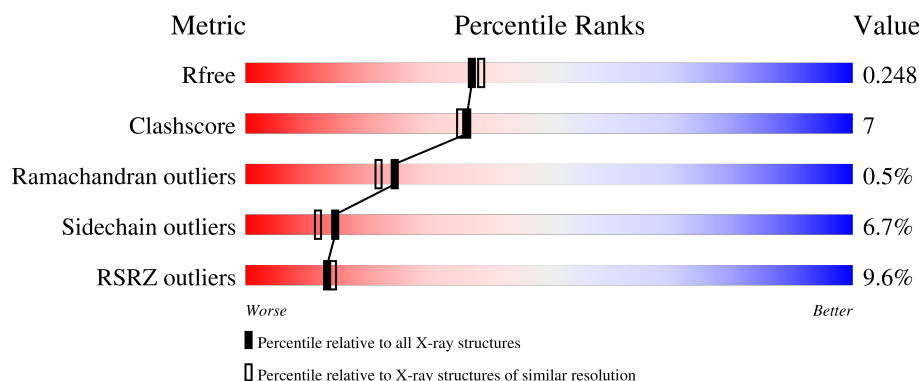
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	367	13% 80% 17% .
1	B	367	10% 78% 18% ..
1	C	367	9% 88% 11% .
1	D	367	7% 80% 15% ..
1	E	367	9% 83% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	367	10% 80% 17%
1	G	367	9% 81% 16%
1	H	367	8% 81% 16%
1	I	367	10% 78% 17%
1	J	367	10% 84% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29573 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 Glutamine synthetase 2 cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2885	1807	508	553	17			
1	B	366	Total	C	N	O	S	0	0	0
			2884	1806	507	554	17			
1	C	366	Total	C	N	O	S	0	0	0
			2880	1804	507	552	17			
1	D	364	Total	C	N	O	S	0	0	0
			2867	1797	505	548	17			
1	E	365	Total	C	N	O	S	0	0	0
			2872	1800	506	549	17			
1	F	367	Total	C	N	O	S	0	0	0
			2889	1809	508	555	17			
1	G	365	Total	C	N	O	S	0	0	0
			2872	1800	506	549	17			
1	H	366	Total	C	N	O	S	0	0	0
			2876	1801	506	552	17			
1	I	365	Total	C	N	O	S	0	0	0
			2875	1801	506	551	17			
1	J	367	Total	C	N	O	S	0	0	0
			2883	1806	505	555	17			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	J	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	65	Total	O	0	0
			65	65		
3	B	50	Total	O	0	0
			50	50		

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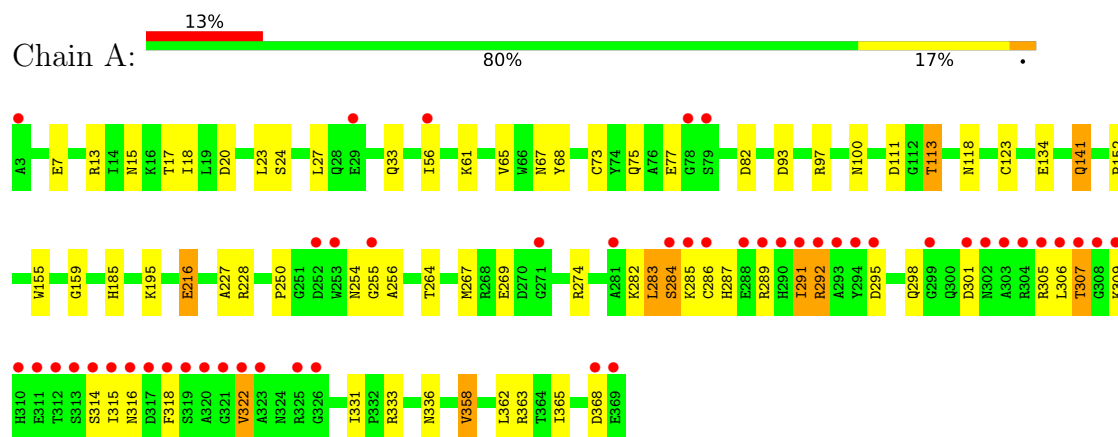
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	34	Total 34	O 34	0	0
3	D	39	Total 39	O 39	0	0
3	E	62	Total 62	O 62	0	0
3	F	56	Total 56	O 56	0	0
3	G	39	Total 39	O 39	0	0
3	H	45	Total 45	O 45	0	0
3	I	62	Total 62	O 62	0	0
3	J	68	Total 68	O 68	0	0

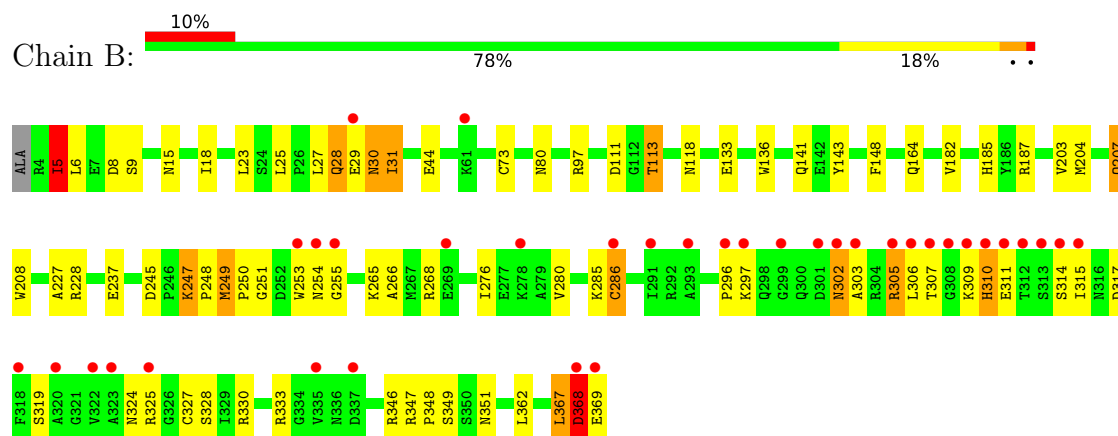
3 Residue-property plots [i](#)

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.

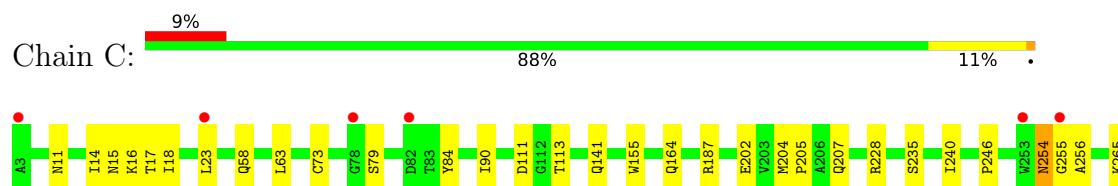
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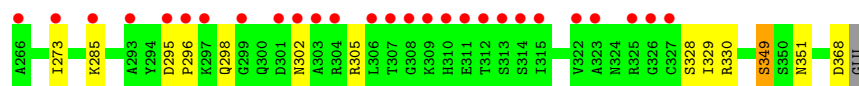


• Molecule 1: Glutamine synthetase 2 cytoplasmic

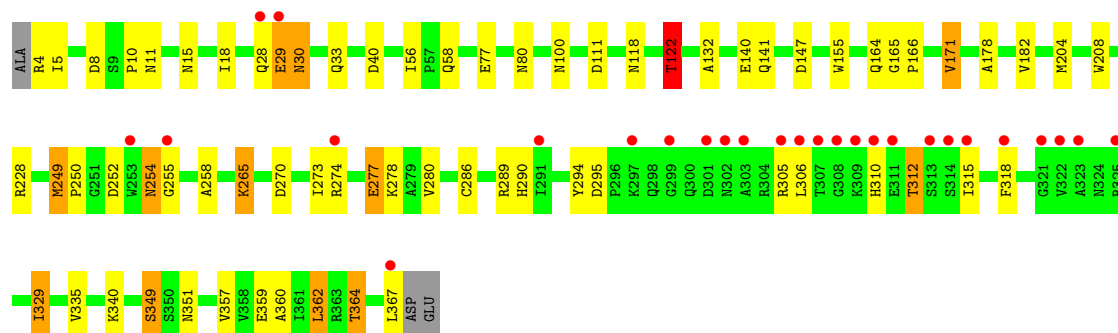
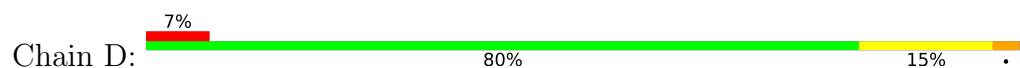


• Molecule 1: Glutamine synthetase 2 cytoplasmic

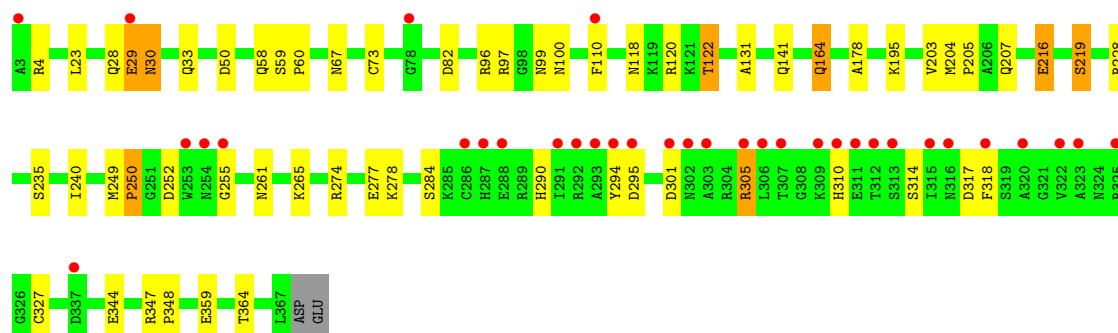
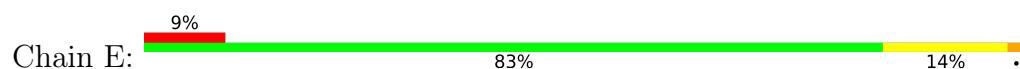




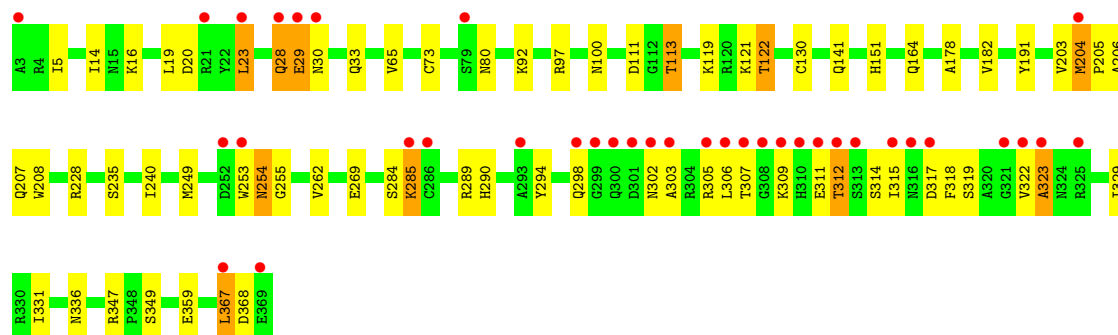
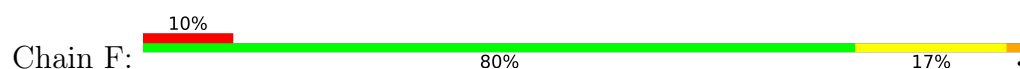
- Molecule 1: Glutamine synthetase 2 cytoplasmic



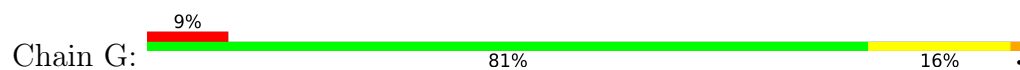
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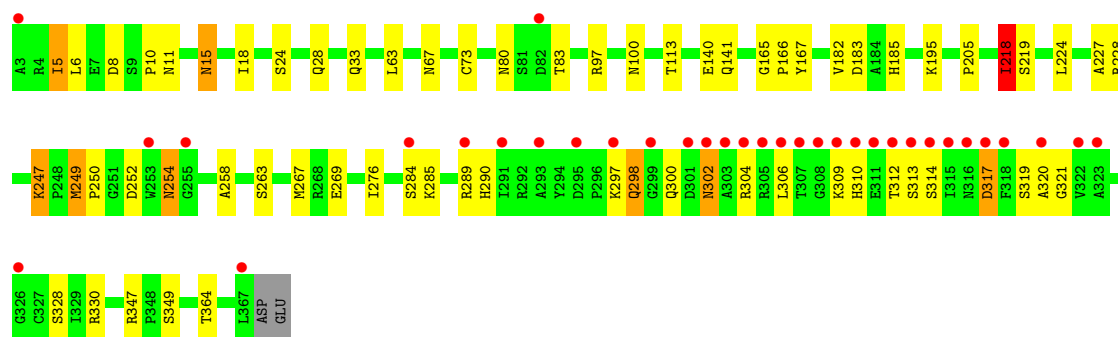


- Molecule 1: Glutamine synthetase 2 cytoplasmic

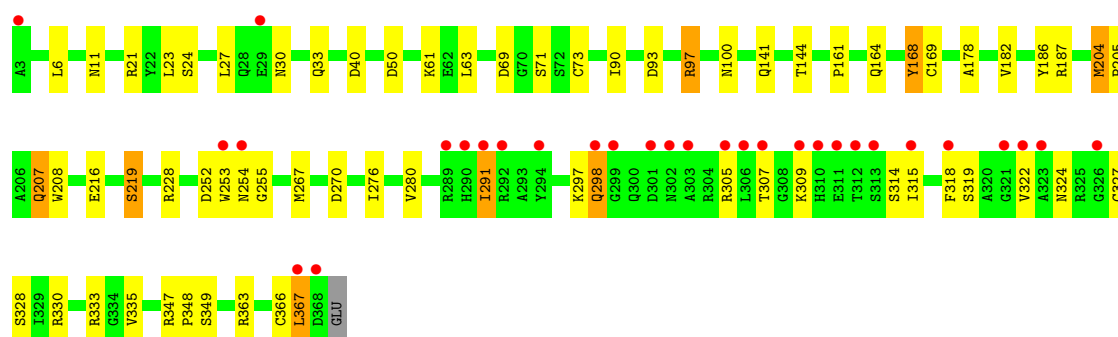
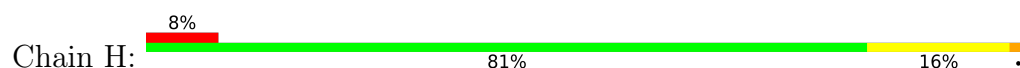


- Molecule 1: Glutamine synthetase 2 cytoplasmic

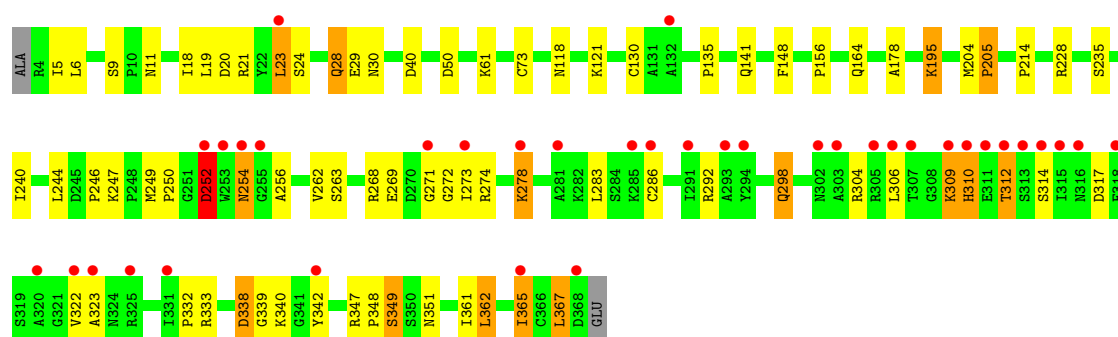
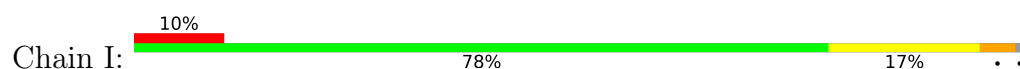




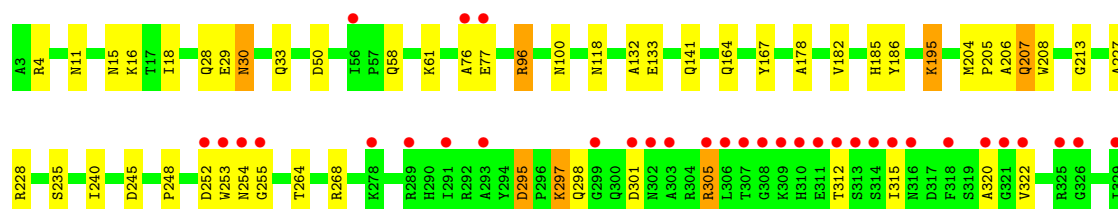
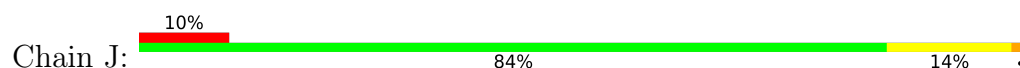
• Molecule 1: Glutamine synthetase 2 cytoplasmic



• Molecule 1: Glutamine synthetase 2 cytoplasmic



• Molecule 1: Glutamine synthetase 2 cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.70Å 102.92Å 206.51Å 90.00° 120.09° 90.00°	Depositor
Resolution (Å)	178.68 – 2.12 178.68 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.6 (178.68-2.12) 96.6 (178.68-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.198 , 0.246 0.203 , 0.248	Depositor DCC
R_{free} test set	11245 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.5	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	0.95	EDS
Total number of atoms	29573	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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	1.02	2/2957 (0.1%)	1.13	8/4013 (0.2%)
1	B	1.00	1/2956 (0.0%)	1.10	5/4011 (0.1%)
1	C	1.07	0/2952	1.12	4/4006 (0.1%)
1	D	1.13	0/2939	1.17	5/3988 (0.1%)
1	E	1.06	1/2944 (0.0%)	1.09	3/3995 (0.1%)
1	F	1.10	0/2961	1.14	13/4018 (0.3%)
1	G	1.15	3/2944 (0.1%)	1.15	12/3995 (0.3%)
1	H	1.09	2/2948 (0.1%)	1.15	8/4002 (0.2%)
1	I	1.02	2/2947 (0.1%)	1.12	6/3999 (0.2%)
1	J	0.97	2/2955 (0.1%)	1.04	4/4011 (0.1%)
All	All	1.06	13/29503 (0.0%)	1.12	68/40038 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	5	ILE	CA-C	6.16	1.59	1.52
1	A	134	GLU	C-O	5.83	1.26	1.23
1	A	134	GLU	N-CA	5.82	1.50	1.46
1	J	320	ALA	CA-C	5.71	1.55	1.52
1	J	207	GLN	C-O	-5.45	1.17	1.23
1	I	205	PRO	CA-C	5.40	1.59	1.52
1	E	205	PRO	CA-C	5.37	1.59	1.52
1	B	5	ILE	CA-C	5.35	1.58	1.52
1	H	366	CYS	CA-C	5.19	1.61	1.53
1	H	168	TYR	CA-C	5.16	1.59	1.52
1	G	284	SER	N-CA	5.14	1.52	1.46
1	G	224	LEU	N-CA	-5.09	1.40	1.46
1	I	195	LYS	N-CA	-5.09	1.40	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	N-CA-C	8.55	123.39	113.38
1	A	56	ILE	N-CA-C	7.94	114.78	107.56
1	C	63	LEU	CA-C-N	-7.24	112.54	119.85
1	C	63	LEU	C-N-CA	-7.24	112.54	119.85
1	A	73	CYS	CB-CA-C	-7.15	100.02	111.18
1	B	73	CYS	N-CA-C	7.13	119.00	110.44
1	C	73	CYS	CB-CA-C	-7.05	99.29	110.85
1	E	73	CYS	CB-CA-C	-6.69	99.88	110.85
1	F	347	ARG	CA-C-N	-6.69	113.07	119.76
1	F	347	ARG	C-N-CA	-6.69	113.07	119.76
1	A	250	PRO	N-CA-C	6.63	121.49	111.14
1	J	295	ASP	CA-C-N	6.59	126.53	119.28
1	J	295	ASP	C-N-CA	6.59	126.53	119.28
1	H	50	ASP	N-CA-C	6.52	119.08	109.24
1	H	73	CYS	CB-CA-C	-6.41	100.63	111.02
1	G	73	CYS	N-CA-C	6.40	118.61	110.61
1	A	298	GLN	N-CA-C	6.36	120.34	112.58
1	B	310	HIS	N-CA-C	6.30	124.22	110.80
1	I	362	LEU	N-CA-C	6.11	117.94	111.28
1	D	56	ILE	N-CA-C	6.02	113.04	107.56
1	B	5	ILE	CB-CA-C	6.00	121.05	111.69
1	G	63	LEU	CA-C-N	-5.92	113.86	120.14
1	G	63	LEU	C-N-CA	-5.92	113.86	120.14
1	D	171	VAL	CB-CA-C	-5.89	101.74	110.33
1	I	29	GLU	N-CA-C	5.85	118.61	111.82
1	H	270	ASP	N-CA-C	5.74	118.28	111.33
1	D	147	ASP	N-CA-C	-5.73	103.14	110.53
1	H	280	VAL	N-CA-C	5.67	115.86	110.42
1	F	73	CYS	CB-CA-C	-5.65	101.58	110.85
1	F	262	VAL	N-CA-C	5.63	116.84	108.46
1	G	347	ARG	CA-C-N	-5.62	113.98	119.76
1	G	347	ARG	C-N-CA	-5.62	113.98	119.76
1	H	24	SER	N-CA-C	5.51	119.11	112.38
1	G	218	ILE	CB-CA-C	-5.50	101.28	111.79
1	E	131	ALA	N-CA-C	5.50	117.71	111.11
1	F	80	ASN	CB-CA-C	-5.50	103.78	111.80
1	A	141	GLN	N-CA-C	5.47	117.15	108.67
1	B	8	ASP	CB-CA-C	-5.44	101.36	110.56
1	F	331	ILE	CB-CA-C	-5.39	104.94	110.71
1	G	15	ASN	N-CA-C	5.27	117.52	110.35
1	I	252	ASP	CB-CA-C	5.27	118.96	111.74
1	H	97	ARG	CB-CA-C	-5.26	108.94	115.89
1	B	30	ASN	N-CA-C	5.22	117.87	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	286	CYS	N-CA-C	5.21	117.09	108.49
1	E	250	PRO	N-CA-C	5.19	120.34	111.68
1	F	30	ASN	CA-C-N	5.19	128.96	121.18
1	F	30	ASN	C-N-CA	5.19	128.96	121.18
1	H	186	TYR	N-CA-C	-5.15	104.92	111.11
1	C	84	TYR	CA-CB-CG	-5.14	104.64	113.90
1	G	312	THR	N-CA-C	5.14	115.13	107.88
1	H	187	ARG	N-CA-C	5.12	116.94	111.36
1	F	303	ALA	N-CA-C	5.12	119.02	112.87
1	I	50	ASP	N-CA-C	5.11	116.96	109.24
1	J	186	TYR	N-CA-C	-5.10	105.61	111.07
1	G	97	ARG	CB-CA-C	-5.10	109.73	115.79
1	J	252	ASP	CB-CA-C	-5.09	104.91	111.22
1	A	65	VAL	N-CA-C	-5.07	102.31	109.21
1	D	122	THR	N-CA-CB	-5.07	102.42	110.22
1	G	182	VAL	N-CA-C	5.05	115.77	110.62
1	D	250	PRO	N-CA-C	5.05	119.40	111.38
1	I	262	VAL	N-CA-C	5.04	115.97	108.46
1	F	121	LYS	CA-C-N	5.03	126.98	120.44
1	F	121	LYS	C-N-CA	5.03	126.98	120.44
1	A	97	ARG	CB-CA-C	-5.02	103.04	111.23
1	G	113	THR	CA-C-N	5.01	124.92	119.76
1	G	113	THR	C-N-CA	5.01	124.92	119.76
1	F	151	HIS	CA-C-N	-5.01	114.62	119.78
1	F	151	HIS	C-N-CA	-5.01	114.62	119.78

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	2885	0	2764	52	0
1	B	2884	0	2763	60	0
1	C	2880	0	2762	24	0
1	D	2867	0	2753	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2872	0	2758	44	0
1	F	2889	0	2768	48	0
1	G	2872	0	2758	34	0
1	H	2876	0	2751	47	0
1	I	2875	0	2757	41	0
1	J	2883	0	2757	39	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
3	A	65	0	0	1	0
3	B	50	0	0	1	0
3	C	34	0	0	0	0
3	D	39	0	0	0	0
3	E	62	0	0	1	0
3	F	56	0	0	1	0
3	G	39	0	0	0	0
3	H	45	0	0	4	0
3	I	62	0	0	1	0
3	J	68	0	0	3	0
All	All	29573	0	27711	405	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 7.

All (405) 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:F:204:MET:HE2	1:F:253:TRP:CZ3	1.96	1.00
1:J:204:MET:HE2	1:J:253:TRP:HB3	1.46	0.97
1:F:204:MET:HB2	1:F:207:GLN:OE1	1.71	0.90
1:E:122:THR:HG22	1:E:359:GLU:OE1	1.77	0.85
1:H:204:MET:HB2	3:H:502:HOH:O	1.78	0.83
1:A:307:THR:OG1	1:A:315:ILE:HG22	1.77	0.82
1:F:204:MET:CE	1:F:253:TRP:CZ3	2.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:ARG:O	1:H:367:LEU:HB3	1.80	0.82
1:A:284:SER:HA	1:A:318:PHE:CZ	2.14	0.82
1:A:307:THR:HA	1:A:314:SER:HA	1.60	0.81
1:E:29:GLU:OE2	1:E:30:ASN:N	2.13	0.81
1:H:204:MET:CB	3:H:502:HOH:O	2.27	0.81
1:E:33:GLN:H	1:E:100:ASN:HD22	1.28	0.81
1:A:33:GLN:H	1:A:100:ASN:HD22	1.28	0.78
1:B:311:GLU:O	1:B:346:ARG:NH2	2.15	0.78
1:I:247:LYS:HE3	1:I:250:PRO:HA	1.65	0.78
1:A:287:HIS:HB2	1:A:318:PHE:HD2	1.47	0.78
1:D:33:GLN:H	1:D:100:ASN:HD22	1.32	0.76
1:J:33:GLN:H	1:J:100:ASN:HD22	1.29	0.76
1:D:29:GLU:O	1:D:30:ASN:ND2	2.18	0.74
1:J:141:GLN:HE22	1:J:228:ARG:HH21	1.35	0.74
1:J:15:ASN:HD21	1:J:18:ILE:H	1.32	0.74
1:B:367:LEU:O	1:B:369:GLU:N	2.21	0.74
1:A:291:ILE:HD13	1:A:315:ILE:HG13	1.70	0.73
1:A:141:GLN:HE22	1:A:228:ARG:HH21	1.36	0.73
1:D:122:THR:HG22	1:D:359:GLU:OE1	1.87	0.73
1:D:141:GLN:HE22	1:D:228:ARG:HH21	1.38	0.72
1:H:204:MET:O	1:H:207:GLN:HB2	1.90	0.72
1:E:255:GLY:HA3	1:E:305:ARG:HD3	1.71	0.72
1:B:15:ASN:HD21	1:B:18:ILE:H	1.37	0.72
1:G:33:GLN:H	1:G:100:ASN:HD22	1.36	0.72
1:B:111:ASP:OD1	1:B:113:THR:HB	1.90	0.71
1:I:141:GLN:HE22	1:I:228:ARG:HH21	1.38	0.71
1:B:247:LYS:HD3	1:B:305:ARG:NH1	2.05	0.71
1:C:111:ASP:OD1	1:C:113:THR:HG22	1.91	0.71
1:B:141:GLN:HE22	1:B:228:ARG:HH21	1.36	0.71
1:E:141:GLN:HE22	1:E:228:ARG:HH21	1.40	0.70
1:G:15:ASN:HD21	1:G:18:ILE:H	1.37	0.69
1:F:164:GLN:HE21	1:F:204:MET:HG2	1.56	0.69
1:G:141:GLN:HE22	1:G:228:ARG:HH21	1.40	0.69
1:G:263:SER:HA	1:G:267:MET:HE2	1.73	0.69
1:F:33:GLN:H	1:F:100:ASN:HD22	1.41	0.69
1:D:290:HIS:CE1	1:D:364:THR:HG21	2.28	0.68
1:F:122:THR:HG22	1:F:359:GLU:OE1	1.93	0.68
1:A:82:ASP:OD2	1:B:333:ARG:NH1	2.26	0.68
1:H:164:GLN:HG3	1:H:204:MET:SD	2.35	0.68
1:F:204:MET:SD	1:F:205:PRO:HD3	2.34	0.67
1:F:141:GLN:HE22	1:F:228:ARG:HH21	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLN:HE22	1:C:228:ARG:HH21	1.42	0.67
1:H:33:GLN:H	1:H:100:ASN:HD22	1.42	0.66
1:B:255:GLY:HA3	1:B:305:ARG:CG	2.26	0.66
1:J:28:GLN:CD	1:J:30:ASN:HD21	2.03	0.66
1:C:164:GLN:HE22	1:C:254:ASN:H	1.44	0.66
1:E:164:GLN:CG	1:E:203:VAL:HG12	2.26	0.66
1:A:287:HIS:HB2	1:A:318:PHE:CD2	2.29	0.66
1:D:306:LEU:O	1:D:315:ILE:HG13	1.96	0.65
1:F:111:ASP:OD1	1:F:113:THR:HG22	1.97	0.65
1:E:255:GLY:HA3	1:E:305:ARG:CD	2.26	0.65
1:B:27:LEU:O	1:B:28:GLN:HB2	1.97	0.64
1:D:290:HIS:HE1	1:D:364:THR:HG21	1.60	0.64
1:J:28:GLN:OE1	1:J:30:ASN:ND2	2.31	0.64
1:F:204:MET:SD	1:F:253:TRP:CZ3	2.90	0.64
1:B:302:ASN:O	1:B:306:LEU:HD12	1.97	0.64
1:B:255:GLY:HA3	1:B:305:ARG:HG2	1.79	0.64
1:D:164:GLN:HE22	1:D:254:ASN:H	1.45	0.64
1:B:247:LYS:CE	1:B:250:PRO:HA	2.27	0.63
1:D:33:GLN:H	1:D:100:ASN:ND2	1.95	0.63
1:H:204:MET:HE2	1:H:253:TRP:CZ3	2.34	0.63
1:B:247:LYS:NZ	1:B:305:ARG:HH12	1.97	0.63
1:A:33:GLN:H	1:A:100:ASN:ND2	1.97	0.63
1:H:164:GLN:HE22	1:H:254:ASN:H	1.46	0.63
1:A:333:ARG:NH1	1:E:82:ASP:OD2	2.32	0.62
1:A:15:ASN:HD21	1:A:18:ILE:H	1.45	0.62
1:H:204:MET:HG3	1:H:205:PRO:HD2	1.80	0.62
1:H:164:GLN:CG	1:H:204:MET:SD	2.88	0.62
1:D:15:ASN:HD21	1:D:18:ILE:H	1.47	0.62
1:A:333:ARG:NH1	1:E:110:PHE:HB2	2.15	0.62
1:F:285:LYS:HD2	1:F:285:LYS:N	2.15	0.61
1:F:249:MET:HG3	3:F:501:HOH:O	2.00	0.61
1:H:324:ASN:HB3	1:H:327:CYS:SG	2.39	0.61
1:H:11:ASN:HD21	1:I:178:ALA:H	1.48	0.61
1:D:286:CYS:HB2	1:D:289:ARG:HD3	1.83	0.61
1:E:29:GLU:OE2	1:E:29:GLU:HA	2.01	0.61
1:A:13:ARG:HB2	1:B:5:ILE:HD12	1.83	0.60
1:A:68:TYR:OH	1:A:75:GLN:NE2	2.35	0.60
1:A:255:GLY:HA3	1:A:305:ARG:HG3	1.84	0.60
1:F:130:CYS:SG	1:F:367:LEU:HD13	2.42	0.59
1:H:204:MET:CE	1:H:253:TRP:CZ3	2.85	0.59
1:I:292:ARG:O	1:I:298:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:SG	1:A:358:VAL:HG22	2.42	0.59
1:A:264:THR:OG1	1:A:267:MET:HG3	2.02	0.59
1:F:204:MET:SD	1:F:253:TRP:HZ3	2.25	0.59
1:J:33:GLN:H	1:J:100:ASN:ND2	1.99	0.59
1:E:249:MET:HE3	1:E:250:PRO:HD2	1.84	0.58
1:H:21:ARG:HD2	1:I:20:ASP:OD2	2.04	0.58
1:B:253:TRP:O	1:B:305:ARG:NH2	2.37	0.58
1:G:267:MET:HE3	1:G:276:ILE:HG12	1.84	0.57
1:A:291:ILE:CD1	1:A:315:ILE:HG13	2.34	0.57
1:I:28:GLN:NE2	1:I:30:ASN:OD1	2.36	0.57
1:I:252:ASP:HB2	1:I:310:HIS:CE1	2.39	0.57
1:G:263:SER:HA	1:G:267:MET:CE	2.34	0.57
1:I:204:MET:HE3	1:I:254:ASN:O	2.03	0.57
1:A:287:HIS:CB	1:A:318:PHE:HD2	2.17	0.57
1:G:298:GLN:HA	1:G:298:GLN:HE21	1.70	0.57
1:E:255:GLY:CA	1:E:305:ARG:HD3	2.33	0.57
1:C:15:ASN:HD21	1:C:18:ILE:H	1.53	0.57
1:E:33:GLN:H	1:E:100:ASN:ND2	2.01	0.57
1:H:255:GLY:HA3	1:H:305:ARG:HD3	1.87	0.56
1:F:122:THR:CG2	1:F:359:GLU:OE1	2.54	0.56
1:D:255:GLY:HA3	1:D:305:ARG:HD2	1.87	0.56
1:H:297:LYS:O	1:H:298:GLN:HB3	2.06	0.56
1:A:24:SER:HB2	1:B:97:ARG:HH12	1.70	0.56
1:J:132:ALA:HB3	3:J:507:HOH:O	2.04	0.56
1:D:140:GLU:O	1:D:258:ALA:HA	2.06	0.56
1:I:19:LEU:HG	1:I:23:LEU:HD22	1.87	0.56
1:A:307:THR:HG1	1:A:315:ILE:HG22	1.69	0.56
1:B:324:ASN:ND2	1:B:327:CYS:SG	2.79	0.56
1:E:29:GLU:OE1	1:E:99:ASN:OD1	2.24	0.56
1:F:33:GLN:H	1:F:100:ASN:ND2	2.04	0.56
1:B:31:ILE:C	1:B:31:ILE:HD12	2.32	0.55
1:B:247:LYS:HE2	1:B:250:PRO:HA	1.88	0.55
1:D:255:GLY:HA3	1:D:305:ARG:CD	2.35	0.55
1:F:14:ILE:O	1:F:16:LYS:HE2	2.06	0.55
1:G:249:MET:HE3	1:G:250:PRO:HD2	1.88	0.55
1:C:11:ASN:HD21	1:D:178:ALA:H	1.55	0.55
1:H:255:GLY:HA3	1:H:305:ARG:CD	2.37	0.55
1:G:33:GLN:H	1:G:100:ASN:ND2	2.04	0.55
1:F:164:GLN:HG3	1:F:204:MET:SD	2.47	0.55
1:A:185:HIS:HD2	3:A:558:HOH:O	1.90	0.55
1:E:29:GLU:OE2	1:E:29:GLU:CA	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:H	1:A:216:GLU:CD	2.15	0.55
1:B:27:LEU:O	1:B:28:GLN:CB	2.55	0.55
1:H:204:MET:SD	1:H:205:PRO:HD3	2.47	0.54
1:F:164:GLN:HE22	1:F:254:ASN:H	1.56	0.54
1:B:164:GLN:HE22	1:B:254:ASN:H	1.55	0.54
1:C:202:GLU:HB3	1:C:207:GLN:HE21	1.72	0.54
1:G:309:LYS:HG3	1:G:310:HIS:H	1.73	0.54
1:D:8:ASP:O	1:D:10:PRO:HD3	2.08	0.54
1:F:20:ASP:HA	1:F:23:LEU:HD22	1.90	0.54
1:F:284:SER:OG	1:F:285:LYS:HD2	2.06	0.54
1:I:141:GLN:NE2	1:I:228:ARG:HE	2.06	0.54
1:H:141:GLN:HE22	1:H:228:ARG:HH21	1.56	0.53
1:I:204:MET:HE1	3:I:508:HOH:O	2.07	0.53
1:I:272:GLY:HA3	1:I:339:GLY:O	2.08	0.53
1:E:118:ASN:C	1:E:118:ASN:OD1	2.50	0.53
1:F:204:MET:CE	1:F:253:TRP:HZ3	2.17	0.52
1:A:111:ASP:OD1	1:A:113:THR:HB	2.09	0.52
1:D:349:SER:OG	1:D:351:ASN:OD1	2.26	0.52
1:F:164:GLN:CG	1:F:204:MET:SD	2.98	0.52
1:H:204:MET:N	3:H:502:HOH:O	2.42	0.52
1:D:252:ASP:HB2	1:D:310:HIS:CE1	2.45	0.52
1:J:204:MET:HE1	3:J:519:HOH:O	2.09	0.52
1:B:44:GLU:CG	1:B:296:PRO:HG2	2.39	0.52
1:B:204:MET:O	1:B:207:GLN:HB2	2.09	0.52
1:G:24:SER:CB	1:H:97:ARG:HH12	2.22	0.52
1:A:141:GLN:NE2	1:A:228:ARG:HE	2.08	0.52
1:D:305:ARG:NH2	1:D:310:HIS:HB2	2.25	0.51
1:F:204:MET:HE3	1:F:205:PRO:CD	2.40	0.51
1:A:284:SER:HA	1:A:318:PHE:CE1	2.46	0.51
1:F:290:HIS:HD2	1:F:294:TYR:OH	1.94	0.51
1:B:367:LEU:O	1:B:368:ASP:C	2.53	0.51
1:D:305:ARG:HH21	1:D:312:THR:HG21	1.76	0.51
1:A:256:ALA:N	1:A:305:ARG:HD3	2.25	0.51
1:F:204:MET:CG	1:F:253:TRP:CE3	2.93	0.51
1:B:255:GLY:HA3	1:B:305:ARG:HG3	1.93	0.51
1:E:164:GLN:CG	1:E:203:VAL:CG1	2.89	0.50
1:F:16:LYS:HD2	1:J:18:ILE:HD11	1.93	0.50
1:G:218:ILE:HD12	1:G:219:SER:N	2.26	0.50
1:J:204:MET:HE3	1:J:254:ASN:O	2.10	0.50
1:D:122:THR:CG2	1:D:359:GLU:OE1	2.57	0.50
1:G:297:LYS:O	1:G:298:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:ASN:HD21	1:J:178:ALA:H	1.58	0.50
1:A:15:ASN:OD1	1:A:17:THR:HG22	2.12	0.50
1:H:216:GLU:O	1:H:219:SER:HB2	2.11	0.50
1:H:347:ARG:N	1:H:348:PRO:CD	2.74	0.50
1:D:11:ASN:HD21	1:E:178:ALA:H	1.58	0.50
1:D:318:PHE:HE2	1:D:329:ILE:HD13	1.77	0.50
1:B:302:ASN:HB3	1:B:306:LEU:HD13	1.94	0.50
1:I:9:SER:HB2	1:I:148:PHE:HB2	1.93	0.50
1:A:118:ASN:C	1:A:118:ASN:OD1	2.55	0.50
1:C:15:ASN:ND2	1:C:18:ILE:H	2.09	0.50
1:C:155:TRP:CZ2	1:C:204:MET:HE3	2.47	0.50
1:B:302:ASN:HD22	1:B:306:LEU:HD11	1.77	0.49
1:G:24:SER:HB2	1:H:97:ARG:HH12	1.77	0.49
1:E:305:ARG:HH21	1:E:310:HIS:HB2	1.77	0.49
1:H:63:LEU:HD12	1:H:90:ILE:HD11	1.93	0.49
1:J:205:PRO:O	1:J:206:ALA:HB3	2.12	0.49
1:A:287:HIS:CG	1:A:318:PHE:HD2	2.30	0.49
1:G:254:ASN:ND2	1:G:310:HIS:HB3	2.28	0.49
1:J:28:GLN:CD	1:J:30:ASN:ND2	2.70	0.49
1:F:130:CYS:SG	1:F:367:LEU:CD1	3.00	0.49
1:F:178:ALA:H	1:J:11:ASN:HD21	1.61	0.49
1:H:307:THR:HG23	1:H:309:LYS:HB2	1.95	0.49
1:J:15:ASN:ND2	1:J:18:ILE:H	2.07	0.49
1:J:255:GLY:HA3	1:J:305:ARG:HG2	1.94	0.49
1:B:245:ASP:O	1:B:248:PRO:HD3	2.12	0.49
1:F:141:GLN:NE2	1:F:228:ARG:HE	2.11	0.48
1:G:11:ASN:HD21	1:H:178:ALA:H	1.60	0.48
1:B:118:ASN:OD1	1:B:118:ASN:C	2.54	0.48
1:E:164:GLN:HG2	1:E:203:VAL:CG1	2.43	0.48
1:E:284:SER:CB	1:E:318:PHE:CE1	2.97	0.48
1:E:284:SER:HB2	1:E:318:PHE:CE1	2.49	0.48
1:I:269:GLU:O	1:I:271:GLY:N	2.43	0.48
1:D:141:GLN:NE2	1:D:228:ARG:HE	2.12	0.48
1:J:167:TYR:CE2	1:J:205:PRO:HG3	2.48	0.48
1:C:329:ILE:HG22	1:C:330:ARG:N	2.29	0.48
1:I:164:GLN:HE22	1:I:254:ASN:H	1.61	0.48
1:I:332:PRO:O	1:I:333:ARG:C	2.57	0.48
1:J:297:LYS:O	1:J:298:GLN:NE2	2.47	0.48
1:H:168:TYR:O	1:H:169:CYS:C	2.56	0.48
1:I:323:ALA:HB2	1:I:333:ARG:HB2	1.96	0.47
1:G:167:TYR:CE2	1:G:205:PRO:HG3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:MET:HG2	1:H:276:ILE:HG13	1.95	0.47
1:I:309:LYS:O	1:I:310:HIS:HB2	2.14	0.47
1:B:302:ASN:ND2	1:B:349:SER:HB2	2.29	0.47
1:E:29:GLU:O	1:E:30:ASN:HB2	2.14	0.47
1:D:155:TRP:CH2	1:D:204:MET:HE3	2.49	0.47
1:A:322:VAL:HG22	1:A:331:ILE:HB	1.97	0.47
1:E:216:GLU:O	1:E:219:SER:HB2	2.14	0.47
1:H:255:GLY:CA	1:H:305:ARG:HD3	2.43	0.47
1:I:247:LYS:HD3	1:I:304:ARG:O	2.14	0.47
1:I:347:ARG:N	1:I:348:PRO:CD	2.78	0.47
1:C:349:SER:OG	1:C:351:ASN:OD1	2.33	0.47
1:E:204:MET:HB3	1:E:207:GLN:HB2	1.95	0.47
1:I:135:PRO:HA	1:I:263:SER:O	2.15	0.47
1:D:280:VAL:HG22	1:D:329:ILE:HG21	1.96	0.47
1:J:195:LYS:HD3	1:J:213:GLY:O	2.14	0.47
1:J:182:VAL:HG21	1:J:208:TRP:CD2	2.50	0.46
1:F:28:GLN:O	1:F:29:GLU:HB2	2.16	0.46
1:F:204:MET:CG	1:F:253:TRP:HE3	2.28	0.46
1:A:287:HIS:ND1	1:A:318:PHE:CD2	2.83	0.46
1:B:25:LEU:O	1:C:187:ARG:NH2	2.47	0.46
1:C:11:ASN:ND2	1:D:178:ALA:H	2.13	0.46
1:F:92:LYS:HE3	1:F:191:TYR:CZ	2.51	0.46
1:B:276:ILE:O	1:B:280:VAL:HG23	2.16	0.46
1:E:122:THR:HG22	1:E:359:GLU:CD	2.40	0.46
1:B:247:LYS:CD	1:B:305:ARG:NH1	2.78	0.46
1:B:302:ASN:C	1:B:306:LEU:CD1	2.89	0.46
1:D:155:TRP:CZ2	1:D:204:MET:HE3	2.51	0.46
1:J:204:MET:HE2	1:J:253:TRP:CB	2.32	0.46
1:B:185:HIS:HE1	1:B:227:ALA:O	1.99	0.46
1:C:235:SER:HB3	1:C:240:ILE:O	2.16	0.46
1:C:302:ASN:OD1	1:C:349:SER:HB3	2.16	0.46
1:I:361:ILE:O	1:I:365:ILE:HB	2.16	0.46
1:G:165:GLY:N	1:G:166:PRO:CD	2.78	0.46
1:B:15:ASN:ND2	1:B:18:ILE:H	2.11	0.46
1:B:44:GLU:HG3	1:B:296:PRO:HG2	1.97	0.46
1:B:310:HIS:NE2	1:B:311:GLU:HB2	2.31	0.46
1:I:18:ILE:HD11	1:J:16:LYS:HD2	1.98	0.46
1:J:118:ASN:C	1:J:118:ASN:OD1	2.57	0.46
1:D:204:MET:HE1	1:D:249:MET:HB2	1.97	0.46
1:G:309:LYS:HG3	1:G:310:HIS:N	2.30	0.46
1:A:295:ASP:OD2	1:A:301:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:GLU:O	1:G:258:ALA:HA	2.16	0.45
1:H:144:THR:OG1	1:H:207:GLN:HG2	2.16	0.45
1:E:235:SER:HB3	1:E:240:ILE:O	2.16	0.45
1:B:9:SER:HB2	1:B:148:PHE:HB2	1.98	0.45
1:B:309:LYS:O	1:B:310:HIS:ND1	2.49	0.45
1:F:322:VAL:O	1:F:323:ALA:C	2.60	0.45
1:I:246:PRO:HA	1:I:256:ALA:HB3	1.98	0.45
1:A:287:HIS:CG	1:A:318:PHE:CD2	3.04	0.45
1:I:338:ASP:N	1:I:338:ASP:OD1	2.48	0.45
1:B:324:ASN:O	1:B:330:ARG:HD2	2.16	0.45
1:D:294:TYR:CD1	1:D:357:VAL:HG22	2.51	0.45
1:G:247:LYS:HG3	1:G:304:ARG:O	2.17	0.45
1:B:302:ASN:ND2	1:B:306:LEU:HD11	2.31	0.45
1:H:164:GLN:HG2	1:H:204:MET:SD	2.56	0.45
1:G:15:ASN:ND2	1:G:15:ASN:C	2.75	0.45
1:H:69:ASP:OD1	1:H:71:SER:OG	2.21	0.45
1:H:297:LYS:O	1:H:298:GLN:CB	2.65	0.45
1:J:235:SER:HB3	1:J:240:ILE:O	2.17	0.45
1:A:27:LEU:HD22	1:B:187:ARG:NH1	2.32	0.44
1:I:204:MET:HG2	1:I:205:PRO:HD2	1.98	0.44
1:E:290:HIS:O	1:E:294:TYR:CG	2.70	0.44
1:H:204:MET:HE2	1:H:253:TRP:CE3	2.52	0.44
1:A:285:LYS:C	1:A:287:HIS:H	2.26	0.44
1:C:204:MET:HB3	1:C:207:GLN:HB2	1.99	0.44
1:H:204:MET:HG3	1:H:205:PRO:CD	2.45	0.44
1:J:345:ASP:OD1	1:J:345:ASP:C	2.61	0.44
1:D:11:ASN:ND2	1:E:178:ALA:H	2.16	0.44
1:F:164:GLN:HG2	1:F:204:MET:SD	2.57	0.44
1:F:255:GLY:HA3	1:F:305:ARG:HD2	1.98	0.44
1:A:93:ASP:OD1	1:A:93:ASP:C	2.61	0.44
1:B:349:SER:OG	1:B:351:ASN:OD1	2.26	0.44
1:A:216:GLU:CD	1:A:216:GLU:N	2.76	0.44
1:B:251:GLY:O	1:B:305:ARG:NH2	2.48	0.44
1:H:207:GLN:HG3	3:H:502:HOH:O	2.18	0.44
1:J:185:HIS:HD2	3:J:556:HOH:O	2.01	0.44
1:A:362:LEU:O	1:A:363:ARG:C	2.61	0.44
1:F:302:ASN:HA	1:F:349:SER:OG	2.17	0.44
1:B:310:HIS:CD2	1:B:310:HIS:C	2.96	0.43
1:E:295:ASP:OD1	1:E:301:ASP:HB2	2.18	0.43
1:G:317:ASP:HB3	1:G:328:SER:HG	1.83	0.43
1:J:264:THR:O	1:J:268:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HB2	1:B:5:ILE:CD1	2.48	0.43
1:F:204:MET:HE3	1:F:205:PRO:HD2	2.00	0.43
1:F:235:SER:HB3	1:F:240:ILE:O	2.19	0.43
1:G:67:ASN:HA	1:G:83:THR:O	2.17	0.43
1:J:4:ARG:NH2	1:J:4:ARG:HG3	2.32	0.43
1:C:15:ASN:ND2	1:C:18:ILE:HG13	2.34	0.43
1:E:261:ASN:OD1	1:E:344:GLU:HG3	2.19	0.43
1:I:306:LEU:HD12	1:I:312:THR:HG21	1.99	0.43
1:E:252:ASP:HA	1:E:310:HIS:HE1	1.84	0.43
1:B:185:HIS:HD2	3:B:533:HOH:O	2.02	0.43
1:E:59:SER:HB2	1:E:60:PRO:HD2	2.01	0.43
1:G:185:HIS:HE1	1:G:227:ALA:O	2.02	0.43
1:H:40:ASP:OD1	1:H:40:ASP:C	2.60	0.43
1:I:249:MET:SD	1:I:250:PRO:HD2	2.59	0.43
1:C:15:ASN:HD21	1:C:18:ILE:N	2.16	0.43
1:E:347:ARG:N	1:E:348:PRO:CD	2.82	0.43
1:I:195:LYS:HE2	1:I:214:PRO:O	2.19	0.43
1:I:342:TYR:CD1	1:I:342:TYR:C	2.97	0.43
1:A:284:SER:O	1:A:318:PHE:CD2	2.72	0.43
1:B:265:LYS:O	1:B:266:ALA:C	2.62	0.43
1:E:67:ASN:ND2	3:E:503:HOH:O	2.47	0.43
1:I:278:LYS:HE3	1:I:278:LYS:HA	2.01	0.42
1:J:185:HIS:HE1	1:J:227:ALA:O	2.02	0.42
1:A:152:PRO:HB2	1:A:155:TRP:CD1	2.54	0.42
1:A:283:LEU:HD11	1:A:365:ILE:HG23	2.01	0.42
1:E:50:ASP:CG	1:E:96:ARG:HH22	2.25	0.42
1:E:290:HIS:O	1:E:294:TYR:CD1	2.72	0.42
1:D:132:ALA:O	1:D:265:LYS:HE2	2.20	0.42
1:F:314:SER:HB3	1:F:317:ASP:HB2	2.01	0.42
1:B:182:VAL:HG21	1:B:208:TRP:CD2	2.54	0.42
1:D:40:ASP:OD1	1:D:40:ASP:C	2.62	0.42
1:E:141:GLN:NE2	1:E:228:ARG:HE	2.17	0.42
1:E:164:GLN:CD	1:E:203:VAL:HG12	2.44	0.42
1:J:164:GLN:HE22	1:J:254:ASN:H	1.68	0.42
1:A:289:ARG:HA	1:A:292:ARG:HH11	1.84	0.42
1:F:182:VAL:HG21	1:F:208:TRP:CD2	2.55	0.42
1:F:204:MET:HG2	1:F:253:TRP:HE3	1.83	0.42
1:G:8:ASP:O	1:G:10:PRO:HD3	2.19	0.42
1:J:245:ASP:O	1:J:248:PRO:HD3	2.19	0.42
1:B:141:GLN:NE2	1:B:228:ARG:HE	2.18	0.42
1:C:255:GLY:HA3	1:C:305:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASN:OD1	1:D:118:ASN:C	2.63	0.42
1:G:11:ASN:ND2	1:H:178:ALA:H	2.16	0.42
1:H:30:ASN:OD1	1:H:30:ASN:N	2.52	0.42
1:I:349:SER:OG	1:I:351:ASN:OD1	2.38	0.42
1:D:15:ASN:ND2	1:D:15:ASN:C	2.78	0.42
1:D:305:ARG:O	1:D:305:ARG:NE	2.53	0.42
1:I:235:SER:HB3	1:I:240:ILE:O	2.20	0.42
1:J:204:MET:HB3	1:J:207:GLN:HB2	2.02	0.42
1:A:185:HIS:HE1	1:A:227:ALA:O	2.03	0.42
1:B:247:LYS:CE	1:B:305:ARG:HH12	2.33	0.42
1:D:182:VAL:HG21	1:D:208:TRP:CD2	2.55	0.42
1:H:305:ARG:O	1:H:307:THR:N	2.52	0.42
1:E:284:SER:HA	1:E:318:PHE:CE2	2.55	0.41
1:E:290:HIS:HE1	1:E:364:THR:OG1	2.02	0.41
1:F:205:PRO:O	1:F:206:ALA:HB3	2.19	0.41
1:I:118:ASN:OD1	1:I:118:ASN:C	2.63	0.41
1:I:130:CYS:SG	1:I:367:LEU:HD13	2.59	0.41
1:C:141:GLN:NE2	1:C:228:ARG:HE	2.18	0.41
1:C:204:MET:HG3	1:C:205:PRO:HD2	2.01	0.41
1:D:360:ALA:O	1:D:364:THR:HG23	2.20	0.41
1:I:195:LYS:CE	1:I:214:PRO:O	2.68	0.41
1:J:50:ASP:CG	1:J:96:ARG:HH22	2.27	0.41
1:J:295:ASP:OD2	1:J:301:ASP:HB2	2.20	0.41
1:E:255:GLY:HA3	1:E:305:ARG:HD2	2.02	0.41
1:I:247:LYS:CE	1:I:250:PRO:HA	2.43	0.41
1:A:282:LYS:NZ	1:A:368:ASP:OD1	2.53	0.41
1:D:15:ASN:ND2	1:D:18:ILE:HD12	2.36	0.41
1:E:305:ARG:NH2	1:E:310:HIS:HB2	2.35	0.41
1:F:178:ALA:H	1:J:11:ASN:ND2	2.19	0.41
1:F:318:PHE:CE2	1:F:329:ILE:HD13	2.55	0.41
1:G:80:ASN:HD22	1:H:333:ARG:HH22	1.68	0.41
1:G:290:HIS:HE1	1:G:364:THR:OG1	2.04	0.41
1:G:309:LYS:HE2	1:G:310:HIS:HB2	2.02	0.41
1:B:143:TYR:CZ	1:B:208:TRP:HB2	2.55	0.41
1:F:306:LEU:HD22	1:F:312:THR:HG23	2.02	0.41
1:I:23:LEU:HD12	1:I:23:LEU:HA	1.96	0.41
1:J:255:GLY:HA3	1:J:305:ARG:CG	2.50	0.41
1:A:283:LEU:CD1	1:A:365:ILE:HG23	2.49	0.41
1:B:136:TRP:CE3	1:B:268:ARG:HD3	2.55	0.41
1:D:273:ILE:O	1:D:277:GLU:HG3	2.21	0.41
1:E:120:ARG:O	1:E:120:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:SER:CB	1:G:328:SER:H	2.34	0.41
1:A:15:ASN:ND2	1:A:18:ILE:HD12	2.36	0.41
1:A:13:ARG:CB	1:B:5:ILE:HD12	2.50	0.41
1:C:11:ASN:HA	1:C:14:ILE:HD12	2.03	0.41
1:F:19:LEU:HG	1:F:23:LEU:HD13	2.02	0.41
1:H:318:PHE:CG	1:H:319:SER:N	2.89	0.41
1:A:159:GLY:HA3	1:I:156:PRO:HG2	2.03	0.41
1:B:164:GLN:CD	1:B:203:VAL:HG12	2.46	0.41
1:C:246:PRO:HA	1:C:256:ALA:HB3	2.01	0.41
1:D:165:GLY:N	1:D:166:PRO:CD	2.84	0.41
1:G:167:TYR:CZ	1:G:205:PRO:HG3	2.55	0.41
1:H:182:VAL:HG21	1:H:208:TRP:CD2	2.56	0.41
1:J:295:ASP:O	1:J:297:LYS:O	2.39	0.41
1:C:295:ASP:HB2	1:C:296:PRO:HD2	2.02	0.41
1:H:161:PRO:HG2	1:H:204:MET:HE3	2.03	0.41
1:H:291:ILE:HD13	1:H:315:ILE:HG13	2.03	0.41
1:G:302:ASN:ND2	1:G:349:SER:OG	2.53	0.40
1:B:249:MET:HE2	1:B:249:MET:HB3	1.98	0.40
1:B:302:ASN:C	1:B:306:LEU:HD12	2.46	0.40
1:B:347:ARG:N	1:B:348:PRO:CD	2.84	0.40
1:F:164:GLN:CD	1:F:203:VAL:HG12	2.46	0.40
1:G:319:SER:C	1:G:321:GLY:H	2.28	0.40
1:I:40:ASP:HB2	1:I:73:CYS:HB2	2.03	0.40
1:J:305:ARG:HD2	1:J:312:THR:HG21	2.04	0.40
1:A:13:ARG:CB	1:B:5:ILE:CD1	2.99	0.40
1:C:16:LYS:HA	1:C:16:LYS:HD3	1.89	0.40
1:H:93:ASP:OD1	1:H:93:ASP:C	2.64	0.40
1:D:111:ASP:C	1:D:111:ASP:OD1	2.64	0.40
1:D:362:LEU:HD12	1:D:362:LEU:HA	1.90	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	365/367 (100%)	343 (94%)	20 (6%)	2 (0%)	24	22
1	B	364/367 (99%)	341 (94%)	18 (5%)	5 (1%)	9	5
1	C	364/367 (99%)	348 (96%)	15 (4%)	1 (0%)	36	36
1	D	362/367 (99%)	345 (95%)	17 (5%)	0	100	100
1	E	363/367 (99%)	340 (94%)	22 (6%)	1 (0%)	36	36
1	F	365/367 (100%)	344 (94%)	18 (5%)	3 (1%)	16	12
1	G	363/367 (99%)	348 (96%)	14 (4%)	1 (0%)	36	36
1	H	364/367 (99%)	345 (95%)	18 (5%)	1 (0%)	36	36
1	I	363/367 (99%)	341 (94%)	20 (6%)	2 (1%)	21	18
1	J	365/367 (100%)	342 (94%)	22 (6%)	1 (0%)	36	36
All	All	3638/3670 (99%)	3437 (94%)	184 (5%)	17 (0%)	24	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	B	286	CYS
1	B	368	ASP
1	C	298	GLN
1	F	298	GLN
1	F	368	ASP
1	H	298	GLN
1	E	30	ASN
1	F	323	ALA
1	I	310	HIS
1	A	286	CYS
1	I	24	SER
1	A	316	ASN
1	B	285	LYS
1	J	76	ALA
1	B	303	ALA
1	G	320	ALA

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	308/309 (100%)	286 (93%)	22 (7%)	13	10
1	B	309/309 (100%)	282 (91%)	27 (9%)	9	6
1	C	308/309 (100%)	296 (96%)	12 (4%)	28	29
1	D	307/309 (99%)	281 (92%)	26 (8%)	10	7
1	E	307/309 (99%)	288 (94%)	19 (6%)	16	14
1	F	309/309 (100%)	287 (93%)	22 (7%)	13	10
1	G	307/309 (99%)	286 (93%)	21 (7%)	14	11
1	H	307/309 (99%)	291 (95%)	16 (5%)	21	19
1	I	308/309 (100%)	281 (91%)	27 (9%)	9	6
1	J	308/309 (100%)	294 (96%)	14 (4%)	24	24
All	All	3078/3090 (100%)	2872 (93%)	206 (7%)	15	12

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	20	ASP
1	A	23	LEU
1	A	61	LYS
1	A	67	ASN
1	A	77	GLU
1	A	113	THR
1	A	195	LYS
1	A	216	GLU
1	A	254	ASN
1	A	269	GLU
1	A	274	ARG
1	A	283	LEU
1	A	284	SER
1	A	291	ILE
1	A	292	ARG
1	A	306	LEU
1	A	307	THR
1	A	309	LYS
1	A	322	VAL
1	A	336	ASN
1	A	358	VAL
1	B	5	ILE

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	23	LEU
1	B	29	GLU
1	B	30	ASN
1	B	31	ILE
1	B	80	ASN
1	B	113	THR
1	B	133	GLU
1	B	207	GLN
1	B	237	GLU
1	B	247	LYS
1	B	249	MET
1	B	286	CYS
1	B	297	LYS
1	B	302	ASN
1	B	305	ARG
1	B	307	THR
1	B	314	SER
1	B	315	ILE
1	B	317	ASP
1	B	319	SER
1	B	325	ARG
1	B	328	SER
1	B	362	LEU
1	B	367	LEU
1	B	368	ASP
1	C	17	THR
1	C	23	LEU
1	C	58	GLN
1	C	79	SER
1	C	90	ILE
1	C	254	ASN
1	C	265	LYS
1	C	273	ILE
1	C	285	LYS
1	C	328	SER
1	C	349	SER
1	C	368	ASP
1	D	4	ARG
1	D	5	ILE
1	D	28	GLN
1	D	29	GLU

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Mol	Chain	Res	Type
1	D	30	ASN
1	D	58	GLN
1	D	77	GLU
1	D	80	ASN
1	D	122	THR
1	D	171	VAL
1	D	249	MET
1	D	254	ASN
1	D	265	LYS
1	D	270	ASP
1	D	274	ARG
1	D	277	GLU
1	D	278	LYS
1	D	295	ASP
1	D	312	THR
1	D	329	ILE
1	D	335	VAL
1	D	340	LYS
1	D	349	SER
1	D	362	LEU
1	D	364	THR
1	D	367	LEU
1	E	4	ARG
1	E	23	LEU
1	E	28	GLN
1	E	29	GLU
1	E	58	GLN
1	E	97	ARG
1	E	122	THR
1	E	164	GLN
1	E	195	LYS
1	E	216	GLU
1	E	219	SER
1	E	265	LYS
1	E	274	ARG
1	E	277	GLU
1	E	278	LYS
1	E	305	ARG
1	E	314	SER
1	E	317	ASP
1	E	327	CYS
1	F	5	ILE

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Mol	Chain	Res	Type
1	F	23	LEU
1	F	28	GLN
1	F	29	GLU
1	F	65	VAL
1	F	97	ARG
1	F	113	THR
1	F	119	LYS
1	F	122	THR
1	F	204	MET
1	F	254	ASN
1	F	269	GLU
1	F	285	LYS
1	F	289	ARG
1	F	307	THR
1	F	309	LYS
1	F	311	GLU
1	F	312	THR
1	F	315	ILE
1	F	319	SER
1	F	336	ASN
1	F	367	LEU
1	G	5	ILE
1	G	6	LEU
1	G	28	GLN
1	G	183	ASP
1	G	195	LYS
1	G	218	ILE
1	G	247	LYS
1	G	249	MET
1	G	252	ASP
1	G	254	ASN
1	G	269	GLU
1	G	285	LYS
1	G	289	ARG
1	G	298	GLN
1	G	300	GLN
1	G	302	ASN
1	G	306	LEU
1	G	313	SER
1	G	314	SER
1	G	317	ASP
1	G	330	ARG

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Mol	Chain	Res	Type
1	H	6	LEU
1	H	23	LEU
1	H	27	LEU
1	H	61	LYS
1	H	204	MET
1	H	207	GLN
1	H	219	SER
1	H	252	ASP
1	H	291	ILE
1	H	314	SER
1	H	322	VAL
1	H	328	SER
1	H	330	ARG
1	H	335	VAL
1	H	349	SER
1	H	367	LEU
1	I	5	ILE
1	I	6	LEU
1	I	21	ARG
1	I	23	LEU
1	I	28	GLN
1	I	61	LYS
1	I	121	LYS
1	I	244	LEU
1	I	252	ASP
1	I	254	ASN
1	I	268	ARG
1	I	273	ILE
1	I	274	ARG
1	I	278	LYS
1	I	283	LEU
1	I	298	GLN
1	I	309	LYS
1	I	312	THR
1	I	314	SER
1	I	317	ASP
1	I	322	VAL
1	I	338	ASP
1	I	340	LYS
1	I	349	SER
1	I	362	LEU
1	I	365	ILE

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Mol	Chain	Res	Type
1	I	367	LEU
1	J	29	GLU
1	J	30	ASN
1	J	58	GLN
1	J	61	LYS
1	J	77	GLU
1	J	96	ARG
1	J	133	GLU
1	J	195	LYS
1	J	297	LYS
1	J	305	ARG
1	J	315	ILE
1	J	322	VAL
1	J	338	ASP
1	J	349	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	15	ASN
1	A	58	GLN
1	A	67	ASN
1	A	75	GLN
1	A	100	ASN
1	A	141	GLN
1	A	158	ASN
1	A	164	GLN
1	A	185	HIS
1	A	290	HIS
1	A	300	GLN
1	B	15	ASN
1	B	99	ASN
1	B	141	GLN
1	B	164	GLN
1	B	185	HIS
1	B	290	HIS
1	B	298	GLN
1	B	302	ASN
1	C	11	ASN
1	C	15	ASN
1	C	141	GLN

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Mol	Chain	Res	Type
1	C	158	ASN
1	C	164	GLN
1	C	207	GLN
1	C	254	ASN
1	C	290	HIS
1	C	316	ASN
1	C	336	ASN
1	D	11	ASN
1	D	15	ASN
1	D	67	ASN
1	D	100	ASN
1	D	141	GLN
1	D	164	GLN
1	D	200	ASN
1	D	207	GLN
1	D	254	ASN
1	D	287	HIS
1	E	15	ASN
1	E	99	ASN
1	E	100	ASN
1	E	141	GLN
1	E	290	HIS
1	E	302	ASN
1	E	310	HIS
1	F	11	ASN
1	F	15	ASN
1	F	30	ASN
1	F	100	ASN
1	F	141	GLN
1	F	164	GLN
1	F	185	HIS
1	F	200	ASN
1	F	254	ASN
1	F	287	HIS
1	F	290	HIS
1	F	310	HIS
1	F	336	ASN
1	G	11	ASN
1	G	15	ASN
1	G	80	ASN
1	G	100	ASN
1	G	141	GLN

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Mol	Chain	Res	Type
1	G	185	HIS
1	G	254	ASN
1	G	261	ASN
1	G	290	HIS
1	G	298	GLN
1	G	302	ASN
1	G	324	ASN
1	H	11	ASN
1	H	58	GLN
1	H	100	ASN
1	H	141	GLN
1	H	151	HIS
1	H	164	GLN
1	H	200	ASN
1	H	207	GLN
1	H	232	HIS
1	H	261	ASN
1	H	290	HIS
1	H	300	GLN
1	I	11	ASN
1	I	80	ASN
1	I	99	ASN
1	I	141	GLN
1	I	158	ASN
1	I	164	GLN
1	I	207	GLN
1	I	254	ASN
1	I	261	ASN
1	I	290	HIS
1	J	11	ASN
1	J	15	ASN
1	J	30	ASN
1	J	67	ASN
1	J	99	ASN
1	J	100	ASN
1	J	141	GLN
1	J	158	ASN
1	J	164	GLN
1	J	185	HIS
1	J	287	HIS
1	J	290	HIS
1	J	298	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](#)

10 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	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
2	ADP	E	401	-	28,29,29	1.45	6 (21%)	43,45,45	2.03	11 (25%)
2	ADP	J	401	-	28,29,29	1.53	5 (17%)	43,45,45	1.91	11 (25%)
2	ADP	F	401	-	28,29,29	1.53	5 (17%)	43,45,45	2.06	11 (25%)
2	ADP	D	401	-	28,29,29	1.47	4 (14%)	43,45,45	1.86	9 (20%)
2	ADP	A	401	-	28,29,29	1.35	4 (14%)	43,45,45	2.13	7 (16%)
2	ADP	I	401	-	28,29,29	1.35	4 (14%)	43,45,45	2.13	7 (16%)
2	ADP	G	401	-	28,29,29	1.34	4 (14%)	43,45,45	2.16	8 (18%)
2	ADP	H	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
2	ADP	B	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)

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	401	-	-	3/16/32/32	0/3/3/3
2	ADP	E	401	-	-	7/16/32/32	0/3/3/3
2	ADP	J	401	-	-	3/16/32/32	0/3/3/3
2	ADP	F	401	-	-	6/16/32/32	0/3/3/3
2	ADP	D	401	-	-	2/16/32/32	0/3/3/3
2	ADP	A	401	-	-	7/16/32/32	0/3/3/3
2	ADP	I	401	-	-	7/16/32/32	0/3/3/3
2	ADP	G	401	-	-	7/16/32/32	0/3/3/3
2	ADP	H	401	-	-	0/16/32/32	0/3/3/3
2	ADP	B	401	-	-	0/16/32/32	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ADP	C5-C4	5.08	1.48	1.39
2	H	401	ADP	C5-C4	4.77	1.47	1.39
2	C	401	ADP	C5-C4	4.74	1.47	1.39
2	B	401	ADP	C5-C4	4.70	1.47	1.39
2	J	401	ADP	C5-C4	4.38	1.46	1.39
2	F	401	ADP	PA-O3A	4.20	1.64	1.59
2	F	401	ADP	C5-C4	4.14	1.46	1.39
2	J	401	ADP	PA-O3A	4.10	1.63	1.59
2	A	401	ADP	C5-C4	3.71	1.45	1.39
2	I	401	ADP	C5-C4	3.66	1.45	1.39
2	G	401	ADP	C5-C4	3.59	1.45	1.39
2	E	401	ADP	C5-N7	-3.37	1.32	1.39
2	G	401	ADP	C5-N7	-3.21	1.33	1.39
2	I	401	ADP	C5-N7	-3.20	1.33	1.39
2	E	401	ADP	C5-C4	3.18	1.44	1.39
2	A	401	ADP	C5-N7	-3.18	1.33	1.39
2	E	401	ADP	C8-N9	-3.08	1.32	1.37
2	F	401	ADP	C5-C6	2.86	1.48	1.41
2	B	401	ADP	C5-C6	2.77	1.48	1.41
2	D	401	ADP	C5-C6	2.77	1.48	1.41
2	C	401	ADP	C5-C6	2.76	1.48	1.41
2	H	401	ADP	C5-C6	2.73	1.48	1.41
2	J	401	ADP	C8-N7	2.56	1.36	1.31
2	E	401	ADP	C4-N9	-2.50	1.32	1.37
2	F	401	ADP	C8-N7	2.49	1.36	1.31
2	A	401	ADP	C5-C6	2.49	1.47	1.41
2	I	401	ADP	C5-C6	2.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	ADP	C5-C6	2.44	1.47	1.41
2	G	401	ADP	C5-C6	2.40	1.47	1.41
2	H	401	ADP	C8-N7	2.38	1.36	1.31
2	C	401	ADP	C8-N7	2.36	1.36	1.31
2	G	401	ADP	C8-N9	-2.35	1.33	1.37
2	D	401	ADP	C8-N7	2.35	1.36	1.31
2	B	401	ADP	C8-N7	2.35	1.36	1.31
2	A	401	ADP	C8-N9	-2.35	1.33	1.37
2	E	401	ADP	PA-O3A	2.34	1.62	1.59
2	I	401	ADP	C8-N9	-2.31	1.33	1.37
2	H	401	ADP	C5-N7	-2.25	1.35	1.39
2	C	401	ADP	C5-N7	-2.23	1.35	1.39
2	B	401	ADP	C5-N7	-2.23	1.35	1.39
2	J	401	ADP	C5-N7	-2.21	1.35	1.39
2	D	401	ADP	C5-N7	-2.20	1.35	1.39
2	E	401	ADP	C5-C6	2.09	1.46	1.41
2	F	401	ADP	C5-N7	-2.04	1.35	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	ADP	C5-C4-N3	-6.82	117.33	126.72
2	I	401	ADP	C5-C4-N3	-6.79	117.37	126.72
2	A	401	ADP	C5-C4-N3	-6.71	117.48	126.72
2	A	401	ADP	O4'-C1'-N9	6.04	119.69	108.09
2	I	401	ADP	O4'-C1'-N9	6.02	119.64	108.09
2	G	401	ADP	O4'-C1'-N9	6.01	119.64	108.09
2	B	401	ADP	C5-C4-N3	-5.88	118.62	126.72
2	C	401	ADP	C5-C4-N3	-5.85	118.66	126.72
2	H	401	ADP	C5-C4-N3	-5.83	118.69	126.72
2	E	401	ADP	C5-C4-N3	-5.80	118.72	126.72
2	D	401	ADP	C5-C4-N3	-5.78	118.76	126.72
2	J	401	ADP	C5-C4-N3	-5.78	118.76	126.72
2	F	401	ADP	C5-C4-N3	-5.52	119.12	126.72
2	A	401	ADP	N3-C4-N9	5.29	136.17	127.17
2	I	401	ADP	N3-C4-N9	5.21	136.03	127.17
2	G	401	ADP	N3-C4-N9	5.20	136.01	127.17
2	F	401	ADP	N3-C2-N1	-5.03	120.97	128.58
2	D	401	ADP	N3-C4-N9	4.74	135.23	127.17
2	E	401	ADP	N3-C4-N9	4.68	135.12	127.17
2	H	401	ADP	N3-C4-N9	4.61	135.01	127.17
2	B	401	ADP	N3-C4-N9	4.61	135.01	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	ADP	N3-C4-N9	4.60	134.98	127.17
2	C	401	ADP	N3-C4-N9	4.59	134.98	127.17
2	F	401	ADP	C2-N3-C4	4.58	123.03	111.83
2	F	401	ADP	N3-C4-N9	4.40	134.64	127.17
2	E	401	ADP	N3-C2-N1	-4.17	122.27	128.58
2	J	401	ADP	N3-C2-N1	-4.12	122.35	128.58
2	E	401	ADP	C2-N3-C4	4.06	121.75	111.83
2	A	401	ADP	C2-N3-C4	4.04	121.71	111.83
2	G	401	ADP	C2-N3-C4	4.03	121.68	111.83
2	J	401	ADP	C2-N3-C4	4.03	121.67	111.83
2	I	401	ADP	C2-N3-C4	4.03	121.67	111.83
2	E	401	ADP	C4-C5-N7	-3.77	106.27	110.58
2	H	401	ADP	C2-N3-C4	3.71	120.90	111.83
2	I	401	ADP	C4-C5-N7	-3.71	106.34	110.58
2	B	401	ADP	C2-N3-C4	3.70	120.88	111.83
2	C	401	ADP	C2-N3-C4	3.70	120.87	111.83
2	D	401	ADP	C2-N3-C4	3.70	120.87	111.83
2	G	401	ADP	C4-C5-N7	-3.70	106.35	110.58
2	F	401	ADP	C4-C5-N7	-3.60	106.47	110.58
2	A	401	ADP	C4-C5-N7	-3.58	106.49	110.58
2	C	401	ADP	C4-C5-N7	-3.53	106.54	110.58
2	B	401	ADP	C4-C5-N7	-3.52	106.56	110.58
2	F	401	ADP	C4-N9-C8	3.47	109.39	105.74
2	H	401	ADP	C4-C5-N7	-3.47	106.62	110.58
2	D	401	ADP	C4-C5-N7	-3.46	106.63	110.58
2	E	401	ADP	O4'-C1'-C2'	-3.30	99.56	106.62
2	D	401	ADP	N3-C2-N1	-3.29	123.61	128.58
2	J	401	ADP	C4-C5-N7	-3.29	106.82	110.58
2	H	401	ADP	N3-C2-N1	-3.24	123.68	128.58
2	C	401	ADP	N3-C2-N1	-3.23	123.69	128.58
2	B	401	ADP	N3-C2-N1	-3.18	123.77	128.58
2	F	401	ADP	C6-C5-N7	3.06	137.99	132.09
2	J	401	ADP	C4-N9-C8	3.05	108.94	105.74
2	A	401	ADP	N3-C2-N1	-3.04	123.97	128.58
2	G	401	ADP	N3-C2-N1	-3.03	123.99	128.58
2	E	401	ADP	C4-N9-C8	3.03	108.92	105.74
2	I	401	ADP	N3-C2-N1	-3.02	124.00	128.58
2	E	401	ADP	C5-N7-C8	2.97	108.11	103.45
2	F	401	ADP	C5-N7-C8	2.95	108.09	103.45
2	F	401	ADP	N9-C8-N7	-2.91	109.81	113.94
2	I	401	ADP	C5-N7-C8	2.89	108.00	103.45
2	A	401	ADP	C5-N7-C8	2.88	107.97	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	ADP	C4-N9-C8	2.87	108.75	105.74
2	G	401	ADP	C5-N7-C8	2.86	107.95	103.45
2	E	401	ADP	C2-N1-C6	2.73	123.22	118.73
2	J	401	ADP	C5-N7-C8	2.66	107.64	103.45
2	H	401	ADP	C4-N9-C8	2.61	108.47	105.74
2	B	401	ADP	C5-N7-C8	2.59	107.51	103.45
2	C	401	ADP	C5-N7-C8	2.57	107.50	103.45
2	B	401	ADP	C4-N9-C8	2.57	108.44	105.74
2	C	401	ADP	C4-N9-C8	2.57	108.44	105.74
2	H	401	ADP	C5-N7-C8	2.56	107.48	103.45
2	D	401	ADP	C5-N7-C8	2.55	107.47	103.45
2	F	401	ADP	C2-N1-C6	2.55	122.91	118.73
2	J	401	ADP	N9-C8-N7	-2.53	110.34	113.94
2	D	401	ADP	C3'-C2'-C1'	2.46	106.12	101.46
2	J	401	ADP	C6-C5-N7	2.39	136.70	132.09
2	E	401	ADP	N9-C8-N7	-2.39	110.55	113.94
2	C	401	ADP	C3'-C2'-C1'	2.33	105.88	101.46
2	E	401	ADP	C6-C5-N7	2.32	136.55	132.09
2	H	401	ADP	C3'-C2'-C1'	2.26	105.73	101.46
2	B	401	ADP	C3'-C2'-C1'	2.23	105.67	101.46
2	J	401	ADP	O4'-C1'-N9	2.20	112.31	108.09
2	G	401	ADP	O3A-PB-O1B	-2.18	99.56	111.04
2	D	401	ADP	C6-C5-N7	2.13	136.20	132.09
2	C	401	ADP	C6-C5-N7	2.09	136.13	132.09
2	H	401	ADP	C6-C5-N7	2.09	136.12	132.09
2	B	401	ADP	C6-C5-N7	2.09	136.12	132.09
2	J	401	ADP	C2-N1-C6	2.03	122.06	118.73
2	F	401	ADP	C4-N9-C1'	-2.00	121.94	126.63

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	ADP	C5'-O5'-PA-O1A
2	F	401	ADP	C5'-O5'-PA-O1A
2	F	401	ADP	C5'-O5'-PA-O3A
2	G	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	O4'-C4'-C5'-O5'
2	C	401	ADP	C3'-C4'-C5'-O5'
2	F	401	ADP	C3'-C4'-C5'-O5'
2	A	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	O4'-C4'-C5'-O5'

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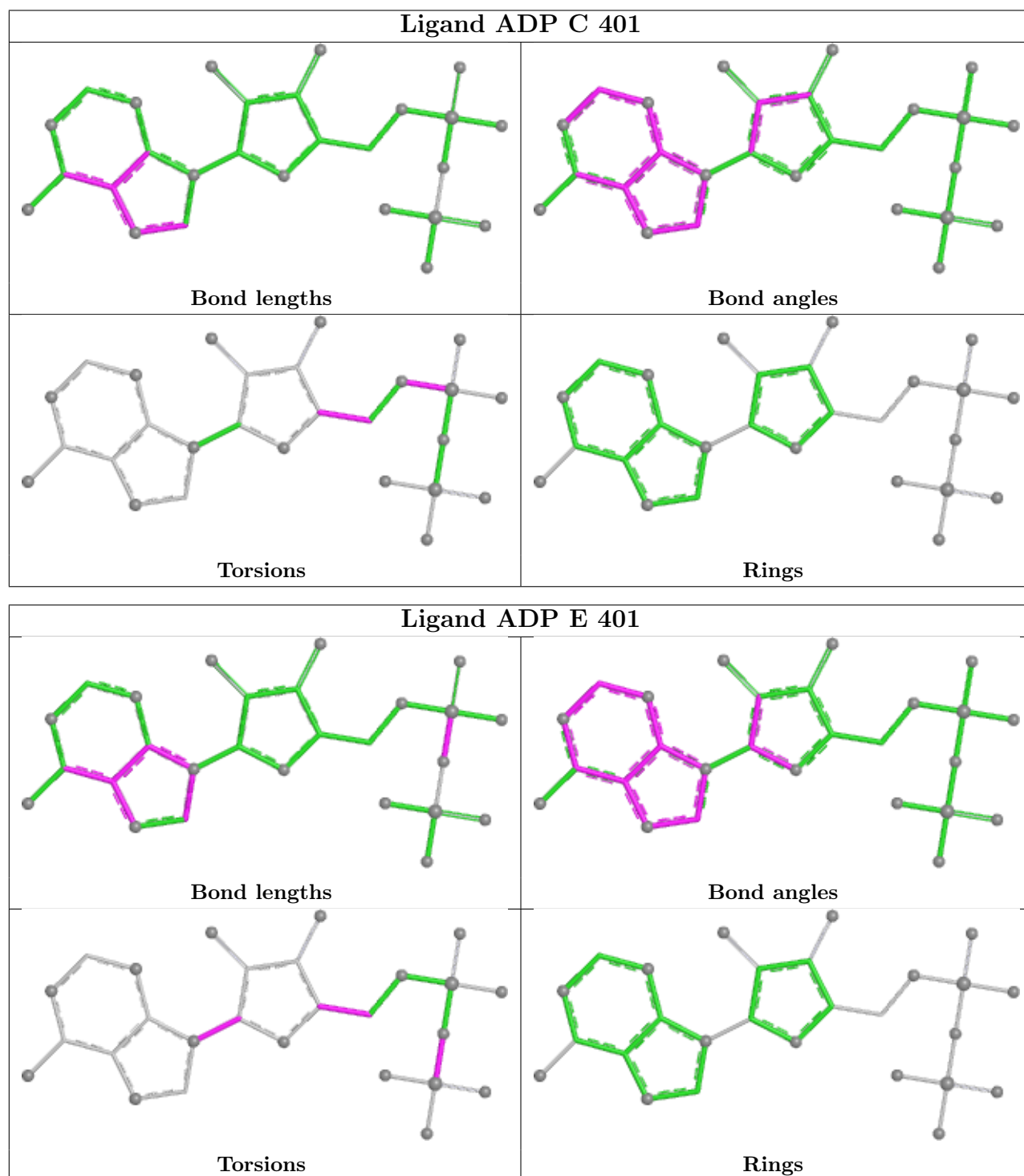
Mol	Chain	Res	Type	Atoms
2	F	401	ADP	O4'-C4'-C5'-O5'
2	G	401	ADP	O4'-C4'-C5'-O5'
2	I	401	ADP	O4'-C4'-C5'-O5'
2	J	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	C3'-C4'-C5'-O5'
2	J	401	ADP	C3'-C4'-C5'-O5'
2	A	401	ADP	C3'-C4'-C5'-O5'
2	G	401	ADP	C3'-C4'-C5'-O5'
2	I	401	ADP	C3'-C4'-C5'-O5'
2	F	401	ADP	C4'-C5'-O5'-PA
2	A	401	ADP	PA-O3A-PB-O1B
2	E	401	ADP	PA-O3A-PB-O1B
2	I	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	C2'-C1'-N9-C8
2	E	401	ADP	C2'-C1'-N9-C8
2	G	401	ADP	C2'-C1'-N9-C8
2	I	401	ADP	C2'-C1'-N9-C8
2	G	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	PA-O3A-PB-O2B
2	A	401	ADP	PA-O3A-PB-O3B
2	E	401	ADP	PA-O3A-PB-O2B
2	E	401	ADP	PA-O3A-PB-O3B
2	G	401	ADP	PA-O3A-PB-O3B
2	I	401	ADP	PA-O3A-PB-O2B
2	I	401	ADP	PA-O3A-PB-O3B
2	A	401	ADP	O4'-C1'-N9-C8
2	G	401	ADP	O4'-C1'-N9-C8
2	I	401	ADP	O4'-C1'-N9-C8
2	E	401	ADP	O4'-C4'-C5'-O5'
2	F	401	ADP	C2'-C1'-N9-C8
2	E	401	ADP	C2'-C1'-N9-C4
2	E	401	ADP	O4'-C1'-N9-C8
2	J	401	ADP	PB-O3A-PA-O2A

There are no ring outliers.

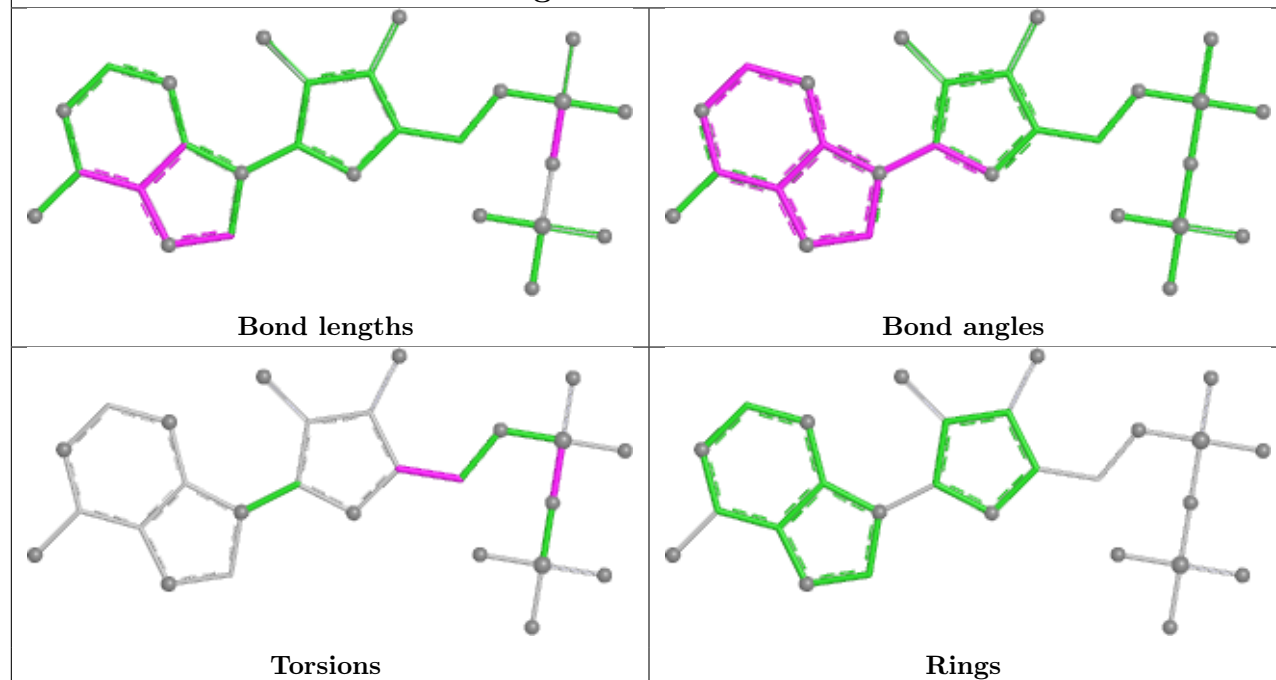
No monomer is involved in short contacts.

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

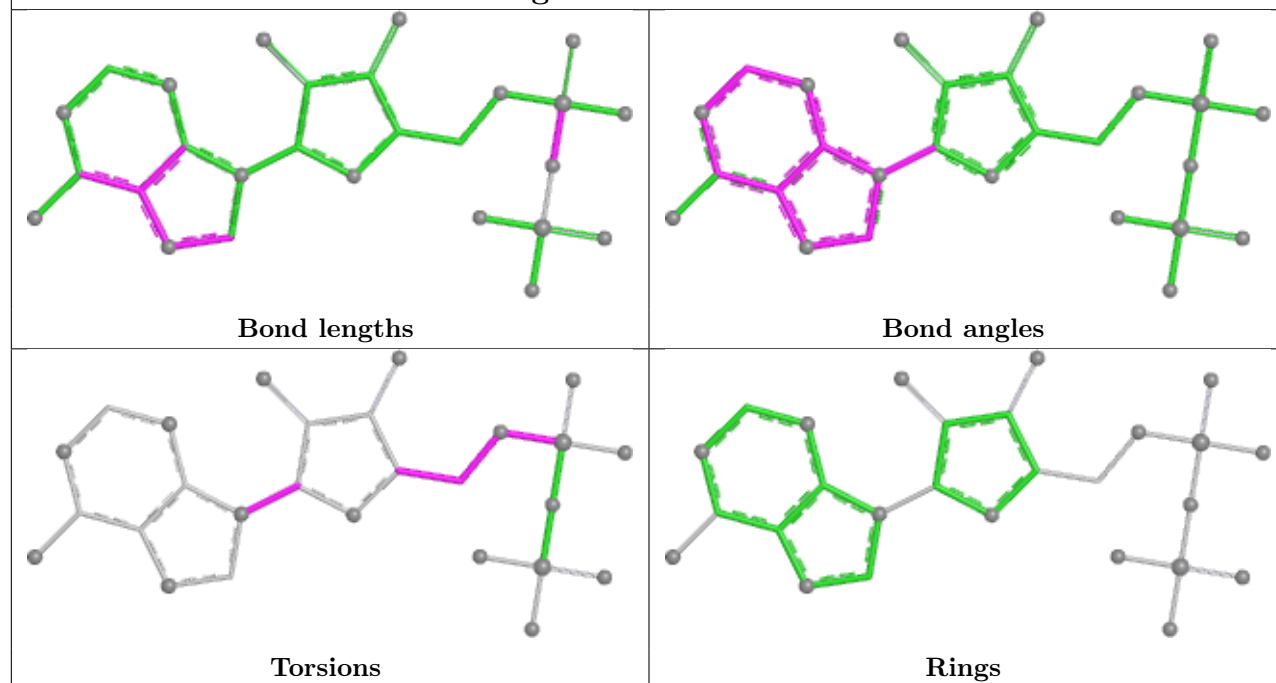
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

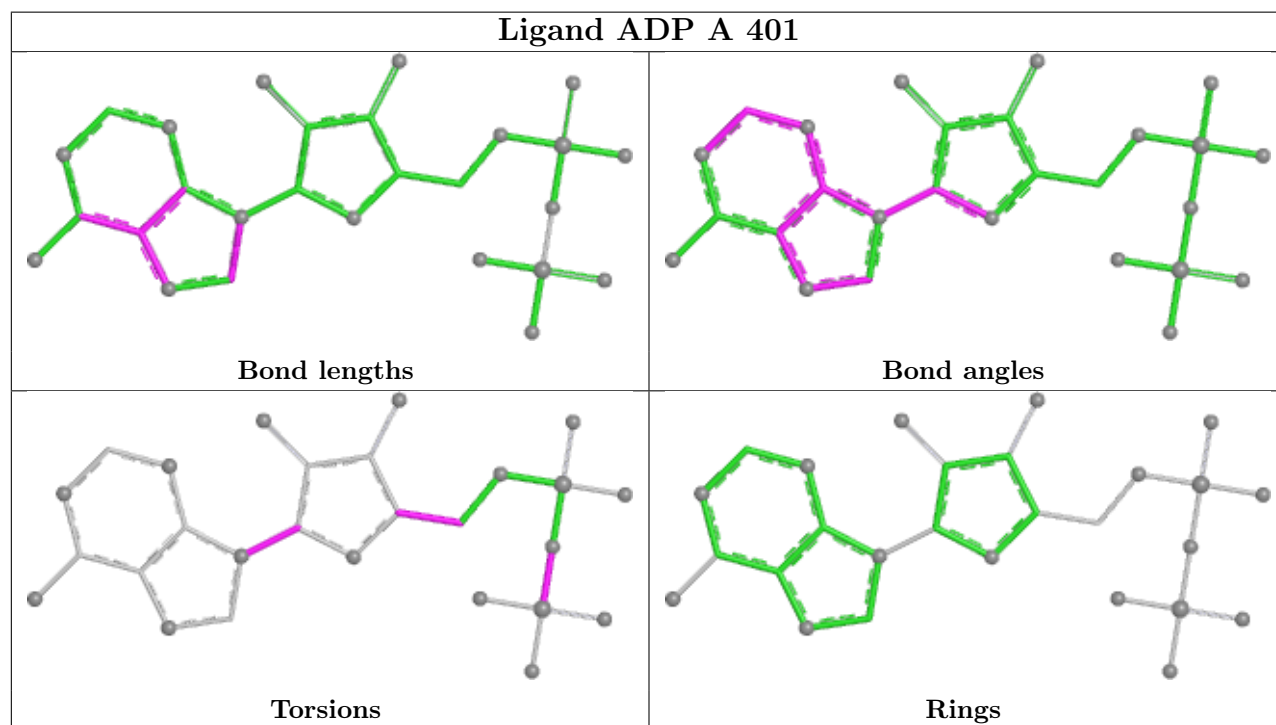
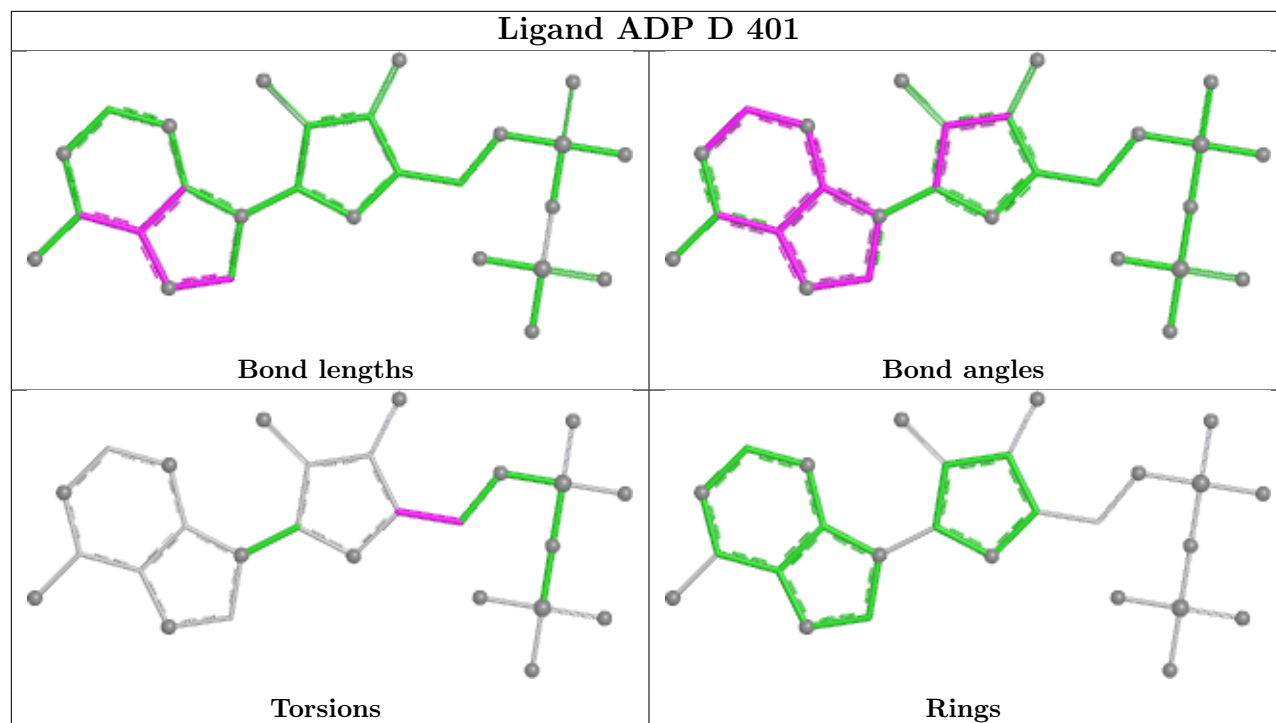


Ligand ADP J 401

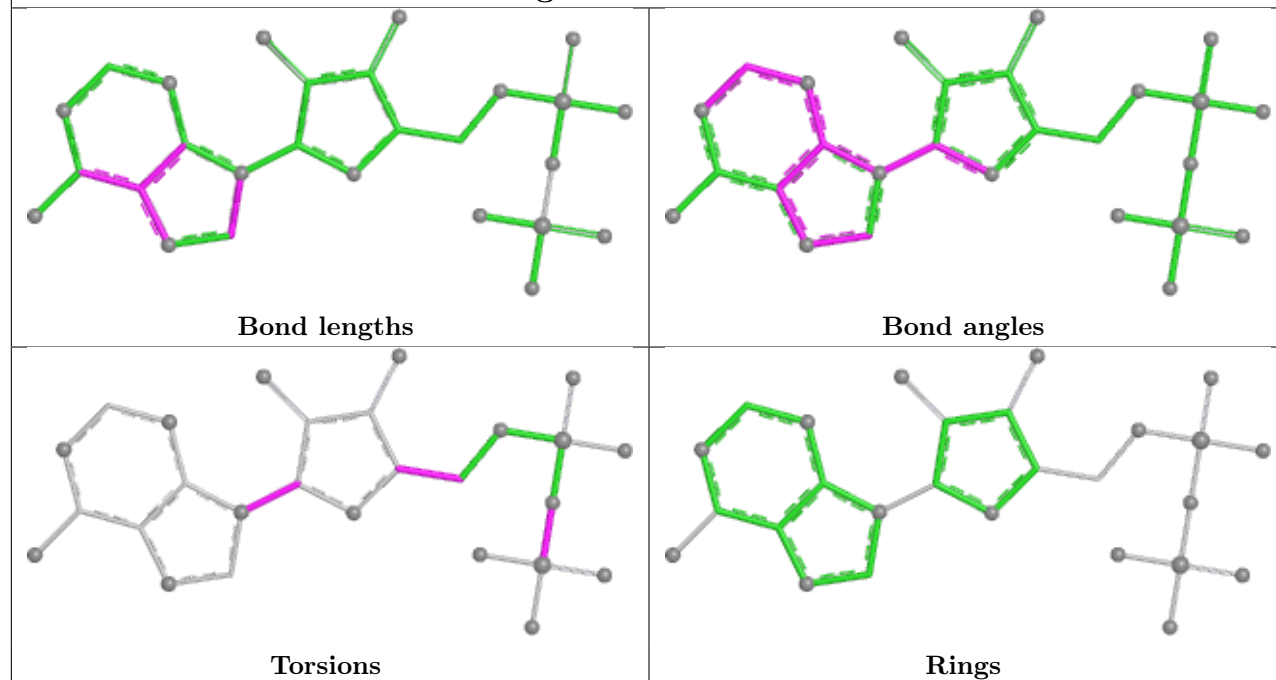


Ligand ADP F 401

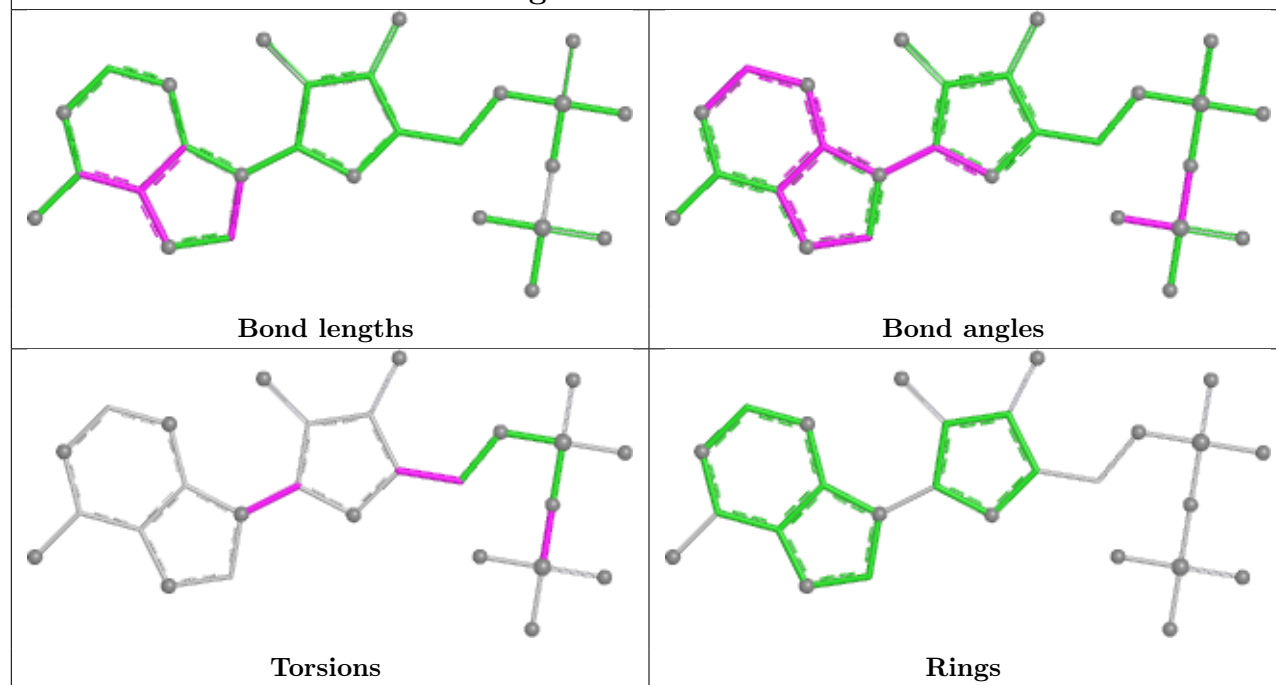


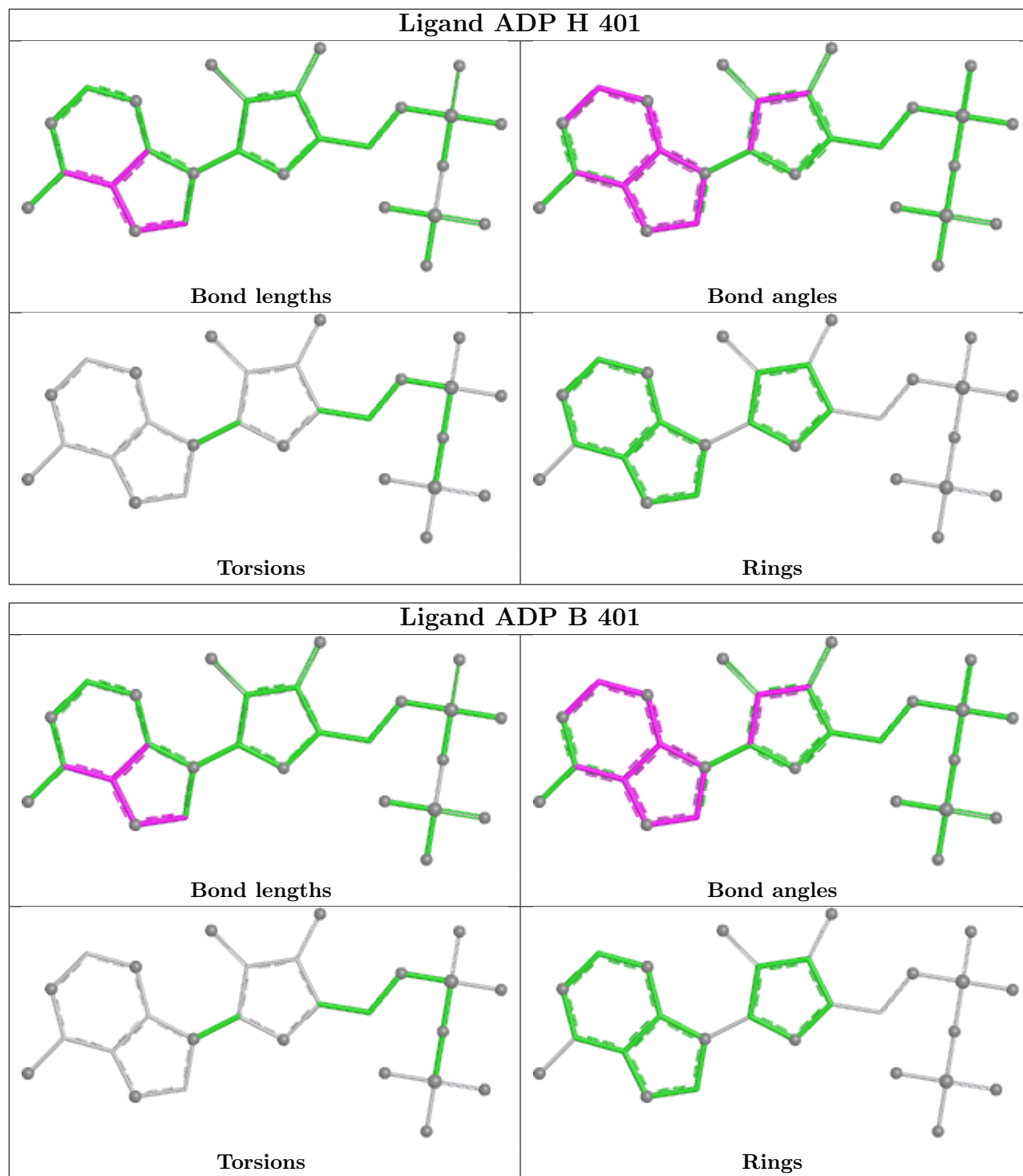


Ligand ADP I 401



Ligand ADP G 401





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	367/367 (100%)	0.50	49 (13%) 7 7	24, 46, 127, 170	0
1	B	366/367 (99%)	0.43	36 (9%) 13 14	23, 46, 110, 166	0
1	C	366/367 (99%)	0.28	33 (9%) 15 16	23, 39, 102, 150	0
1	D	364/367 (99%)	0.16	27 (7%) 20 22	23, 36, 96, 126	0
1	E	365/367 (99%)	0.35	34 (9%) 14 15	24, 42, 125, 183	0
1	F	367/367 (100%)	0.25	37 (10%) 12 13	24, 39, 101, 136	0
1	G	365/367 (99%)	0.30	34 (9%) 14 15	21, 37, 114, 155	0
1	H	366/367 (99%)	0.38	30 (8%) 17 19	22, 41, 116, 190	0
1	I	365/367 (99%)	0.48	37 (10%) 12 13	24, 47, 109, 163	0
1	J	367/367 (100%)	0.45	35 (9%) 14 15	26, 48, 118, 157	0
All	All	3658/3670 (99%)	0.36	352 (9%) 13 14	21, 42, 114, 190	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	8.7
1	G	318	PHE	8.1
1	E	306	LEU	6.3
1	G	315	ILE	6.0
1	H	367	LEU	5.9
1	F	315	ILE	5.8
1	B	315	ILE	5.6
1	B	312	THR	5.6
1	G	320	ALA	5.6
1	G	367	LEU	5.4
1	A	311	GLU	5.4
1	J	315	ILE	5.2
1	C	3	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	H	313	SER	5.2
1	E	322	VAL	5.2
1	G	305	ARG	5.0
1	A	253	TRP	4.9
1	F	322	VAL	4.9
1	H	322	VAL	4.9
1	D	303	ALA	4.8
1	C	306	LEU	4.8
1	G	306	LEU	4.8
1	B	306	LEU	4.7
1	D	305	ARG	4.7
1	H	310	HIS	4.7
1	A	306	LEU	4.7
1	H	312	THR	4.6
1	A	310	HIS	4.5
1	D	315	ILE	4.5
1	J	307	THR	4.5
1	C	322	VAL	4.5
1	G	312	THR	4.4
1	G	302	ASN	4.4
1	A	293	ALA	4.4
1	J	322	VAL	4.4
1	A	301	ASP	4.4
1	J	306	LEU	4.4
1	A	302	ASN	4.3
1	H	306	LEU	4.3
1	J	302	ASN	4.3
1	B	310	HIS	4.3
1	I	310	HIS	4.3
1	B	308	GLY	4.3
1	E	323	ALA	4.2
1	J	303	ALA	4.2
1	H	305	ARG	4.2
1	A	305	ARG	4.2
1	B	301	ASP	4.2
1	G	322	VAL	4.2
1	F	28	GLN	4.2
1	F	311	GLU	4.2
1	A	291	ILE	4.2
1	E	303	ALA	4.2
1	A	312	THR	4.1
1	A	315	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	302	ASN	4.1
1	D	306	LEU	4.1
1	C	307	THR	4.1
1	I	311	GLU	4.1
1	I	322	VAL	4.1
1	A	322	VAL	4.0
1	F	3	ALA	4.0
1	H	253	TRP	4.0
1	F	306	LEU	3.9
1	I	315	ILE	3.9
1	A	326	GLY	3.9
1	G	323	ALA	3.9
1	D	311	GLU	3.9
1	A	318	PHE	3.9
1	F	305	ARG	3.9
1	J	253	TRP	3.8
1	F	299	GLY	3.8
1	J	321	GLY	3.8
1	F	301	ASP	3.7
1	A	299	GLY	3.7
1	E	310	HIS	3.7
1	E	253	TRP	3.7
1	A	309	LYS	3.7
1	C	312	THR	3.7
1	A	286	CYS	3.6
1	F	309	LYS	3.6
1	G	303	ALA	3.6
1	J	320	ALA	3.6
1	E	315	ILE	3.6
1	I	331	ILE	3.6
1	J	299	GLY	3.6
1	C	301	ASP	3.5
1	H	302	ASN	3.5
1	C	311	GLU	3.5
1	D	253	TRP	3.5
1	I	303	ALA	3.5
1	B	313	SER	3.5
1	F	313	SER	3.5
1	F	310	HIS	3.5
1	F	30	ASN	3.5
1	G	307	THR	3.4
1	C	303	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	299	GLY	3.4
1	C	310	HIS	3.4
1	A	307	THR	3.4
1	E	305	ARG	3.4
1	F	323	ALA	3.4
1	E	318	PHE	3.4
1	A	313	SER	3.3
1	E	313	SER	3.3
1	D	323	ALA	3.3
1	J	310	HIS	3.3
1	I	318	PHE	3.3
1	F	285	LYS	3.3
1	H	307	THR	3.3
1	J	312	THR	3.3
1	C	326	GLY	3.3
1	H	318	PHE	3.3
1	E	309	LYS	3.3
1	I	309	LYS	3.3
1	F	307	THR	3.2
1	D	255	GLY	3.2
1	A	325	ARG	3.2
1	C	302	ASN	3.2
1	E	291	ILE	3.2
1	H	315	ILE	3.2
1	C	82	ASP	3.2
1	J	301	ASP	3.2
1	D	310	HIS	3.2
1	F	321	GLY	3.2
1	B	303	ALA	3.2
1	F	293	ALA	3.2
1	H	3	ALA	3.2
1	H	303	ALA	3.1
1	A	295	ASP	3.1
1	C	313	SER	3.1
1	C	325	ARG	3.1
1	D	322	VAL	3.1
1	H	368	ASP	3.1
1	I	281	ALA	3.1
1	D	307	THR	3.1
1	C	304	ARG	3.1
1	H	311	GLU	3.1
1	F	253	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	313	SER	3.1
1	I	307	THR	3.1
1	G	311	GLU	3.1
1	B	293	ALA	3.1
1	F	303	ALA	3.1
1	F	312	THR	3.0
1	G	310	HIS	3.0
1	J	305	ARG	3.0
1	A	369	GLU	3.0
1	F	317	ASP	3.0
1	B	322	VAL	3.0
1	B	302	ASN	3.0
1	C	253	TRP	3.0
1	G	301	ASP	3.0
1	F	21	ARG	3.0
1	I	23	LEU	3.0
1	D	302	ASN	3.0
1	G	299	GLY	3.0
1	F	298	GLN	2.9
1	G	314	SER	2.9
1	H	323	ALA	2.9
1	I	365	ILE	2.9
1	J	291	ILE	2.9
1	E	312	THR	2.9
1	H	301	ASP	2.9
1	A	294	TYR	2.9
1	A	303	ALA	2.9
1	C	315	ILE	2.9
1	I	314	SER	2.9
1	A	285	LYS	2.9
1	J	309	LYS	2.9
1	F	300	GLN	2.9
1	I	305	ARG	2.9
1	E	287	HIS	2.9
1	F	325	ARG	2.8
1	D	291	ILE	2.8
1	B	254	ASN	2.8
1	F	252	ASP	2.8
1	J	254	ASN	2.8
1	E	307	THR	2.8
1	G	291	ILE	2.8
1	I	273	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	304	ARG	2.8
1	I	320	ALA	2.8
1	F	23	LEU	2.8
1	I	325	ARG	2.7
1	E	301	ASP	2.7
1	H	326	GLY	2.7
1	B	318	PHE	2.7
1	G	309	LYS	2.7
1	D	367	LEU	2.7
1	B	325	ARG	2.7
1	D	313	SER	2.7
1	J	255	GLY	2.7
1	A	320	ALA	2.7
1	C	323	ALA	2.7
1	I	323	ALA	2.7
1	B	309	LYS	2.7
1	J	326	GLY	2.7
1	G	3	ALA	2.7
1	G	293	ALA	2.7
1	G	253	TRP	2.7
1	E	288	GLU	2.6
1	E	337	ASP	2.6
1	B	305	ARG	2.6
1	J	311	GLU	2.6
1	F	204	MET	2.6
1	B	323	ALA	2.6
1	E	320	ALA	2.6
1	I	312	THR	2.6
1	A	292	ARG	2.6
1	I	291	ILE	2.6
1	C	308	GLY	2.6
1	G	316	ASN	2.6
1	B	307	THR	2.6
1	J	313	SER	2.6
1	A	255	GLY	2.6
1	C	327	CYS	2.6
1	D	321	GLY	2.6
1	F	308	GLY	2.6
1	I	286	CYS	2.6
1	B	278	LYS	2.6
1	A	323	ALA	2.6
1	I	252	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	311	GLU	2.5
1	A	321	GLY	2.5
1	H	254	ASN	2.5
1	I	294	TYR	2.5
1	A	304	ARG	2.5
1	D	301	ASP	2.5
1	F	79	SER	2.5
1	I	313	SER	2.5
1	I	306	LEU	2.5
1	E	293	ALA	2.5
1	J	278	LYS	2.5
1	I	255	GLY	2.5
1	A	288	GLU	2.4
1	J	293	ALA	2.4
1	A	289	ARG	2.4
1	H	289	ARG	2.4
1	C	299	GLY	2.4
1	C	273	ILE	2.4
1	J	77	GLU	2.4
1	E	325	ARG	2.4
1	G	289	ARG	2.4
1	A	308	GLY	2.4
1	E	110	PHE	2.4
1	G	82	ASP	2.4
1	B	335	VAL	2.4
1	B	314	SER	2.4
1	E	286	CYS	2.4
1	I	342	TYR	2.4
1	H	29	GLU	2.4
1	A	316	ASN	2.4
1	I	302	ASN	2.4
1	G	295	ASP	2.4
1	B	297	LYS	2.4
1	E	292	ARG	2.4
1	G	284	SER	2.4
1	B	29	GLU	2.3
1	E	3	ALA	2.3
1	J	308	GLY	2.3
1	D	325	ARG	2.3
1	H	292	ARG	2.3
1	J	325	ARG	2.3
1	E	29	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	321	GLY	2.3
1	I	271	GLY	2.3
1	J	289	ARG	2.3
1	C	297	LYS	2.3
1	J	318	PHE	2.3
1	F	302	ASN	2.3
1	C	266	ALA	2.3
1	G	255	GLY	2.3
1	G	308	GLY	2.3
1	C	285	LYS	2.3
1	A	290	HIS	2.3
1	B	311	GLU	2.3
1	B	296	PRO	2.3
1	B	299	GLY	2.3
1	D	309	LYS	2.3
1	I	278	LYS	2.3
1	I	285	LYS	2.3
1	E	294	TYR	2.3
1	B	269	GLU	2.2
1	F	369	GLU	2.2
1	C	314	SER	2.2
1	B	337	ASP	2.2
1	G	317	ASP	2.2
1	D	299	GLY	2.2
1	A	29	GLU	2.2
1	H	291	ILE	2.2
1	B	368	ASP	2.2
1	J	252	ASP	2.2
1	C	255	GLY	2.2
1	D	29	GLU	2.2
1	F	29	GLU	2.2
1	C	23	LEU	2.2
1	H	309	LYS	2.2
1	F	316	ASN	2.2
1	I	254	ASN	2.2
1	A	252	ASP	2.2
1	C	295	ASP	2.2
1	J	329	ILE	2.2
1	C	78	GLY	2.2
1	B	320	ALA	2.2
1	H	290	HIS	2.2
1	H	298	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	286	CYS	2.2
1	F	367	LEU	2.2
1	D	297	LYS	2.2
1	J	316	ASN	2.2
1	B	253	TRP	2.2
1	I	368	ASP	2.2
1	J	335	VAL	2.1
1	A	271	GLY	2.1
1	G	326	GLY	2.1
1	C	293	ALA	2.1
1	B	286	CYS	2.1
1	A	79	SER	2.1
1	A	314	SER	2.1
1	A	319	SER	2.1
1	G	297	LYS	2.1
1	H	294	TYR	2.1
1	I	316	ASN	2.1
1	A	317	ASP	2.1
1	I	253	TRP	2.1
1	B	291	ILE	2.1
1	J	56	ILE	2.1
1	A	284	SER	2.1
1	D	314	SER	2.1
1	B	369	GLU	2.1
1	D	308	GLY	2.1
1	D	318	PHE	2.1
1	C	309	LYS	2.1
1	I	132	ALA	2.1
1	J	76	ALA	2.1
1	J	314	SER	2.1
1	C	296	PRO	2.1
1	A	78	GLY	2.1
1	E	78	GLY	2.1
1	E	255	GLY	2.1
1	A	56	ILE	2.1
1	E	254	ASN	2.0
1	E	316	ASN	2.0
1	D	274	ARG	2.0
1	B	61	LYS	2.0
1	A	281	ALA	2.0
1	I	293	ALA	2.0
1	D	28	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	368	ASP	2.0
1	E	295	ASP	2.0
1	B	255	GLY	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](#)

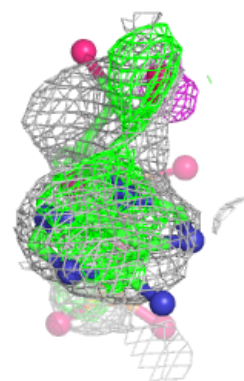
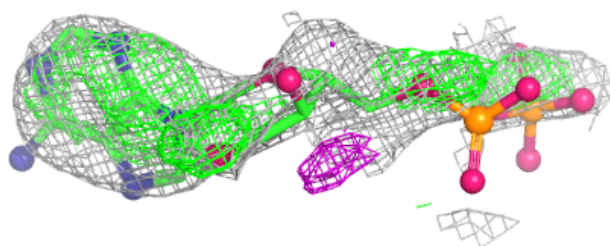
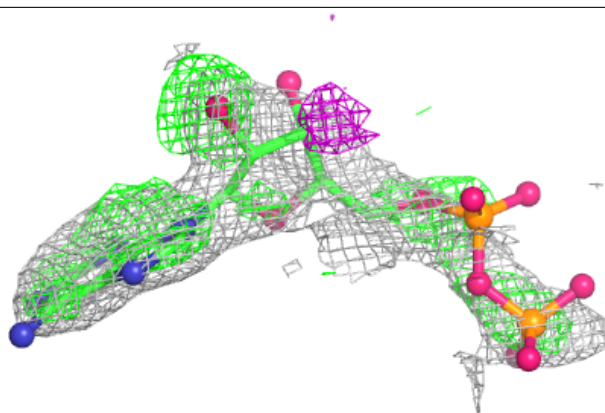
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	401	27/27	-	-	45,56,69,80	27
2	ADP	B	401	27/27	-	-	29,43,60,82	27
2	ADP	C	401	27/27	-	-	60,71,79,92	27
2	ADP	D	401	27/27	-	-	53,65,68,77	27
2	ADP	E	401	27/27	-	-	56,77,88,100	27
2	ADP	J	401	27/27	0.75	0.16	79,105,135,138	0
2	ADP	G	401	27/27	-	-	45,56,69,80	27
2	ADP	H	401	27/27	-	-	44,68,80,86	27
2	ADP	I	401	27/27	-	-	45,56,69,80	27
2	ADP	F	401	27/27	0.81	0.14	52,87,132,133	0

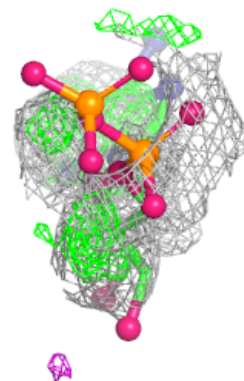
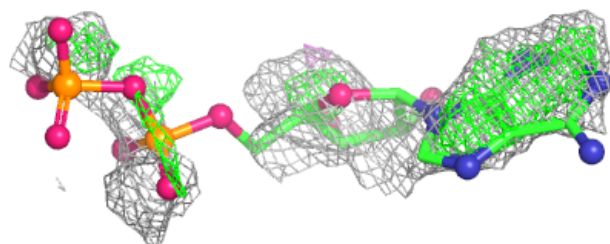
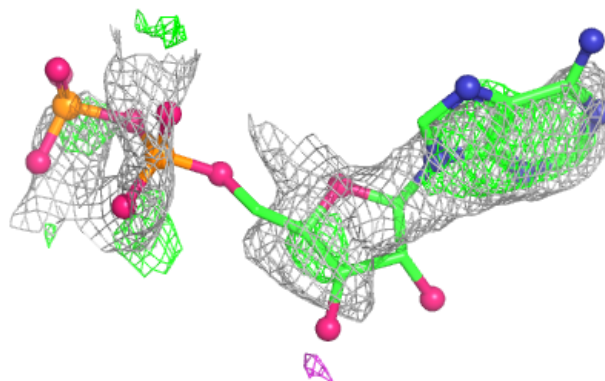
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 401:

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

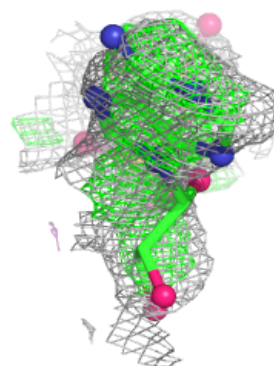
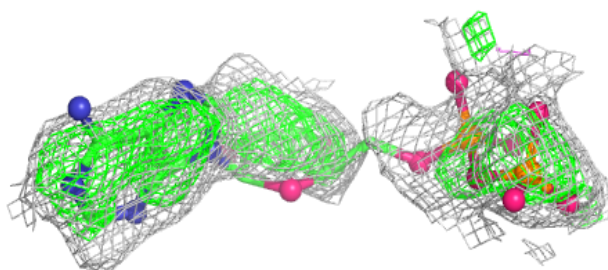
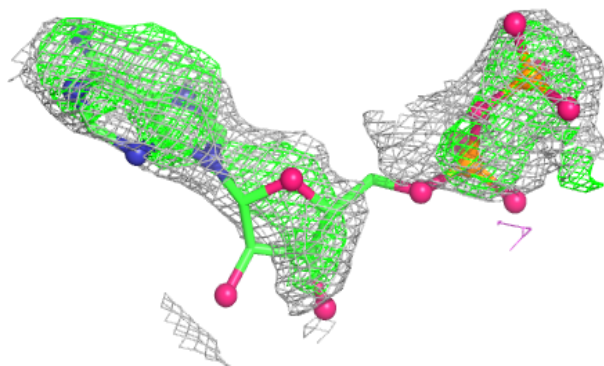
**Electron density around ADP B 401:**

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

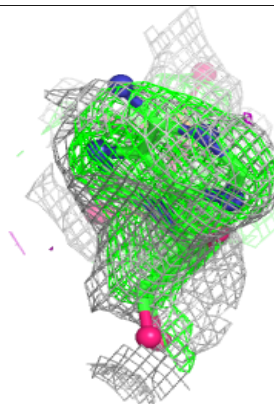
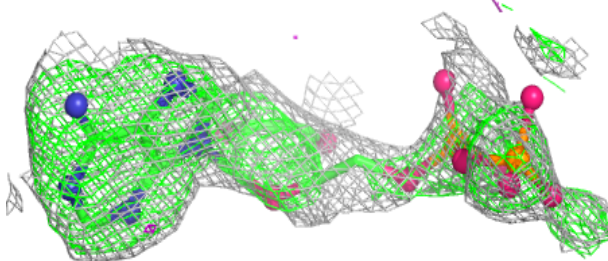
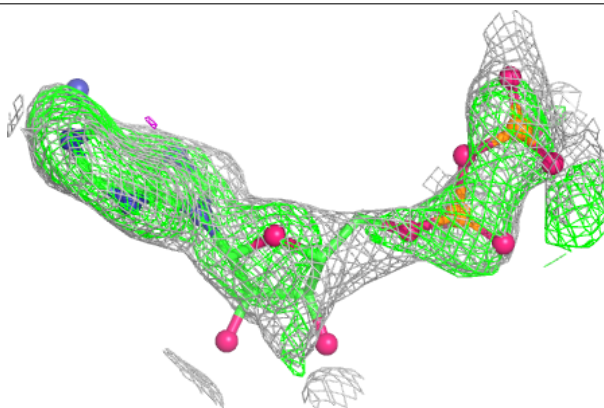


Electron density around ADP C 401:

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

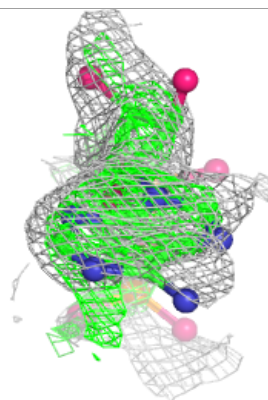
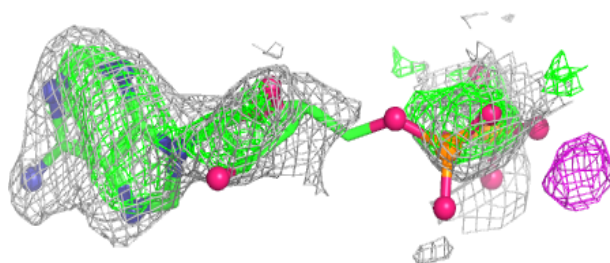
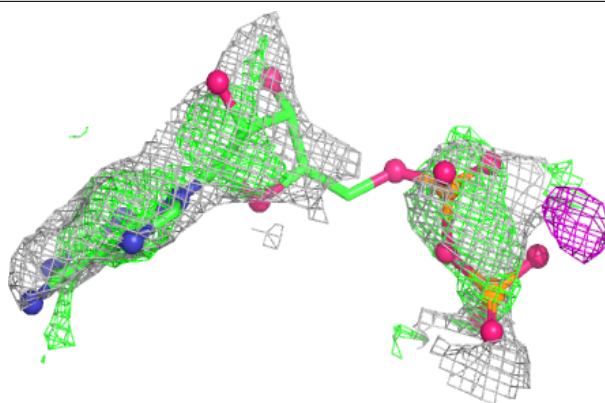
**Electron density around ADP D 401:**

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

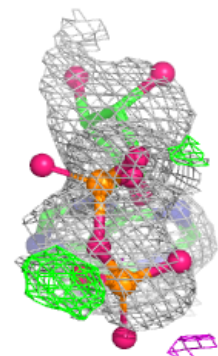
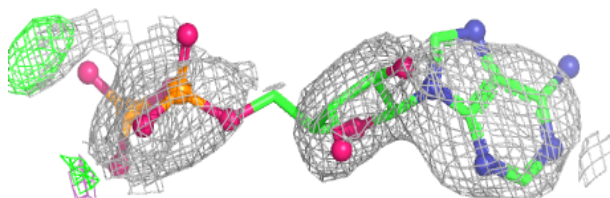
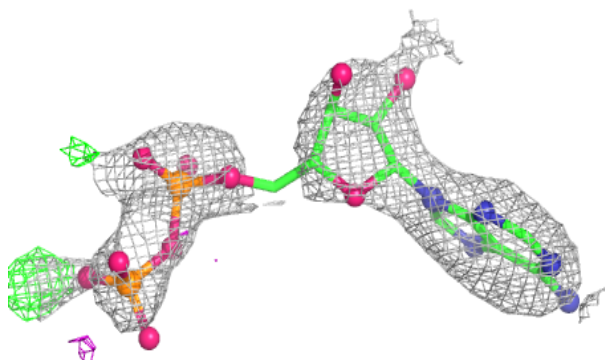


Electron density around ADP E 401:

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

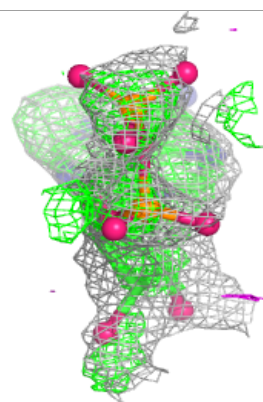
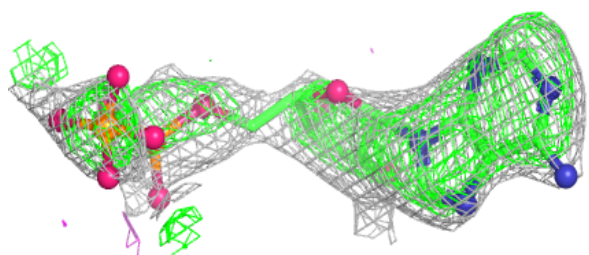
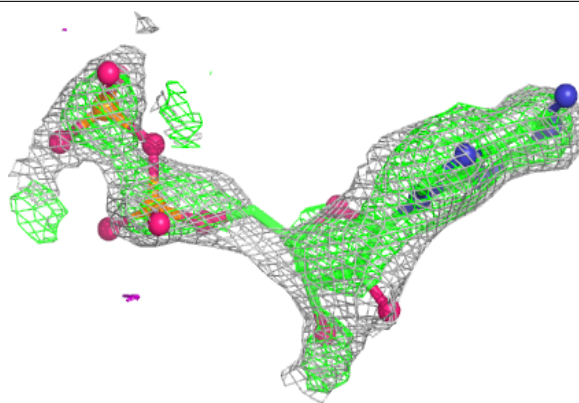
**Electron density around ADP J 401:**

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

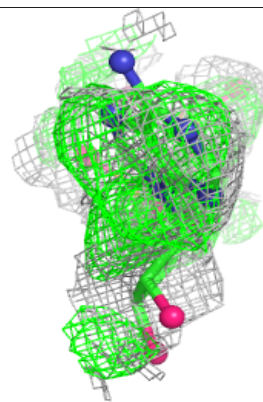
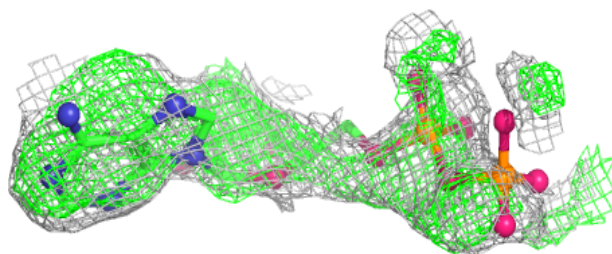
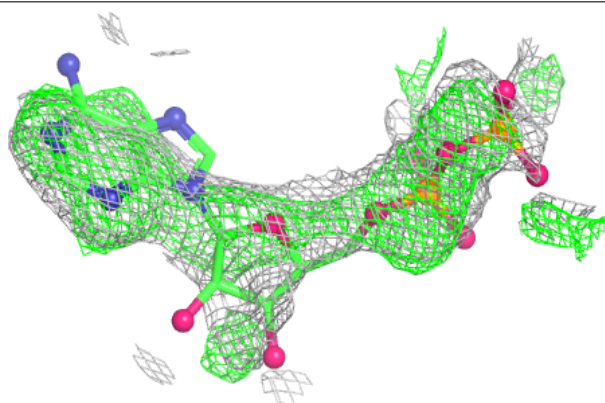


Electron density around ADP G 401:

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

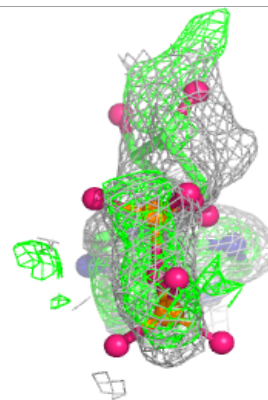
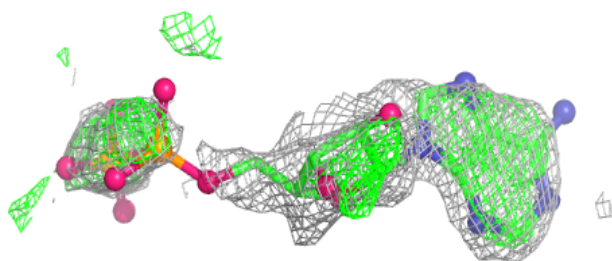
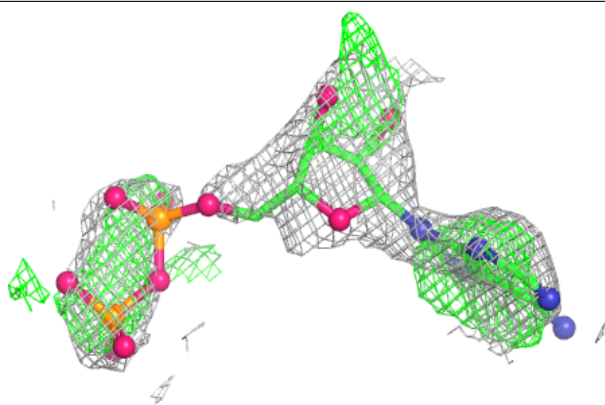
**Electron density around ADP H 401:**

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

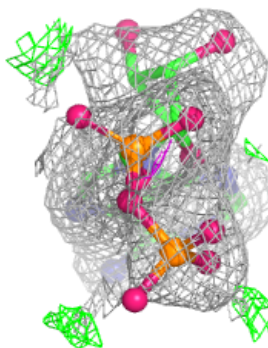
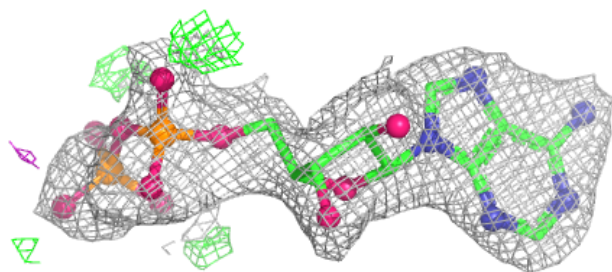
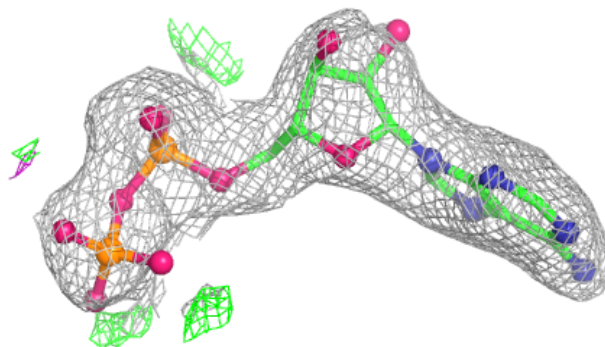


Electron density around ADP I 401:

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

**Electron density around ADP F 401:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.