



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 12:35 PM JST

PDB ID : 7CPR
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

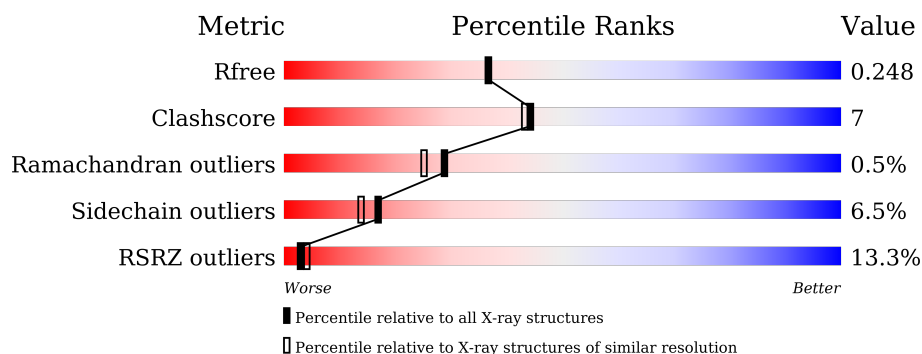
1 Overall quality at a glance

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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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	<div> <div>15%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	367	<div> <div>13%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	C	367	<div> <div>11%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	D	367	<div> <div>10%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	E	367	<div> <div>12%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	F	367	<div> <div>11%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	367	<div><div></div><div>12%</div><div>82%</div><div>15%</div><div>..</div></div>
1	H	367	<div><div></div><div>11%</div><div>83%</div><div>15%</div><div>.</div></div>
1	I	367	<div><div></div><div>19%</div><div>80%</div><div>16%</div><div>..</div></div>
1	J	367	<div><div></div><div>16%</div><div>86%</div><div>13%</div><div>.</div></div>

2 Entry composition

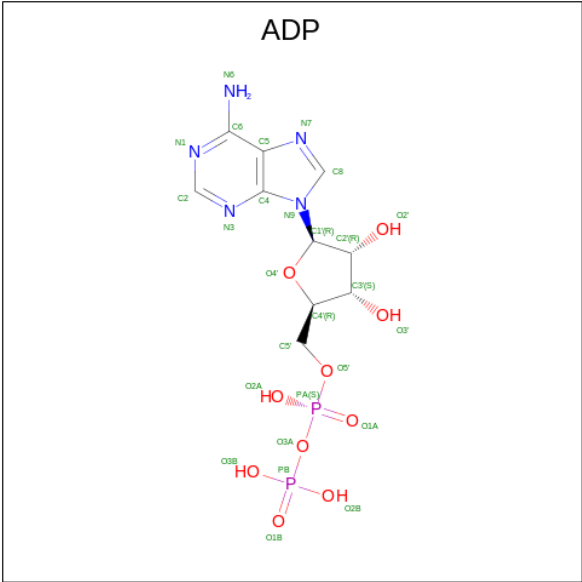
There are 3 unique types of molecules in this entry. The entry contains 29573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (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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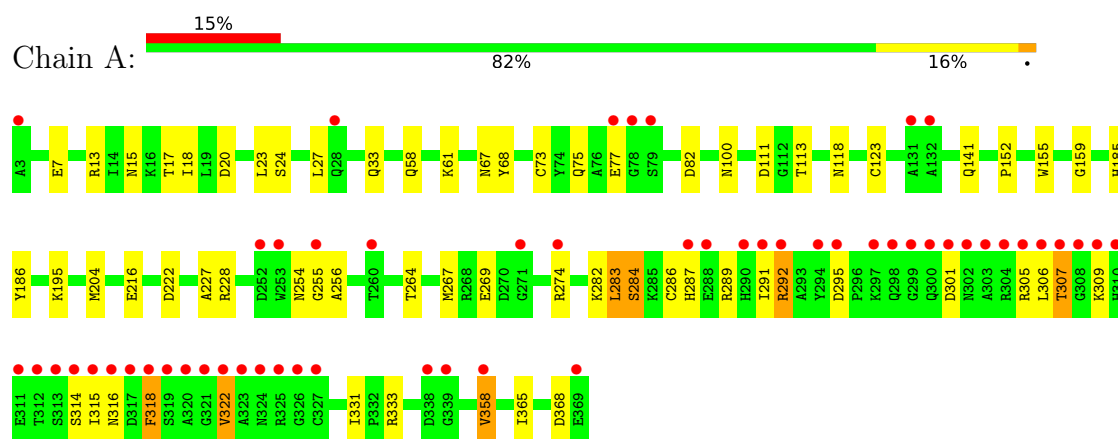
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	34	Total 34	O 34	0	0
3	D	39	Total 39	O 39	0	0
3	E	62	Total 62	O 62	0	0
3	F	56	Total 56	O 56	0	0
3	G	39	Total 39	O 39	0	0
3	H	45	Total 45	O 45	0	0
3	I	62	Total 62	O 62	0	0
3	J	68	Total 68	O 68	0	0

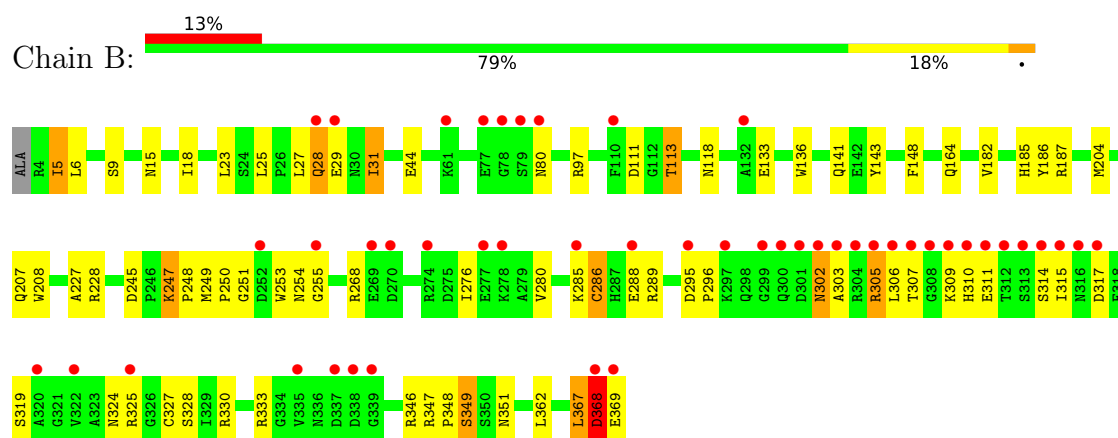
3 Residue-property plots [i](#)

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.

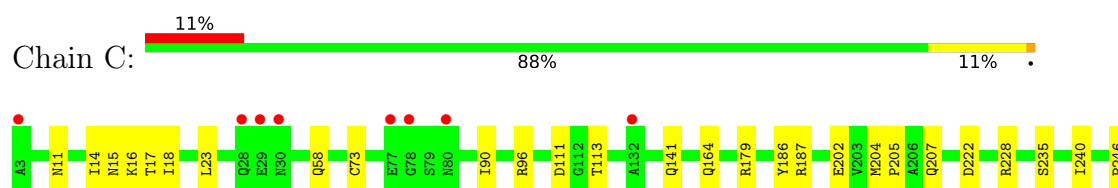
• Molecule 1: Glutamine synthetase 2 cytoplasmic

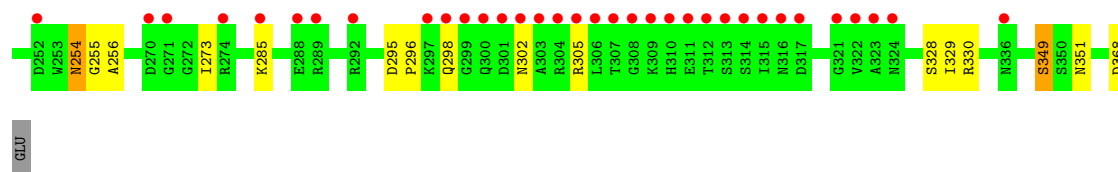


• Molecule 1: Glutamine synthetase 2 cytoplasmic

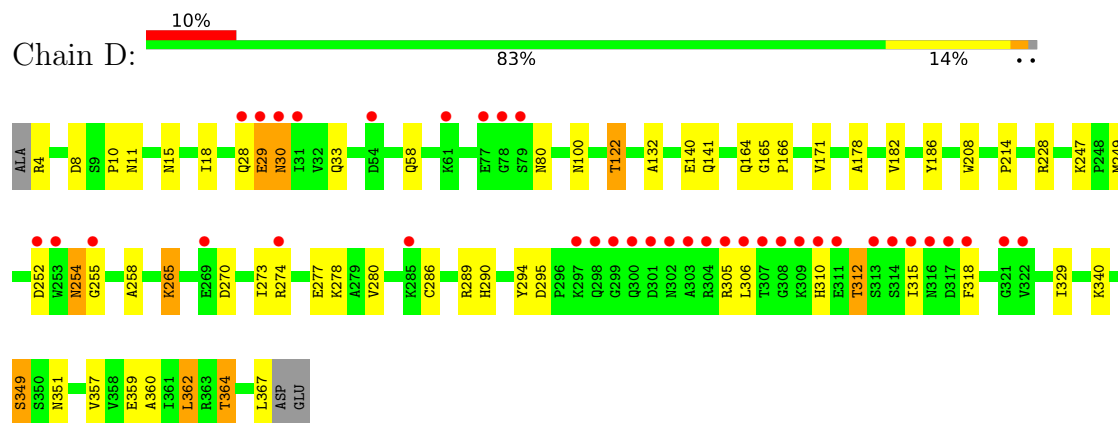


• Molecule 1: Glutamine synthetase 2 cytoplasmic

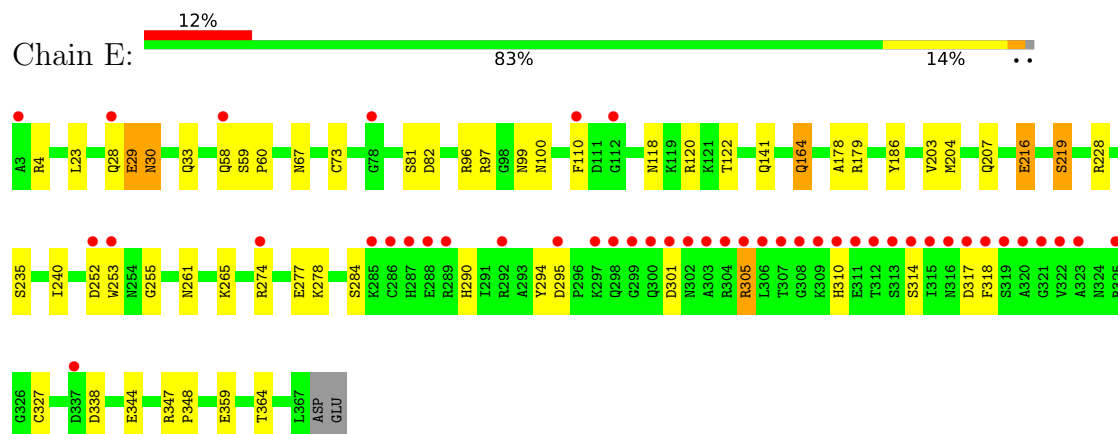




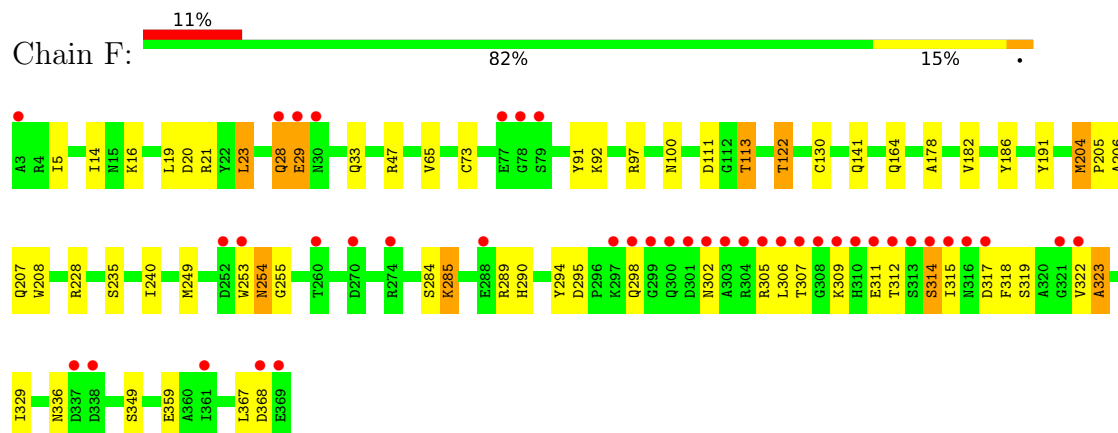
- Molecule 1: Glutamine synthetase 2 cytoplasmic



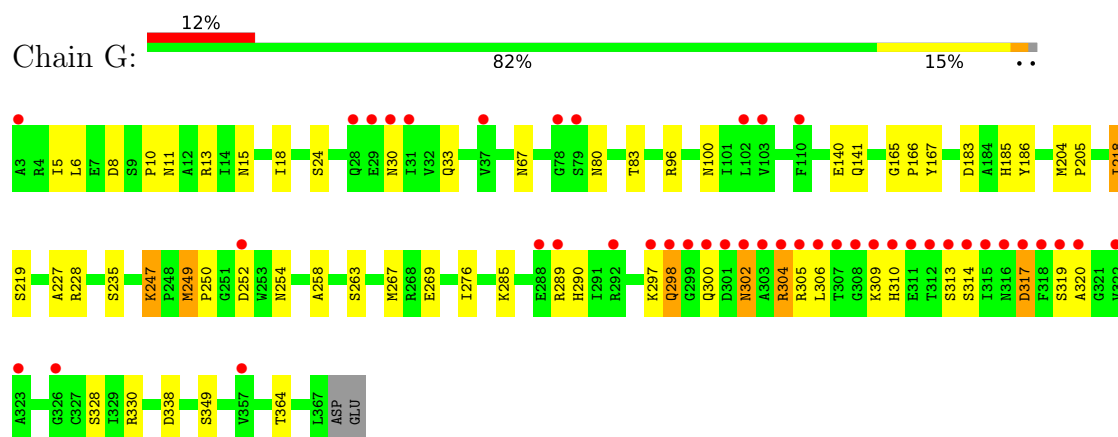
- Molecule 1: Glutamine synthetase 2 cytoplasmic



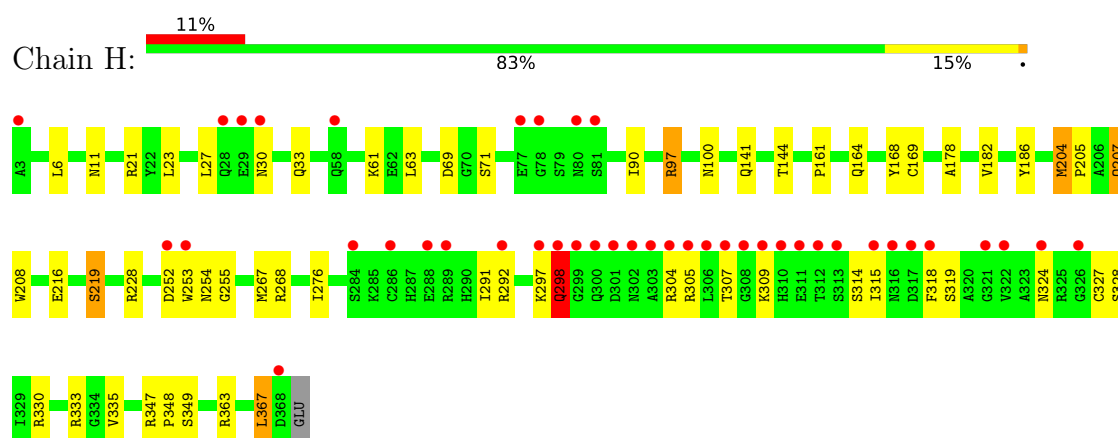
- Molecule 1: Glutamine synthetase 2 cytoplasmic



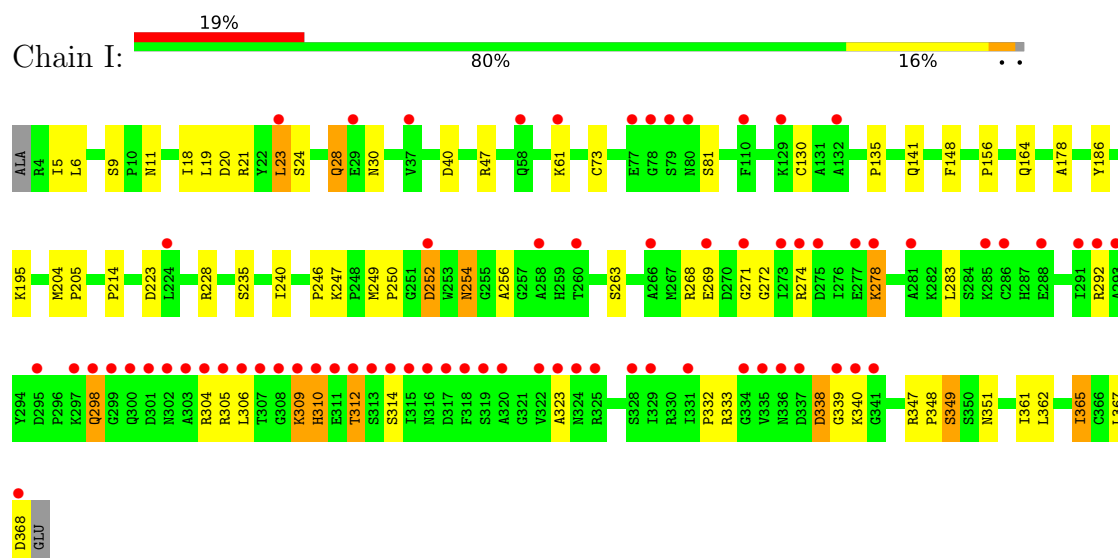
- Molecule 1: Glutamine synthetase 2 cytoplasmic



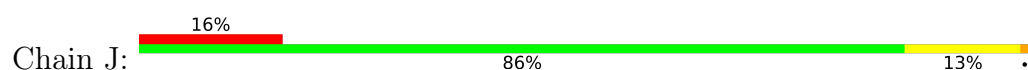
- Molecule 1: Glutamine synthetase 2 cytoplasmic

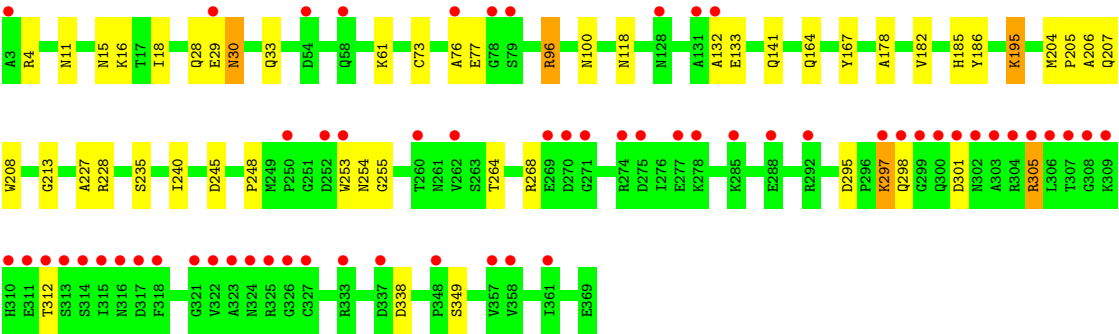


- Molecule 1: Glutamine synthetase 2 cytoplasmic



- 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 27.37 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.6 (178.68-2.12) 96.6 (27.37-2.12)	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 (4.94%)	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 , 37.6	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.76	1/2957 (0.0%)	0.89	4/4013 (0.1%)
1	B	0.75	0/2956	0.86	0/4011
1	C	0.82	1/2952 (0.0%)	0.86	5/4006 (0.1%)
1	D	0.87	0/2939	0.93	1/3988 (0.0%)
1	E	0.80	2/2944 (0.1%)	0.89	4/3995 (0.1%)
1	F	0.84	2/2961 (0.1%)	0.91	1/4018 (0.0%)
1	G	0.88	1/2944 (0.0%)	0.91	3/3995 (0.1%)
1	H	0.81	0/2948	0.91	4/4002 (0.1%)
1	I	0.75	0/2947	0.87	2/3999 (0.1%)
1	J	0.71	1/2955 (0.0%)	0.80	1/4011 (0.0%)
All	All	0.80	8/29503 (0.0%)	0.88	25/40038 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	CYS	CB-SG	-7.50	1.69	1.82
1	F	73	CYS	CB-SG	-6.97	1.70	1.82
1	J	73	CYS	CB-SG	-6.96	1.70	1.82
1	A	73	CYS	CB-SG	-6.31	1.71	1.82
1	G	235	SER	CB-OG	-5.61	1.34	1.42
1	E	73	CYS	CB-SG	-5.45	1.73	1.81
1	E	253	TRP	CB-CG	-5.45	1.40	1.50
1	F	91	TYR	CE1-CZ	-5.17	1.31	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	96	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	H	268	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	E	179	ARG	NE-CZ-NH1	6.27	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ASP	CB-CG-OD1	5.80	123.52	118.30
1	G	96	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	73	CYS	CB-CA-C	-5.56	99.29	110.40
1	H	97	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	C	96	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	G	204	MET	CA-CB-CG	5.47	122.60	113.30
1	F	47	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	96	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	I	47	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	73	CYS	CB-CA-C	-5.26	99.88	110.40
1	C	222	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	73	CYS	CB-CA-C	-5.19	100.02	110.40
1	H	304	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	G	218	ILE	CB-CA-C	-5.16	101.28	111.60
1	A	222	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	D	171	VAL	CB-CA-C	-5.09	101.74	111.40
1	E	96	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	H	268	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	179	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	204	MET	CG-SD-CE	5.04	108.26	100.20
1	I	223	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	179	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	48	0
1	B	2884	0	2763	56	0
1	C	2880	0	2762	23	0
1	D	2867	0	2753	37	0
1	E	2872	0	2758	41	0
1	F	2889	0	2768	48	0
1	G	2872	0	2758	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2876	0	2751	44	0
1	I	2875	0	2757	38	0
1	J	2883	0	2757	34	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	0	0
3	J	68	0	0	2	0
All	All	29573	0	27711	374	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 (374) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:204:MET:HE1	1:F:253:TRP:CZ3	2.32	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: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:J:28:GLN:CD	1:J:30:ASN:HD21	2.03	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
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:H:204:MET:HE1	1:H:253:TRP:CZ3	2.38	0.59
1:H:21:ARG:HD2	1:I:20:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:TRP:O	1:B:305:ARG:NH2	2.37	0.58
1:G:263:SER:HA	1:G:267:MET:CE	2.34	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: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: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: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
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:G:263:SER:HA	1:G:267:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:272:GLY:HA3	1:I:339:GLY:O	2.08	0.53
1:G:267:MET:HE3	1:G:276:ILE:HG12	1.90	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:J:204:MET:HE1	1:J:253:TRP:HB3	1.92	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: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: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: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:B:31:ILE:C	1:B:31:ILE:HD12	2.32	0.50
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: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
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:A:216:GLU:H	1:A:216:GLU:CD	2.15	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:C:15:ASN:ND2	1:C:18:ILE:H	2.09	0.50
1:B:302:ASN:HD22	1:B:306:LEU:HD11	1.77	0.49
1:E:118:ASN:C	1:E:118:ASN:OD1	2.50	0.49
1:G:24:SER:HB2	1:H:97:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:204:MET:CE	1:J:253:TRP:HB3	2.42	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: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: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:F:204:MET:HE2	1:F:253:TRP:CZ3	2.47	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:J:297:LYS:O	1:J:298:GLN:NE2	2.47	0.48
1:G:249:MET:HE3	1:G:250:PRO:HD2	1.94	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:367:LEU:O	1:B:368:ASP:C	2.53	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:B:247:LYS:CD	1:B:305:ARG:NH1	2.78	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: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
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: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:A:118:ASN:C	1:A:118:ASN:OD1	2.55	0.45
1:B:302:ASN:ND2	1:B:306:LEU:HD11	2.31	0.45
1:F:204:MET:HE3	1:F:205:PRO:CD	2.46	0.45
1:H:164:GLN:HG2	1:H:204:MET:SD	2.56	0.45
1:I:204:MET:HE2	1:I:254:ASN:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:118:ASN:OD1	1:B:118:ASN:C	2.54	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:B:349:SER:OG	1:B:351:ASN:OD1	2.26	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:F:302:ASN:HA	1:F:349:SER:OG	2.17	0.44
1:E:295:ASP:OD1	1:E:301:ASP:HB2	2.18	0.43
1:J:264:THR:O	1:J:268:ARG:HG3	2.18	0.43
1:A:13:ARG:HB2	1:B:5:ILE:CD1	2.48	0.43
1:F:204:MET:HE1	1:F:253:TRP:HZ3	1.81	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:I:332:PRO:O	1:I:333:ARG:C	2.57	0.43
1:D:247:LYS:HZ3	1:D:305:ARG:NH1	2.16	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:168:TYR:O	1:H:169:CYS:C	2.56	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:G:317:ASP:HB3	1:G:328:SER:HG	1.84	0.43
1:I:195:LYS:HE2	1:I:214:PRO:O	2.19	0.43
1:A:284:SER:O	1:A:318:PHE:CD2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:141:GLN:NE2	1:E:228:ARG:HE	2.17	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
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: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: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:E:122:THR:HG22	1:E:359:GLU:CD	2.40	0.41
1:I:195:LYS:CE	1:I:214:PRO:O	2.68	0.41
1:J:295:ASP:OD2	1:J:301:ASP:HB2	2.20	0.41
1:B:302:ASN:C	1:B:306:LEU:CD1	2.89	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:B:295:ASP:N	1:B:295:ASP:OD1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:161:PRO:HG2	1:H:204:MET:HE3	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
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:H:318:PHE:CG	1:H:319:SER:N	2.89	0.41
1:J:118:ASN:C	1:J:118:ASN:OD1	2.57	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:A:159:GLY:HA3	1:I:156:PRO:HG2	2.03	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:F:322:VAL:O	1:F:323:ALA:C	2.60	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:347:ARG:N	1:B:348:PRO:CD	2.84	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: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%)	29	25
1	B	364/367 (99%)	341 (94%)	18 (5%)	5 (1%)	11	6
1	C	364/367 (99%)	348 (96%)	15 (4%)	1 (0%)	41	40
1	D	362/367 (99%)	345 (95%)	17 (5%)	0	100	100
1	E	363/367 (99%)	340 (94%)	22 (6%)	1 (0%)	41	40
1	F	365/367 (100%)	344 (94%)	18 (5%)	3 (1%)	19	14
1	G	363/367 (99%)	348 (96%)	14 (4%)	1 (0%)	41	40
1	H	364/367 (99%)	345 (95%)	18 (5%)	1 (0%)	41	40
1	I	363/367 (99%)	341 (94%)	20 (6%)	2 (1%)	25	20
1	J	365/367 (100%)	342 (94%)	22 (6%)	1 (0%)	41	40
All	All	3638/3670 (99%)	3437 (94%)	184 (5%)	17 (0%)	29	25

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

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Mol	Chain	Res	Type
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%)	287 (93%)	21 (7%)	16	12
1	B	309/309 (100%)	282 (91%)	27 (9%)	10	6
1	C	308/309 (100%)	297 (96%)	11 (4%)	35	35
1	D	307/309 (99%)	285 (93%)	22 (7%)	14	11
1	E	307/309 (99%)	287 (94%)	20 (6%)	17	14
1	F	309/309 (100%)	287 (93%)	22 (7%)	14	11
1	G	307/309 (99%)	284 (92%)	23 (8%)	13	10
1	H	307/309 (99%)	290 (94%)	17 (6%)	21	18
1	I	308/309 (100%)	283 (92%)	25 (8%)	11	8
1	J	308/309 (100%)	296 (96%)	12 (4%)	32	32
All	All	3078/3090 (100%)	2878 (94%)	200 (6%)	17	14

All (200) 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	58	GLN
1	A	61	LYS
1	A	67	ASN
1	A	77	GLU
1	A	186	TYR
1	A	195	LYS
1	A	254	ASN

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Mol	Chain	Res	Type
1	A	269	GLU
1	A	274	ARG
1	A	283	LEU
1	A	284	SER
1	A	292	ARG
1	A	306	LEU
1	A	307	THR
1	A	309	LYS
1	A	318	PHE
1	A	322	VAL
1	A	358	VAL
1	B	5	ILE
1	B	6	LEU
1	B	23	LEU
1	B	29	GLU
1	B	31	ILE
1	B	80	ASN
1	B	113	THR
1	B	133	GLU
1	B	186	TYR
1	B	247	LYS
1	B	249	MET
1	B	286	CYS
1	B	288	GLU
1	B	289	ARG
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	349	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	90	ILE

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Mol	Chain	Res	Type
1	C	186	TYR
1	C	254	ASN
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	28	GLN
1	D	29	GLU
1	D	30	ASN
1	D	58	GLN
1	D	80	ASN
1	D	122	THR
1	D	186	TYR
1	D	214	PRO
1	D	249	MET
1	D	254	ASN
1	D	265	LYS
1	D	270	ASP
1	D	274	ARG
1	D	278	LYS
1	D	295	ASP
1	D	312	THR
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	81	SER
1	E	97	ARG
1	E	164	GLN
1	E	186	TYR
1	E	216	GLU
1	E	219	SER
1	E	265	LYS
1	E	274	ARG

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Mol	Chain	Res	Type
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	E	338	ASP
1	F	5	ILE
1	F	21	ARG
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	122	THR
1	F	186	TYR
1	F	204	MET
1	F	254	ASN
1	F	285	LYS
1	F	289	ARG
1	F	295	ASP
1	F	307	THR
1	F	309	LYS
1	F	311	GLU
1	F	314	SER
1	F	315	ILE
1	F	319	SER
1	F	336	ASN
1	G	5	ILE
1	G	6	LEU
1	G	13	ARG
1	G	30	ASN
1	G	183	ASP
1	G	186	TYR
1	G	247	LYS
1	G	249	MET
1	G	252	ASP
1	G	269	GLU
1	G	285	LYS
1	G	289	ARG
1	G	298	GLN

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Mol	Chain	Res	Type
1	G	300	GLN
1	G	302	ASN
1	G	304	ARG
1	G	305	ARG
1	G	306	LEU
1	G	313	SER
1	G	314	SER
1	G	317	ASP
1	G	330	ARG
1	G	338	ASP
1	H	6	LEU
1	H	23	LEU
1	H	27	LEU
1	H	61	LYS
1	H	186	TYR
1	H	204	MET
1	H	207	GLN
1	H	219	SER
1	H	252	ASP
1	H	292	ARG
1	H	298	GLN
1	H	314	SER
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	81	SER
1	I	186	TYR
1	I	252	ASP
1	I	254	ASN
1	I	268	ARG
1	I	274	ARG
1	I	278	LYS
1	I	283	LEU
1	I	298	GLN

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Mol	Chain	Res	Type
1	I	305	ARG
1	I	309	LYS
1	I	312	THR
1	I	314	SER
1	I	338	ASP
1	I	340	LYS
1	I	349	SER
1	I	362	LEU
1	I	365	ILE
1	I	368	ASP
1	J	29	GLU
1	J	30	ASN
1	J	61	LYS
1	J	77	GLU
1	J	96	ARG
1	J	133	GLU
1	J	186	TYR
1	J	195	LYS
1	J	297	LYS
1	J	305	ARG
1	J	338	ASP
1	J	349	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) 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	164	GLN
1	A	185	HIS
1	A	290	HIS
1	A	300	GLN
1	B	15	ASN
1	B	141	GLN
1	B	164	GLN
1	B	185	HIS
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	254	ASN
1	B	290	HIS
1	B	298	GLN
1	B	302	ASN
1	C	11	ASN
1	C	15	ASN
1	C	141	GLN
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	100	ASN
1	D	141	GLN
1	D	164	GLN
1	D	200	ASN
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	254	ASN
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	261	ASN
1	F	287	HIS
1	F	290	HIS

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Mol	Chain	Res	Type
1	F	310	HIS
1	F	336	ASN
1	G	11	ASN
1	G	15	ASN
1	G	30	ASN
1	G	80	ASN
1	G	100	ASN
1	G	141	GLN
1	G	185	HIS
1	G	254	ASN
1	G	290	HIS
1	G	298	GLN
1	G	302	ASN
1	H	11	ASN
1	H	100	ASN
1	H	141	GLN
1	H	164	GLN
1	H	200	ASN
1	H	207	GLN
1	H	232	HIS
1	H	290	HIS
1	H	298	GLN
1	H	300	GLN
1	I	11	ASN
1	I	80	ASN
1	I	141	GLN
1	I	164	GLN
1	I	207	GLN
1	I	254	ASN
1	I	290	HIS
1	J	11	ASN
1	J	15	ASN
1	J	30	ASN
1	J	100	ASN
1	J	141	GLN
1	J	164	GLN
1	J	185	HIS
1	J	200	ASN
1	J	290	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	401	-	24,29,29	0.96	0	29,45,45	1.30	3 (10%)
2	ADP	G	401	-	24,29,29	0.95	0	29,45,45	1.34	4 (13%)
2	ADP	E	401	-	24,29,29	0.91	0	29,45,45	1.70	4 (13%)
2	ADP	H	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	J	401	-	24,29,29	0.96	2 (8%)	29,45,45	1.30	3 (10%)
2	ADP	I	401	-	24,29,29	0.96	0	29,45,45	1.31	3 (10%)
2	ADP	F	401	-	24,29,29	0.93	2 (8%)	29,45,45	1.49	4 (13%)
2	ADP	B	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
2	ADP	D	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	C	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)

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	A	401	-	-	5/12/32/32	0/3/3/3
2	ADP	G	401	-	-	5/12/32/32	0/3/3/3
2	ADP	E	401	-	-	5/12/32/32	0/3/3/3
2	ADP	H	401	-	-	0/12/32/32	0/3/3/3
2	ADP	J	401	-	-	2/12/32/32	0/3/3/3
2	ADP	I	401	-	-	5/12/32/32	0/3/3/3
2	ADP	F	401	-	-	5/12/32/32	0/3/3/3
2	ADP	B	401	-	-	0/12/32/32	0/3/3/3
2	ADP	D	401	-	-	2/12/32/32	0/3/3/3
2	ADP	C	401	-	-	4/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ADP	C5-C4	2.73	1.48	1.40
2	H	401	ADP	C5-C4	2.52	1.47	1.40
2	C	401	ADP	C5-C4	2.50	1.47	1.40
2	B	401	ADP	C5-C4	2.47	1.47	1.40
2	J	401	ADP	C5-C4	2.26	1.46	1.40
2	J	401	ADP	O4'-C1'	2.20	1.44	1.41
2	F	401	ADP	O4'-C1'	2.16	1.44	1.41
2	F	401	ADP	C5-C4	2.10	1.46	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	ADP	O4'-C1'-C2'	-5.04	99.56	106.93
2	F	401	ADP	N3-C2-N1	-4.93	120.97	128.68
2	E	401	ADP	N3-C2-N1	-4.10	122.27	128.68
2	J	401	ADP	N3-C2-N1	-4.05	122.35	128.68
2	H	401	ADP	PA-O3A-PB	-3.61	120.44	132.83
2	C	401	ADP	PA-O3A-PB	-3.57	120.59	132.83
2	D	401	ADP	PA-O3A-PB	-3.57	120.59	132.83
2	B	401	ADP	PA-O3A-PB	-3.53	120.71	132.83
2	D	401	ADP	C3'-C2'-C1'	3.41	106.12	100.98
2	C	401	ADP	C3'-C2'-C1'	3.25	105.88	100.98
2	D	401	ADP	N3-C2-N1	-3.25	123.61	128.68
2	H	401	ADP	N3-C2-N1	-3.20	123.68	128.68
2	C	401	ADP	N3-C2-N1	-3.19	123.69	128.68
2	H	401	ADP	C3'-C2'-C1'	3.16	105.73	100.98
2	B	401	ADP	N3-C2-N1	-3.14	123.77	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ADP	C3'-C2'-C1'	3.12	105.67	100.98
2	A	401	ADP	N3-C2-N1	-3.01	123.97	128.68
2	E	401	ADP	C4-C5-N7	-3.00	106.27	109.40
2	G	401	ADP	N3-C2-N1	-3.00	123.99	128.68
2	I	401	ADP	N3-C2-N1	-2.99	124.00	128.68
2	I	401	ADP	C4-C5-N7	-2.93	106.34	109.40
2	G	401	ADP	C4-C5-N7	-2.93	106.35	109.40
2	F	401	ADP	C4-C5-N7	-2.81	106.47	109.40
2	A	401	ADP	C4-C5-N7	-2.79	106.49	109.40
2	C	401	ADP	C4-C5-N7	-2.74	106.54	109.40
2	B	401	ADP	C4-C5-N7	-2.73	106.56	109.40
2	F	401	ADP	C1'-N9-C4	-2.67	121.94	126.64
2	H	401	ADP	C4-C5-N7	-2.67	106.62	109.40
2	D	401	ADP	C4-C5-N7	-2.66	106.63	109.40
2	E	401	ADP	C2-N1-C6	2.61	123.22	118.75
2	J	401	ADP	C4-C5-N7	-2.47	106.82	109.40
2	F	401	ADP	C2-N1-C6	2.43	122.91	118.75
2	I	401	ADP	O4'-C1'-C2'	-2.38	103.45	106.93
2	A	401	ADP	O4'-C1'-C2'	-2.36	103.48	106.93
2	G	401	ADP	O4'-C1'-C2'	-2.36	103.48	106.93
2	G	401	ADP	O3A-PB-O1B	-2.10	99.56	111.19
2	J	401	ADP	C1'-N9-C4	-2.06	123.03	126.64

There are no chirality outliers.

All (33) torsion outliers are listed below:

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

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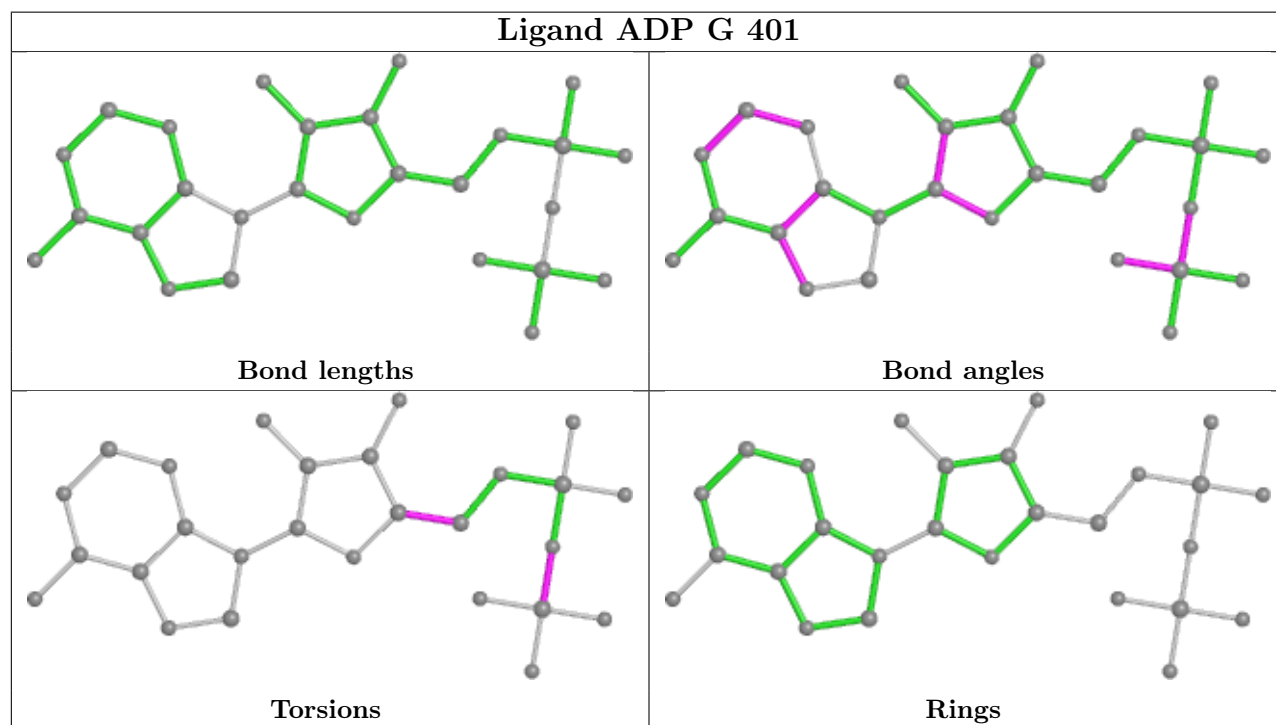
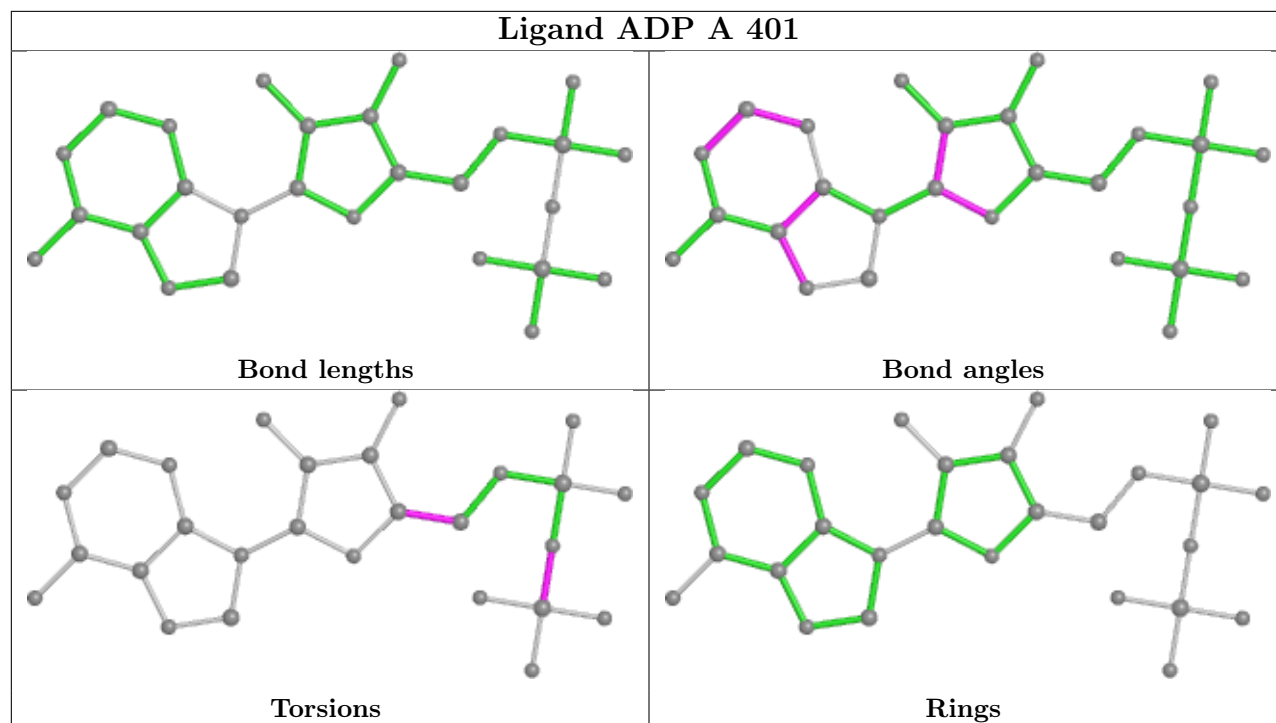
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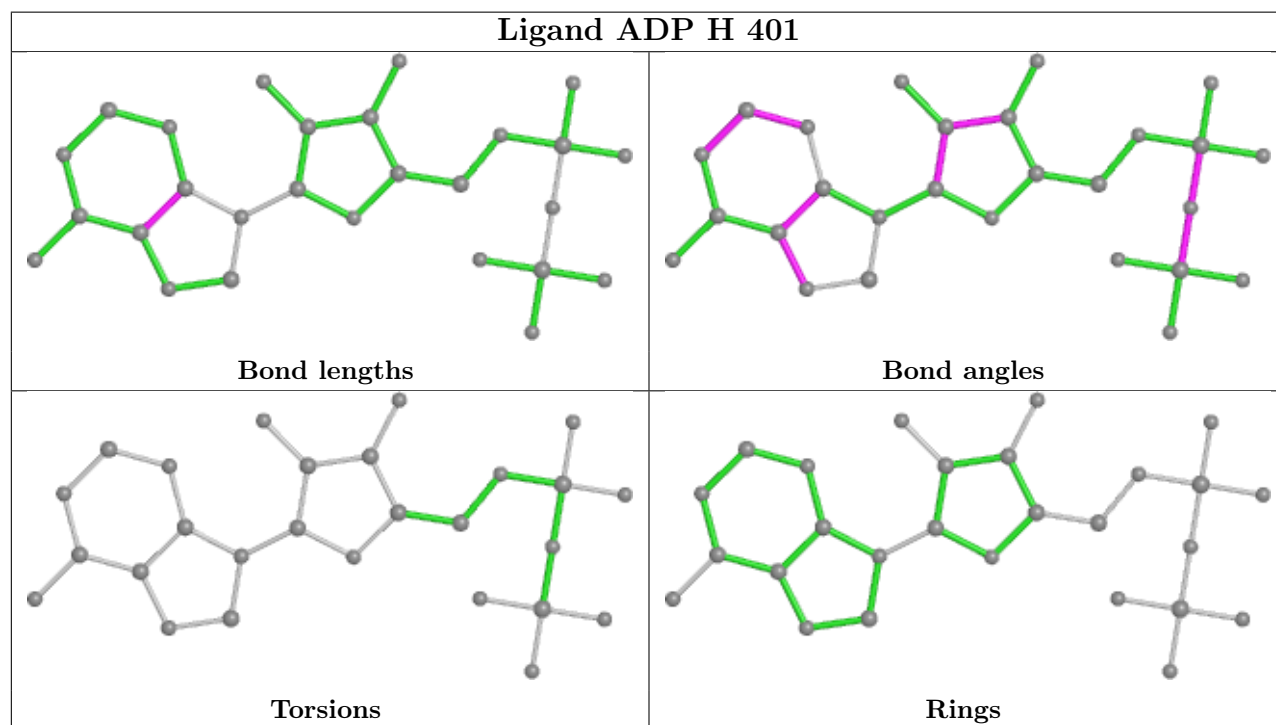
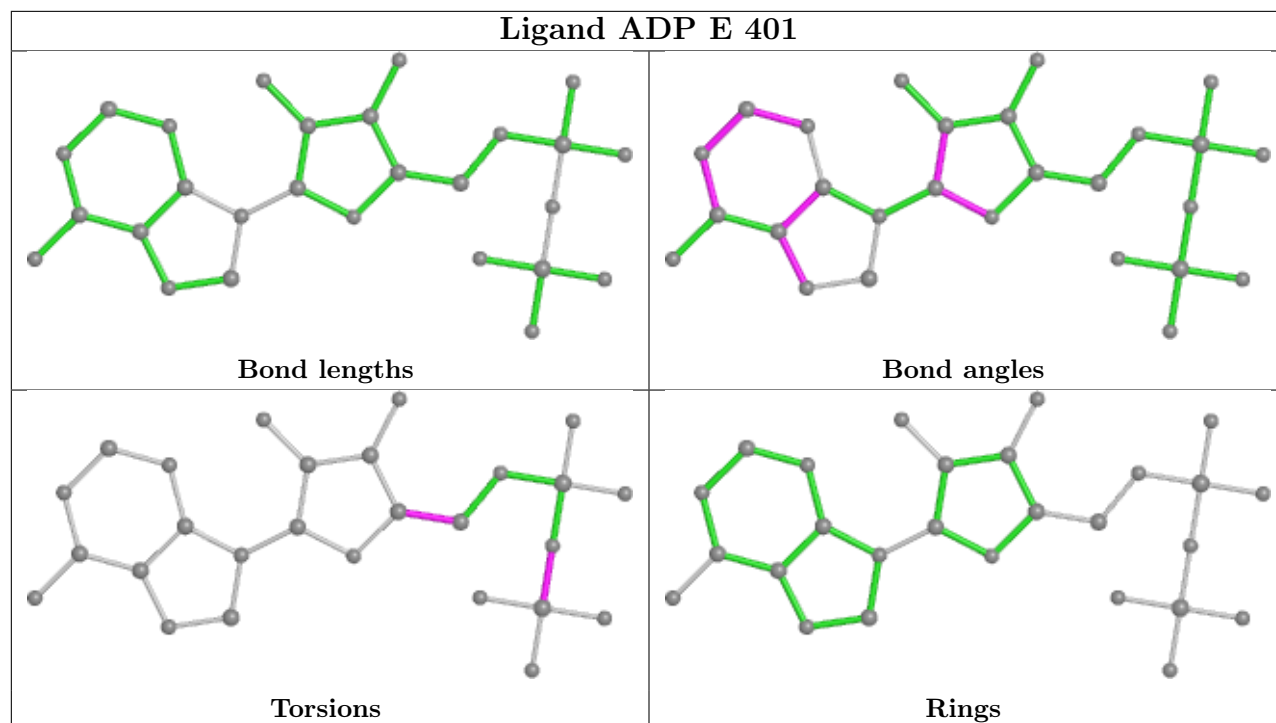
Mol	Chain	Res	Type	Atoms
2	J	401	ADP	O4'-C4'-C5'-O5'
2	J	401	ADP	C3'-C4'-C5'-O5'
2	F	401	ADP	O4'-C4'-C5'-O5'
2	F	401	ADP	C4'-C5'-O5'-PA
2	A	401	ADP	PA-O3A-PB-O1B
2	E	401	ADP	PA-O3A-PB-O1B
2	I	401	ADP	PA-O3A-PB-O1B
2	E	401	ADP	O4'-C4'-C5'-O5'
2	G	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	PA-O3A-PB-O2B
2	A	401	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	C	401	ADP	C5'-O5'-PA-O3A
2	E	401	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

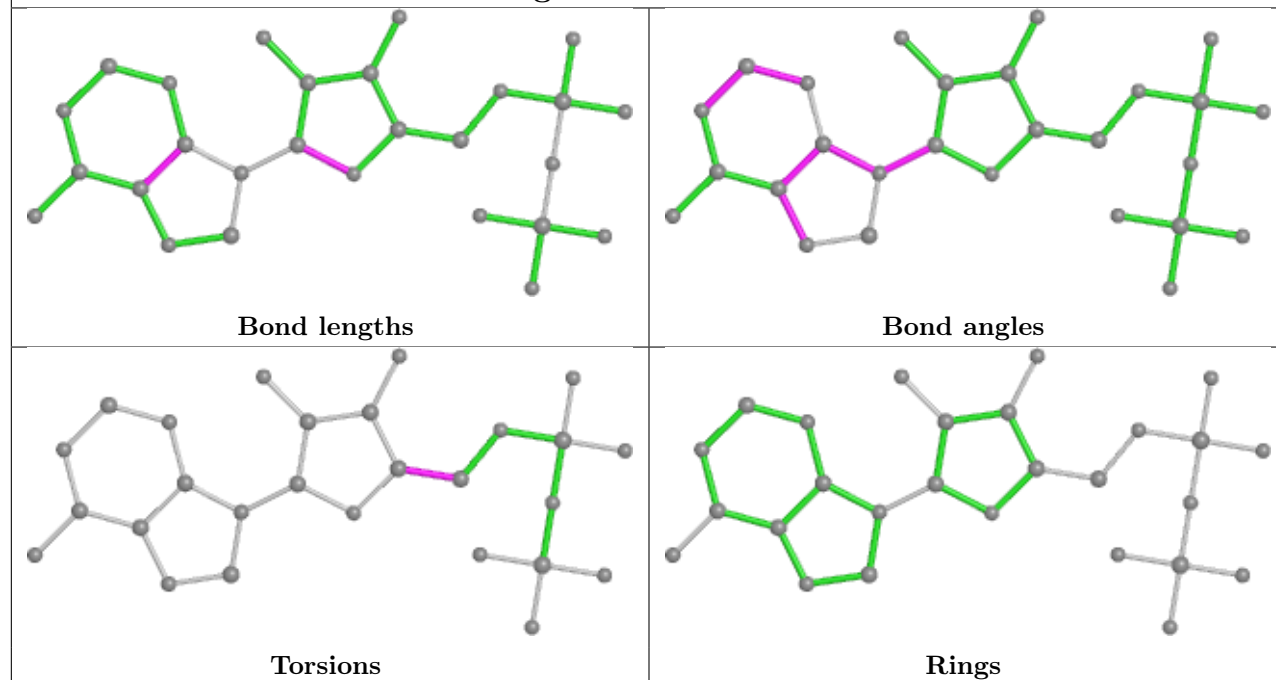
No monomer is involved in short contacts.

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.

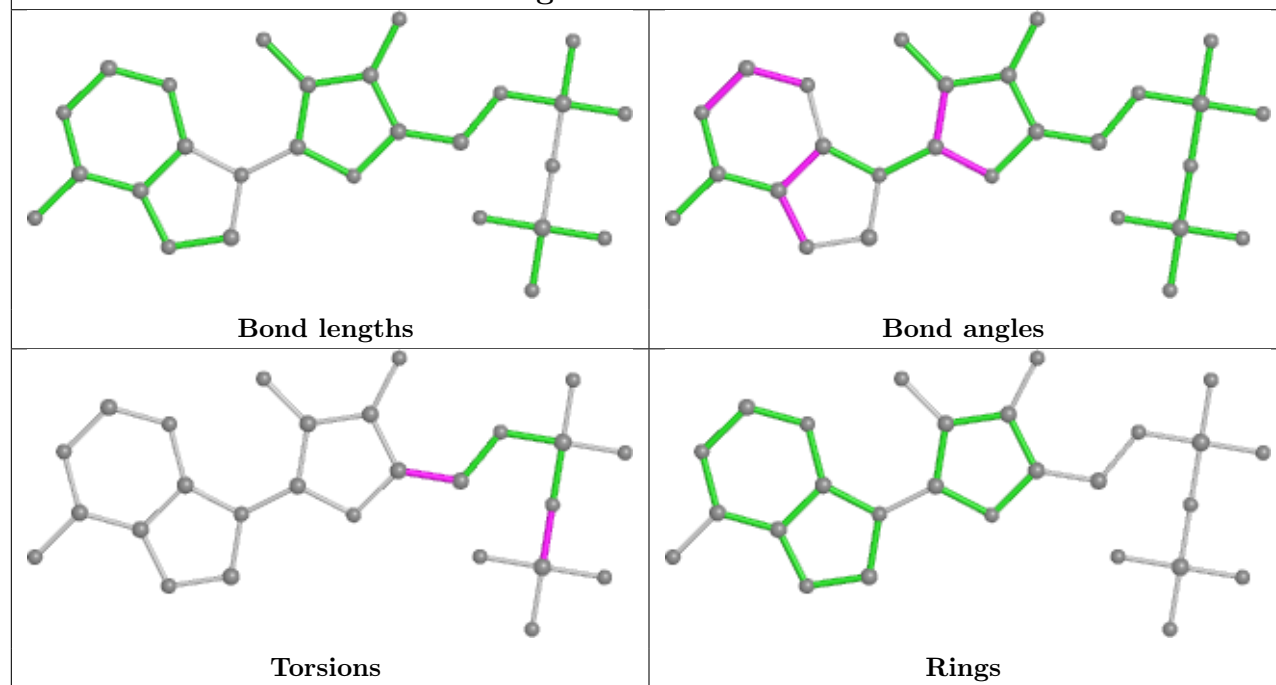


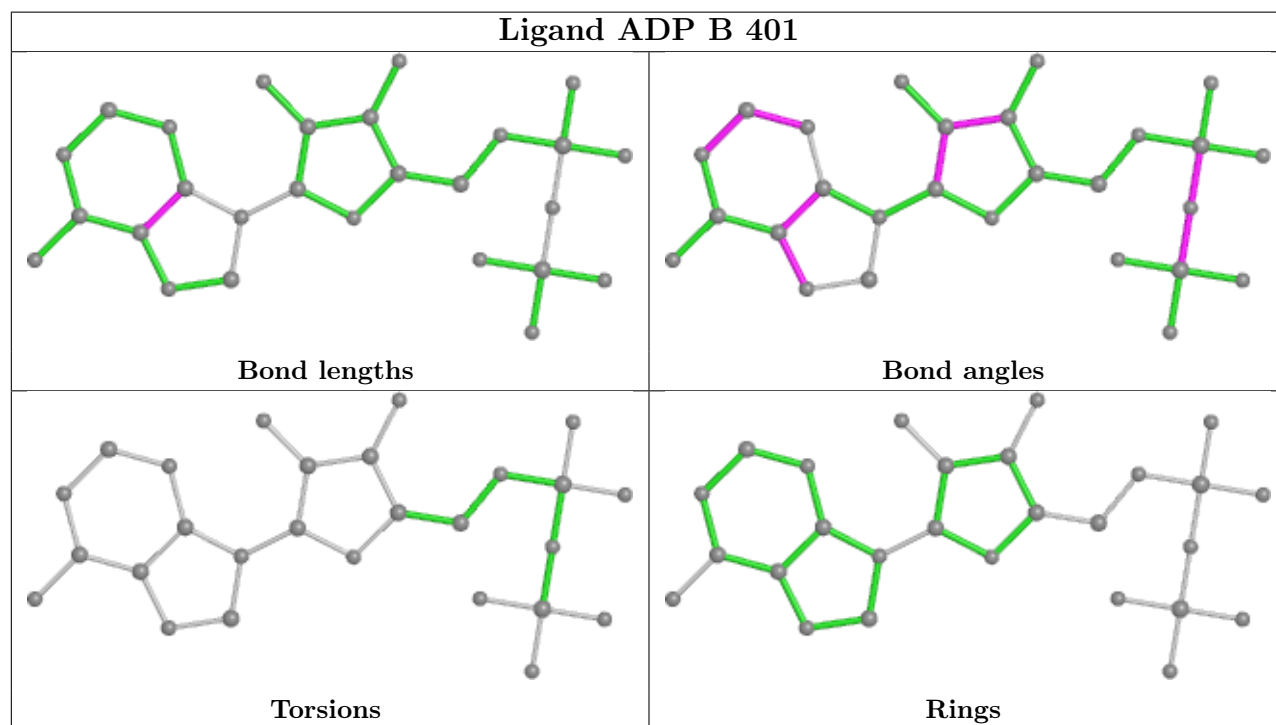
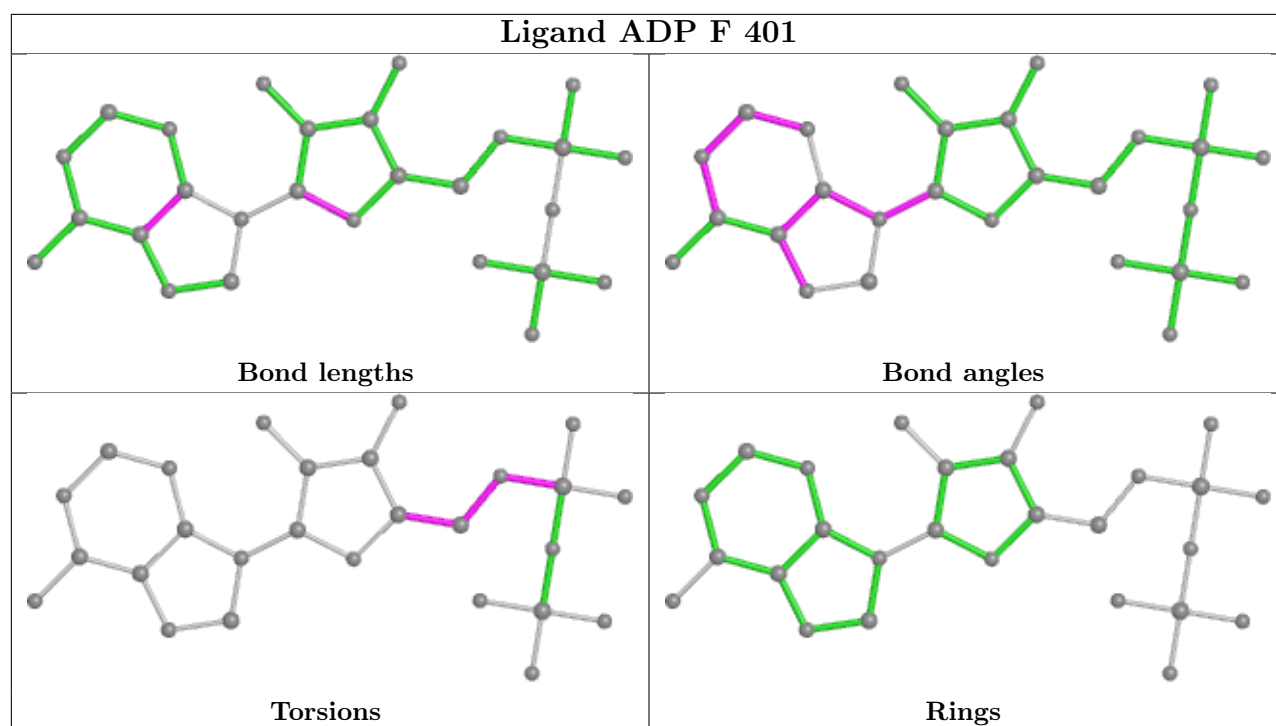


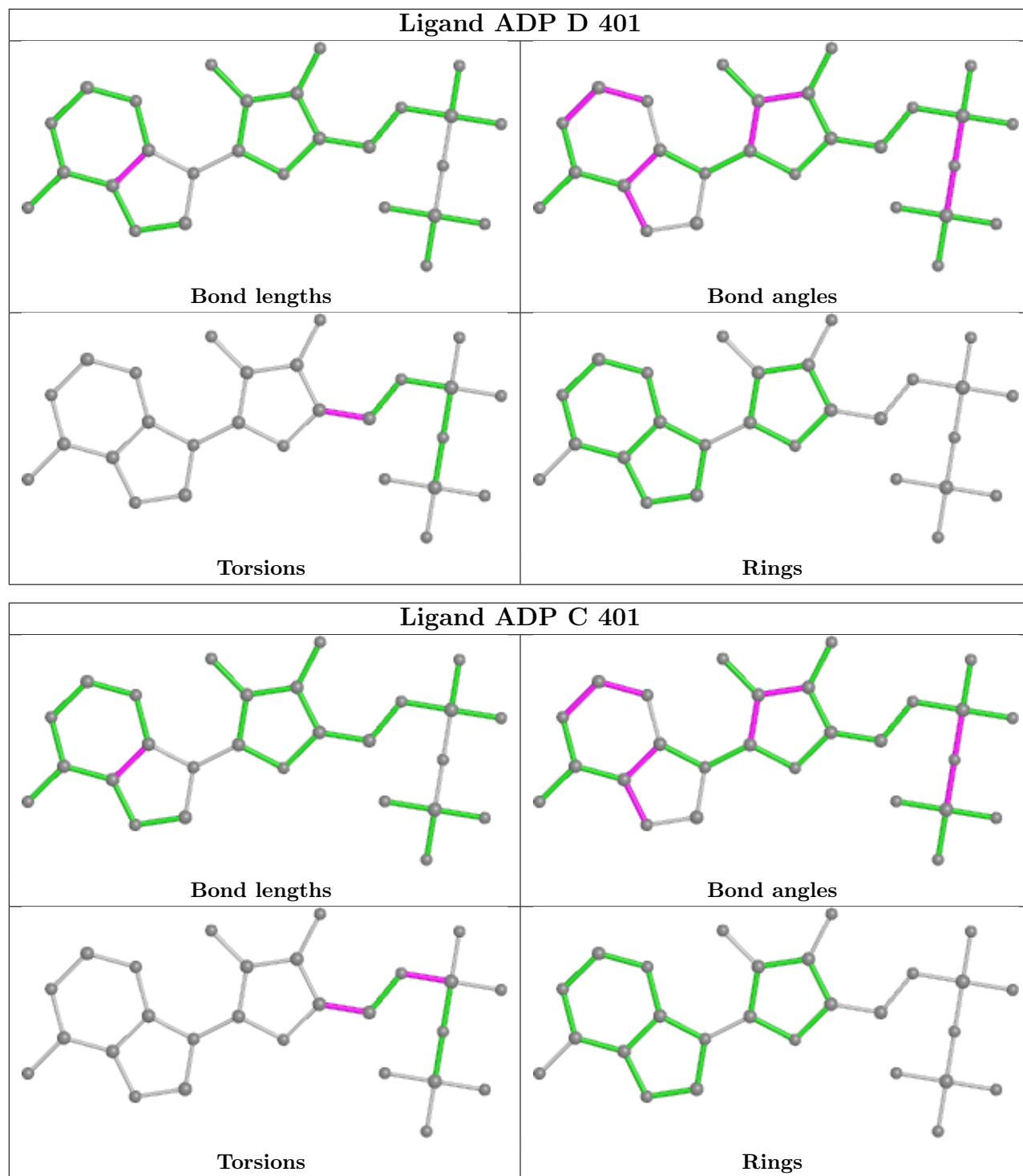
Ligand ADP J 401



Ligand ADP I 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%)	0.74	55 (14%) 2 3	24, 46, 127, 170	0
1	B	366/367 (99%)	0.55	48 (13%) 3 4	23, 46, 110, 166	0
1	C	366/367 (99%)	0.43	42 (11%) 4 6	23, 39, 102, 150	0
1	D	364/367 (99%)	0.20	38 (10%) 6 8	23, 36, 96, 126	0
1	E	365/367 (99%)	0.61	45 (12%) 4 5	24, 42, 125, 183	0
1	F	367/367 (100%)	0.40	41 (11%) 5 6	24, 39, 101, 136	0
1	G	365/367 (99%)	0.50	43 (11%) 4 5	21, 37, 114, 155	0
1	H	366/367 (99%)	0.44	42 (11%) 4 6	22, 41, 116, 190	0
1	I	365/367 (99%)	0.73	71 (19%) 1 1	24, 47, 109, 163	0
1	J	367/367 (100%)	0.72	60 (16%) 1 2	26, 48, 118, 157	0
All	All	3658/3670 (99%)	0.53	485 (13%) 3 4	21, 42, 114, 190	0

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	312	THR	19.8
1	G	318	PHE	19.0
1	E	310	HIS	14.7
1	E	307	THR	13.8
1	E	302	ASN	13.6
1	C	307	THR	13.2
1	E	322	VAL	13.0
1	E	306	LEU	12.2
1	G	315	ILE	12.1
1	J	308	GLY	10.8
1	G	307	THR	10.8
1	H	310	HIS	10.6
1	E	311	GLU	10.5

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Mol	Chain	Res	Type	RSRZ
1	C	308	GLY	10.5
1	J	307	THR	10.2
1	E	303	ALA	10.2
1	I	310	HIS	10.1
1	C	312	THR	9.9
1	H	298	GLN	9.9
1	J	309	LYS	9.8
1	H	300	GLN	9.5
1	A	310	HIS	9.5
1	A	312	THR	9.4
1	G	320	ALA	9.4
1	H	299	GLY	9.2
1	I	308	GLY	9.2
1	F	307	THR	9.1
1	A	302	ASN	9.1
1	B	316	ASN	8.9
1	F	308	GLY	8.9
1	A	311	GLU	8.9
1	H	311	GLU	8.8
1	E	309	LYS	8.8
1	I	309	LYS	8.8
1	A	299	GLY	8.6
1	I	316	ASN	8.6
1	I	315	ILE	8.5
1	G	304	ARG	8.5
1	A	309	LYS	8.4
1	E	318	PHE	8.4
1	A	307	THR	8.3
1	C	322	VAL	8.3
1	A	316	ASN	8.2
1	J	316	ASN	8.2
1	E	312	THR	8.2
1	G	303	ALA	8.1
1	F	299	GLY	8.0
1	B	313	SER	8.0
1	A	306	LEU	8.0
1	H	322	VAL	7.8
1	A	308	GLY	7.8
1	E	300	GLN	7.8
1	F	322	VAL	7.8
1	B	301	ASP	7.8
1	D	299	GLY	7.8

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Mol	Chain	Res	Type	RSRZ
1	F	300	GLN	7.7
1	E	317	ASP	7.7
1	D	303	ALA	7.7
1	C	310	HIS	7.6
1	I	311	GLU	7.6
1	J	300	GLN	7.6
1	B	309	LYS	7.5
1	B	308	GLY	7.5
1	A	322	VAL	7.5
1	G	302	ASN	7.4
1	J	315	ILE	7.4
1	I	299	GLY	7.3
1	C	3	ALA	7.2
1	G	300	GLN	7.2
1	B	310	HIS	7.2
1	F	317	ASP	7.2
1	G	308	GLY	7.2
1	G	312	THR	7.1
1	A	298	GLN	7.1
1	C	306	LEU	7.1
1	H	309	LYS	7.1
1	H	307	THR	7.1
1	A	301	ASP	7.0
1	H	305	ARG	7.0
1	F	311	GLU	6.9
1	A	313	SER	6.8
1	J	303	ALA	6.7
1	D	300	GLN	6.7
1	C	309	LYS	6.7
1	E	315	ILE	6.7
1	J	306	LEU	6.6
1	I	314	SER	6.6
1	J	299	GLY	6.6
1	C	311	GLU	6.5
1	A	300	GLN	6.4
1	B	300	GLN	6.4
1	D	315	ILE	6.4
1	C	316	ASN	6.3
1	E	313	SER	6.3
1	F	309	LYS	6.3
1	E	299	GLY	6.2
1	H	308	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	G	316	ASN	6.1
1	J	317	ASP	6.1
1	B	299	GLY	6.0
1	B	312	THR	6.0
1	I	322	VAL	6.0
1	E	316	ASN	6.0
1	A	315	ILE	6.0
1	E	308	GLY	6.0
1	G	305	ARG	5.9
1	B	303	ALA	5.9
1	I	274	ARG	5.9
1	A	318	PHE	5.9
1	B	307	THR	5.9
1	J	310	HIS	5.9
1	F	28	GLN	5.8
1	I	271	GLY	5.8
1	J	302	ASN	5.8
1	E	301	ASP	5.8
1	F	312	THR	5.8
1	C	300	GLN	5.7
1	F	310	HIS	5.7
1	B	78	GLY	5.7
1	F	303	ALA	5.6
1	B	302	ASN	5.5
1	F	298	GLN	5.5
1	I	320	ALA	5.5
1	F	78	GLY	5.5
1	J	301	ASP	5.5
1	G	310	HIS	5.4
1	H	368	ASP	5.4
1	H	313	SER	5.4
1	A	303	ALA	5.4
1	I	292	ARG	5.4
1	I	303	ALA	5.4
1	A	295	ASP	5.4
1	I	300	GLN	5.3
1	H	303	ALA	5.3
1	A	305	ARG	5.3
1	G	309	LYS	5.2
1	B	337	ASP	5.2
1	C	303	ALA	5.2
1	H	301	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	I	78	GLY	5.2
1	A	314	SER	5.2
1	G	306	LEU	5.2
1	C	285	LYS	5.2
1	A	304	ARG	5.1
1	E	298	GLN	5.1
1	I	336	ASN	5.0
1	D	306	LEU	5.0
1	B	315	ILE	5.0
1	C	78	GLY	5.0
1	H	318	PHE	5.0
1	F	369	GLU	5.0
1	H	3	ALA	5.0
1	G	301	ASP	5.0
1	F	301	ASP	4.9
1	D	301	ASP	4.9
1	A	317	ASP	4.8
1	D	310	HIS	4.8
1	H	302	ASN	4.8
1	I	317	ASP	4.8
1	F	321	GLY	4.8
1	A	369	GLU	4.8
1	B	369	GLU	4.8
1	E	304	ARG	4.8
1	E	323	ALA	4.8
1	A	3	ALA	4.8
1	A	292	ARG	4.7
1	C	299	GLY	4.7
1	J	312	THR	4.7
1	B	314	SER	4.7
1	I	306	LEU	4.7
1	E	305	ARG	4.7
1	D	29	GLU	4.6
1	E	321	GLY	4.6
1	H	317	ASP	4.6
1	F	306	LEU	4.5
1	E	252	ASP	4.5
1	A	319	SER	4.5
1	D	305	ARG	4.5
1	F	315	ILE	4.5
1	B	322	VAL	4.5
1	D	302	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	297	LYS	4.5
1	G	78	GLY	4.5
1	D	316	ASN	4.5
1	J	314	SER	4.5
1	I	275	ASP	4.5
1	I	285	LYS	4.5
1	E	288	GLU	4.5
1	I	307	THR	4.4
1	I	335	VAL	4.4
1	A	323	ALA	4.4
1	E	319	SER	4.4
1	A	252	ASP	4.3
1	G	110	PHE	4.3
1	B	297	LYS	4.2
1	J	304	ARG	4.2
1	G	298	GLN	4.2
1	B	317	ASP	4.2
1	G	314	SER	4.2
1	J	252	ASP	4.2
1	J	321	GLY	4.2
1	D	307	THR	4.2
1	A	324	ASN	4.2
1	C	304	ARG	4.1
1	A	288	GLU	4.1
1	J	278	LYS	4.1
1	B	269	GLU	4.0
1	B	339	GLY	4.0
1	B	306	LEU	4.0
1	I	298	GLN	4.0
1	F	316	ASN	4.0
1	H	252	ASP	4.0
1	H	297	LYS	4.0
1	C	314	SER	4.0
1	D	311	GLU	4.0
1	I	297	LYS	4.0
1	B	278	LYS	3.9
1	J	285	LYS	3.9
1	H	316	ASN	3.9
1	D	309	LYS	3.9
1	J	311	GLU	3.9
1	H	292	ARG	3.9
1	I	339	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	274	ARG	3.9
1	F	79	SER	3.9
1	J	357	VAL	3.9
1	J	132	ALA	3.8
1	B	288	GLU	3.8
1	D	317	ASP	3.8
1	G	289	ARG	3.8
1	G	3	ALA	3.8
1	J	325	ARG	3.8
1	B	77	GLU	3.8
1	C	313	SER	3.8
1	J	260	THR	3.7
1	A	297	LYS	3.7
1	F	314	SER	3.7
1	E	274	ARG	3.7
1	I	304	ARG	3.7
1	J	305	ARG	3.7
1	D	322	VAL	3.7
1	A	78	GLY	3.7
1	G	299	GLY	3.7
1	H	306	LEU	3.7
1	H	77	GLU	3.6
1	F	3	ALA	3.6
1	F	302	ASN	3.6
1	C	298	GLN	3.6
1	J	326	GLY	3.6
1	C	274	ARG	3.6
1	I	324	ASN	3.6
1	J	313	SER	3.6
1	C	323	ALA	3.6
1	B	304	ARG	3.6
1	I	286	CYS	3.5
1	A	320	ALA	3.5
1	H	253	TRP	3.5
1	J	76	ALA	3.5
1	H	78	GLY	3.5
1	C	315	ILE	3.4
1	C	301	ASP	3.4
1	H	324	ASN	3.4
1	C	297	LYS	3.4
1	B	311	GLU	3.4
1	F	252	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	301	ASP	3.4
1	J	274	ARG	3.4
1	C	317	ASP	3.4
1	E	297	LYS	3.4
1	B	132	ALA	3.4
1	J	361	ILE	3.4
1	F	29	GLU	3.4
1	E	287	HIS	3.4
1	J	3	ALA	3.3
1	I	368	ASP	3.3
1	H	315	ILE	3.3
1	I	288	GLU	3.3
1	D	274	ARG	3.2
1	A	77	GLU	3.2
1	J	297	LYS	3.2
1	C	29	GLU	3.2
1	F	288	GLU	3.2
1	I	269	GLU	3.2
1	J	322	VAL	3.2
1	H	304	ARG	3.2
1	J	277	GLU	3.1
1	G	311	GLU	3.1
1	I	318	PHE	3.1
1	G	317	ASP	3.1
1	F	304	ARG	3.1
1	B	320	ALA	3.1
1	D	285	LYS	3.1
1	I	29	GLU	3.1
1	I	281	ALA	3.1
1	B	274	ARG	3.1
1	E	58	GLN	3.0
1	H	288	GLU	3.0
1	G	29	GLU	3.0
1	B	295	ASP	3.0
1	E	295	ASP	3.0
1	A	260	THR	3.0
1	C	302	ASN	3.0
1	A	339	GLY	3.0
1	G	28	GLN	3.0
1	J	270	ASP	3.0
1	A	327	CYS	3.0
1	I	278	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	253	TRP	3.0
1	D	79	SER	3.0
1	D	298	GLN	2.9
1	H	80	ASN	2.9
1	I	319	SER	2.9
1	A	325	ARG	2.9
1	I	252	ASP	2.9
1	D	30	ASN	2.9
1	D	304	ARG	2.9
1	F	313	SER	2.9
1	B	338	ASP	2.9
1	C	288	GLU	2.9
1	G	288	GLU	2.9
1	D	31	ILE	2.9
1	I	273	ILE	2.9
1	E	253	TRP	2.9
1	I	79	SER	2.9
1	F	305	ARG	2.8
1	B	252	ASP	2.8
1	J	275	ASP	2.8
1	E	314	SER	2.8
1	A	131	ALA	2.8
1	B	110	PHE	2.8
1	E	337	ASP	2.8
1	G	30	ASN	2.8
1	C	336	ASN	2.8
1	I	305	ARG	2.8
1	A	79	SER	2.8
1	B	79	SER	2.8
1	E	325	ARG	2.8
1	J	262	VAL	2.8
1	A	291	ILE	2.8
1	D	78	GLY	2.8
1	D	308	GLY	2.7
1	H	321	GLY	2.7
1	I	329	ILE	2.7
1	I	277	GLU	2.7
1	J	269	GLU	2.7
1	J	358	VAL	2.7
1	E	292	ARG	2.7
1	D	318	PHE	2.7
1	A	326	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	132	ALA	2.7
1	B	285	LYS	2.7
1	D	321	GLY	2.7
1	I	334	GLY	2.7
1	C	132	ALA	2.7
1	I	323	ALA	2.7
1	A	253	TRP	2.7
1	F	297	LYS	2.7
1	I	312	THR	2.7
1	C	80	ASN	2.7
1	I	61	LYS	2.7
1	I	266	ALA	2.7
1	G	292	ARG	2.7
1	I	328	SER	2.6
1	C	77	GLU	2.6
1	B	29	GLU	2.6
1	E	289	ARG	2.6
1	J	54	ASP	2.6
1	B	80	ASN	2.6
1	F	368	ASP	2.6
1	B	305	ARG	2.6
1	E	78	GLY	2.6
1	G	313	SER	2.6
1	H	58	GLN	2.6
1	I	77	GLU	2.6
1	E	285	LYS	2.6
1	I	110	PHE	2.6
1	I	341	GLY	2.6
1	I	337	ASP	2.6
1	J	271	GLY	2.6
1	E	110	PHE	2.6
1	B	270	ASP	2.5
1	J	78	GLY	2.5
1	D	297	LYS	2.5
1	D	253	TRP	2.5
1	A	132	ALA	2.5
1	A	338	ASP	2.5
1	H	29	GLU	2.5
1	I	340	LYS	2.5
1	A	274	ARG	2.5
1	F	30	ASN	2.5
1	I	313	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	324	ASN	2.5
1	J	323	ALA	2.5
1	B	28	GLN	2.4
1	J	253	TRP	2.4
1	C	252	ASP	2.4
1	F	270	ASP	2.4
1	J	327	CYS	2.4
1	B	325	ARG	2.4
1	I	331	ILE	2.4
1	D	269	GLU	2.4
1	E	112	GLY	2.4
1	J	29	GLU	2.4
1	J	298	GLN	2.4
1	B	61	LYS	2.4
1	G	323	ALA	2.4
1	D	28	GLN	2.4
1	C	321	GLY	2.4
1	A	294	TYR	2.4
1	I	80	ASN	2.3
1	J	318	PHE	2.3
1	G	319	SER	2.3
1	C	270	ASP	2.3
1	G	31	ILE	2.3
1	C	289	ARG	2.3
1	E	28	GLN	2.3
1	A	255	GLY	2.3
1	D	252	ASP	2.3
1	G	326	GLY	2.3
1	F	260	THR	2.3
1	I	58	GLN	2.3
1	D	313	SER	2.3
1	F	337	ASP	2.3
1	B	335	VAL	2.3
1	E	320	ALA	2.3
1	C	28	GLN	2.3
1	J	292	ARG	2.3
1	A	287	HIS	2.3
1	A	321	GLY	2.3
1	D	61	LYS	2.3
1	H	284	SER	2.3
1	A	358	VAL	2.3
1	H	289	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	325	ARG	2.3
1	J	333	ARG	2.3
1	I	258	ALA	2.3
1	G	37	VAL	2.3
1	G	322	VAL	2.3
1	D	314	SER	2.3
1	B	277	GLU	2.3
1	H	28	GLN	2.3
1	B	368	ASP	2.2
1	D	77	GLU	2.2
1	A	271	GLY	2.2
1	D	255	GLY	2.2
1	J	324	ASN	2.2
1	H	30	ASN	2.2
1	C	271	GLY	2.2
1	J	79	SER	2.2
1	C	292	ARG	2.2
1	G	102	LEU	2.2
1	J	58	GLN	2.2
1	A	290	HIS	2.2
1	F	361	ILE	2.2
1	G	103	VAL	2.2
1	I	291	ILE	2.2
1	C	305	ARG	2.2
1	B	255	GLY	2.2
1	G	79	SER	2.1
1	I	260	THR	2.1
1	J	131	ALA	2.1
1	J	288	GLU	2.1
1	F	77	GLU	2.1
1	C	30	ASN	2.1
1	H	286	CYS	2.1
1	F	338	ASP	2.1
1	I	224	LEU	2.1
1	J	128	ASN	2.1
1	D	54	ASP	2.1
1	J	337	ASP	2.1
1	E	286	CYS	2.1
1	I	302	ASN	2.1
1	G	252	ASP	2.0
1	I	295	ASP	2.0
1	A	28	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	348	PRO	2.0
1	G	357	VAL	2.0
1	H	326	GLY	2.0
1	I	23	LEU	2.0
1	E	3	ALA	2.0
1	I	37	VAL	2.0
1	H	81	SER	2.0
1	I	129	LYS	2.0
1	J	250	PRO	2.0
1	I	293	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.