



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:53 PM UTC

PDB ID : 2HYI / pdb_00002hyi
Title : Structure of the human exon junction complex with a trapped DEAD-box helicase bound to RNA
Authors : Andersen, C.B.F.; Le Hir, H.; Andersen, G.R.
Deposited on : 2006-08-06
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

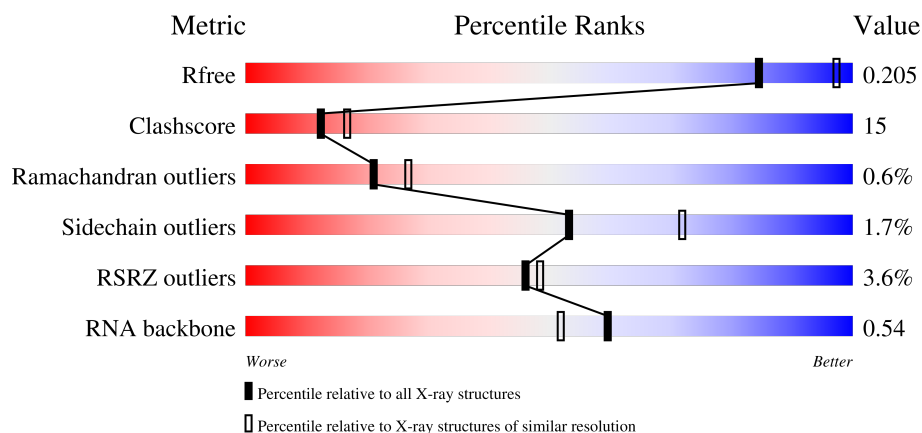
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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	F	6	100%
1	L	6	83% 17%
2	A	146	5% 77% 21% ..
2	G	146	3% 70% 27% ..

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Mol	Chain	Length	Quality of chain
3	B	91	
3	H	91	
4	C	413	
4	I	413	
5	D	77	
5	J	77	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12033 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 RNA chain called 5'-R(*UP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			
1	L	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 2 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	144	Total	C	N	O	S	0	0	0
			1196	772	200	221	3			
2	G	144	Total	C	N	O	S	0	0	0
			1196	772	200	221	3			

- Molecule 3 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	91	Total	C	N	O	S	0	0	0
			731	463	122	143	3			
3	H	91	Total	C	N	O	S	0	0	0
			731	463	122	143	3			

- Molecule 4 is a protein called Probable ATP-dependent RNA helicase DDX48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	392	Total	C	N	O	S	0	0	0
			3148	1987	548	594	19			
4	I	392	Total	C	N	O	S	0	0	0
			3148	1987	548	594	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	412	LEU	-	cloning artifact	UNP P38919
C	413	GLU	-	cloning artifact	UNP P38919
I	412	LEU	-	cloning artifact	UNP P38919
I	413	GLU	-	cloning artifact	UNP P38919

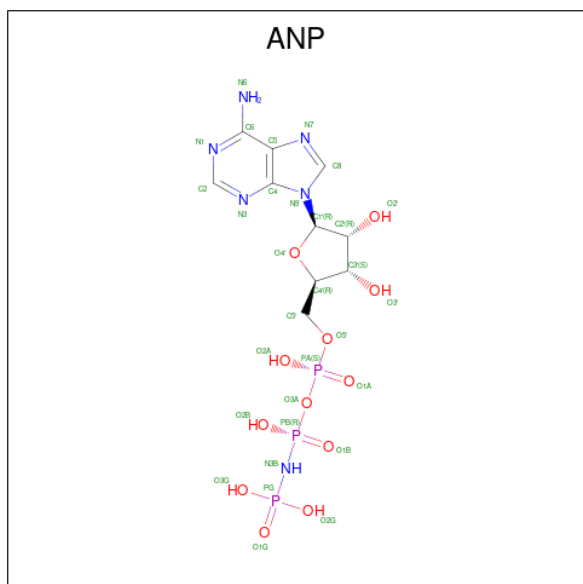
- Molecule 5 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	56	Total	C	N	O	0	0	0
			485	303	89	93			
5	J	51	Total	C	N	O	0	0	0
			440	278	84	78			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	12	Total	O	0	0
			12	12		
8	L	4	Total	O	0	0
			4	4		
8	A	55	Total	O	0	0
			55	55		
8	B	46	Total	O	0	0
			46	46		
8	C	229	Total	O	0	0
			229	229		
8	D	26	Total	O	0	0
			26	26		
8	G	65	Total	O	0	0
			65	65		
8	H	20	Total	O	0	0
			20	20		
8	I	190	Total	O	0	0
			190	190		
8	J	13	Total	O	0	0
			13	13		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5'-R(*UP*UP*UP*UP*UP*U)-3'

Chain F:  100%

There are no outlier residues recorded for this chain.

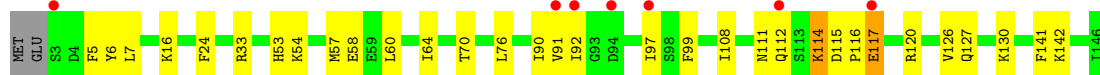
- Molecule 1: 5'-R(*UP*UP*UP*UP*UP*U)-3'

Chain L:  83% 17%



- Molecule 2: Protein mago nashi homolog

Chain A:  5% 77% 21% ..



- Molecule 2: Protein mago nashi homolog

Chain G:  3% 70% 27% ..

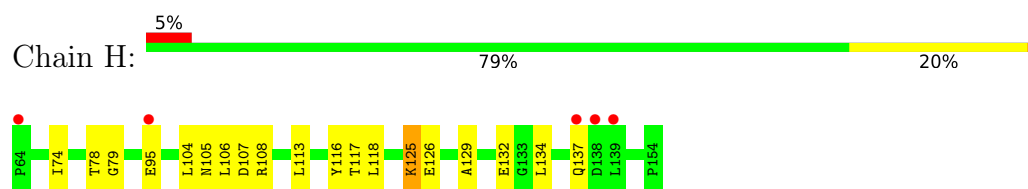


- Molecule 3: RNA-binding protein 8A

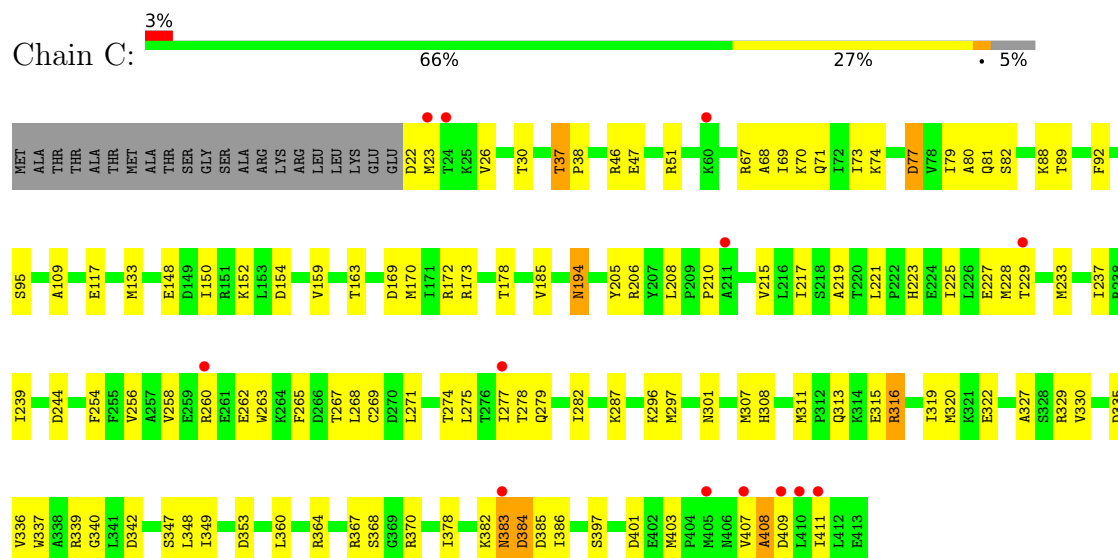
Chain B:  4% 70% 26% .



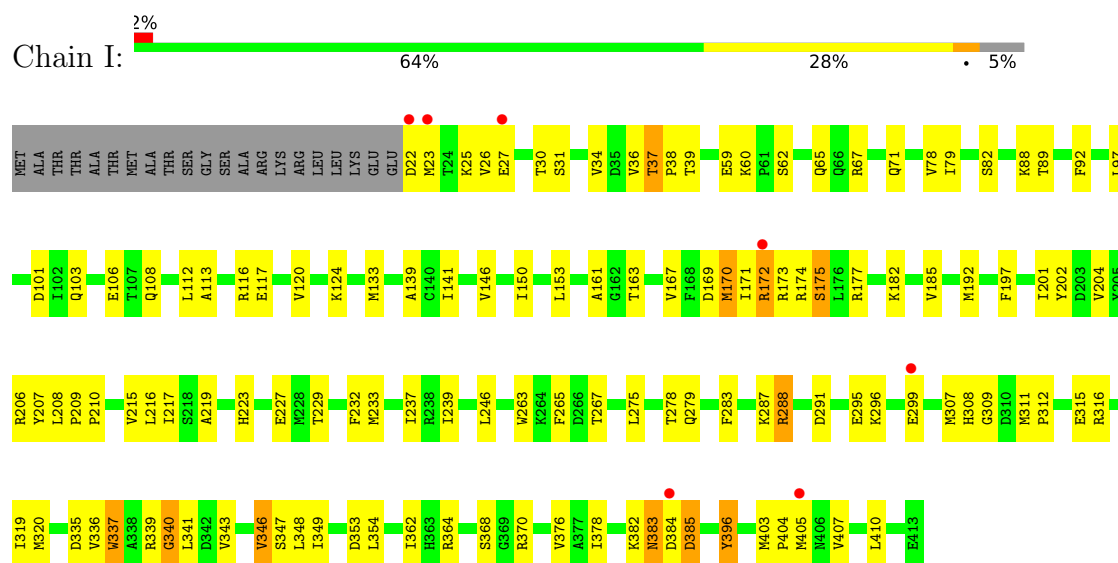
- Molecule 3: RNA-binding protein 8A



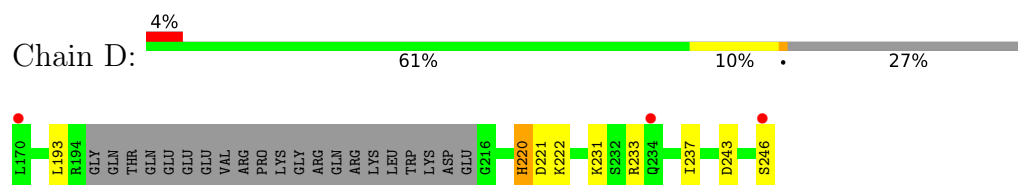
- Molecule 4: Probable ATP-dependent RNA helicase DDX48



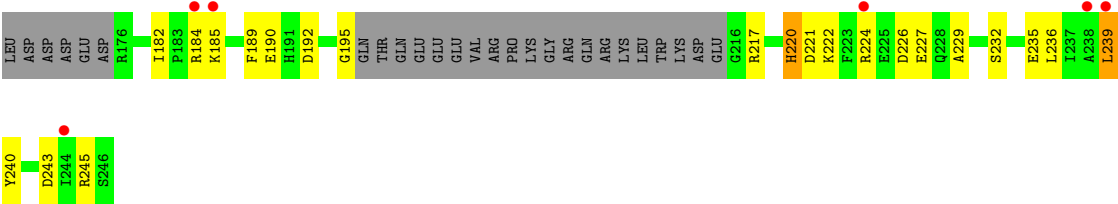
- Molecule 4: Probable ATP-dependent RNA helicase DDX48



- Molecule 5: Protein CASC3



● Molecule 5: Protein CASC3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.83Å 88.26Å 145.77Å 90.00° 110.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 99.8 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.231 0.199 , 0.205	Depositor DCC
R_{free} test set	1948 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12033	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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: MG, ANP

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	F	0.63	0/128	0.79	0/196
1	L	0.75	0/128	0.75	0/196
2	A	0.40	0/1225	0.84	3/1648 (0.2%)
2	G	0.42	0/1225	0.88	2/1648 (0.1%)
3	B	0.40	0/749	0.98	4/1012 (0.4%)
3	H	0.33	0/749	0.83	2/1012 (0.2%)
4	C	0.45	0/3197	1.00	14/4314 (0.3%)
4	I	0.44	0/3197	0.99	18/4314 (0.4%)
5	D	0.41	0/496	0.93	1/662 (0.2%)
5	J	0.38	0/451	0.86	1/600 (0.2%)
All	All	0.43	0/11545	0.94	45/15602 (0.3%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	37	THR	CA-C-N	10.61	130.38	119.56
4	C	37	THR	C-N-CA	10.61	130.38	119.56
4	I	396	TYR	N-CA-C	-10.57	96.89	110.53
3	B	114	LYS	N-CA-C	-10.46	93.67	110.20
4	I	384	ASP	N-CA-C	8.62	120.68	111.28
4	C	408	ALA	N-CA-C	7.20	118.77	111.07
4	C	77	ASP	N-CA-C	-7.06	99.83	110.28
4	I	78	VAL	N-CA-C	6.83	118.63	108.46
4	C	38	PRO	N-CA-C	6.59	122.41	113.84
4	I	175	SER	N-CA-C	-6.47	105.52	113.41
4	C	68	ALA	N-CA-C	6.29	119.43	111.69
4	I	396	TYR	CA-C-N	-6.15	114.54	122.79
4	I	396	TYR	C-N-CA	-6.15	114.54	122.79
2	A	142	LYS	N-CA-C	6.14	118.65	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	38	PRO	N-CA-C	6.06	121.72	113.84
4	C	339	ARG	N-CA-C	6.05	119.57	109.95
4	C	178	THR	N-CA-C	6.00	120.73	113.17
4	I	339	ARG	N-CA-C	5.88	119.06	109.59
4	I	36	VAL	N-CA-C	5.85	116.37	108.17
4	C	336	VAL	N-CA-C	-5.74	104.01	112.04
3	H	105	ASN	N-CA-C	5.73	118.88	109.76
4	I	209	PRO	CA-C-N	5.68	126.06	119.47
4	I	209	PRO	C-N-CA	5.68	126.06	119.47
4	C	210	PRO	N-CA-C	5.64	121.37	113.53
2	A	114	LYS	N-CA-C	-5.62	100.52	109.96
4	I	37	THR	CA-C-N	5.59	125.27	119.56
4	I	37	THR	C-N-CA	5.59	125.27	119.56
4	I	340	GLY	N-CA-C	5.58	126.42	113.18
2	G	142	LYS	N-CA-C	5.57	117.77	109.25
4	C	384	ASP	N-CA-C	5.50	117.70	111.11
3	B	115	GLY	N-CA-C	5.47	126.14	113.18
5	J	220	HIS	N-CA-C	-5.43	105.33	112.72
4	I	210	PRO	N-CA-C	5.26	121.44	113.81
5	D	220	HIS	N-CA-C	-5.24	104.27	111.81
4	C	367	ARG	N-CA-C	-5.22	106.17	112.54
4	I	309	GLY	N-CA-C	5.22	120.08	113.24
4	I	336	VAL	N-CA-C	-5.18	104.79	112.04
4	C	163	THR	N-CA-C	-5.17	103.66	110.39
4	I	246	LEU	N-CA-C	5.15	118.03	111.69
3	B	107	ASP	N-CA-C	-5.12	102.07	109.59
4	C	342	ASP	N-CA-C	5.12	117.05	107.99
2	A	141	PHE	N-CA-C	5.11	120.16	113.88
3	H	107	ASP	N-CA-C	-5.10	102.10	109.59
3	B	148	TRP	N-CA-C	-5.08	103.33	110.50
2	G	57	MET	N-CA-C	-5.06	105.77	111.28

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	F	117	0	62	0	0
1	L	117	0	62	1	0
2	A	1196	0	1182	35	0
2	G	1196	0	1182	46	0
3	B	731	0	690	28	0
3	H	731	0	690	15	0
4	C	3148	0	3190	101	0
4	I	3148	0	3190	116	0
5	D	485	0	452	11	0
5	J	440	0	422	24	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
7	C	31	0	13	4	0
7	I	31	0	13	3	0
8	A	55	0	0	2	0
8	B	46	0	0	1	0
8	C	229	0	0	12	0
8	D	26	0	0	0	0
8	F	12	0	0	0	0
8	G	65	0	0	1	0
8	H	20	0	0	1	0
8	I	190	0	0	8	0
8	J	13	0	0	1	0
8	L	4	0	0	0	0
All	All	12033	0	11148	347	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 15.

All (347) 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)
2:G:58:GLU:HA	2:G:61:LYS:HE2	1.23	1.20
4:I:229:THR:HG23	4:I:233:MET:HE3	1.25	1.15
2:A:70:THR:HG21	2:A:92:ILE:HD11	1.29	1.08
2:G:58:GLU:HA	2:G:61:LYS:CE	1.82	1.08
4:I:172:ARG:HG3	4:I:172:ARG:HH11	0.95	1.05
5:J:224:ARG:HG3	5:J:227:GLU:HG3	1.32	1.05
4:C:278:THR:HG23	4:C:279:GLN:H	1.26	1.00
5:J:224:ARG:CG	5:J:227:GLU:HG3	1.94	0.98
2:A:90:ILE:HG22	2:A:92:ILE:HG23	1.46	0.96
4:I:278:THR:HG23	4:I:279:GLN:H	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:97:ILE:HD12	2:G:99:PHE:HE1	1.31	0.94
4:I:172:ARG:HG3	4:I:172:ARG:NH1	1.74	0.94
4:I:185:VAL:HG22	4:I:215:VAL:CG2	1.99	0.93
4:C:278:THR:HG23	4:C:279:GLN:N	1.84	0.91
3:H:134:LEU:HD23	3:H:137:GLN:OE1	1.72	0.90
2:G:97:ILE:HD12	2:G:99:PHE:CE1	2.07	0.90
2:A:108:ILE:O	2:A:112:GLN:HG2	1.74	0.85
2:G:57:MET:O	2:G:61:LYS:HG2	1.76	0.83
2:A:70:THR:CG2	2:A:92:ILE:HD11	2.08	0.83
2:G:27:ARG:HG2	2:G:28:PRO:HD2	1.57	0.83
4:I:278:THR:HG23	4:I:279:GLN:N	1.94	0.80
4:C:383:ASN:CG	4:C:384:ASP:H	1.89	0.80
2:G:58:GLU:CA	2:G:61:LYS:HE2	2.07	0.80
2:A:127:GLN:HB3	3:B:108:ARG:HG3	1.64	0.80
4:C:79:ILE:HD11	4:C:229:THR:HG21	1.64	0.80
2:G:7:LEU:HD12	2:G:64:ILE:HD11	1.62	0.79
4:I:370:ARG:HH22	7:I:802:ANP:HNB1	1.31	0.79
4:I:172:ARG:HH11	4:I:172:ARG:CG	1.88	0.78
4:I:362:ILE:HD11	4:I:396:TYR:CE1	2.19	0.77
4:I:278:THR:CG2	4:I:279:GLN:H	1.98	0.77
3:H:125:LYS:HG3	3:H:126:GLU:N	1.98	0.76
2:G:82:ARG:NH1	5:J:195:GLY:HA2	2.00	0.75
2:G:27:ARG:CG	2:G:28:PRO:HD2	2.16	0.75
4:C:278:THR:HG21	4:C:347:SER:HB2	1.69	0.74
4:C:206:ARG:HD2	5:D:221:ASP:OD1	1.88	0.74
3:B:109:ARG:HG3	3:B:110:THR:N	2.03	0.74
4:C:370:ARG:HH22	7:C:801:ANP:HNB1	1.37	0.73
2:A:97:ILE:HD12	2:A:99:PHE:CE1	2.24	0.72
4:C:275:LEU:HG	4:C:348:LEU:HD23	1.71	0.72
4:I:170:MET:HE3	4:I:170:MET:HA	1.72	0.72
4:I:185:VAL:HG22	4:I:215:VAL:HG21	1.71	0.72
4:I:405:MET:HE2	4:I:405:MET:HA	1.71	0.71
2:A:70:THR:HG21	2:A:92:ILE:CD1	2.16	0.71
4:I:216:LEU:HD22	4:I:233:MET:HE1	1.71	0.71
4:I:170:MET:HG3	4:I:175:SER:HB2	1.73	0.71
4:C:275:LEU:HD23	4:C:275:LEU:O	1.90	0.70
2:A:117:GLU:OE1	2:A:117:GLU:HA	1.91	0.70
2:A:90:ILE:CG2	2:A:92:ILE:HG23	2.21	0.69
5:J:236:LEU:HD11	5:J:245:ARG:NH1	2.06	0.69
4:C:69:ILE:O	4:C:73:ILE:HG12	1.91	0.69
4:I:370:ARG:NH2	7:I:802:ANP:HNB1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:26:VAL:HB	8:C:818:HOH:O	1.90	0.69
4:C:73:ILE:HD11	4:C:95:SER:HA	1.75	0.68
2:G:70:THR:HG22	2:G:97:ILE:HD13	1.74	0.68
3:B:106:LEU:HD23	3:B:113:LEU:HD23	1.77	0.67
4:C:335:ASP:OD1	4:C:364:ARG:HD2	1.95	0.67
2:G:6:TYR:HB3	2:G:91:VAL:HB	1.76	0.66
2:G:139:LEU:HB3	3:H:74:ILE:HD13	1.76	0.66
2:G:58:GLU:O	2:G:61:LYS:HG3	1.96	0.65
4:I:37:THR:HB	8:I:811:HOH:O	1.96	0.65
4:I:185:VAL:HG13	4:I:215:VAL:HG23	1.78	0.65
2:G:44:VAL:HG21	4:I:27:GLU:OE1	1.97	0.65
3:B:125:LYS:HG3	3:B:126:GLU:N	2.12	0.64
4:C:278:THR:HG22	8:C:969:HOH:O	1.97	0.64
4:I:362:ILE:CD1	4:I:396:TYR:CZ	2.81	0.64
2:G:27:ARG:HG2	2:G:28:PRO:CD	2.28	0.64
4:I:278:THR:CG2	4:I:347:SER:OG	2.46	0.63
4:I:278:THR:HG21	4:I:347:SER:OG	1.97	0.63
4:I:362:ILE:HD11	4:I:396:TYR:CZ	2.33	0.63
2:A:120:ARG:HH11	2:A:120:ARG:HG2	1.61	0.63
4:C:223:HIS:O	4:C:227:GLU:HG3	1.99	0.63
4:I:229:THR:HG23	4:I:233:MET:CE	2.17	0.63
2:A:7:LEU:CD1	2:A:90:ILE:HG12	2.29	0.63
4:C:278:THR:HG21	4:C:347:SER:CB	2.29	0.63
3:B:78:THR:CG2	3:B:145:SER:HB2	2.29	0.62
4:C:370:ARG:NH2	7:C:801:ANP:HNB1	1.97	0.62
3:B:78:THR:HG22	3:B:145:SER:HB2	1.80	0.62
4:I:288:ARG:NH1	4:I:291:ASP:HB2	2.15	0.62
4:C:275:LEU:CD2	4:C:330:VAL:HG22	2.30	0.61
4:C:383:ASN:CG	4:C:384:ASP:N	2.58	0.61
2:G:7:LEU:CD1	2:G:64:ILE:HD11	2.31	0.61
4:C:229:THR:HG23	4:C:233:MET:SD	2.41	0.61
2:A:117:GLU:OE1	2:A:117:GLU:CA	2.49	0.61
4:I:307:MET:HE1	4:I:320:MET:SD	2.41	0.61
4:C:148:GLU:OE1	4:C:148:GLU:HA	2.01	0.60
4:I:153:LEU:CD1	4:I:170:MET:HG2	2.31	0.60
2:G:58:GLU:HA	2:G:61:LYS:HE3	1.77	0.60
4:I:335:ASP:OD1	4:I:364:ARG:HD2	2.01	0.60
5:J:224:ARG:HG2	5:J:227:GLU:OE2	2.01	0.60
4:C:278:THR:O	4:C:329:ARG:HD2	2.01	0.60
4:I:404:PRO:O	4:I:405:MET:HE2	2.01	0.60
2:A:6:TYR:HB3	2:A:91:VAL:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:278:THR:CG2	4:C:279:GLN:N	2.57	0.60
4:I:343:VAL:O	4:I:346:VAL:HG13	2.02	0.60
4:I:172:ARG:HH12	4:I:173:ARG:HG2	1.67	0.59
4:C:382:LYS:HE2	8:C:986:HOH:O	2.02	0.59
4:I:106:GLU:O	4:I:108:GLN:HG3	2.02	0.59
2:A:97:ILE:HD12	2:A:99:PHE:CZ	2.38	0.59
4:I:208:LEU:O	5:J:220:HIS:HB3	2.02	0.59
3:B:77:VAL:HB	3:B:117:THR:CG2	2.33	0.58
2:G:139:LEU:HB3	3:H:74:ILE:CD1	2.32	0.58
4:I:308:HIS:CD2	4:I:311:MET:HE3	2.38	0.58
4:I:97:LEU:O	4:I:133:MET:HE1	2.04	0.58
3:B:109:ARG:HG3	3:B:110:THR:HG23	1.86	0.57
4:C:23:MET:HB3	8:C:818:HOH:O	2.04	0.57
4:I:382:LYS:O	4:I:383:ASN:C	2.48	0.57
4:C:46:ARG:HD3	4:C:133:MET:HE3	1.85	0.57
5:J:217:ARG:HD3	8:J:259:HOH:O	2.03	0.57
4:I:169:ASP:O	4:I:173:ARG:HG3	2.03	0.57
4:I:206:ARG:NH2	5:J:222:LYS:HE3	2.20	0.57
4:I:295:GLU:O	4:I:299:GLU:HG3	2.03	0.57
5:J:185:LYS:O	5:J:185:LYS:HG3	2.05	0.56
3:H:78:THR:HG22	3:H:79:GLY:N	2.19	0.56
4:C:268:LEU:HD11	4:C:282:ILE:HD13	1.87	0.56
2:A:115:ASP:N	2:A:116:PRO:HD3	2.21	0.56
4:C:315:GLU:O	4:C:319:ILE:HG12	2.05	0.56
4:C:275:LEU:HD23	4:C:275:LEU:C	2.31	0.56
4:I:37:THR:HG23	8:I:817:HOH:O	2.04	0.56
4:C:77:ASP:HB3	4:C:233:MET:HE2	1.86	0.55
2:A:97:ILE:HD12	2:A:99:PHE:HE1	1.70	0.55
4:C:51:ARG:CZ	4:I:59:GLU:HG2	2.36	0.55
4:I:31:SER:HB2	4:I:34:VAL:HG23	1.87	0.55
4:I:62:SER:OG	4:I:65:GLN:HG3	2.06	0.55
5:J:232:SER:OG	5:J:235:GLU:HG3	2.07	0.55
4:I:362:ILE:CD1	4:I:396:TYR:CE1	2.90	0.55
4:C:89:THR:HB	7:C:801:ANP:O1A	2.06	0.55
4:C:30:THR:HG23	4:C:239:ILE:HA	1.89	0.54
4:I:177:ARG:NH1	5:J:229:ALA:O	2.40	0.54
4:C:287:LYS:HG2	4:C:308:HIS:HB2	1.89	0.54
2:G:97:ILE:CD1	2:G:99:PHE:HE1	2.11	0.54
2:G:146:ILE:OXT	2:G:146:ILE:HG22	2.06	0.54
2:A:53:HIS:CE1	2:A:54:LYS:HG2	2.43	0.54
2:G:59:GLU:OE1	2:G:59:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:22:ASP:OD2	4:I:25:LYS:HB2	2.08	0.54
2:G:116:PRO:O	2:G:120:ARG:HB2	2.07	0.54
4:C:275:LEU:HD21	4:C:330:VAL:HG22	1.90	0.54
4:C:47:GLU:OE1	4:I:39:THR:HB	2.08	0.54
2:A:127:GLN:CB	3:B:108:ARG:HG3	2.36	0.54
2:G:58:GLU:HG2	2:G:61:LYS:CE	2.37	0.54
3:H:137:GLN:HB3	8:H:157:HOH:O	2.08	0.54
3:B:123:THR:OG1	3:B:126:GLU:HG3	2.07	0.53
3:H:125:LYS:HG3	3:H:126:GLU:H	1.73	0.53
4:I:89:THR:HB	7:I:802:ANP:O1A	2.08	0.53
4:C:23:MET:HE1	8:C:896:HOH:O	2.08	0.53
4:I:278:THR:CG2	4:I:279:GLN:N	2.61	0.53
4:C:46:ARG:NH1	4:C:133:MET:HE3	2.24	0.53
4:C:383:ASN:OD1	4:C:384:ASP:N	2.38	0.53
3:B:125:LYS:CG	3:B:126:GLU:N	2.71	0.53
4:I:223:HIS:O	4:I:227:GLU:HG3	2.08	0.53
4:C:307:MET:HE1	4:C:320:MET:HG2	1.90	0.53
4:C:383:ASN:O	4:C:386:ILE:HG22	2.09	0.53
4:I:362:ILE:HD13	4:I:396:TYR:CZ	2.44	0.52
4:C:80:ALA:HB3	4:C:217:ILE:HD13	1.91	0.52
4:C:307:MET:HA	4:C:311:MET:SD	2.49	0.52
2:G:91:VAL:HG22	2:G:96:HIS:HD2	1.74	0.52
4:C:277:ILE:HG13	8:C:882:HOH:O	2.10	0.52
3:B:104:LEU:HD22	3:B:113:LEU:HD13	1.91	0.52
4:C:313:GLN:HA	4:C:316:ARG:HG3	1.90	0.52
4:I:216:LEU:HD22	4:I:233:MET:CE	2.39	0.52
2:A:92:ILE:HG13	2:A:92:ILE:O	2.09	0.52
4:C:71:GLN:HG3	4:C:237:ILE:HG21	1.92	0.52
2:G:58:GLU:HG2	2:G:61:LYS:NZ	2.24	0.52
4:I:23:MET:HA	4:I:26:VAL:HG23	1.92	0.52
2:G:110:VAL:HG13	2:G:119:LEU:HB3	1.91	0.52
4:C:225:ILE:HD13	4:C:228:MET:HE3	1.93	0.51
2:G:143:ILE:HD13	4:I:67:ARG:NH2	2.25	0.51
4:I:30:THR:HG23	4:I:239:ILE:HA	1.92	0.51
3:B:82:GLU:CG	3:B:112:TYR:HB3	2.40	0.51
3:B:74:ILE:HD13	3:B:120:GLU:HG3	1.93	0.51
4:C:307:MET:HE1	4:C:320:MET:SD	2.51	0.51
4:C:322:GLU:HG3	4:C:327:ALA:HB3	1.94	0.50
4:I:348:LEU:HD13	4:I:376:VAL:HB	1.93	0.50
4:C:256:VAL:CG2	4:C:403:MET:HE2	2.41	0.50
4:C:185:VAL:HG22	4:C:215:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:117:GLU:OE2	4:I:316:ARG:HD2	2.09	0.50
4:I:120:VAL:O	4:I:124:LYS:HG2	2.11	0.50
4:I:79:ILE:HD11	4:I:229:THR:HG21	1.94	0.50
4:I:288:ARG:HH12	4:I:291:ASP:CB	2.25	0.50
2:A:5:PHE:CE1	2:A:92:ILE:HG22	2.46	0.49
5:J:224:ARG:CG	5:J:227:GLU:CG	2.80	0.49
4:I:146:VAL:O	4:I:150:ILE:HG13	2.13	0.49
2:A:7:LEU:HD22	2:A:64:ILE:HD11	1.93	0.49
2:A:126:VAL:HG12	2:A:130:LYS:HE2	1.93	0.49
4:C:244:ASP:HB2	4:C:397:SER:HB2	1.95	0.48
4:I:206:ARG:HD2	5:J:221:ASP:OD1	2.12	0.48
2:A:111:ASN:HA	2:A:116:PRO:HB3	1.95	0.48
3:B:77:VAL:HB	3:B:117:THR:HG23	1.95	0.48
4:C:89:THR:HA	4:C:92:PHE:CE2	2.48	0.48
4:C:277:ILE:N	8:C:882:HOH:O	2.46	0.48
4:I:267:THR:HG23	8:I:934:HOH:O	2.12	0.48
3:B:142:GLN:HG2	8:B:160:HOH:O	2.12	0.48
4:C:206:ARG:HB3	5:D:222:LYS:HG3	1.95	0.48
3:B:77:VAL:HB	3:B:117:THR:HG22	1.95	0.48
2:A:24:PHE:HA	2:A:33:ARG:O	2.14	0.48
5:J:224:ARG:HG2	5:J:227:GLU:HG3	1.90	0.48
4:C:172:ARG:NH2	8:C:1010:HOH:O	2.47	0.48
4:C:206:ARG:CZ	5:D:222:LYS:HE3	2.44	0.48
3:B:82:GLU:HG3	3:B:112:TYR:HB3	1.96	0.47
4:C:349:ILE:HG12	4:C:368:SER:HB3	1.95	0.47
4:C:307:MET:HE2	4:C:319:ILE:CG2	2.44	0.47
4:I:26:VAL:HG23	8:I:976:HOH:O	2.13	0.47
4:I:204:VAL:O	4:I:208:LEU:HD13	2.13	0.47
4:I:207:TYR:CZ	5:J:222:LYS:HD3	2.49	0.47
4:C:70:LYS:O	4:C:74:LYS:HG3	2.13	0.47
2:A:70:THR:HG23	8:A:182:HOH:O	2.13	0.47
3:B:125:LYS:NZ	3:B:126:GLU:HG3	2.29	0.47
2:G:10:TYR:HB3	2:G:87:GLU:HB2	1.96	0.47
3:B:107:ASP:OD1	3:B:109:ARG:HG2	2.15	0.47
4:C:154:ASP:OD1	5:D:231:LYS:HD2	2.15	0.47
2:A:7:LEU:HD12	2:A:90:ILE:HG12	1.95	0.47
4:C:206:ARG:NH2	5:D:222:LYS:HE3	2.29	0.47
4:C:225:ILE:HA	4:C:228:MET:HE3	1.96	0.47
4:I:206:ARG:CZ	5:J:222:LYS:HE3	2.44	0.47
2:A:97:ILE:CD1	2:A:99:PHE:HE1	2.27	0.47
2:G:90:ILE:HG22	2:G:92:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:125:LYS:HZ3	3:B:126:GLU:CG	2.27	0.46
8:C:926:HOH:O	4:I:60:LYS:HA	2.15	0.46
2:A:16:LYS:NZ	8:A:160:HOH:O	2.48	0.46
2:A:120:ARG:HG2	2:A:120:ARG:NH1	2.30	0.46
5:D:193:LEU:HD23	5:D:193:LEU:HA	1.68	0.46
4:I:167:VAL:O	4:I:171:ILE:HG13	2.15	0.46
4:C:269:CYS:SG	4:C:297:MET:HE1	2.56	0.46
4:I:182:LYS:HE3	8:I:916:HOH:O	2.15	0.46
4:I:288:ARG:HH12	4:I:291:ASP:HB2	1.80	0.46
3:B:131:MET:HE1	3:B:148:TRP:CD1	2.51	0.46
4:I:172:ARG:NH1	4:I:173:ARG:HG2	2.31	0.46
5:J:226:ASP:OD1	5:J:226:ASP:O	2.32	0.46
2:A:5:PHE:HE1	2:A:92:ILE:HG22	1.80	0.46
3:H:129:ALA:O	3:H:132:GLU:HG2	2.15	0.46
2:A:54:LYS:O	2:A:58:GLU:HG2	2.15	0.46
4:I:27:GLU:OE1	4:I:27:GLU:HA	2.16	0.46
2:G:102:SER:HB2	8:G:172:HOH:O	2.14	0.46
4:I:82:SER:O	4:I:219:ALA:HA	2.16	0.46
4:C:267:THR:O	4:C:271:LEU:HD13	2.17	0.45
2:G:132:LEU:HD13	3:H:116:TYR:CZ	2.52	0.45
4:C:275:LEU:CD2	4:C:330:VAL:CG2	2.94	0.45
2:G:146:ILE:HG13	8:I:899:HOH:O	2.16	0.45
4:C:265:PHE:CZ	4:C:296:LYS:HG2	2.51	0.45
4:C:307:MET:HA	4:C:311:MET:CE	2.47	0.45
4:I:307:MET:HE2	4:I:319:ILE:CG2	2.47	0.45
4:C:51:ARG:NH2	4:I:59:GLU:HG2	2.31	0.45
5:D:243:ASP:HB3	5:D:246:SER:OG	2.17	0.45
4:I:378:ILE:HD13	4:I:403:MET:SD	2.56	0.45
3:B:125:LYS:HZ3	3:B:126:GLU:HG3	1.81	0.45
4:I:89:THR:HG21	8:I:912:HOH:O	2.17	0.45
2:A:5:PHE:HE2	2:A:60:LEU:HD23	1.82	0.44
3:B:109:ARG:CG	3:B:110:THR:N	2.77	0.44
4:I:185:VAL:HG22	4:I:215:VAL:HG22	1.94	0.44
4:C:148:GLU:OE2	4:C:152:LYS:HE2	2.17	0.44
4:C:73:ILE:CD1	4:C:95:SER:HA	2.46	0.44
4:I:112:LEU:HD11	4:I:204:VAL:HG21	2.00	0.44
4:I:275:LEU:HD23	4:I:348:LEU:HD23	1.98	0.44
2:G:127:GLN:HB3	3:H:108:ARG:HG3	2.00	0.44
3:H:117:THR:HG22	3:H:118:LEU:N	2.32	0.44
1:L:5:U:H1'	4:I:169:ASP:HB2	1.99	0.44
3:H:104:LEU:HG	3:H:113:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:82:SER:O	4:C:219:ALA:HA	2.17	0.44
4:C:403:MET:HG3	4:C:411:ILE:HD12	2.00	0.44
4:I:362:ILE:N	4:I:362:ILE:HD12	2.32	0.44
3:B:123:THR:OG1	3:B:126:GLU:CG	2.66	0.44
2:G:54:LYS:O	2:G:58:GLU:HG3	2.17	0.44
4:I:353:ASP:OD2	5:J:182:ILE:HD11	2.18	0.44
4:C:260:ARG:HG2	4:C:262:GLU:H	1.83	0.44
4:C:274:THR:HG21	4:C:409:ASP:OD1	2.17	0.44
4:I:312:PRO:HD2	4:I:315:GLU:OE1	2.18	0.44
4:C:265:PHE:CE1	4:C:297:MET:HE3	2.53	0.43
2:G:115:ASP:O	2:G:115:ASP:CG	2.61	0.43
4:C:22:ASP:OD1	4:C:22:ASP:C	2.61	0.43
4:C:81:GLN:HB2	4:C:221:LEU:HD12	1.99	0.43
3:H:78:THR:CG2	3:H:79:GLY:N	2.81	0.43
2:G:85:ARG:HD3	2:G:87:GLU:OE2	2.18	0.43
4:I:172:ARG:NH1	4:I:172:ARG:CG	2.58	0.43
4:I:116:ARG:HG2	4:I:141:ILE:HB	2.00	0.43
4:I:197:PHE:O	4:I:201:ILE:HG12	2.17	0.43
4:I:287:LYS:HG2	4:I:308:HIS:HB2	2.00	0.43
4:C:23:MET:O	4:C:227:GLU:HG2	2.18	0.43
4:C:254:PHE:HA	4:C:401:ASP:O	2.18	0.43
4:C:271:LEU:HD11	4:C:408:ALA:HB1	2.00	0.43
2:A:5:PHE:HD2	2:A:57:MET:HE3	1.84	0.43
4:C:194:ASN:HB3	8:C:870:HOH:O	2.17	0.43
4:C:208:LEU:O	5:D:220:HIS:HB3	2.19	0.43
4:C:307:MET:HE1	4:C:320:MET:CG	2.49	0.43
3:B:131:MET:HE2	3:B:147:ASP:C	2.44	0.43
3:B:137:GLN:O	3:B:143:PRO:HA	2.19	0.42
2:G:5:PHE:CZ	2:G:64:ILE:HD12	2.53	0.42
2:G:7:LEU:HD12	2:G:64:ILE:CD1	2.42	0.42
4:I:201:ILE:O	4:I:204:VAL:HG22	2.20	0.42
4:I:405:MET:HE2	4:I:405:MET:CA	2.46	0.42
4:I:265:PHE:CE1	4:I:296:LYS:HB3	2.55	0.42
4:I:295:GLU:HA	4:I:295:GLU:OE1	2.19	0.42
5:D:233:ARG:HG3	5:D:243:ASP:OD2	2.19	0.42
4:I:112:LEU:C	4:I:192:MET:HE2	2.45	0.42
4:C:173:ARG:CB	4:C:173:ARG:HH21	2.33	0.42
4:I:112:LEU:HB3	4:I:192:MET:CE	2.50	0.42
4:I:153:LEU:HD11	4:I:170:MET:HG2	2.02	0.42
4:I:403:MET:HG2	4:I:407:VAL:HG21	2.01	0.42
4:C:307:MET:HE2	4:C:319:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:101:ASP:OD1	4:I:103:GLN:HB2	2.19	0.42
4:I:202:TYR:CZ	4:I:206:ARG:HD3	2.55	0.42
2:G:5:PHE:HZ	2:G:64:ILE:HD12	1.84	0.42
4:I:407:VAL:O	4:I:410:LEU:HB2	2.18	0.42
4:C:148:GLU:OE1	4:C:148:GLU:CA	2.65	0.42
4:C:265:PHE:CE1	4:C:297:MET:CE	3.03	0.42
4:I:71:GLN:HG3	4:I:237:ILE:HG21	2.02	0.42
5:J:184:ARG:HH11	5:J:189:PHE:HE1	1.67	0.42
4:I:174:ARG:HH12	5:J:227:GLU:HB3	1.85	0.42
4:I:232:PHE:CE1	4:I:233:MET:HE2	2.55	0.42
4:I:337:TRP:CD2	4:I:341:LEU:HD12	2.55	0.42
5:J:239:LEU:CD1	5:J:240:TYR:CE2	3.02	0.42
4:C:205:TYR:O	5:D:220:HIS:HD2	2.03	0.41
4:C:378:ILE:HD13	4:C:403:MET:HE1	2.02	0.41
4:I:113:ALA:O	4:I:163:THR:HG22	2.19	0.41
4:I:89:THR:HA	4:I:92:PHE:CE2	2.55	0.41
4:I:404:PRO:O	4:I:407:VAL:HG23	2.20	0.41
5:J:182:ILE:O	5:J:184:ARG:HG2	2.21	0.41
2:A:76:LEU:HB3	2:A:114:LYS:HB2	2.02	0.41
2:A:90:ILE:CG2	2:A:92:ILE:CG2	2.95	0.41
2:G:15:GLY:O	2:G:16:LYS:C	2.63	0.41
2:G:55:SER:O	2:G:58:GLU:HB2	2.20	0.41
4:C:67:ARG:HG3	4:C:67:ARG:HH11	1.86	0.41
4:C:353:ASP:O	4:C:364:ARG:NH2	2.53	0.41
4:C:258:VAL:HB	4:C:263:TRP:HB2	2.02	0.41
4:C:117:GLU:HB2	8:C:971:HOH:O	2.19	0.41
4:I:278:THR:O	4:I:279:GLN:HG3	2.20	0.41
4:C:46:ARG:HD3	4:C:133:MET:CE	2.51	0.41
4:C:88:LYS:NZ	7:C:801:ANP:O1G	2.50	0.41
4:C:109:ALA:HB3	4:C:159:VAL:HG22	2.02	0.41
4:C:271:LEU:O	4:C:275:LEU:HB2	2.21	0.41
2:G:146:ILE:HG21	8:I:863:HOH:O	2.19	0.41
4:I:139:ALA:HA	4:I:161:ALA:O	2.20	0.41
4:I:283:PHE:CE1	4:I:364:ARG:HG2	2.56	0.41
4:I:354:LEU:CD1	4:I:385:ASP:HB3	2.51	0.41
4:I:404:PRO:C	4:I:405:MET:HE2	2.45	0.41
3:H:95:GLU:HA	3:H:95:GLU:OE1	2.21	0.41
4:I:312:PRO:HG2	4:I:315:GLU:HB2	2.02	0.41
3:B:131:MET:HE1	3:B:148:TRP:CG	2.56	0.40
5:D:233:ARG:O	5:D:237:ILE:HG13	2.22	0.40
2:G:17:PHE:CE2	5:J:192:ASP:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:ASN:HA	2:G:116:PRO:HB3	2.03	0.40
4:I:88:LYS:HB3	4:I:217:ILE:CG2	2.51	0.40
4:I:349:ILE:HG12	4:I:368:SER:HB3	2.03	0.40
4:C:169:ASP:OD1	4:C:170:MET:HE2	2.21	0.40
3:H:106:LEU:HD23	3:H:113:LEU:HD23	2.04	0.40
4:C:89:THR:HG21	8:C:897:HOH:O	2.22	0.40
4:C:150:ILE:HD11	4:C:173:ARG:HH22	1.86	0.40
2:G:41:LYS:HE2	5:J:190:GLU:OE2	2.21	0.40
4:I:288:ARG:HA	4:I:288:ARG:HD2	1.82	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	
2	A	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
2	G	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
3	B	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	11	13
3	H	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
4	C	390/413 (94%)	378 (97%)	9 (2%)	3 (1%)	16	20
4	I	390/413 (94%)	374 (96%)	13 (3%)	3 (1%)	16	20
5	D	52/77 (68%)	50 (96%)	2 (4%)	0	100	100
5	J	47/77 (61%)	42 (89%)	4 (8%)	1 (2%)	5	4
All	All	1341/1454 (92%)	1294 (96%)	39 (3%)	8 (1%)	21	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	383	ASN

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Mol	Chain	Res	Type
4	I	383	ASN
3	B	115	GLY
4	C	340	GLY
4	C	385	ASP
4	I	340	GLY
5	J	243	ASP
4	I	385	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	132/134 (98%)	131 (99%)	1 (1%)	73	86
2	G	132/134 (98%)	129 (98%)	3 (2%)	44	63
3	B	76/76 (100%)	75 (99%)	1 (1%)	61	77
3	H	76/76 (100%)	75 (99%)	1 (1%)	61	77
4	C	347/363 (96%)	340 (98%)	7 (2%)	48	67
4	I	347/363 (96%)	341 (98%)	6 (2%)	53	72
5	D	50/69 (72%)	50 (100%)	0	100	100
5	J	44/69 (64%)	43 (98%)	1 (2%)	44	63
All	All	1204/1284 (94%)	1184 (98%)	20 (2%)	53	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	117	GLU
3	B	118	LEU
4	C	37	THR
4	C	194	ASN
4	C	301	ASN
4	C	316	ARG
4	C	337	TRP
4	C	360	LEU

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Mol	Chain	Res	Type
4	C	407	VAL
2	G	115	ASP
2	G	119	LEU
2	G	125	LEU
3	H	125	LYS
4	I	170	MET
4	I	172	ARG
4	I	263	TRP
4	I	288	ARG
4	I	337	TRP
4	I	346	VAL
5	J	239	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	37	ASN
4	C	136	GLN
4	C	157	GLN
4	C	301	ASN
4	C	345	GLN
4	C	394	GLN
2	G	86	GLN
3	H	67	GLN
4	I	138	HIS
4	I	345	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	F	5/6 (83%)	0	0
1	L	5/6 (83%)	0	0
All	All	10/12 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	ANP	C	801	6	33,33,33	1.24	4 (12%)	45,52,52	1.94	9 (20%)
7	ANP	I	802	6	33,33,33	1.19	4 (12%)	45,52,52	1.77	8 (17%)

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
7	ANP	C	801	6	-	3/18/38/38	0/3/3/3
7	ANP	I	802	6	-	3/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	801	ANP	C4-N9	-3.18	1.31	1.37
7	I	802	ANP	C5-N7	-3.00	1.33	1.39
7	C	801	ANP	PB-O1B	2.32	1.49	1.46
7	I	802	ANP	PA-O3A	2.23	1.61	1.59
7	I	802	ANP	C4-N9	-2.18	1.33	1.37
7	C	801	ANP	C5-N7	-2.16	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	801	ANP	PG-O1G	2.10	1.49	1.46
7	I	802	ANP	C8-N9	-2.08	1.34	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	801	ANP	C5-C4-N3	-6.36	117.96	126.72
7	I	802	ANP	C5-C4-N3	-5.46	119.19	126.72
7	I	802	ANP	N3-C2-N1	-4.42	121.89	128.58
7	C	801	ANP	N3-C2-N1	-4.16	122.28	128.58
7	C	801	ANP	N3-C4-N9	4.06	134.07	127.17
7	C	801	ANP	C4-C5-N7	-4.04	105.97	110.58
7	I	802	ANP	N3-C4-N9	3.67	133.41	127.17
7	C	801	ANP	C2-N3-C4	3.64	120.72	111.83
7	I	802	ANP	C2-N3-C4	3.48	120.33	111.83
7	C	801	ANP	N9-C8-N7	-3.14	109.48	113.94
7	C	801	ANP	C5-N7-C8	3.11	108.33	103.45
7	I	802	ANP	N9-C8-N7	-3.02	109.65	113.94
7	I	802	ANP	O1G-PG-N3B	2.81	115.91	111.77
7	C	801	ANP	O1G-PG-N3B	2.72	115.78	111.77
7	I	802	ANP	C4-C5-N7	-2.70	107.49	110.58
7	I	802	ANP	C5-N7-C8	2.69	107.67	103.45
7	C	801	ANP	C4-N9-C8	2.39	108.25	105.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

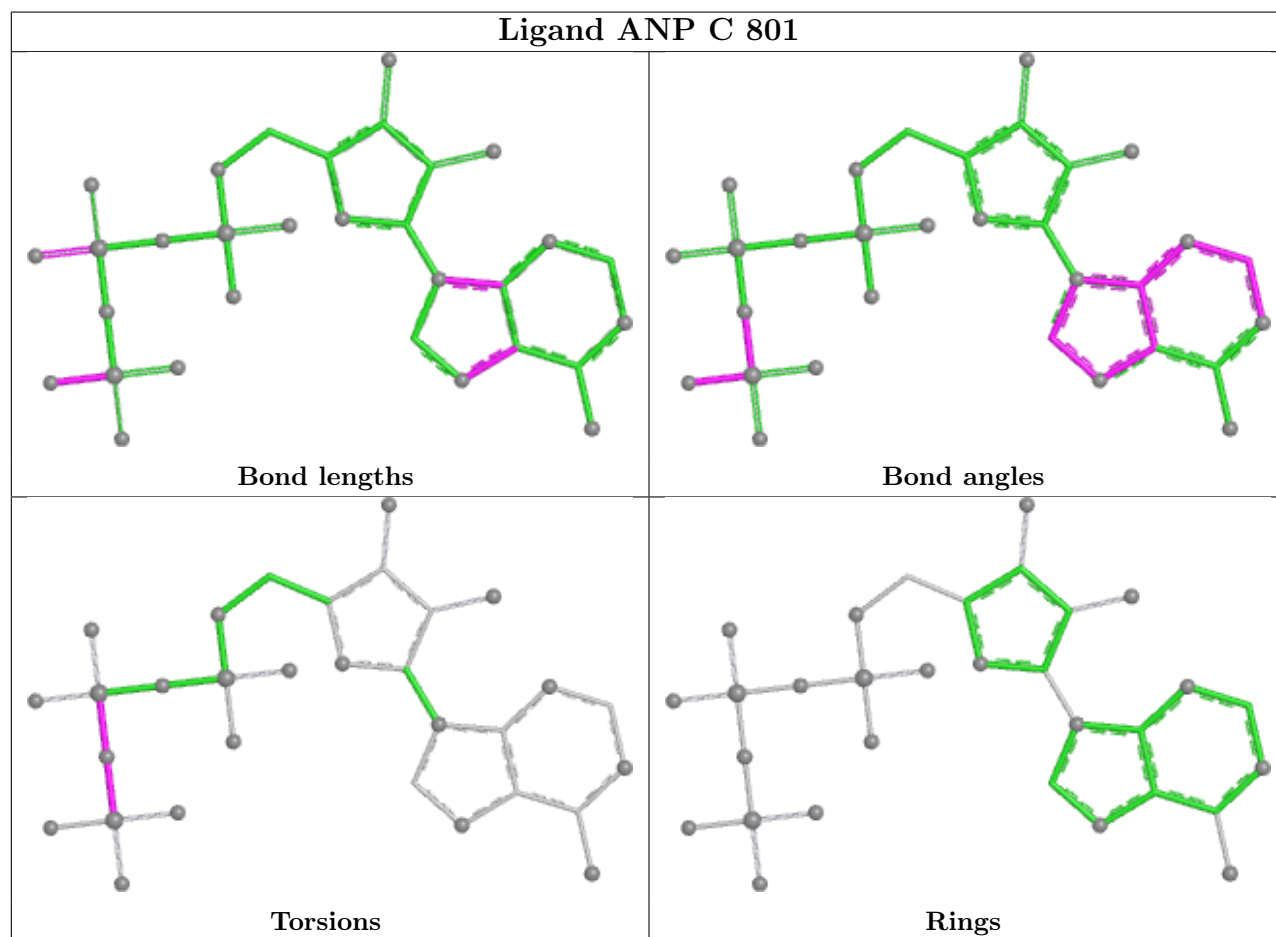
Mol	Chain	Res	Type	Atoms
7	C	801	ANP	PB-N3B-PG-O1G
7	C	801	ANP	PG-N3B-PB-O1B
7	C	801	ANP	PG-N3B-PB-O3A
7	I	802	ANP	PB-N3B-PG-O1G
7	I	802	ANP	PG-N3B-PB-O1B
7	I	802	ANP	PG-N3B-PB-O3A

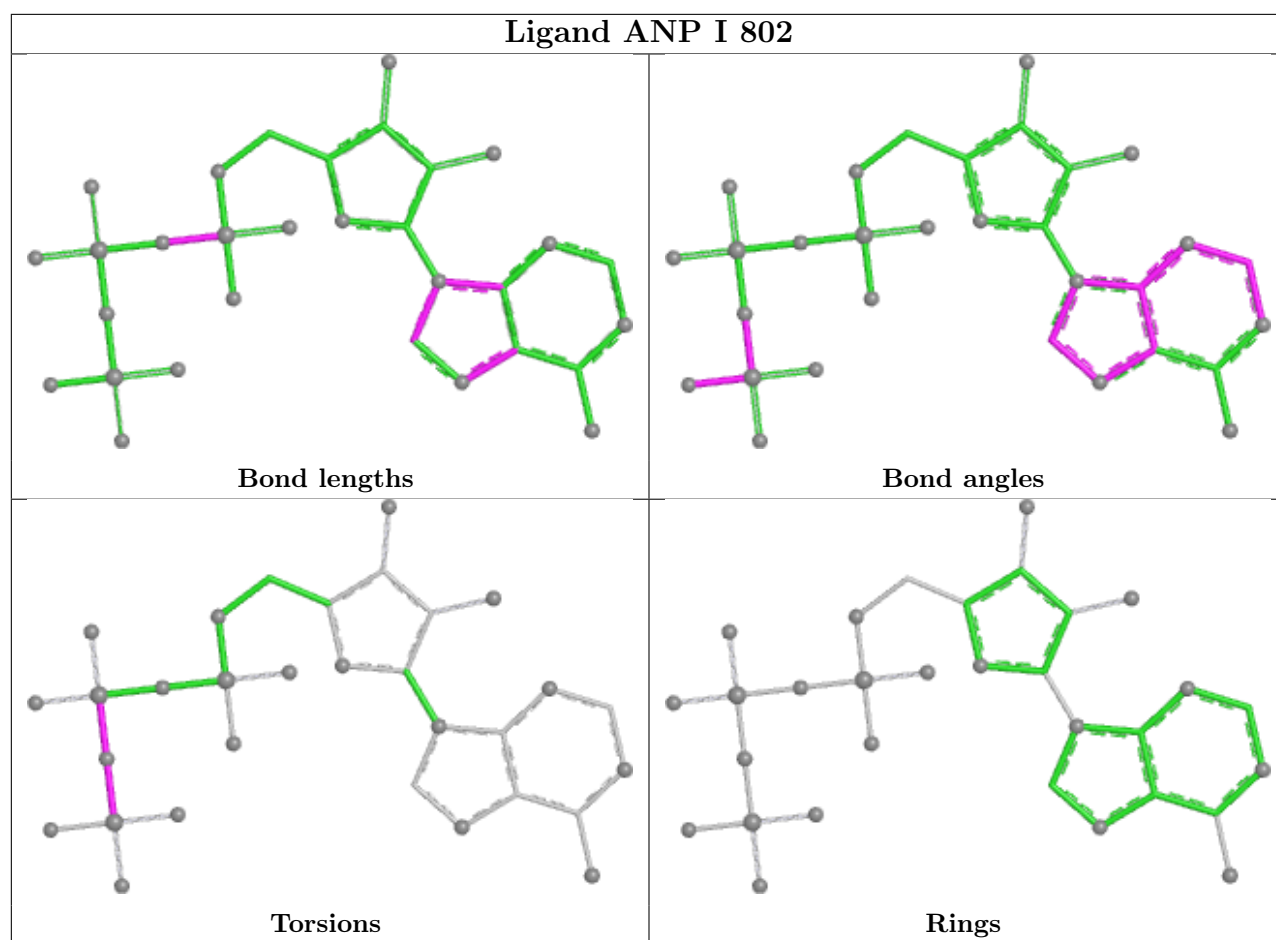
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	801	ANP	4	0
7	I	802	ANP	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	F	6/6 (100%)	-0.09	0 100 100	39, 44, 59, 67	0
1	L	6/6 (100%)	0.16	0 100 100	46, 49, 62, 79	0
2	A	144/146 (98%)	0.24	7 (4%) 35 36	35, 55, 80, 98	0
2	G	144/146 (98%)	-0.03	4 (2%) 55 57	37, 48, 74, 99	0
3	B	91/91 (100%)	0.19	4 (4%) 39 41	38, 52, 70, 80	0
3	H	91/91 (100%)	0.74	5 (5%) 30 32	46, 74, 86, 92	0
4	C	392/413 (94%)	-0.07	13 (3%) 49 51	30, 44, 75, 98	0
4	I	392/413 (94%)	0.09	7 (1%) 67 69	31, 50, 72, 99	0
5	D	56/77 (72%)	0.39	3 (5%) 31 33	44, 55, 77, 81	0
5	J	51/77 (66%)	1.03	6 (11%) 9 10	39, 69, 83, 84	0
All	All	1373/1466 (93%)	0.14	49 (3%) 46 48	30, 50, 81, 99	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	92	ILE	4.8
2	A	94	ASP	4.0
4	I	27	GLU	4.0
3	H	64	PRO	3.9
4	C	23	MET	3.7
2	G	92	ILE	3.6
4	C	409	ASP	3.6
2	G	94	ASP	3.3
4	C	383	ASN	3.3
3	B	64	PRO	3.2
4	I	23	MET	3.1
5	D	234	GLN	3.1
3	H	137	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
4	C	260	ARG	3.0
4	C	407	VAL	2.9
4	C	277	ILE	2.8
5	D	246	SER	2.7
5	J	239	LEU	2.7
3	B	109	ARG	2.7
5	J	184	ARG	2.7
5	D	170	LEU	2.7
4	C	24	THR	2.6
4	I	22	ASP	2.5
4	I	172	ARG	2.5
4	I	384	ASP	2.5
2	A	97	ILE	2.4
5	J	244	ILE	2.4
5	J	185	LYS	2.4
3	H	138	ASP	2.4
4	C	411	ILE	2.4
4	C	405	MET	2.4
4	C	410	LEU	2.3
2	A	112	GLN	2.3
3	B	154	PRO	2.2
2	G	93	GLY	2.2
4	I	405	MET	2.2
5	J	224	ARG	2.2
4	C	211	ALA	2.2
4	I	299	GLU	2.2
3	B	152	ARG	2.1
2	A	117	GLU	2.1
2	A	91	VAL	2.1
2	A	3	SER	2.1
4	C	229	THR	2.1
3	H	95	GLU	2.0
3	H	139	LEU	2.0
2	G	61	LYS	2.0
4	C	60	LYS	2.0
5	J	238	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

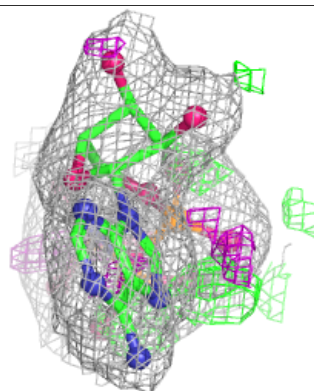
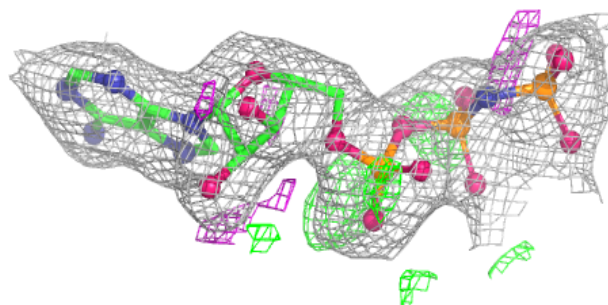
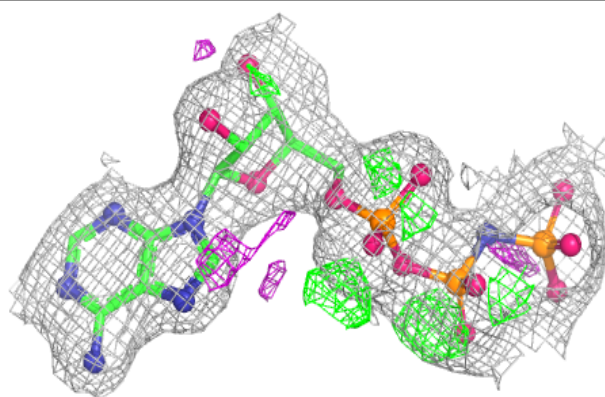
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

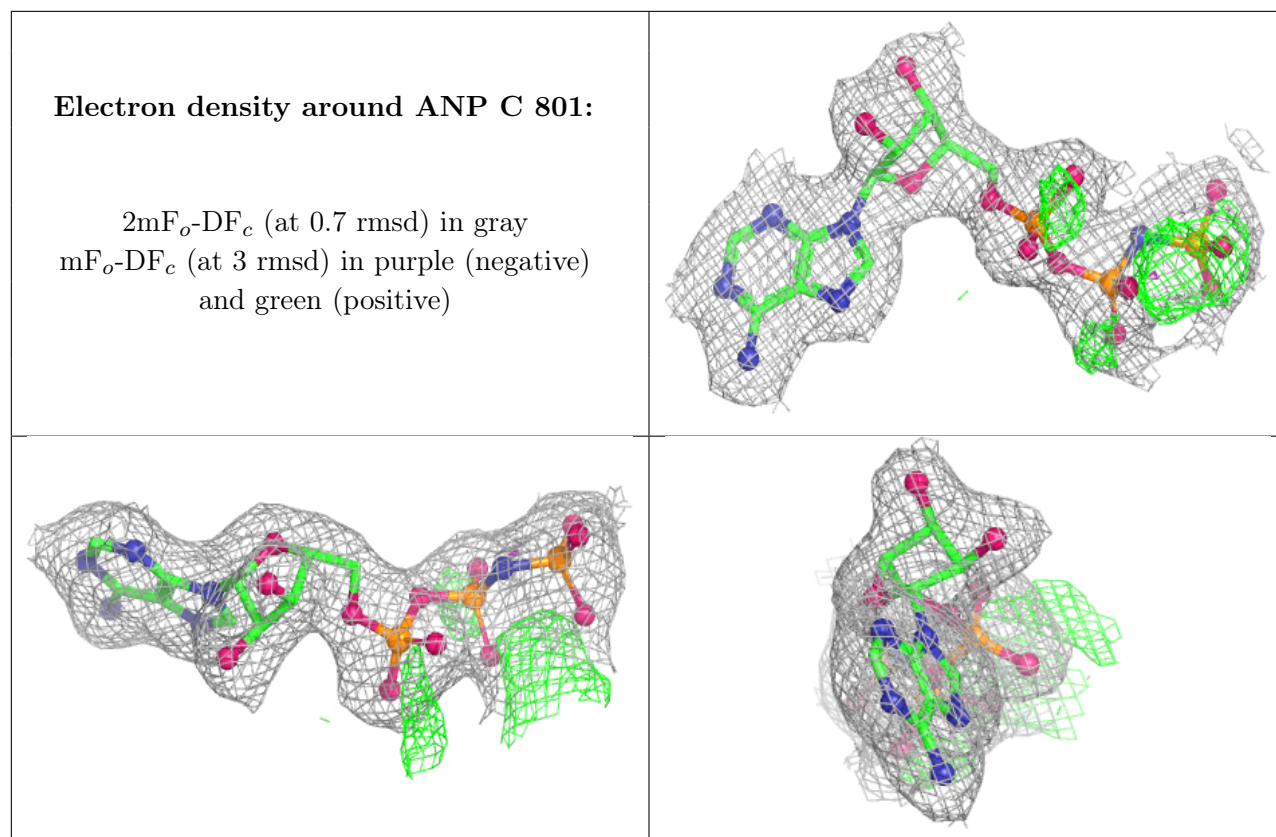
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	701	1/1	0.96	0.17	35,35,35,35	0
6	MG	I	702	1/1	0.97	0.10	39,39,39,39	0
7	ANP	I	802	31/31	0.97	0.07	33,40,43,44	0
7	ANP	C	801	31/31	0.98	0.06	31,34,35,37	0

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 ANP I 802:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.