



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 AM UTC

PDB ID : 2JDI / pdb_00002jdi
Title : Ground state structure of F1-ATPase from bovine heart mitochondria (Bovine F1-ATPase crystallised in the absence of azide)
Authors : Bowler, M.W.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2007-01-09
Resolution : 1.90 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

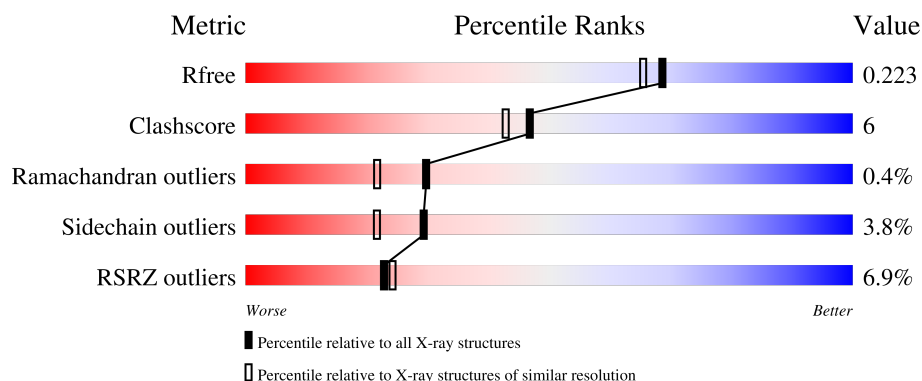
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	510	3% 86% 9% • 5%
1	B	510	8% 85% 8% • 6%
1	C	510	3% 86% 8% • 5%
2	D	482	2% 87% 8% • •
2	E	482	7% 82% 11% • 5%

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Mol	Chain	Length	Quality of chain
2	F	482	4% 87% 8%
3	G	273	19% 51% 14% 33%
4	H	146	18% 41% 16% 40%
5	I	50	8% 44% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26426 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	2	0
			3726	2348	659	707	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	SEE REMARK 999	UNP P19483
B	481	GLY	SER	SEE REMARK 999	UNP P19483
C	481	GLY	SER	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	3	1	0
			3544	2248	601	684	11			
2	E	458	Total	C	N	O	S	5	2	0
			3481	2207	593	671	10			
2	F	466	Total	C	N	O	S	1	2	0
			3538	2246	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	184	Total	C	N	O	S	0	0	0
			1417	894	252	265	6			

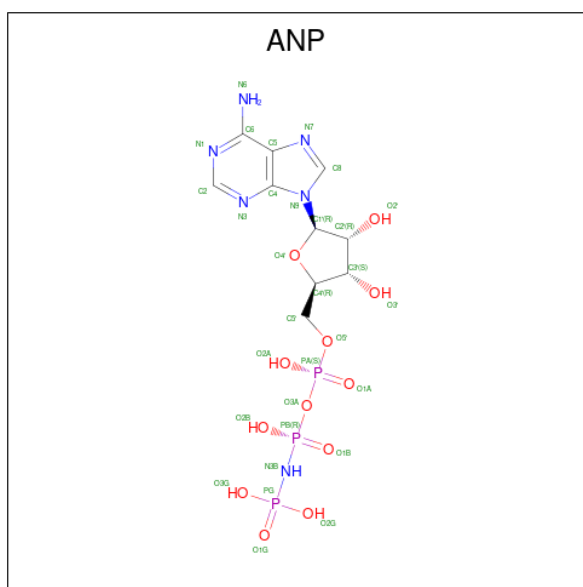
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	88	Total	C	N	O	S	0	0	0
			657	417	108	131	1			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	25	Total	C	N	O	S	0	0	0
			203	130	38	34	1			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

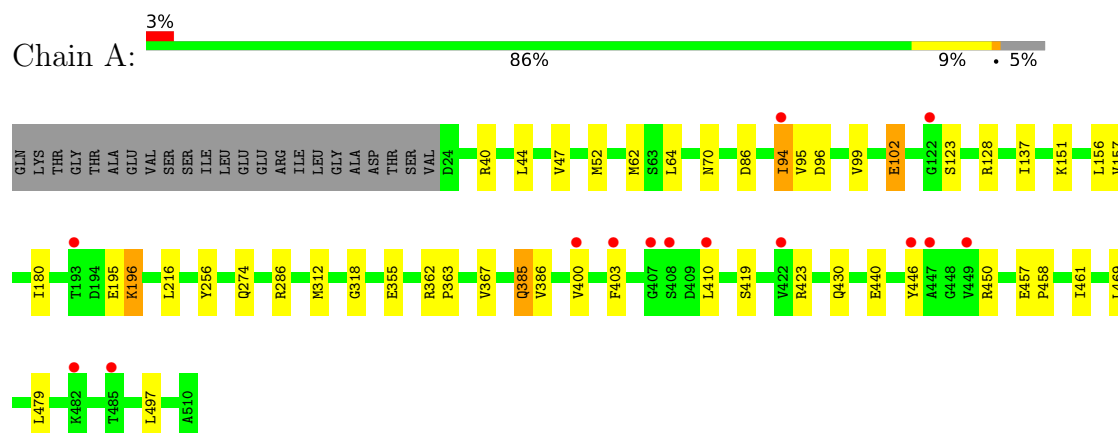
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	B	348	Total O 348 348	0	0
8	C	367	Total O 367 367	0	0
8	D	389	Total O 389 389	0	0
8	E	267	Total O 267 267	0	0
8	F	436	Total O 436 436	0	0
8	G	114	Total O 114 114	0	0
8	H	31	Total O 31 31	0	0
8	I	16	Total O 16 16	0	0

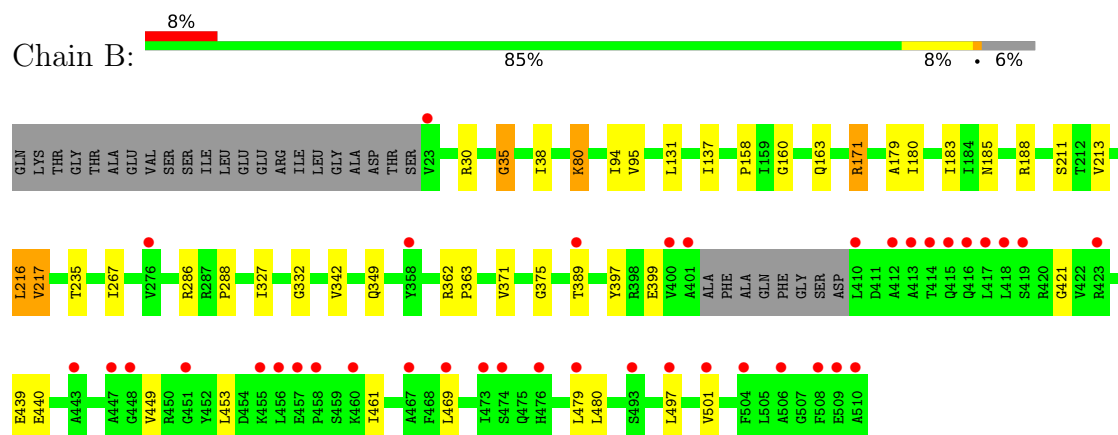
3 Residue-property plots [i](#)

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.

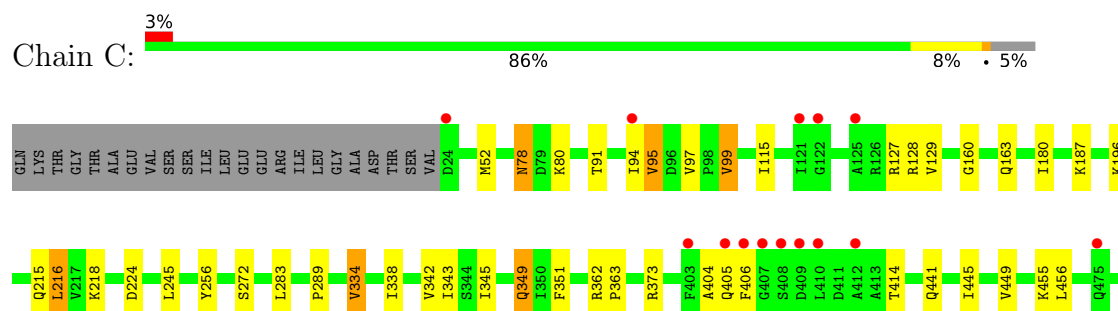
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

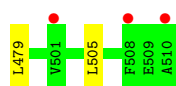


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

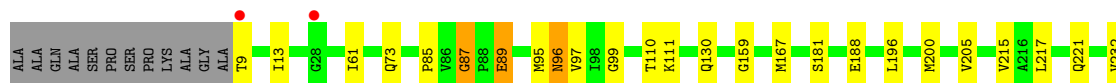
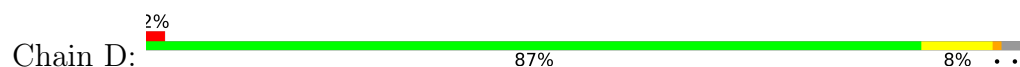


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

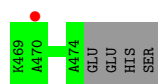
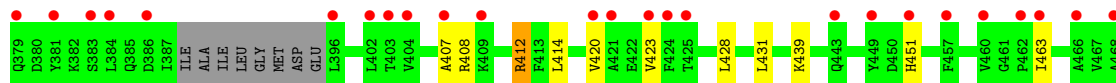
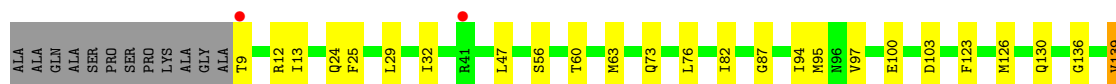
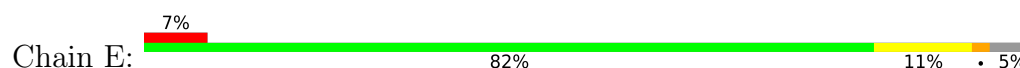




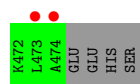
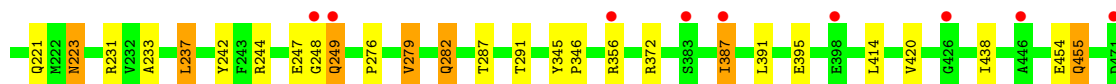
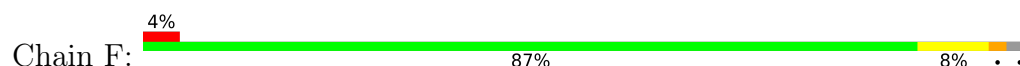
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• Molecule 2: ATP SYNTHASE SUBUNIT BETA

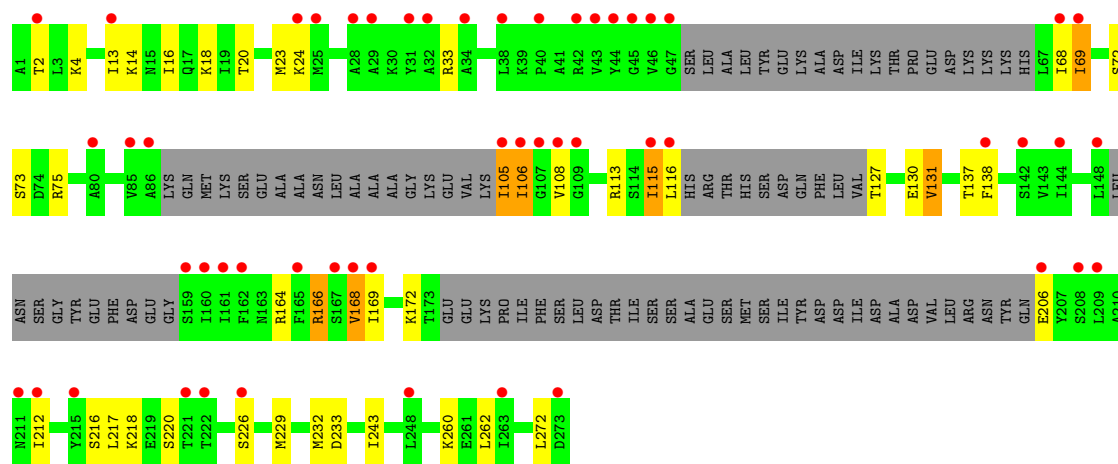


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

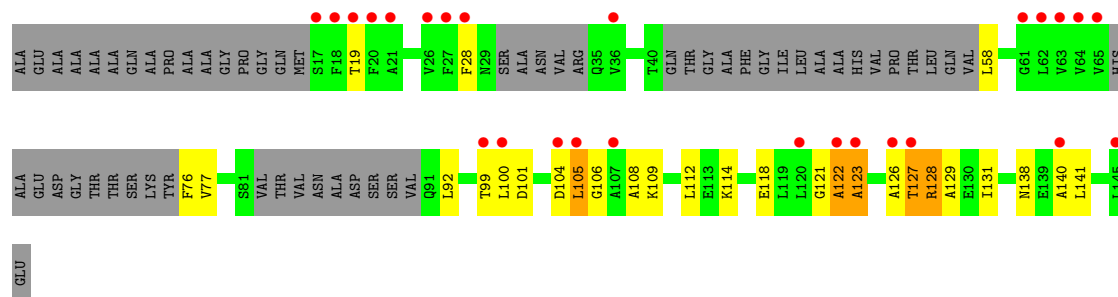


• Molecule 3: ATP SYNTHASE GAMMA CHAIN

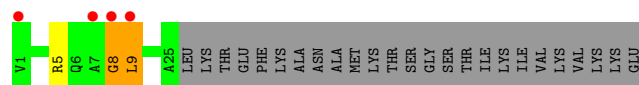
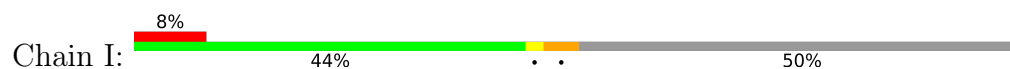




• Molecule 4: ATP SYNTHASE DELTA CHAIN



• Molecule 5: ATP SYNTHASE EPSILON CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.61Å 123.13Å 261.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	72.7 (20.00-1.90) 72.6 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.220 0.178 , 0.223	Depositor DCC
R_{free} test set	9843 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26426	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: ANP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3783	0.80	0/5102
1	B	0.53	0/3711	0.80	0/5005
1	C	0.53	0/3766	0.84	0/5080
2	D	0.52	0/3604	0.78	2/4891 (0.0%)
2	E	0.50	0/3543	0.78	1/4807 (0.0%)
2	F	0.54	0/3601	1.14	5/4887 (0.1%)
3	G	0.49	0/1426	0.85	0/1907
4	H	0.48	0/660	0.96	3/890 (0.3%)
5	I	0.41	0/207	0.91	1/279 (0.4%)
All	All	0.52	0/24301	0.87	12/32848 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	97[A]	VAL	CG1-CB-CG2	-40.34	22.06	110.80
2	F	97[B]	VAL	CG1-CB-CG2	-40.34	22.06	110.80
2	F	139	VAL	CB-CA-C	-7.10	102.88	111.97
4	H	127	THR	CA-C-N	5.76	132.06	121.70
4	H	127	THR	C-N-CA	5.76	132.06	121.70
4	H	106	GLY	N-CA-C	-5.71	107.58	114.66
2	D	87	GLY	CA-C-N	5.56	125.92	119.47
2	D	87	GLY	C-N-CA	5.56	125.92	119.47
5	I	8	GLY	N-CA-C	-5.13	102.93	112.37
2	E	215	VAL	CB-CA-C	-5.02	102.77	110.50
2	F	87	GLY	CA-C-N	5.01	126.10	119.84
2	F	87	GLY	C-N-CA	5.01	126.10	119.84

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	3726	0	3832	33	0
1	B	3663	0	3774	32	0
1	C	3715	0	3814	34	0
2	D	3544	0	3603	41	0
2	E	3481	0	3539	45	0
2	F	3538	0	3604	44	0
3	G	1417	0	1501	35	0
4	H	657	0	663	28	0
5	I	203	0	205	2	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	D	31	0	13	3	0
6	F	31	0	13	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	354	0	0	6	0
8	B	348	0	0	5	0
8	C	367	0	0	11	0
8	D	389	0	0	5	0
8	E	267	0	0	5	0
8	F	436	0	0	8	0
8	G	114	0	0	3	0
8	H	31	0	0	1	0
8	I	16	0	0	0	0
All	All	26426	0	24600	276	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 6.

All (276) 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)
3:G:68:ILE:HB	3:G:69:ILE:HA	1.29	1.11
4:H:104:ASP:HA	4:H:105:LEU:CB	1.80	1.10
4:H:104:ASP:CA	4:H:105:LEU:HB2	1.82	1.08
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.31	1.07
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.09	1.05
4:H:122:ALA:HA	4:H:123:ALA:CB	1.82	1.04
2:E:282:GLN:H	2:E:282:GLN:HE21	1.04	1.01
2:F:356:ARG:HD2	8:F:2347:HOH:O	1.64	0.98
4:H:99:THR:HB	4:H:101:ASP:H	1.31	0.93
2:D:282:GLN:H	2:D:282:GLN:HE21	1.01	0.93
4:H:99:THR:HA	4:H:100:LEU:HB2	1.48	0.93
1:A:99:VAL:HG11	1:A:256:TYR:HB2	1.52	0.91
2:D:159:GLY:H	6:D:1480:ANP:HNB1	1.14	0.89
2:F:282:GLN:H	2:F:282:GLN:HE21	0.91	0.87
2:F:282:GLN:HE21	2:F:282:GLN:N	1.73	0.87
1:C:52:MET:SD	8:C:2016:HOH:O	2.32	0.85
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.57	0.84
8:A:2187:HOH:O	2:D:291:THR:HG22	1.76	0.84
1:C:449:VAL:HB	8:C:2323:HOH:O	1.78	0.83
2:F:167:MET:HE1	2:F:196:LEU:HD13	1.58	0.83
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.59	0.82
1:C:338:ILE:HG21	8:C:2195:HOH:O	1.81	0.80
4:H:126:ALA:HA	4:H:129:ALA:HB3	1.62	0.80
2:F:282:GLN:H	2:F:282:GLN:NE2	1.76	0.78
1:C:95:VAL:HG22	8:C:2025:HOH:O	1.80	0.78
4:H:104:ASP:HA	4:H:105:LEU:HB2	0.88	0.78
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.64	0.78
4:H:121:GLY:HA3	4:H:122:ALA:HB3	1.66	0.77
1:A:151:LYS:H	1:A:430:GLN:HE22	1.32	0.76
2:D:97:VAL:HG23	8:D:2198:HOH:O	1.87	0.73
8:A:2213:HOH:O	2:D:275[A]:ILE:HG23	1.88	0.73
3:G:23:MET:SD	3:G:232:MET:HE2	2.28	0.73
2:D:196:LEU:HG	2:D:200:MET:HE2	1.69	0.73
1:A:44:LEU:O	1:A:47:VAL:HG22	1.89	0.73
2:F:438:ILE:HG13	8:F:2361:HOH:O	1.87	0.73
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.19	0.72
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.71	0.71
2:F:196:LEU:HD11	2:F:200:MET:HE3	1.71	0.71
4:H:99:THR:HB	4:H:101:ASP:N	2.04	0.71
3:G:68:ILE:CB	3:G:69:ILE:HA	2.12	0.71
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.26	0.70
2:F:223:ASN:HD22	2:F:223:ASN:H	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:ALA:HB3	8:E:2134:HOH:O	1.92	0.70
4:H:99:THR:CA	4:H:100:LEU:HB2	2.20	0.69
4:H:122:ALA:CA	4:H:123:ALA:CB	2.66	0.69
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.40	0.69
1:C:362:ARG:HH12	2:F:372:ARG:CZ	2.06	0.69
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.23	0.69
2:D:282:GLN:H	2:D:282:GLN:NE2	1.85	0.68
1:C:94:ILE:HG22	8:C:2068:HOH:O	1.93	0.68
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.29	0.68
2:F:395:GLU:HB3	8:F:2384:HOH:O	1.94	0.67
1:A:419:SER:O	1:A:423:ARG:HD3	1.93	0.67
2:D:97:VAL:HG22	2:D:232:VAL:HB	1.77	0.67
4:H:127:THR:N	4:H:128:ARG:HB2	2.10	0.66
1:B:217:VAL:HG11	2:E:123:PHE:HZ	1.60	0.66
1:C:160:GLY:H	1:C:163:GLN:NE2	1.92	0.66
4:H:105:LEU:H	4:H:108:ALA:H	1.43	0.65
2:F:249:GLN:OE1	2:F:249:GLN:HA	1.95	0.65
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.77	0.65
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.79	0.65
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.77	0.65
1:C:272:SER:HA	8:C:2195:HOH:O	1.96	0.65
1:B:35:GLY:O	8:B:2011:HOH:O	2.14	0.64
2:D:85:PRO:HB3	2:D:110:THR:HG21	1.78	0.64
2:F:287:THR:O	2:F:291:THR:HG23	1.97	0.64
3:G:20:THR:HG22	3:G:232:MET:HE3	1.81	0.63
1:A:86:ASP:HB3	8:A:2068:HOH:O	1.99	0.63
2:F:96:ASN:C	2:F:96:ASN:HD22	2.06	0.63
4:H:126:ALA:HA	4:H:129:ALA:CB	2.28	0.62
1:C:95:VAL:CG2	8:C:2025:HOH:O	2.43	0.62
2:E:157:GLY:HA2	2:E:162:LYS:HE3	1.81	0.62
2:E:63:MET:HE2	2:E:82:ILE:CD1	2.28	0.62
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.08	0.62
2:D:275[A]:ILE:HG22	3:G:272:LEU:HD13	1.81	0.62
4:H:127:THR:H	4:H:128:ARG:HB2	1.65	0.61
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.35	0.61
2:F:223:ASN:HD22	2:F:223:ASN:N	1.99	0.60
1:C:95:VAL:O	8:C:2068:HOH:O	2.16	0.60
2:E:223:ASN:HD22	2:E:223:ASN:H	1.48	0.60
3:G:20:THR:HG22	3:G:232:MET:CE	2.32	0.60
1:A:446:TYR:CE1	1:A:450:ARG:HD2	2.35	0.60
3:G:168:VAL:HG23	3:G:169:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:CG1	1:A:256:TYR:CB	2.81	0.59
4:H:99:THR:HA	4:H:100:LEU:CB	2.28	0.59
4:H:99:THR:CB	4:H:101:ASP:H	2.12	0.59
3:G:23:MET:HE3	3:G:75:ARG:NH2	2.18	0.59
2:E:356:ARG:NH2	8:E:2249:HOH:O	2.34	0.58
2:D:96:ASN:C	2:D:96:ASN:HD22	2.11	0.58
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.84	0.58
2:E:282:GLN:H	2:E:282:GLN:NE2	1.87	0.58
1:C:215:GLN:HB3	2:F:356:ARG:HH22	1.69	0.57
2:D:393:MET:HE3	2:D:401:LYS:HB2	1.84	0.57
2:E:377:ILE:HG12	2:E:407:ALA:HB2	1.85	0.57
2:D:159:GLY:N	6:D:1480:ANP:HNB1	1.93	0.57
8:C:2175:HOH:O	2:F:291:THR:HG22	2.04	0.57
3:G:166:ARG:HE	3:G:172:LYS:HB2	1.70	0.57
4:H:127:THR:H	4:H:128:ARG:CB	2.17	0.57
3:G:113:ARG:HD3	3:G:127:THR:HG21	1.87	0.56
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.56
1:B:160:GLY:H	1:B:163:GLN:HE21	1.53	0.56
2:F:139:VAL:HG13	2:F:414:LEU:HD22	1.86	0.56
3:G:73:SER:HA	3:G:131:VAL:CG2	2.36	0.56
2:E:47:LEU:HB3	2:E:60[B]:THR:CG2	2.37	0.55
2:E:282:GLN:HE21	2:E:282:GLN:N	1.89	0.55
2:E:47:LEU:HB3	2:E:60[B]:THR:HG21	1.88	0.55
1:A:446:TYR:CE2	1:A:497:LEU:HB3	2.42	0.55
1:C:362:ARG:HA	1:C:363:PRO:C	2.31	0.55
2:D:287:THR:O	2:D:291:THR:HG23	2.07	0.55
1:B:179:ALA:HB1	1:B:267:ILE:HG12	1.88	0.54
3:G:2:THR:HG22	3:G:4:LYS:H	1.72	0.54
2:F:233:ALA:O	2:F:237:LEU:HD13	2.07	0.54
1:A:40:ARG:HD2	1:A:70:ASN:OD1	2.08	0.54
4:H:122:ALA:HB3	8:H:2007:HOH:O	2.07	0.54
2:E:223:ASN:HD22	2:E:223:ASN:N	2.05	0.54
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.38	0.54
2:D:390:ILE:HD12	3:G:16:ILE:CD1	2.37	0.54
2:E:258:ILE:HG21	2:E:310:ILE:HD13	1.90	0.54
1:A:423:ARG:HG3	1:A:461:ILE:HD11	1.89	0.54
1:A:355:GLU:HG3	8:A:2131:HOH:O	2.08	0.53
2:D:188:GLU:O	2:D:221:GLN:HB3	2.08	0.53
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.44	0.53
2:D:390:ILE:HD12	3:G:16:ILE:HD13	1.91	0.53
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:HG3	1:A:123:SER:HA	1.91	0.52
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.91	0.52
3:G:229:MET:HB2	8:G:2014:HOH:O	2.09	0.52
3:G:23:MET:HE3	3:G:75:ARG:HH21	1.75	0.52
1:B:158:PRO:O	1:B:375:GLY:HA3	2.10	0.52
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.93	0.51
1:B:213:VAL:O	1:B:217:VAL:HG12	2.10	0.51
3:G:115:ILE:HG22	3:G:116:LEU:HD12	1.92	0.51
4:H:58:LEU:HD21	4:H:92:LEU:HD11	1.93	0.51
1:C:52:MET:HE2	1:C:95:VAL:HG13	1.93	0.51
1:C:441:GLN:O	1:C:445:ILE:HG12	2.10	0.51
2:D:89:GLU:CD	2:D:89:GLU:H	2.19	0.51
1:B:183:ILE:HD11	1:B:267:ILE:HD13	1.93	0.50
1:C:218:LYS:HD3	2:F:128:VAL:HG21	1.93	0.50
3:G:168:VAL:HB	3:G:229:MET:HE1	1.92	0.50
4:H:127:THR:H	4:H:129:ALA:H	1.59	0.50
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.45	0.50
2:E:63:MET:HE1	2:E:97:VAL:HG21	1.94	0.50
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.93	0.50
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.76	0.50
2:F:244:ARG:O	2:F:248:GLY:HA2	2.10	0.50
1:B:171:ARG:HD3	8:E:2234:HOH:O	2.10	0.50
2:D:275[A]:ILE:CG2	3:G:272:LEU:HD13	2.41	0.50
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.94	0.50
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.77	0.50
2:D:85:PRO:HB3	2:D:110:THR:CG2	2.41	0.49
2:F:175:LYS:C	2:F:177:HIS:H	2.18	0.49
1:B:362:ARG:HA	1:B:363:PRO:C	2.36	0.49
5:I:5:ARG:HA	5:I:9:LEU:H	1.76	0.49
2:E:408:ARG:O	2:E:412:ARG:NE	2.45	0.49
2:F:455:GLN:H	2:F:455:GLN:CD	2.20	0.49
1:A:286:ARG:HG2	2:D:275[A]:ILE:HG21	1.94	0.49
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.77	0.49
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.39	0.49
2:D:414:LEU:HD23	2:D:441:PHE:CZ	2.48	0.49
2:F:159:GLY:HA2	6:F:1479:ANP:HNB1	1.77	0.48
1:B:30:ARG:HB3	8:B:2062:HOH:O	2.13	0.48
2:D:61:ILE:HD13	8:D:2057:HOH:O	2.12	0.48
1:B:349:GLN:NE2	8:B:2298:HOH:O	2.31	0.48
2:E:229:ARG:NH2	2:E:267:GLU:OE1	2.39	0.48
1:B:497:LEU:O	1:B:501:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:137:THR:HG22	3:G:138:PHE:N	2.29	0.47
3:G:68:ILE:HB	3:G:69:ILE:CA	2.21	0.47
3:G:164:ARG:HH12	3:G:172:LYS:HE2	1.79	0.47
1:B:211:SER:CA	2:E:126:MET:HE2	2.44	0.47
1:B:332:GLY:HA2	8:B:2283:HOH:O	2.13	0.47
2:F:188:GLU:O	2:F:221:GLN:HB3	2.14	0.47
2:F:454:GLU:HG2	8:F:2388:HOH:O	2.13	0.47
4:H:128:ARG:H	4:H:131:ILE:HD12	1.80	0.47
3:G:24:LYS:HG3	3:G:233:ASP:HB2	1.97	0.47
2:E:47:LEU:CB	2:E:60[B]:THR:HG21	2.45	0.46
2:F:223:ASN:H	2:F:223:ASN:ND2	2.11	0.46
3:G:260:LYS:HD2	8:G:2043:HOH:O	2.14	0.46
3:G:69:ILE:HG21	3:G:106:ILE:HD12	1.98	0.46
1:C:78:ASN:HD22	1:C:80:LYS:H	1.61	0.46
2:F:139:VAL:CG1	2:F:414:LEU:HD22	2.46	0.46
1:A:362:ARG:NH1	8:A:2283:HOH:O	2.48	0.46
3:G:14:LYS:O	3:G:18:LYS:HE3	2.14	0.46
1:A:457:GLU:HA	1:A:458:PRO:HD2	1.79	0.46
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.98	0.45
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.99	0.45
1:C:115:ILE:O	2:F:124:VAL:HG13	2.16	0.45
2:D:205:VAL:CG1	2:D:215:VAL:CG2	2.95	0.45
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.80	0.45
2:D:275[A]:ILE:CG2	2:D:275[A]:ILE:H	2.28	0.45
2:F:13:ILE:HD12	2:F:73:GLN:HB3	1.97	0.45
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.97	0.45
1:A:400:VAL:HG13	1:A:403:PHE:CE1	2.52	0.45
4:H:121:GLY:CA	4:H:122:ALA:HB3	2.40	0.45
2:E:9:THR:N	8:E:2001:HOH:O	2.49	0.45
1:A:286:ARG:CZ	2:D:275[A]:ILE:HG21	2.47	0.45
1:C:94:ILE:HD11	8:C:2023:HOH:O	2.16	0.45
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.98	0.45
3:G:69:ILE:HG13	3:G:106:ILE:HG13	1.99	0.45
2:F:231:ARG:NH1	8:F:2250:HOH:O	2.50	0.44
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.99	0.44
2:F:345:TYR:HA	2:F:346:PRO:C	2.42	0.44
3:G:73:SER:HA	3:G:131:VAL:HG23	1.98	0.44
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.98	0.44
3:G:106:ILE:HG22	3:G:127:THR:N	2.31	0.44
1:A:128:ARG:NE	8:A:2105:HOH:O	2.48	0.44
1:B:371:VAL:HG21	8:F:2436:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLN:HG3	1:A:386:VAL:HG13	1.99	0.44
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.98	0.44
2:D:242:TYR:CD1	2:D:246:GLN:HG3	2.53	0.44
2:F:96:ASN:C	2:F:96:ASN:ND2	2.75	0.44
1:C:99:VAL:HG21	1:C:127:ARG:HB2	1.99	0.44
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.00	0.44
1:C:404:ALA:O	1:C:406:PHE:N	2.51	0.44
2:F:27:GLU:HG2	8:F:2013:HOH:O	2.18	0.44
1:C:128:ARG:NH1	8:C:2101:HOH:O	2.51	0.43
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.49	0.43
2:E:126:MET:HE1	2:E:297:THR:OG1	2.19	0.43
1:C:52:MET:O	1:C:91:THR:HB	2.17	0.43
1:B:440:GLU:HB3	1:B:469:LEU:HD11	2.00	0.43
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.01	0.43
3:G:216:SER:O	3:G:220:SER:HB2	2.18	0.43
1:A:195:GLU:O	1:A:196:LYS:HB2	2.19	0.43
2:E:25:PHE:O	2:E:56:SER:HB3	2.19	0.43
2:E:95:MET:HA	2:E:100:GLU:O	2.18	0.43
2:F:291:THR:HG21	8:F:2161:HOH:O	2.17	0.43
1:C:160:GLY:H	1:C:163:GLN:HE21	1.61	0.43
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.49	0.43
2:E:256:ASP:HA	2:E:257[A]:ASN:HA	1.67	0.43
1:C:187:LYS:HE2	1:C:224:ASP:HB3	2.00	0.43
1:B:327:ILE:HD11	1:B:342:VAL:HG21	2.02	0.42
1:A:312:MET:O	1:A:318:GLY:HA2	2.19	0.42
2:F:249:GLN:OE1	2:F:249:GLN:CA	2.66	0.42
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.54	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.42
3:G:69:ILE:HD11	3:G:105:ILE:N	2.34	0.42
4:H:19:THR:HA	4:H:28:PHE:O	2.18	0.42
2:E:63:MET:HE2	2:E:82:ILE:HD13	2.01	0.42
5:I:8:GLY:HA3	5:I:9:LEU:CD1	2.50	0.42
1:A:94:ILE:CD1	1:A:96:ASP:HB3	2.49	0.42
1:B:180:ILE:HG13	1:B:216:LEU:HD21	2.02	0.42
3:G:166:ARG:HH21	3:G:172:LYS:HB2	1.85	0.42
1:C:343:ILE:HG23	1:C:349:GLN:NE2	2.34	0.42
1:C:373:ARG:HA	6:D:1480:ANP:O3'	2.20	0.42
2:E:63:MET:CE	2:E:97:VAL:HG21	2.49	0.42
3:G:13:ILE:HG22	3:G:243:ILE:HG13	2.02	0.42
2:D:96:ASN:C	2:D:96:ASN:ND2	2.76	0.41
1:B:286:ARG:HA	2:E:275:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:THR:HG21	8:D:2367:HOH:O	2.19	0.41
2:D:167:MET:HE3	8:D:2174:HOH:O	2.20	0.41
4:H:138:ASN:HA	4:H:141:LEU:HD12	2.00	0.41
1:B:235:THR:HG22	8:B:2182:HOH:O	2.20	0.41
4:H:58:LEU:HD13	4:H:77:VAL:HG11	2.02	0.41
2:E:345:TYR:HA	2:E:346:PRO:C	2.44	0.41
2:F:89:GLU:HG3	2:F:110:THR:HA	2.02	0.41
1:C:99:VAL:HG13	1:C:256:TYR:HB2	2.02	0.41
1:B:94:ILE:O	1:B:95:VAL:C	2.64	0.41
1:B:211:SER:HA	2:E:126:MET:HE2	2.03	0.41
2:D:285:LEU:C	2:D:285:LEU:HD23	2.46	0.41
2:E:196:LEU:HD11	2:E:200:MET:HE3	2.03	0.41
2:E:260:ARG:HD2	8:E:2086:HOH:O	2.20	0.41
2:F:387:ILE:H	2:F:387:ILE:HG13	1.70	0.41
1:B:288:PRO:HB3	2:F:276:PRO:HG3	2.03	0.41
4:H:76:PHE:CZ	4:H:140:ALA:O	2.73	0.41
1:A:137:ILE:HD11	2:E:103:ASP:HA	2.04	0.40
1:A:362:ARG:HA	1:A:363:PRO:C	2.45	0.40
1:B:439:GLU:HG3	1:B:480:LEU:HB3	2.02	0.40
3:G:226:SER:HB2	8:G:2075:HOH:O	2.21	0.40
1:A:151:LYS:H	1:A:430:GLN:NE2	2.10	0.40
1:B:80:LYS:HA	2:E:32:ILE:HB	2.02	0.40
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.03	0.40
3:G:69:ILE:O	3:G:69:ILE:HG23	2.20	0.40
1:C:78:ASN:HD22	1:C:78:ASN:C	2.29	0.40
2:D:9:THR:N	8:D:2001:HOH:O	2.54	0.40
2:D:200:MET:HE1	2:D:217:LEU:HD11	2.03	0.40
1:A:62:MET:CE	1:A:64:LEU:HD21	2.45	0.40
1:B:453:LEU:HB3	1:B:461:ILE:HD12	2.04	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	487/510 (96%)	475 (98%)	11 (2%)	1 (0%)	43	36
1	B	476/510 (93%)	463 (97%)	12 (2%)	1 (0%)	43	36
1	C	485/510 (95%)	474 (98%)	10 (2%)	1 (0%)	43	36
2	D	466/482 (97%)	450 (97%)	16 (3%)	0	100	100
2	E	456/482 (95%)	442 (97%)	12 (3%)	2 (0%)	30	22
2	F	466/482 (97%)	453 (97%)	12 (3%)	1 (0%)	43	36
3	G	172/273 (63%)	163 (95%)	8 (5%)	1 (1%)	21	13
4	H	78/146 (53%)	65 (83%)	9 (12%)	4 (5%)	1	0
5	I	23/50 (46%)	22 (96%)	1 (4%)	0	100	100
All	All	3109/3445 (90%)	3007 (97%)	91 (3%)	11 (0%)	30	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	C	405	GLN
4	H	105	LEU
4	H	123	ALA
1	B	35	GLY
4	H	128	ARG
3	G	72	SER
4	H	122	ALA
2	E	279	VAL
2	F	279	VAL
2	E	157	GLY

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	395/412 (96%)	388 (98%)	7 (2%)	51	50
1	B	389/412 (94%)	379 (97%)	10 (3%)	40	35
1	C	393/412 (95%)	381 (97%)	12 (3%)	35	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	378/386 (98%)	364 (96%)	14 (4%)	30	22
2	E	372/386 (96%)	352 (95%)	20 (5%)	20	12
2	F	378/386 (98%)	363 (96%)	15 (4%)	28	20
3	G	154/231 (67%)	139 (90%)	15 (10%)	8	3
4	H	70/109 (64%)	66 (94%)	4 (6%)	18	11
5	I	19/41 (46%)	18 (95%)	1 (5%)	20	12
All	All	2548/2775 (92%)	2450 (96%)	98 (4%)	29	21

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	102	GLU
1	A	157	VAL
1	A	274	GLN
1	A	385	GLN
1	A	410	LEU
1	A	479	LEU
1	B	38	ILE
1	B	80	LYS
1	B	131	LEU
1	B	171	ARG
1	B	216	LEU
1	B	217	VAL
1	B	389	THR
1	B	399	GLU
1	B	449	VAL
1	B	479	LEU
1	C	78	ASN
1	C	95	VAL
1	C	97	VAL
1	C	99	VAL
1	C	196	LYS
1	C	216	LEU
1	C	334	VAL
1	C	349	GLN
1	C	455	LYS
1	C	456	LEU
1	C	479	LEU
1	C	505	LEU

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Mol	Chain	Res	Type
2	D	89	GLU
2	D	96	ASN
2	D	111	LYS
2	D	237	LEU
2	D	246	GLN
2	D	247	GLU
2	D	249	GLN
2	D	275[A]	ILE
2	D	275[B]	ILE
2	D	279	VAL
2	D	282	GLN
2	D	341	GLU
2	D	393	MET
2	D	428	LEU
2	E	76	LEU
2	E	130	GLN
2	E	139	VAL
2	E	163	THR
2	E	215	VAL
2	E	223	ASN
2	E	257[A]	ASN
2	E	257[B]	ASN
2	E	279	VAL
2	E	282	GLN
2	E	293	GLN
2	E	301	LYS
2	E	310	ILE
2	E	412	ARG
2	E	420	VAL
2	E	423	VAL
2	E	428	LEU
2	E	439	LYS
2	E	451	HIS
2	E	463	ILE
2	F	10	THR
2	F	89	GLU
2	F	96	ASN
2	F	112	GLN
2	F	139	VAL
2	F	205	VAL
2	F	223	ASN
2	F	237	LEU

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Mol	Chain	Res	Type
2	F	247	GLU
2	F	249	GLN
2	F	279	VAL
2	F	282	GLN
2	F	387	ILE
2	F	420	VAL
2	F	455	GLN
3	G	33	ARG
3	G	69	ILE
3	G	105	ILE
3	G	106	ILE
3	G	108	VAL
3	G	115	ILE
3	G	130	GLU
3	G	131	VAL
3	G	166	ARG
3	G	168	VAL
3	G	206	GLU
3	G	212	ILE
3	G	217	LEU
3	G	218	LYS
3	G	262	LEU
4	H	109	LYS
4	H	112	LEU
4	H	114	LYS
4	H	118	GLU
5	I	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	186	GLN
1	A	274	GLN
1	A	330	GLN
1	A	396	GLN
1	A	430	GLN
1	A	471	HIS
1	B	65	ASN
1	B	163	GLN
1	B	172	GLN
1	B	186	GLN

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Mol	Chain	Res	Type
1	B	208	GLN
1	B	330	GLN
1	B	466	ASN
1	B	471	HIS
1	B	475	GLN
1	B	503	ASN
1	C	42	HIS
1	C	78	ASN
1	C	163	GLN
1	C	186	GLN
1	C	263	HIS
1	C	341	ASN
1	C	349	GLN
1	C	416	GLN
1	C	476	HIS
2	D	73	GLN
2	D	96	ASN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	D	385	GLN
2	D	419	GLN
2	D	427	HIS
2	E	130	GLN
2	E	171	ASN
2	E	194	ASN
2	E	223	ASN
2	E	249	GLN
2	E	282	GLN
2	E	293	GLN
2	E	375	GLN
2	E	379	GLN
2	E	385	GLN
2	E	419	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	177	HIS
2	F	194	ASN
2	F	198	HIS

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Mol	Chain	Res	Type
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	379	GLN
2	F	427	HIS
2	F	443	GLN
3	G	211	ASN
4	H	91	GLN
4	H	138	ASN
5	I	16	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
6	ANP	F	1479	7	33,33,33	1.94	11 (33%)	45,52,52	2.14	13 (28%)
6	ANP	A	1511	7	33,33,33	2.04	11 (33%)	45,52,52	2.22	12 (26%)
6	ANP	B	1511	7	33,33,33	1.98	11 (33%)	45,52,52	2.07	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ANP	D	1480	7	33,33,33	1.99	10 (30%)	45,52,52	2.26	13 (28%)
6	ANP	C	1511	7	33,33,33	2.07	12 (36%)	45,52,52	2.14	12 (26%)

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
6	ANP	F	1479	7	-	3/18/38/38	0/3/3/3
6	ANP	A	1511	7	-	3/18/38/38	0/3/3/3
6	ANP	B	1511	7	-	2/18/38/38	0/3/3/3
6	ANP	D	1480	7	-	3/18/38/38	0/3/3/3
6	ANP	C	1511	7	-	3/18/38/38	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1480	ANP	C5-C4	4.98	1.48	1.39
6	C	1511	ANP	C5-C4	4.83	1.47	1.39
6	F	1479	ANP	C5-C4	4.83	1.47	1.39
6	A	1511	ANP	C5-C4	4.82	1.47	1.39
6	B	1511	ANP	C5-C4	4.75	1.47	1.39
6	F	1479	ANP	PB-O1B	4.47	1.52	1.46
6	C	1511	ANP	PB-N3B	4.40	1.74	1.63
6	B	1511	ANP	PB-N3B	4.40	1.74	1.63
6	C	1511	ANP	PG-N3B	4.38	1.74	1.63
6	B	1511	ANP	PG-N3B	4.11	1.74	1.63
6	A	1511	ANP	PB-N3B	4.10	1.74	1.63
6	A	1511	ANP	PG-N3B	3.95	1.73	1.63
6	D	1480	ANP	PG-N3B	3.93	1.73	1.63
6	C	1511	ANP	PB-O1B	3.86	1.52	1.46
6	D	1480	ANP	PB-O1B	3.82	1.52	1.46
6	A	1511	ANP	PG-O1G	3.73	1.51	1.46
6	D	1480	ANP	PB-N3B	3.68	1.73	1.63
6	F	1479	ANP	PG-N3B	3.68	1.73	1.63
6	F	1479	ANP	PB-N3B	3.61	1.72	1.63
6	A	1511	ANP	PB-O1B	3.58	1.51	1.46
6	D	1480	ANP	PG-O1G	3.52	1.51	1.46
6	B	1511	ANP	PG-O1G	3.51	1.51	1.46
6	C	1511	ANP	PG-O1G	3.50	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1511	ANP	PB-O1B	3.22	1.51	1.46
6	F	1479	ANP	PG-O1G	2.92	1.50	1.46
6	F	1479	ANP	C5-C6	2.85	1.48	1.41
6	B	1511	ANP	C5-C6	2.84	1.48	1.41
6	A	1511	ANP	PA-O3A	2.80	1.62	1.59
6	A	1511	ANP	C5-C6	2.74	1.48	1.41
6	C	1511	ANP	C5-C6	2.68	1.48	1.41
6	D	1480	ANP	PB-O2B	-2.65	1.49	1.56
6	F	1479	ANP	PG-O2G	-2.60	1.49	1.56
6	D	1480	ANP	C5-C6	2.58	1.48	1.41
6	A	1511	ANP	C5-N7	-2.57	1.34	1.39
6	C	1511	ANP	PA-O3A	2.47	1.62	1.59
6	A	1511	ANP	PG-O2G	-2.44	1.50	1.56
6	B	1511	ANP	C5-N7	-2.35	1.34	1.39
6	D	1480	ANP	C5-N7	-2.35	1.34	1.39
6	B	1511	ANP	C8-N7	2.35	1.36	1.31
6	C	1511	ANP	C8-N7	2.34	1.36	1.31
6	F	1479	ANP	PB-O2B	-2.33	1.50	1.56
6	A	1511	ANP	PB-O2B	-2.31	1.50	1.56
6	D	1480	ANP	C8-N7	2.31	1.36	1.31
6	F	1479	ANP	C8-N7	2.28	1.36	1.31
6	B	1511	ANP	PB-O2B	-2.27	1.50	1.56
6	F	1479	ANP	C5-N7	-2.26	1.35	1.39
6	C	1511	ANP	PG-O3G	-2.24	1.50	1.56
6	C	1511	ANP	C5-N7	-2.23	1.35	1.39
6	C	1511	ANP	PB-O2B	-2.22	1.50	1.56
6	D	1480	ANP	PG-O2G	-2.21	1.50	1.56
6	A	1511	ANP	C8-N7	2.18	1.35	1.31
6	B	1511	ANP	PG-O2G	-2.15	1.51	1.56
6	F	1479	ANP	PG-O3G	-2.12	1.51	1.56
6	B	1511	ANP	PG-O3G	-2.12	1.51	1.56
6	C	1511	ANP	PG-O2G	-2.06	1.51	1.56

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1480	ANP	O1G-PG-N3B	-9.07	98.41	111.77
6	C	1511	ANP	O1G-PG-N3B	-7.84	100.22	111.77
6	F	1479	ANP	O1G-PG-N3B	-7.63	100.54	111.77
6	A	1511	ANP	O1G-PG-N3B	-7.54	100.67	111.77
6	B	1511	ANP	O1G-PG-N3B	-6.53	102.15	111.77
6	A	1511	ANP	C5-C4-N3	-5.70	118.86	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1511	ANP	C5-C4-N3	-5.69	118.88	126.72
6	C	1511	ANP	C5-C4-N3	-5.50	119.14	126.72
6	F	1479	ANP	C5-C4-N3	-5.45	119.21	126.72
6	D	1480	ANP	C5-C4-N3	-5.35	119.35	126.72
6	A	1511	ANP	N3-C4-N9	4.60	134.98	127.17
6	C	1511	ANP	N3-C4-N9	4.59	134.97	127.17
6	B	1511	ANP	N3-C4-N9	4.50	134.81	127.17
6	D	1480	ANP	N3-C4-N9	4.36	134.59	127.17
6	F	1479	ANP	N3-C4-N9	4.30	134.49	127.17
6	A	1511	ANP	O2B-PB-O1B	4.04	118.54	109.87
6	B	1511	ANP	C2-N3-C4	3.80	121.11	111.83
6	A	1511	ANP	C2-N3-C4	3.78	121.07	111.83
6	A	1511	ANP	N3-C2-N1	-3.71	122.97	128.58
6	C	1511	ANP	C2-N3-C4	3.67	120.78	111.83
6	F	1479	ANP	C2-N3-C4	3.62	120.68	111.83
6	B	1511	ANP	N3-C2-N1	-3.59	123.14	128.58
6	B	1511	ANP	C4-C5-N7	-3.54	106.53	110.58
6	C	1511	ANP	N3-C2-N1	-3.47	123.32	128.58
6	D	1480	ANP	N3-C2-N1	-3.47	123.33	128.58
6	F	1479	ANP	N3-C2-N1	-3.46	123.34	128.58
6	D	1480	ANP	C2-N3-C4	3.41	120.17	111.83
6	A	1511	ANP	C4-C5-N7	-3.35	106.75	110.58
6	F	1479	ANP	O2B-PB-O1B	3.30	116.94	109.87
6	B	1511	ANP	O2B-PB-O1B	3.27	116.88	109.87
6	F	1479	ANP	C4-C5-N7	-3.22	106.90	110.58
6	C	1511	ANP	C4-C5-N7	-3.19	106.93	110.58
6	A	1511	ANP	O1B-PB-N3B	-3.17	107.10	111.77
6	D	1480	ANP	C2'-C1'-N9	-3.12	105.55	113.30
6	C	1511	ANP	C4-N9-C8	3.09	108.98	105.74
6	D	1480	ANP	C4-C5-N7	-3.06	107.08	110.58
6	F	1479	ANP	O3A-PB-N3B	-2.96	98.37	106.59
6	C	1511	ANP	O2B-PB-O1B	2.86	116.00	109.87
6	B	1511	ANP	C4-N9-C8	2.68	108.55	105.74
6	B	1511	ANP	C5-N7-C8	2.64	107.60	103.45
6	A	1511	ANP	C5-N7-C8	2.55	107.46	103.45
6	A	1511	ANP	C4-N9-C8	2.54	108.41	105.74
6	D	1480	ANP	C2-N1-C6	2.45	122.75	118.73
6	D	1480	ANP	O2B-PB-O1B	2.45	115.11	109.87
6	C	1511	ANP	C5-N7-C8	2.45	107.29	103.45
6	D	1480	ANP	C4-N9-C8	2.39	108.25	105.74
6	F	1479	ANP	C5-N7-C8	2.33	107.11	103.45
6	B	1511	ANP	C6-C5-N7	2.26	136.44	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1511	ANP	C2-N1-C6	2.23	122.39	118.73
6	D	1480	ANP	C5-N7-C8	2.23	106.95	103.45
6	D	1480	ANP	O2B-PB-O3A	2.18	111.91	104.64
6	F	1479	ANP	C4-N9-C8	2.14	107.98	105.74
6	C	1511	ANP	C6-C5-N7	2.13	136.20	132.09
6	F	1479	ANP	C2-N1-C6	2.13	122.23	118.73
6	C	1511	ANP	N9-C8-N7	-2.13	110.92	113.94
6	F	1479	ANP	C6-C5-N7	2.12	136.18	132.09
6	D	1480	ANP	O2G-PG-O3G	2.09	113.20	107.59
6	B	1511	ANP	N9-C8-N7	-2.06	111.01	113.94
6	B	1511	ANP	C2-N1-C6	2.05	122.11	118.73
6	F	1479	ANP	C2'-C1'-N9	-2.03	108.27	113.30
6	C	1511	ANP	C2-N1-C6	2.02	122.04	118.73
6	A	1511	ANP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

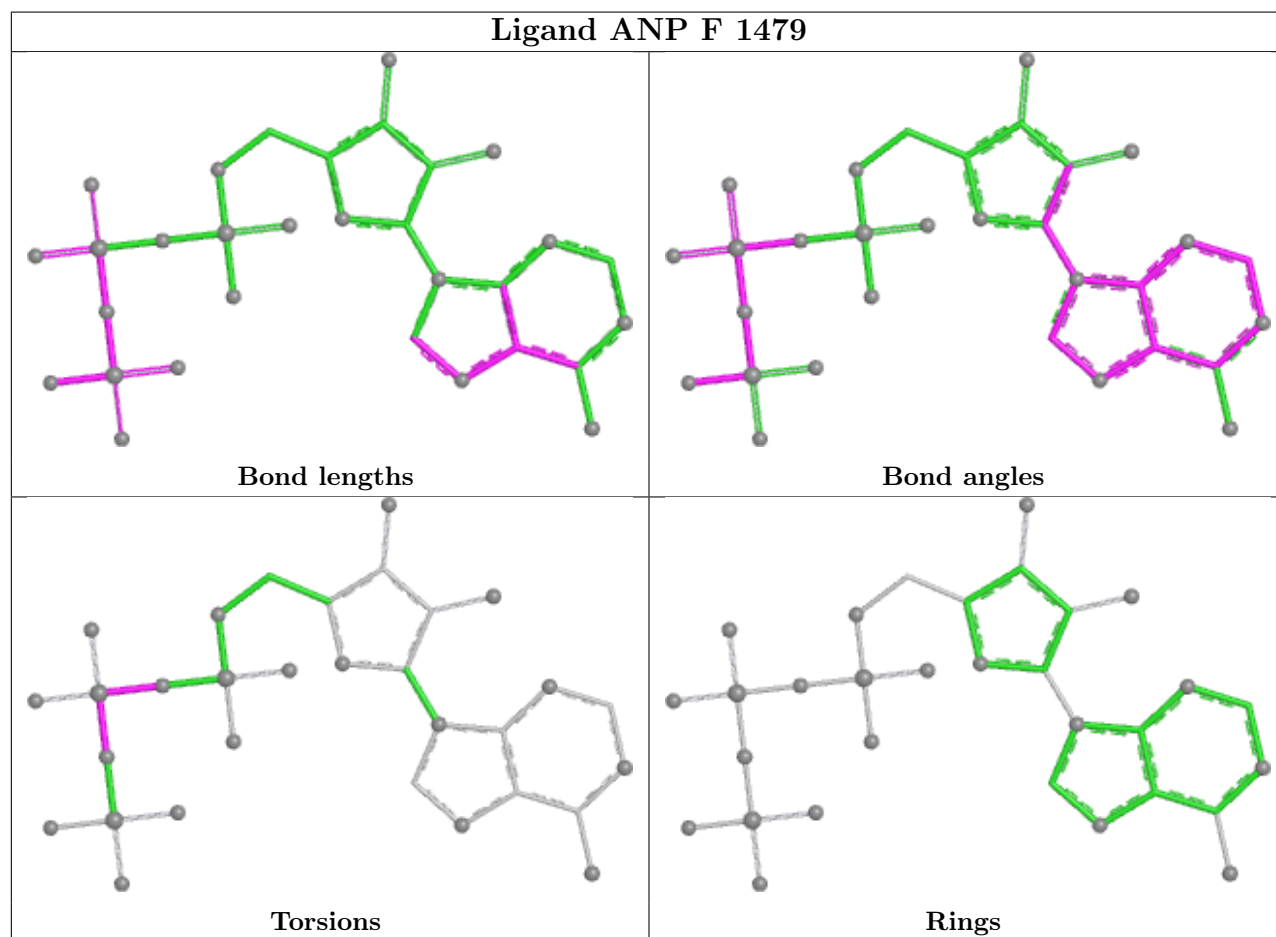
Mol	Chain	Res	Type	Atoms
6	A	1511	ANP	PG-N3B-PB-O1B
6	A	1511	ANP	PG-N3B-PB-O3A
6	B	1511	ANP	PG-N3B-PB-O1B
6	B	1511	ANP	PG-N3B-PB-O3A
6	C	1511	ANP	PB-N3B-PG-O1G
6	C	1511	ANP	PG-N3B-PB-O1B
6	D	1480	ANP	PG-N3B-PB-O1B
6	D	1480	ANP	PA-O3A-PB-O2B
6	F	1479	ANP	PG-N3B-PB-O1B
6	F	1479	ANP	PA-O3A-PB-O2B
6	F	1479	ANP	PA-O3A-PB-O1B
6	A	1511	ANP	PB-N3B-PG-O1G
6	C	1511	ANP	PG-N3B-PB-O3A
6	D	1480	ANP	PB-N3B-PG-O1G

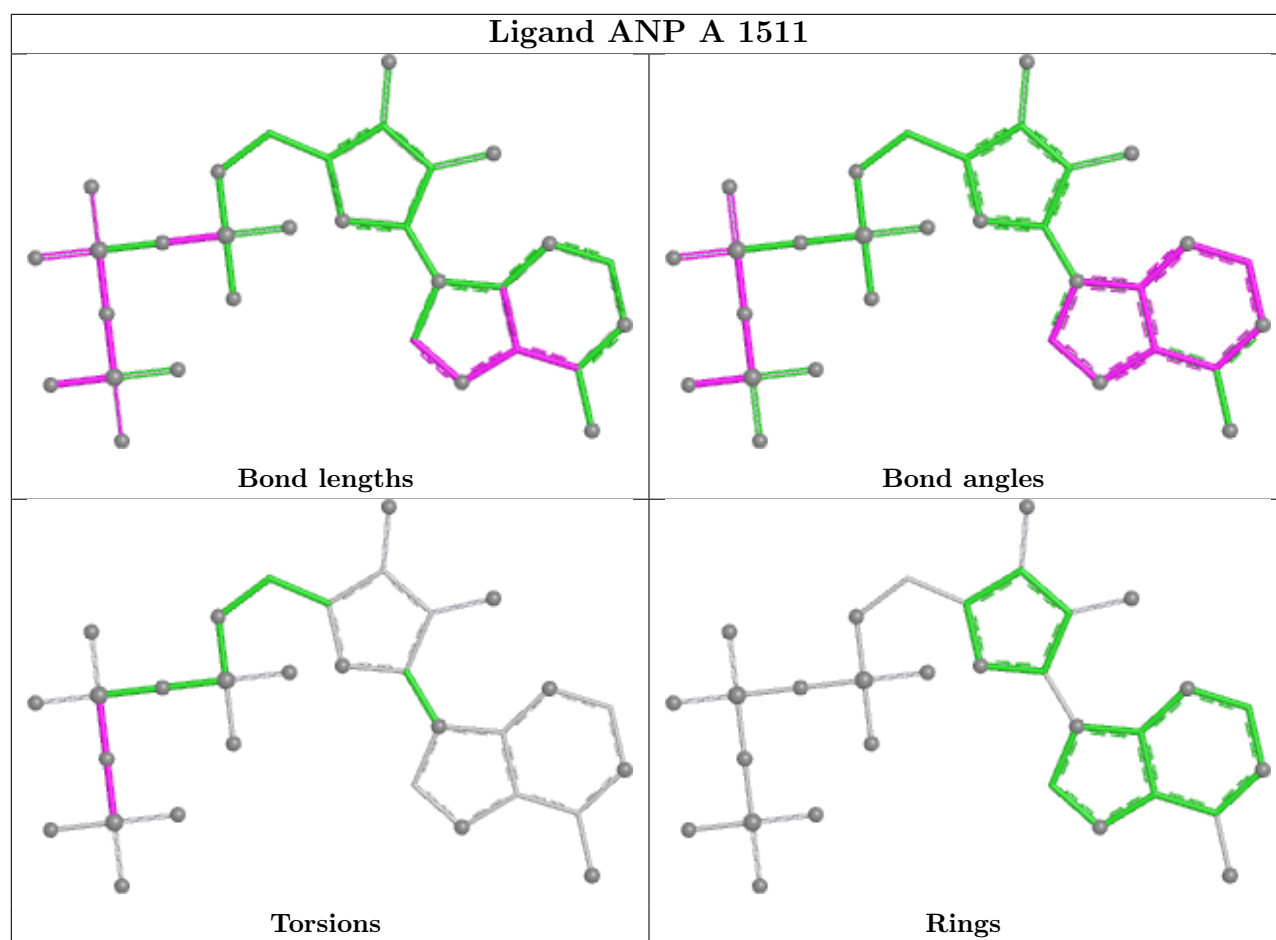
There are no ring outliers.

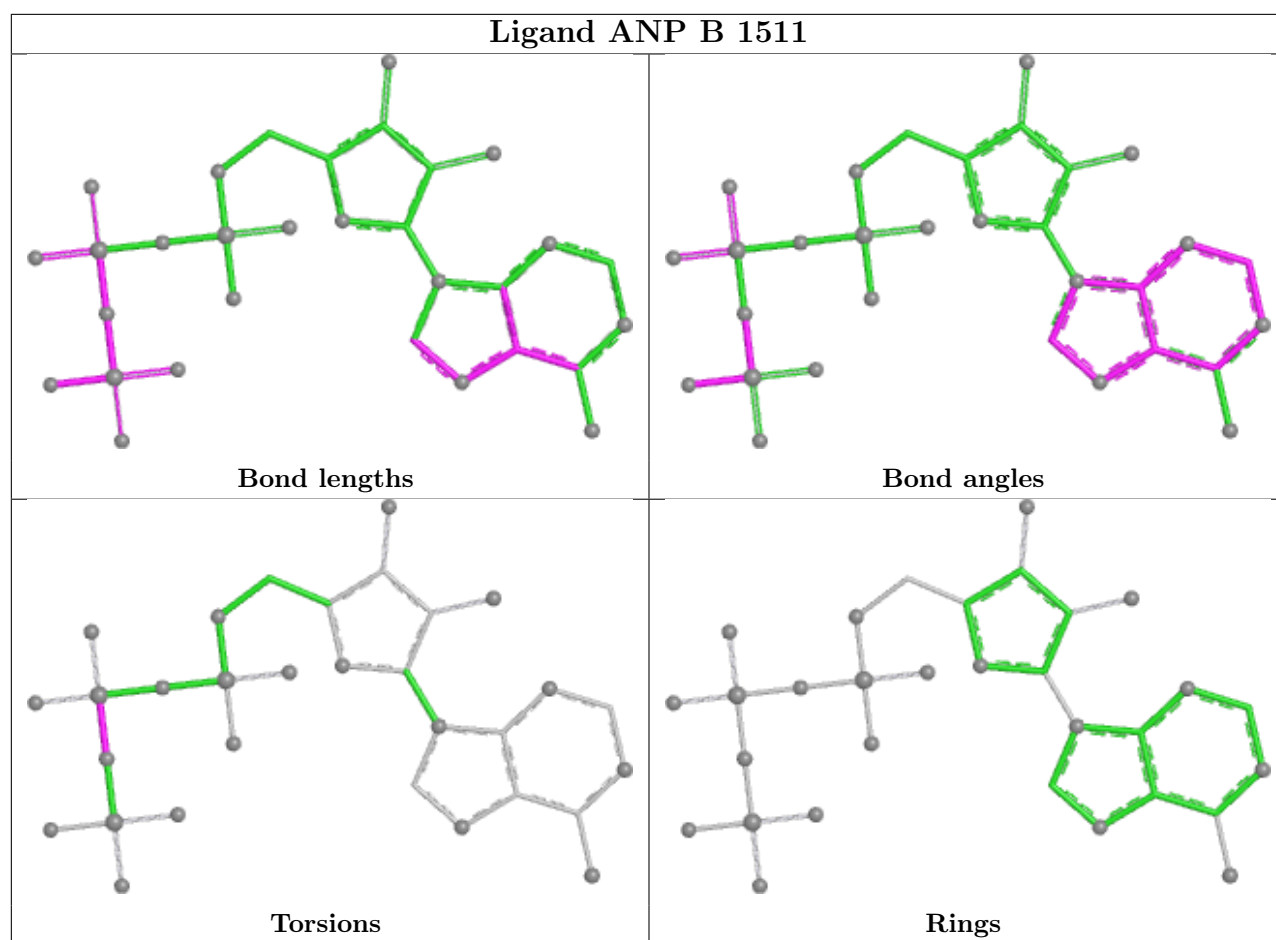
2 monomers are involved in 4 short contacts:

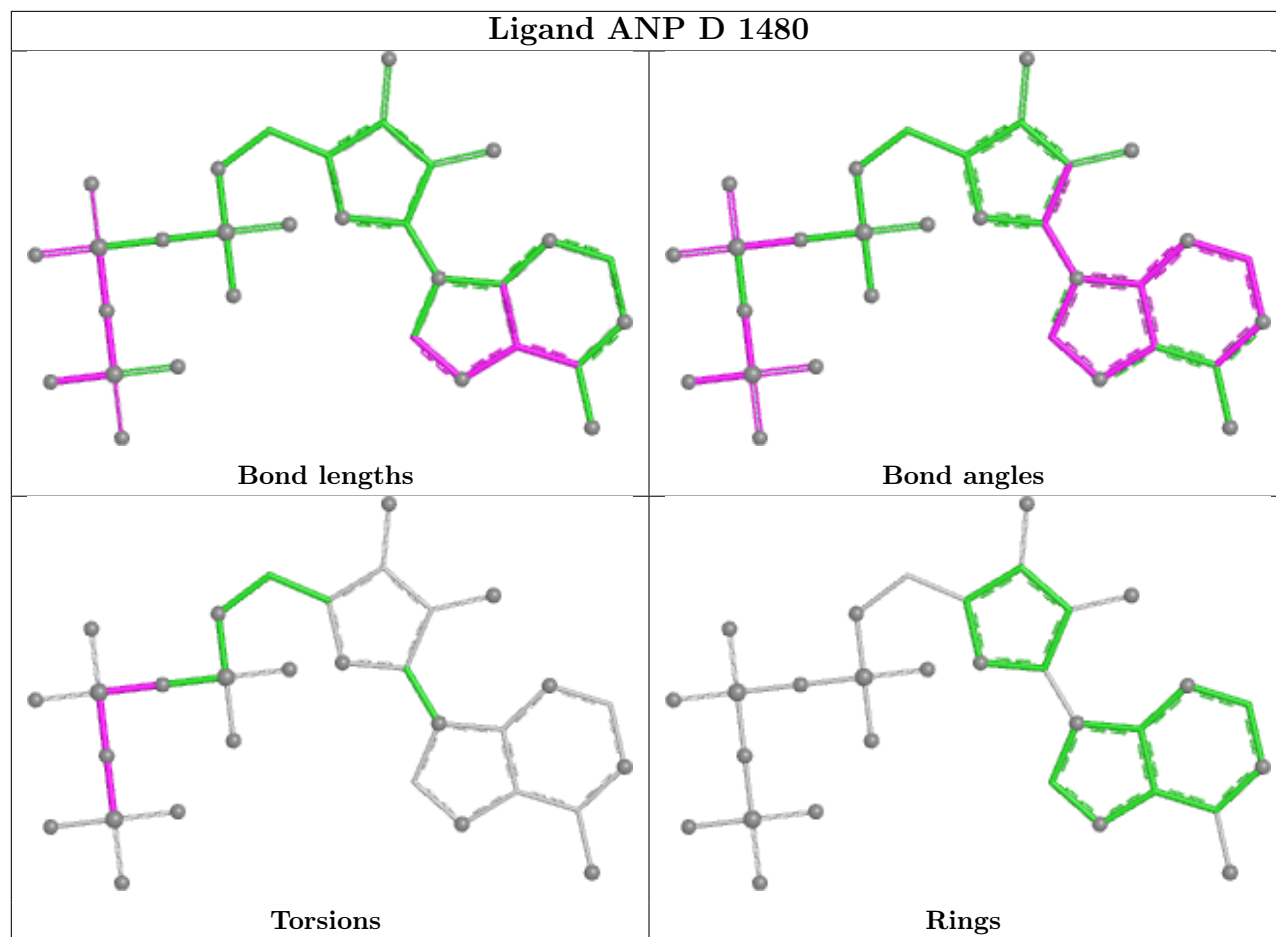
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1479	ANP	1	0
6	D	1480	ANP	3	0

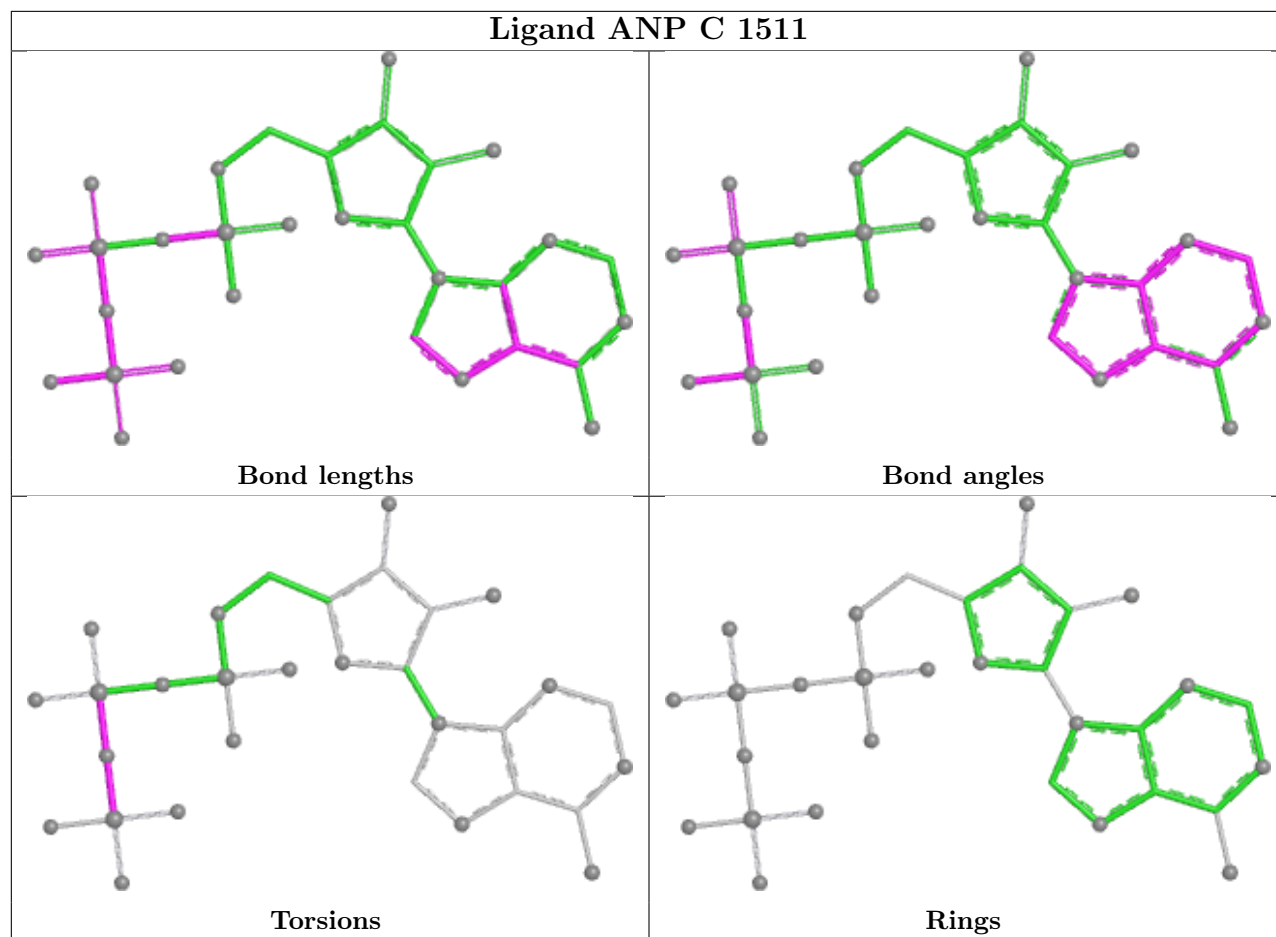
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	A	487/510 (95%)	0.14	14 (2%)	53	57	5, 15, 36, 66	5 (1%)
1	B	480/510 (94%)	0.32	39 (8%)	18	19	5, 14, 48, 78	1 (0%)
1	C	487/510 (95%)	0.13	17 (3%)	47	50	8, 15, 32, 70	0
2	D	467/482 (96%)	-0.01	11 (2%)	59	63	6, 14, 34, 71	1 (0%)
2	E	458/482 (95%)	0.46	36 (7%)	18	20	5, 18, 60, 81	3 (0%)
2	F	466/482 (96%)	0.13	17 (3%)	46	49	6, 14, 38, 59	3 (0%)
3	G	184/273 (67%)	1.45	53 (28%)	1	1	5, 32, 48, 54	1 (0%)
4	H	88/146 (60%)	1.57	26 (29%)	1	1	2, 20, 42, 50	0
5	I	25/50 (50%)	1.11	4 (16%)	5	5	2, 7, 32, 34	0
All	All	3142/3445 (91%)	0.31	217 (6%)	23	24	2, 15, 45, 81	14 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	275[A]	ILE	7.3
1	C	406	PHE	7.0
2	F	248	GLY	6.2
1	B	417	LEU	5.1
3	G	106	ILE	4.9
1	B	410	LEU	4.7
1	B	400	VAL	4.4
3	G	25	MET	4.3
3	G	105	ILE	4.3
4	H	20	PHE	4.3
4	H	28	PHE	4.2
2	D	248	GLY	4.2
2	E	424	PHE	4.2
1	B	419	SER	4.1
3	G	43	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	384	LEU	4.1
3	G	160	ILE	4.1
3	G	29	ALA	4.0
4	H	64	VAL	4.0
2	E	404	VAL	4.0
3	G	85	VAL	4.0
2	E	396	LEU	4.0
2	E	470	ALA	4.0
2	E	402	LEU	3.9
1	B	510	ALA	3.9
3	G	69	ILE	3.9
3	G	222	THR	3.8
3	G	46	VAL	3.8
1	C	407	GLY	3.7
1	B	479	LEU	3.7
5	I	9	LEU	3.7
4	H	21	ALA	3.7
1	B	504	PHE	3.7
1	B	414	THR	3.7
2	E	41	ARG	3.7
1	B	474	SER	3.7
1	B	418	LEU	3.6
2	D	9	THR	3.6
4	H	19	THR	3.6
1	B	413	ALA	3.6
3	G	161	ILE	3.6
1	A	422	VAL	3.6
1	B	412	ALA	3.6
1	C	122	GLY	3.5
3	G	273	ASP	3.5
2	E	157	GLY	3.5
4	H	63	VAL	3.5
1	B	506	ALA	3.5
3	G	32	ALA	3.5
3	G	31	TYR	3.4
3	G	212	ILE	3.4
3	G	24	LYS	3.4
2	E	407	ALA	3.4
5	I	1	VAL	3.3
1	B	447	ALA	3.3
2	D	249	GLN	3.3
1	A	446	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	176	ALA	3.3
3	G	165	PHE	3.3
2	F	474	ALA	3.3
4	H	18	PHE	3.3
3	G	208	SER	3.2
1	B	358	TYR	3.2
1	B	389	THR	3.2
5	I	8	GLY	3.2
4	H	105	LEU	3.1
2	D	474	ALA	3.1
1	B	501	VAL	3.1
3	G	107	GLY	3.1
2	F	178	GLY	3.1
1	B	455	LYS	3.0
4	H	99	THR	3.0
2	D	28	GLY	3.0
2	E	364	GLY	3.0
1	C	405	GLN	3.0
3	G	209	LEU	3.0
2	E	451	HIS	3.0
2	E	468	ALA	3.0
4	H	107	ALA	3.0
2	F	40	GLY	2.9
2	F	426	GLY	2.9
1	C	408	SER	2.9
2	E	420	VAL	2.9
2	E	460	VAL	2.9
4	H	145	LEU	2.9
1	C	501	VAL	2.9
1	A	408	SER	2.9
3	G	148	LEU	2.9
4	H	62	LEU	2.9
2	E	423	VAL	2.8
3	G	108	VAL	2.8
2	E	381	TYR	2.8
4	H	140	ALA	2.8
1	A	122	GLY	2.8
1	B	23	VAL	2.8
3	G	215	TYR	2.8
2	F	446	ALA	2.8
2	E	463	ILE	2.8
2	F	473	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	9	THR	2.8
2	E	158	ALA	2.8
3	G	162	PHE	2.8
4	H	27	PHE	2.8
1	A	193	THR	2.8
4	H	65	VAL	2.8
1	B	416	GLN	2.7
2	F	249	GLN	2.7
4	H	36	VAL	2.7
3	G	45	GLY	2.7
3	G	138	PHE	2.7
3	G	13	ILE	2.7
2	F	356	ARG	2.7
1	C	121	ILE	2.7
1	B	497	LEU	2.6
4	H	26	VAL	2.6
2	E	345	TYR	2.6
2	F	383	SER	2.6
1	B	473	ILE	2.6
4	H	122	ALA	2.6
1	B	415	GLN	2.5
3	G	68	ILE	2.5
3	G	115	ILE	2.5
1	B	401	ALA	2.5
3	G	2	THR	2.5
4	H	127	THR	2.5
2	E	378	LEU	2.5
3	G	38	LEU	2.5
1	B	423	ARG	2.5
3	G	159	SER	2.5
3	G	168	VAL	2.5
2	D	471	ASP	2.5
2	F	471	ASP	2.5
3	G	206	GLU	2.5
3	G	221	THR	2.5
2	F	210	ASP	2.5
1	A	410	LEU	2.4
1	B	508	PHE	2.4
1	C	508	PHE	2.4
2	D	402	LEU	2.4
1	B	457	GLU	2.4
1	C	94	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	263	ILE	2.4
2	D	446	ALA	2.4
1	C	24	ASP	2.4
2	E	379	GLN	2.4
1	B	456	LEU	2.4
2	E	409	LYS	2.4
2	E	386	ASP	2.4
3	G	144	ILE	2.4
1	B	467	ALA	2.4
1	C	409	ASP	2.4
2	F	177	HIS	2.4
2	E	343	GLY	2.4
3	G	47	GLY	2.4
3	G	248	LEU	2.3
1	C	475	GLN	2.3
1	C	412	ALA	2.3
3	G	34	ALA	2.3
3	G	169	ILE	2.3
5	I	7	ALA	2.3
2	E	462	PRO	2.3
3	G	167	SER	2.3
4	H	126	ALA	2.3
1	B	451	GLY	2.3
3	G	116	LEU	2.3
2	E	403	THR	2.3
3	G	40	PRO	2.3
1	A	94	ILE	2.3
1	A	449	VAL	2.3
3	G	211	ASN	2.3
3	G	86	ALA	2.2
4	H	17	SER	2.2
1	A	447	ALA	2.2
1	C	510	ALA	2.2
1	B	476	HIS	2.2
1	A	482	LYS	2.2
1	B	509	GLU	2.2
2	E	9	THR	2.2
2	E	425	THR	2.2
4	H	100	LEU	2.2
3	G	142	SER	2.2
4	H	61	GLY	2.2
1	B	443	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	387	ILE	2.2
1	A	485	THR	2.2
1	A	407	GLY	2.2
1	C	410	LEU	2.2
4	H	123	ALA	2.2
1	A	403	PHE	2.1
2	D	399	GLU	2.1
1	A	400	VAL	2.1
1	B	276	VAL	2.1
2	E	383	SER	2.1
3	G	109	GLY	2.1
1	B	469	LEU	2.1
4	H	120	LEU	2.1
1	B	460	LYS	2.1
2	E	443	GLN	2.1
3	G	226	SER	2.1
1	B	458	PRO	2.1
1	C	125	ALA	2.1
2	E	421	ALA	2.1
3	G	28	ALA	2.1
2	E	457	PHE	2.1
2	E	449	TYR	2.1
2	D	246	GLN	2.1
3	G	80	ALA	2.1
3	G	44	TYR	2.0
2	E	466	ALA	2.0
4	H	104	ASP	2.0
2	F	398	GLU	2.0
1	B	493	SER	2.0
1	C	403	PHE	2.0
1	B	448	GLY	2.0
2	E	159	GLY	2.0
2	E	363	VAL	2.0
3	G	42	ARG	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](#)

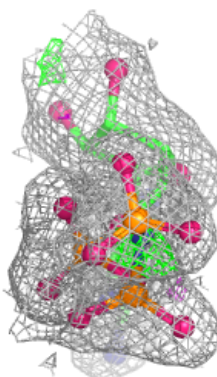
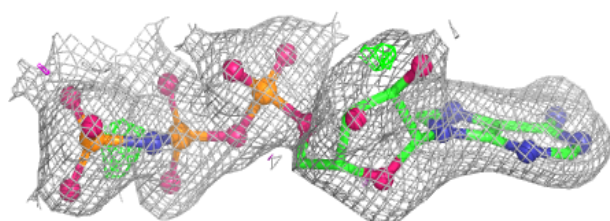
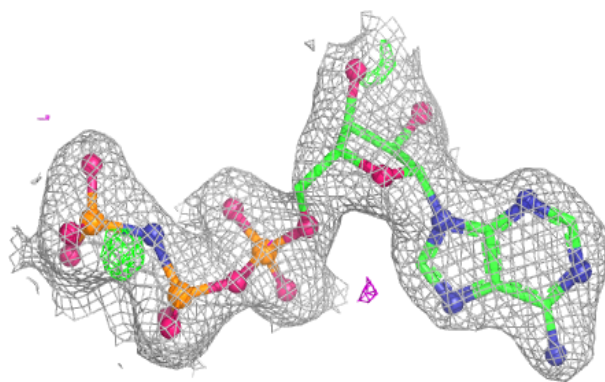
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	MG	A	1512	1/1	0.82	0.07	16,16,16,16	0
7	MG	B	1512	1/1	0.89	0.04	15,15,15,15	0
7	MG	D	1481	1/1	0.91	0.07	14,14,14,14	0
7	MG	F	1480	1/1	0.92	0.08	13,13,13,13	0
6	ANP	B	1511	31/31	0.97	0.06	8,15,24,33	0
6	ANP	C	1511	31/31	0.97	0.06	8,12,17,25	0
6	ANP	A	1511	31/31	0.97	0.05	8,12,19,21	0
7	MG	C	1512	1/1	0.98	0.05	13,13,13,13	0
6	ANP	D	1480	31/31	0.98	0.05	6,10,14,16	0
6	ANP	F	1479	31/31	0.98	0.06	8,12,18,21	0

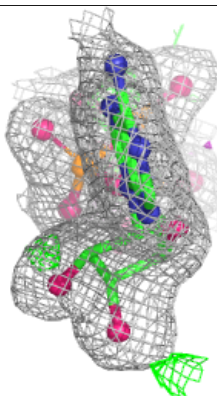
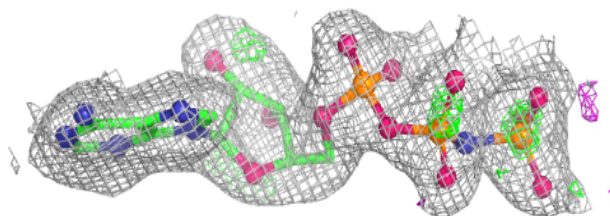
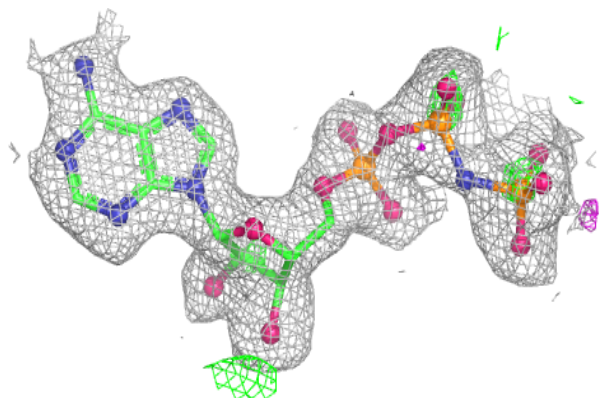
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 1511:

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

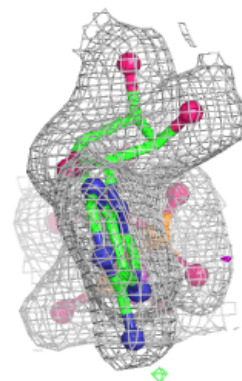
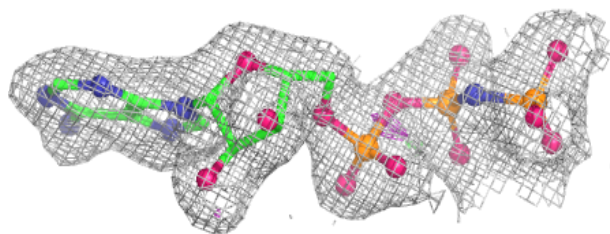
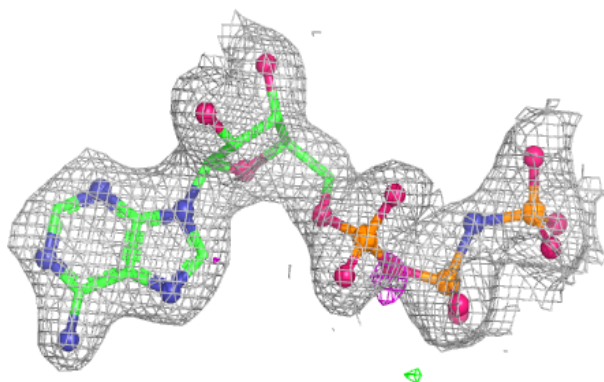
**Electron density around ANP C 1511:**

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

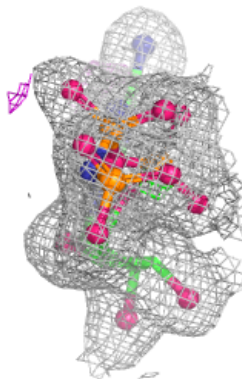
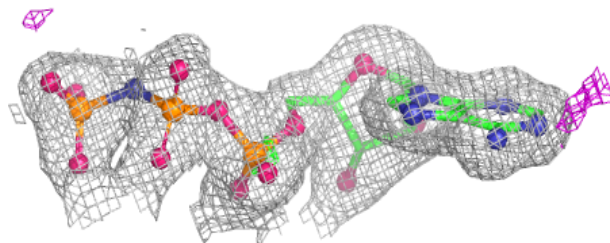
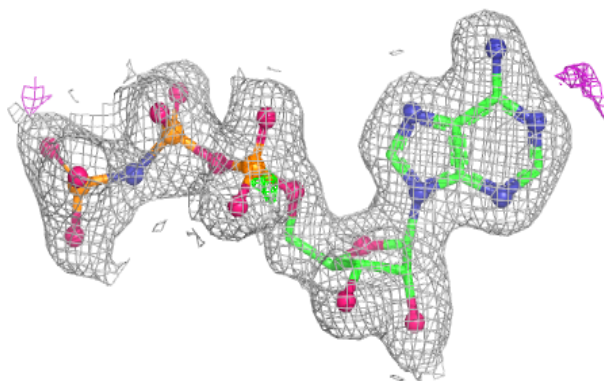


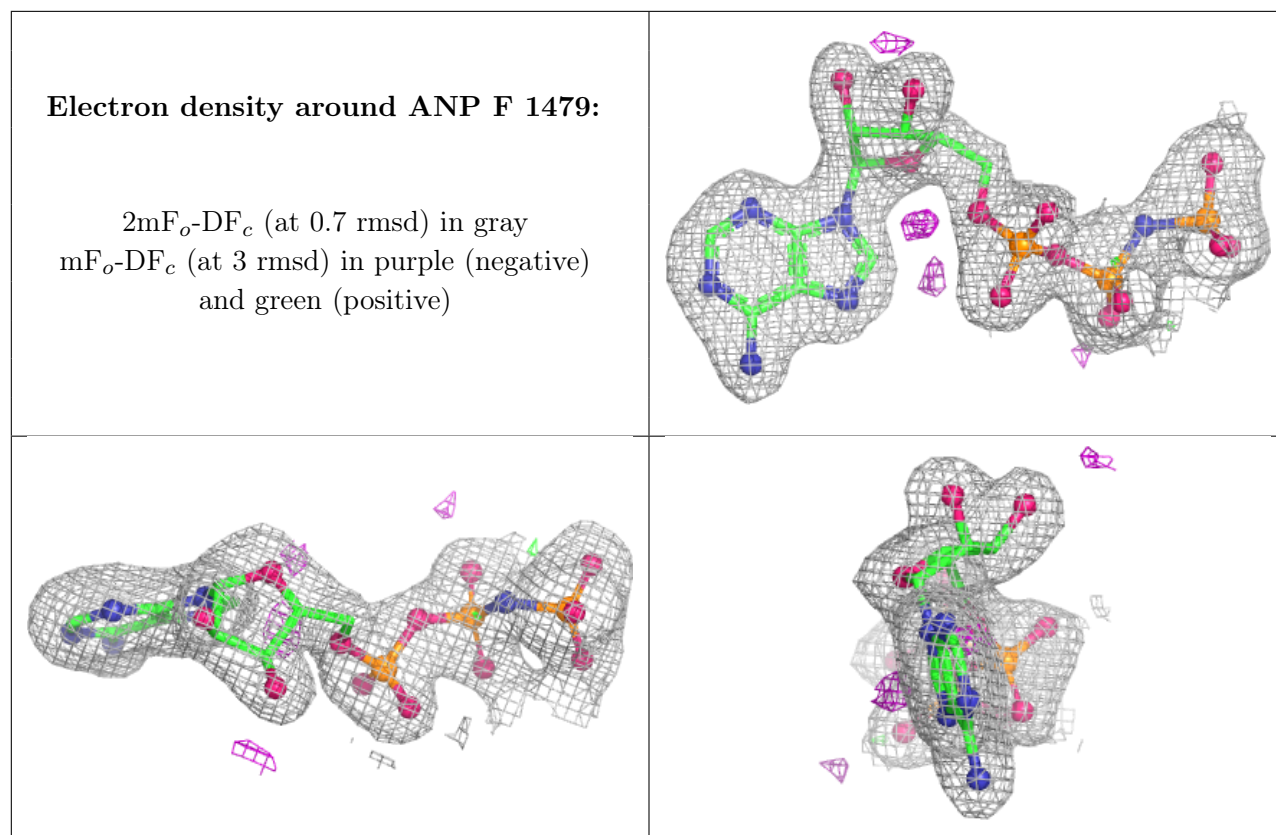
Electron density around ANP A 1511:

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

**Electron density around ANP D 1480:**

$2mF_o-DF_c$ (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.