



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 03:52 PM UTC

PDB ID : 1JQH / pdb_00001jqh
Title : IGF-1 receptor kinase domain
Authors : Pautsch, A.; Zoephel, A.; Ahorn, H.; Spevak, W.; Hauptmann, R.; Nar, H.
Deposited on : 2001-08-07
Resolution : 2.10 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

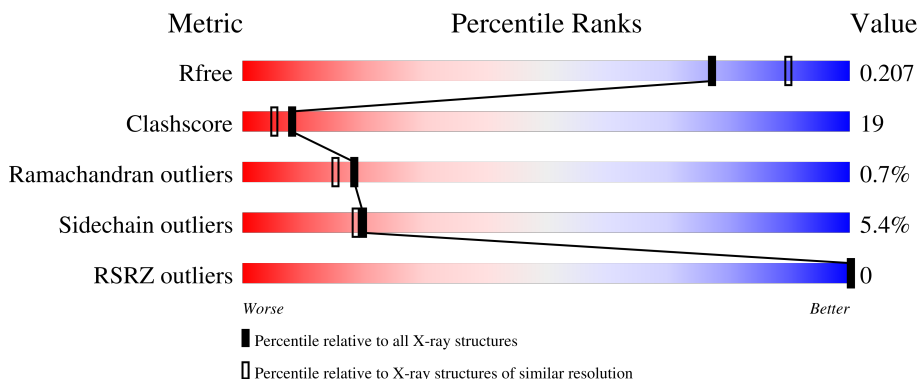
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	308	 62% 29% • 6%
1	B	308	 59% 30% • • 7%
1	C	308	 61% 29% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7292 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 IGF-1 receptor kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2320	1477	387	434	22			
1	B	287	Total	C	N	O	S	0	0	0
			2291	1458	383	428	22			
1	C	291	Total	C	N	O	S	0	0	0
			2320	1477	387	434	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	GLU	engineered mutation	UNP P08069
A	980	SER	TYR	engineered mutation	UNP P08069
B	979	GLY	GLU	engineered mutation	UNP P08069
B	980	SER	TYR	engineered mutation	UNP P08069
C	979	GLY	GLU	engineered mutation	UNP P08069
C	980	SER	TYR	engineered mutation	UNP P08069

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

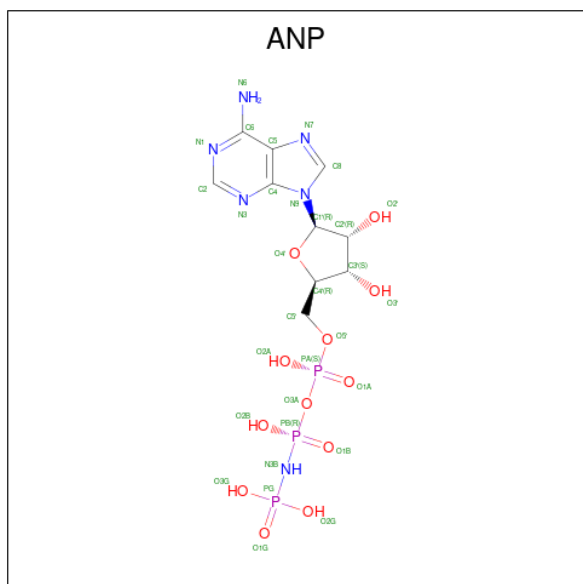
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

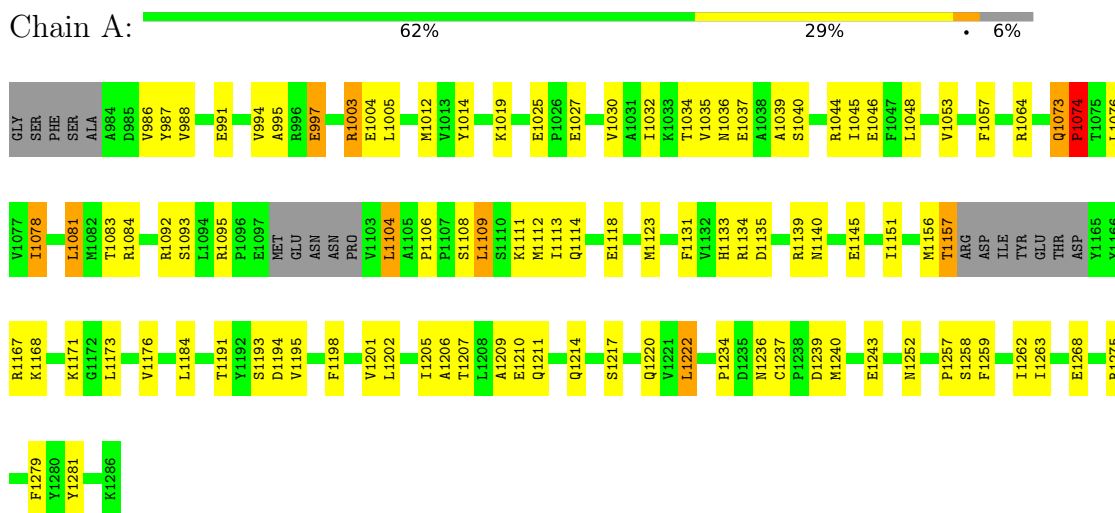
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	91	Total	O	0	0
			91	91		
5	C	77	Total	O	0	0
			77	77		

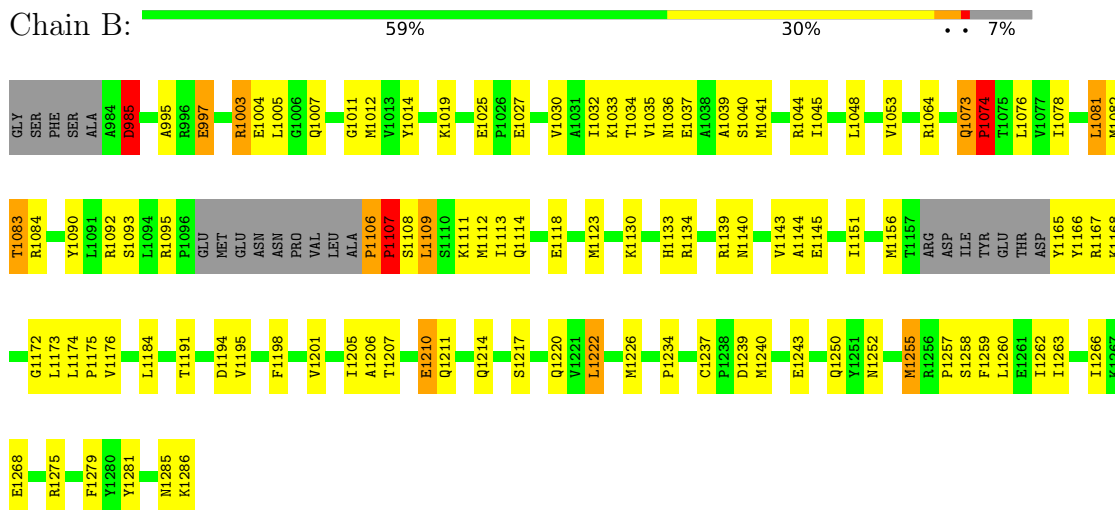
3 Residue-property plots

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: IGF-1 receptor kinase



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GLY	T1075	K1168	F1279
SER	L1076	K1171	Y1280
PHE	V1077	G1172	Y1281
SER	I1078		K1286
ALA			
A984	L1081	V1176	
D985	M1082	L1184	
	T1083	T1191	
Y994	R1084	D1194	
A995	R1092	V1195	
A996			
E997	R1095	F1198	
	P1096	V1201	
R1003	E1097	I1205	
E1004	MET	A1206	
L1005	GLU	T1207	
G1006	ASN	L1208	
Q1007	ASN	A1209	
G1008	PRO	E1210	
	V1103	Q1211	
G1011	L1104		
M1012	A1105	Q1214	
V1013	P1106	S1217	
Y1014		Q1220	
	L1109	V1221	
K1019		L1222	
	M1112	R1223	
E1025	I1113	P1234	
P1026	Q1114	C1237	
E1027		F1238	
	E1118	D1239	
V1030	M1123	M1240	
A1031	F1131	E1243	
K1033	V1132	Q1250	
T1034	H1133	Y1251	
V1035	R1134	N1252	
M1036	D1135	M1255	
E1037		R1256	
A1038	R1139	P1257	
A1039	N1140	S1258	
S1040	E1145	F1259	
M1041	I1151	I1262	
	M1156	I1263	
R1044	T1157	E1268	
	ARG		
L1048	ASP		
N1049	ILE		
E1050	TYR		
	E1056		
V1053			
	R1064		
	L1065		
	L1066		
	ASP		
	Y1165		
	Y1166		
	Q1073		
	P1074		
	R1167		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	85.96Å 85.96Å 132.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.10 19.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.85-2.10) 99.3 (19.85-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.01Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.195 , 0.219 0.190 , 0.207	Depositor DCC
R_{free} test set	3527 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.085 for -h,-k,l 0.288 for h,-h-k,-l 0.088 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, SO4, 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	0.47	0/2368	1.42	17/3190 (0.5%)
1	B	0.47	0/2339	1.35	18/3149 (0.6%)
1	C	0.48	0/2368	1.42	20/3190 (0.6%)
All	All	0.47	0/7075	1.40	55/9529 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1073	GLN	CA-C-N	35.81	164.60	119.84
1	A	1073	GLN	C-N-CA	35.81	164.60	119.84
1	C	1073	GLN	CA-C-N	34.68	163.19	119.84
1	C	1073	GLN	C-N-CA	34.68	163.19	119.84
1	B	1073	GLN	CA-C-N	33.70	161.97	119.84
1	B	1073	GLN	C-N-CA	33.70	161.97	119.84
1	C	1106	PRO	CA-C-N	-17.36	101.23	119.99
1	C	1106	PRO	C-N-CA	-17.36	101.23	119.99
1	A	1106	PRO	CA-C-N	-15.29	99.60	120.25
1	A	1106	PRO	C-N-CA	-15.29	99.60	120.25
1	A	1073	GLN	C-N-CD	-12.07	75.52	125.00
1	C	1073	GLN	C-N-CD	-11.97	75.92	125.00
1	B	1073	GLN	C-N-CD	-11.82	76.52	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1106	PRO	CA-C-N	8.66	130.67	119.84
1	B	1106	PRO	C-N-CA	8.66	130.67	119.84
1	B	1074	PRO	CA-N-CD	-8.66	99.88	112.00
1	A	1074	PRO	CA-N-CD	-8.64	99.90	112.00
1	C	1074	PRO	CA-N-CD	-7.52	101.47	112.00
1	B	1252	ASN	CA-C-N	6.98	126.50	119.24
1	B	1252	ASN	C-N-CA	6.98	126.50	119.24
1	C	1105	ALA	CA-C-N	6.38	126.95	120.38
1	C	1105	ALA	C-N-CA	6.38	126.95	120.38
1	B	1064	ARG	N-CA-C	6.26	120.03	109.76
1	C	1064	ARG	N-CA-C	6.08	120.18	109.96
1	B	1176	VAL	N-CA-C	5.84	116.50	110.36
1	A	1064	ARG	N-CA-C	5.76	119.20	109.76
1	A	1194	ASP	N-CA-C	-5.76	105.08	111.36
1	A	1252	ASN	CA-C-N	5.75	125.88	119.32
1	A	1252	ASN	C-N-CA	5.75	125.88	119.32
1	A	1025	GLU	CA-C-N	5.64	125.11	119.24
1	A	1025	GLU	C-N-CA	5.64	125.11	119.24
1	B	985	ASP	N-CA-C	-5.64	105.08	112.41
1	C	1252	ASN	CA-C-N	5.62	125.73	119.32
1	C	1252	ASN	C-N-CA	5.62	125.73	119.32
1	A	1279	PHE	N-CA-C	-5.50	105.37	111.36
1	B	1279	PHE	N-CA-C	-5.48	105.39	111.36
1	B	1025	GLU	CA-C-N	5.47	124.93	119.24
1	B	1025	GLU	C-N-CA	5.47	124.93	119.24
1	C	1279	PHE	N-CA-C	-5.47	105.40	111.36
1	C	1194	ASP	N-CA-C	-5.45	105.42	111.36
1	A	1209	ALA	N-CA-C	5.44	118.62	111.28
1	C	1025	GLU	CA-C-N	5.42	124.87	119.24
1	C	1025	GLU	C-N-CA	5.42	124.87	119.24
1	A	1005	LEU	N-CA-C	-5.41	106.73	113.55
1	C	1005	LEU	N-CA-C	-5.38	106.77	113.55
1	B	1005	LEU	N-CA-C	-5.32	106.85	113.55
1	B	1194	ASP	N-CA-C	-5.31	105.57	111.36
1	C	1209	ALA	N-CA-C	5.18	118.27	111.28
1	B	1083	THR	N-CA-C	5.17	118.36	111.75
1	A	1202	LEU	N-CA-C	-5.15	105.75	111.36
1	B	1210	GLU	N-CA-C	-5.12	103.17	110.59
1	C	1095	ARG	CA-C-N	5.11	126.22	119.84
1	C	1095	ARG	C-N-CA	5.11	126.22	119.84
1	C	1176	VAL	N-CA-C	5.07	116.39	110.62
1	A	1176	VAL	N-CA-C	5.05	116.38	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1223	ARG	Sidechain

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	2320	0	2295	91	0
1	B	2291	0	2265	99	0
1	C	2320	0	2295	99	1
2	A	1	0	0	0	0
3	A	5	0	0	0	1
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	31	0	13	0	0
4	B	31	0	13	1	0
4	C	31	0	13	1	0
5	A	84	0	0	6	0
5	B	91	0	0	2	0
5	C	77	0	0	0	0
All	All	7292	0	6894	270	1

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 19.

All (270) 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:C:1053:VAL:HG12	1:C:1156:MET:CE	1.78	1.14
1:C:1092:ARG:HH21	1:C:1095:ARG:NE	1.48	1.11
1:C:1053:VAL:HG12	1:C:1156:MET:HE2	1.39	1.03
1:A:1157:THR:HG21	1:C:984:ALA:HA	1.37	1.02
1:B:1003:ARG:HG3	1:B:1003:ARG:HH11	1.28	0.93
1:A:1157:THR:HG21	1:C:984:ALA:CA	2.02	0.90
1:C:1053:VAL:HG12	1:C:1156:MET:HE3	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:ARG:HH21	1:B:1095:ARG:NE	1.69	0.89
1:B:1045:ILE:HD11	1:C:1172:GLY:HA2	1.55	0.89
1:C:1050:GLU:O	1:C:1053:VAL:HG22	1.75	0.84
1:A:1095:ARG:HH22	1:A:1210:GLU:HG2	1.41	0.84
1:A:1104:LEU:N	1:A:1104:LEU:HD22	1.96	0.81
1:A:1003:ARG:HG3	1:A:1003:ARG:HH11	1.42	0.81
1:A:986:VAL:HG23	1:B:1172:GLY:O	1.82	0.80
1:C:1092:ARG:HH21	1:C:1095:ARG:HE	1.28	0.78
1:C:1167:ARG:HH11	1:C:1167:ARG:HB2	1.46	0.77
1:B:1184:LEU:HD22	1:B:1222:LEU:HD22	1.67	0.77
1:C:1184:LEU:HD22	1:C:1222:LEU:HD22	1.67	0.76
1:C:1092:ARG:HH21	1:C:1095:ARG:CZ	1.99	0.76
1:C:1004:GLU:CD	1:C:1012:MET:HE3	2.11	0.75
1:B:1234:PRO:HB2	1:B:1237:CYS:HB2	1.69	0.75
1:C:1003:ARG:HG3	1:C:1003:ARG:HH11	1.51	0.75
1:A:1184:LEU:HD22	1:A:1222:LEU:HD22	1.69	0.75
1:B:1092:ARG:HH21	1:B:1095:ARG:CZ	1.99	0.75
1:A:1004:GLU:CD	1:A:1012:MET:HE3	2.12	0.75
1:A:987:TYR:HB3	1:B:1173:LEU:HD23	1.68	0.75
1:C:1234:PRO:HB2	1:C:1237:CYS:HB2	1.70	0.74
1:B:1004:GLU:CD	1:B:1012:MET:HE3	2.13	0.73
1:C:1104:LEU:HD23	3:C:306:SO4:O2	1.89	0.73
1:C:1074:PRO:O	1:C:1076:LEU:HG	1.88	0.72
1:A:1003:ARG:HG3	1:A:1003:ARG:NH1	2.03	0.72
1:B:1074:PRO:O	1:B:1076:LEU:HG	1.90	0.72
1:A:1234:PRO:HB2	1:A:1237:CYS:HB2	1.72	0.72
1:C:995:ALA:HB1	1:C:997:GLU:OE2	1.90	0.71
1:C:1092:ARG:NH2	1:C:1095:ARG:NE	2.32	0.71
1:C:1053:VAL:HG11	1:C:1156:MET:HG3	1.73	0.71
1:A:1074:PRO:O	1:A:1076:LEU:HG	1.90	0.70
1:A:995:ALA:HB1	1:A:997:GLU:OE2	1.90	0.70
1:A:1092:ARG:HH21	1:A:1095:ARG:HE	1.39	0.70
1:B:1073:GLN:HB3	1:B:1074:PRO:HD2	1.74	0.70
1:B:1003:ARG:HG3	1:B:1003:ARG:NH1	2.03	0.70
1:B:995:ALA:HB1	1:B:997:GLU:OE2	1.92	0.69
1:C:1053:VAL:CG1	1:C:1156:MET:CE	2.66	0.69
1:B:1106:PRO:O	1:B:1107:PRO:O	2.10	0.69
1:C:1040:SER:O	1:C:1044:ARG:HG3	1.93	0.68
1:A:1131:PHE:CD2	1:A:1156:MET:HE2	2.29	0.67
1:B:1145:GLU:HA	1:B:1145:GLU:OE2	1.95	0.67
1:B:1040:SER:O	1:B:1044:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:GLN:O	1:B:1118:GLU:HG3	1.95	0.66
1:C:1145:GLU:OE2	1:C:1145:GLU:HA	1.97	0.65
1:A:1207:THR:HB	1:A:1210:GLU:HG3	1.78	0.65
1:C:1053:VAL:CG1	1:C:1156:MET:HE2	2.22	0.65
1:A:1045:ILE:HG12	1:B:1173:LEU:HD21	1.79	0.64
1:B:1239:ASP:O	1:B:1243:GLU:HG2	1.98	0.64
1:C:1239:ASP:O	1:C:1243:GLU:HG2	1.98	0.64
1:A:1040:SER:O	1:A:1044:ARG:HG3	1.96	0.64
1:C:1114:GLN:O	1:C:1118:GLU:HG3	1.96	0.64
1:B:1207:THR:HB	1:B:1210:GLU:HG3	1.79	0.63
1:A:1045:ILE:HG12	1:B:1173:LEU:CD2	2.29	0.62
1:A:1145:GLU:OE2	1:A:1145:GLU:HA	1.99	0.62
1:A:1113:ILE:HD11	1:A:1240:MET:HE1	1.82	0.62
1:A:1114:GLN:O	1:A:1118:GLU:HG3	1.99	0.62
1:A:1078:ILE:N	1:A:1078:ILE:HD12	2.15	0.61
1:C:1167:ARG:HH11	1:C:1167:ARG:CB	2.14	0.61
1:C:1207:THR:HB	1:C:1210:GLU:HG3	1.82	0.61
1:C:1078:ILE:N	1:C:1078:ILE:HD12	2.16	0.60
1:A:1045:ILE:HD11	1:B:1172:GLY:HA2	1.82	0.60
1:C:1113:ILE:HD11	1:C:1240:MET:HE1	1.84	0.60
1:C:1171:LYS:HG3	1:C:1171:LYS:O	2.01	0.60
1:C:1050:GLU:O	1:C:1053:VAL:CG2	2.48	0.59
1:A:1156:MET:O	1:A:1157:THR:HB	2.02	0.59
1:B:1078:ILE:HD12	1:B:1078:ILE:N	2.17	0.59
1:C:1092:ARG:NH2	1:C:1095:ARG:HE	1.95	0.59
1:C:1003:ARG:HG3	1:C:1003:ARG:NH1	2.17	0.59
1:A:1239:ASP:O	1:A:1243:GLU:HG2	2.02	0.59
1:B:1113:ILE:HD11	1:B:1240:MET:HE1	1.83	0.59
1:B:1198:PHE:O	1:B:1201:VAL:HG22	2.03	0.58
1:A:1157:THR:HG21	1:C:984:ALA:N	2.18	0.58
1:A:1109:LEU:O	1:A:1113:ILE:HG12	2.04	0.58
1:C:1056:GLU:OE1	1:C:1167:ARG:NH2	2.36	0.58
1:C:1198:PHE:O	1:C:1201:VAL:HG22	2.04	0.57
1:A:1134:ARG:HD3	1:A:1168:LYS:HD2	1.86	0.57
1:A:1173:LEU:H	1:C:1041:MET:HE3	1.69	0.57
1:C:1123:MET:HG2	1:C:1151:ILE:HD11	1.87	0.57
1:C:1007:GLN:HE22	1:C:1011:GLY:HA2	1.69	0.57
1:C:1030:VAL:HG23	1:C:1032:ILE:HD11	1.86	0.57
1:A:1112:MET:HE2	1:A:1205:ILE:HG22	1.87	0.56
1:B:1175:PRO:HG3	5:B:54:HOH:O	2.05	0.56
1:B:1030:VAL:HG23	1:B:1032:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:LEU:O	1:B:1113:ILE:HG12	2.04	0.56
1:A:1030:VAL:HG23	1:A:1032:ILE:HD11	1.86	0.56
1:A:1045:ILE:CD1	1:B:1172:GLY:HA2	2.35	0.56
1:B:1123:MET:HG2	1:B:1151:ILE:HD11	1.87	0.56
1:A:1045:ILE:HG22	5:A:221:HOH:O	2.07	0.55
1:B:1167:ARG:HH11	1:B:1167:ARG:HG2	1.71	0.55
1:B:1275:ARG:HA	1:B:1281:TYR:CD1	2.41	0.55
1:B:1090:TYR:O	1:B:1093:SER:OG	2.25	0.55
1:C:1095:ARG:O	1:C:1097:GLU:N	2.37	0.55
1:A:988:VAL:HG22	1:B:1174:LEU:HD12	1.89	0.54
1:B:1073:GLN:CB	1:B:1074:PRO:HD2	2.35	0.54
1:B:1257:PRO:HG2	1:B:1262:ILE:HD11	1.89	0.54
1:A:1123:MET:HG2	1:A:1151:ILE:HD11	1.90	0.54
1:B:1134:ARG:HD3	1:B:1168:LYS:HD2	1.89	0.54
1:B:985:ASP:N	1:B:985:ASP:OD1	2.40	0.54
1:A:1104:LEU:HD22	1:A:1104:LEU:H	1.67	0.54
1:A:1257:PRO:HG2	1:A:1262:ILE:HD11	1.90	0.54
1:A:1198:PHE:O	1:A:1201:VAL:HG22	2.08	0.54
1:C:1109:LEU:O	1:C:1113:ILE:HG12	2.08	0.54
1:C:1275:ARG:HA	1:C:1281:TYR:CD1	2.43	0.54
1:B:1003:ARG:NH1	1:B:1003:ARG:CG	2.68	0.53
1:B:1073:GLN:HB3	1:B:1074:PRO:CD	2.38	0.53
1:B:1082:MET:HE3	1:B:1144:ALA:N	2.23	0.53
1:A:1139:ARG:HG3	1:A:1139:ARG:HH11	1.74	0.53
1:A:987:TYR:HB3	1:B:1173:LEU:CD2	2.36	0.53
1:C:1112:MET:HE2	1:C:1205:ILE:HG22	1.90	0.53
1:C:1056:GLU:OE2	1:C:1167:ARG:NH2	2.42	0.53
1:A:1104:LEU:N	1:A:1104:LEU:CD2	2.68	0.52
1:B:1045:ILE:HD11	1:C:1172:GLY:CA	2.34	0.52
1:A:1275:ARG:HA	1:A:1281:TYR:CD1	2.44	0.52
1:C:1007:GLN:NE2	1:C:1011:GLY:HA2	2.23	0.52
1:C:1134:ARG:HD3	1:C:1168:LYS:HD2	1.90	0.52
1:B:1165:TYR:HE1	1:B:1168:LYS:HZ1	1.55	0.52
1:C:1252:ASN:O	1:C:1255:MET:HB2	2.10	0.52
1:B:1041:MET:HE3	1:C:1172:GLY:HA3	1.92	0.51
1:C:1056:GLU:CD	1:C:1167:ARG:HH22	2.18	0.51
1:A:1113:ILE:CD1	1:A:1240:MET:HE1	2.40	0.51
1:C:1053:VAL:CG1	1:C:1156:MET:HE3	2.31	0.51
1:C:1123:MET:SD	1:C:1151:ILE:HD13	2.51	0.51
1:C:1250:GLN:CB	1:C:1255:MET:HB3	2.41	0.51
1:A:1193:SER:HB2	5:A:151:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1113:ILE:CD1	1:C:1240:MET:HE1	2.41	0.51
1:A:1201:VAL:O	1:A:1205:ILE:HG13	2.10	0.50
1:B:1092:ARG:NH2	1:B:1095:ARG:CZ	2.71	0.50
1:B:1112:MET:HE2	1:B:1205:ILE:HG22	1.93	0.50
1:C:1056:GLU:CD	1:C:1167:ARG:NH2	2.70	0.50
1:C:1257:PRO:HG2	1:C:1262:ILE:HD11	1.93	0.50
1:A:1195:VAL:O	1:A:1198:PHE:HB3	2.12	0.50
1:B:1113:ILE:CD1	1:B:1240:MET:HE1	2.42	0.50
1:C:1092:ARG:HE	1:C:1095:ARG:HE	1.58	0.50
1:A:1123:MET:SD	1:A:1151:ILE:HD13	2.52	0.49
1:B:1082:MET:HE3	1:B:1143:VAL:C	2.37	0.49
1:C:1113:ILE:HD11	1:C:1240:MET:SD	2.51	0.49
1:B:1113:ILE:HD11	1:B:1240:MET:SD	2.53	0.49
1:B:1184:LEU:HD22	1:B:1222:LEU:CD2	2.41	0.49
1:B:1004:GLU:HG2	1:B:1014:TYR:CE1	2.46	0.49
1:B:1036:ASN:OD1	1:B:1037:GLU:HG2	2.13	0.49
1:C:1139:ARG:HG2	1:C:1139:ARG:HH11	1.78	0.49
1:A:1004:GLU:HG2	1:A:1014:TYR:CE1	2.48	0.48
1:B:1258:SER:O	1:B:1262:ILE:HG12	2.13	0.48
1:A:1134:ARG:NE	1:A:1168:LYS:HB3	2.28	0.48
1:B:1083:THR:OG1	1:B:1145:GLU:OE2	2.27	0.48
1:C:1008:GLY:CA	4:C:303:ANP:O2B	2.62	0.48
1:C:1036:ASN:OD1	1:C:1037:GLU:HG2	2.13	0.48
1:A:1083:THR:OG1	1:A:1145:GLU:OE2	2.25	0.48
1:B:1123:MET:SD	1:B:1151:ILE:HD13	2.53	0.48
1:B:1260:LEU:HD11	1:B:1286:LYS:NZ	2.28	0.48
1:B:1082:MET:HE1	1:B:1144:ALA:HB2	1.95	0.47
1:C:1019:LYS:HG2	1:C:1027:GLU:HG2	1.96	0.47
1:A:1053:VAL:HG12	1:A:1057:PHE:HE2	1.78	0.47
1:A:1173:LEU:HG	1:C:1041:MET:CE	2.44	0.47
1:B:1106:PRO:HB2	1:B:1107:PRO:HD2	1.96	0.47
1:A:1092:ARG:HH21	1:A:1095:ARG:NE	2.09	0.47
1:A:1133:HIS:O	1:A:1134:ARG:HB2	2.14	0.47
1:A:1184:LEU:HD22	1:A:1222:LEU:CD2	2.43	0.47
1:B:1019:LYS:HG2	1:B:1027:GLU:HG2	1.96	0.47
1:A:1113:ILE:HD11	1:A:1240:MET:SD	2.54	0.47
1:B:1113:ILE:HG23	1:B:1266:ILE:CG1	2.45	0.47
1:B:1130:LYS:HA	1:B:1166:TYR:CD1	2.50	0.47
1:C:1004:GLU:HG2	1:C:1014:TYR:CE1	2.50	0.47
1:C:1184:LEU:HD22	1:C:1222:LEU:CD2	2.39	0.47
1:C:1201:VAL:O	1:C:1205:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:SER:O	1:A:1262:ILE:HG12	2.14	0.47
1:A:1053:VAL:HA	5:A:235:HOH:O	2.15	0.47
1:C:1195:VAL:O	1:C:1198:PHE:HB3	2.15	0.47
1:A:1046:GLU:HA	5:A:221:HOH:O	2.14	0.46
1:A:1139:ARG:HH12	1:A:1140:ASN:HD21	1.62	0.46
1:B:1033:LYS:NZ	4:B:302:ANP:O1B	2.45	0.46
1:B:1106:PRO:C	1:B:1107:PRO:O	2.56	0.46
1:C:1073:GLN:HB3	1:C:1074:PRO:HD2	1.72	0.46
1:B:1195:VAL:O	1:B:1198:PHE:HB3	2.15	0.46
1:C:1034:THR:HG22	1:C:1076:LEU:CD2	2.46	0.46
1:B:1167:ARG:HG2	1:B:1167:ARG:NH1	2.30	0.46
1:A:1112:MET:HE1	1:A:1206:ALA:HA	1.97	0.46
1:C:1035:VAL:HG12	1:C:1039:ALA:CB	2.45	0.46
1:A:1036:ASN:OD1	1:A:1037:GLU:HG2	2.15	0.46
1:B:1095:ARG:NH2	1:B:1210:GLU:HG2	2.30	0.46
1:A:1081:LEU:HD13	1:A:1083:THR:HG23	1.98	0.46
1:B:1259:PHE:O	1:B:1263:ILE:HG13	2.16	0.46
1:B:1053:VAL:CG1	1:B:1156:MET:HE3	2.46	0.46
1:C:1112:MET:HE1	1:C:1206:ALA:HA	1.98	0.46
1:C:1133:HIS:O	1:C:1134:ARG:HB2	2.16	0.46
1:B:1109:LEU:HD11	1:B:1240:MET:HE3	1.98	0.45
1:B:1211:GLN:O	1:B:1214:GLN:HB2	2.16	0.45
1:A:1019:LYS:HG2	1:A:1027:GLU:HG2	1.98	0.45
1:A:1035:VAL:HG12	1:A:1039:ALA:CB	2.47	0.45
1:A:1113:ILE:HD11	1:A:1240:MET:CE	2.47	0.45
1:A:1211:GLN:O	1:A:1214:GLN:HB2	2.17	0.45
1:A:1078:ILE:N	1:A:1078:ILE:CD1	2.79	0.45
1:C:1019:LYS:HE3	1:C:1027:GLU:CG	2.46	0.45
1:C:1211:GLN:O	1:C:1214:GLN:HB2	2.17	0.45
1:B:1217:SER:OG	1:B:1220:GLN:HG3	2.17	0.45
1:C:1078:ILE:N	1:C:1078:ILE:CD1	2.80	0.45
1:B:1112:MET:HE1	1:B:1206:ALA:HA	1.99	0.45
1:B:1286:LYS:H	1:B:1286:LYS:HD2	1.82	0.45
1:C:1250:GLN:HB3	1:C:1255:MET:HB3	1.97	0.45
1:C:1258:SER:O	1:C:1262:ILE:HG12	2.17	0.45
1:A:1167:ARG:HG2	1:A:1167:ARG:HH11	1.83	0.44
1:A:1217:SER:OG	1:A:1220:GLN:HG3	2.18	0.44
1:C:1217:SER:OG	1:C:1220:GLN:HG3	2.18	0.44
1:A:1034:THR:HG22	1:A:1076:LEU:CD2	2.47	0.44
1:B:1084:ARG:HG2	1:B:1084:ARG:HH11	1.82	0.44
1:C:1081:LEU:HD13	1:C:1083:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:ARG:NH1	1:A:1140:ASN:ND2	2.65	0.44
1:B:1030:VAL:HG23	1:B:1032:ILE:CD1	2.47	0.44
1:B:1035:VAL:HG12	1:B:1039:ALA:CB	2.47	0.44
1:B:1041:MET:HE3	1:C:1172:GLY:CA	2.47	0.44
1:B:1113:ILE:HD11	1:B:1240:MET:CE	2.47	0.44
1:C:1030:VAL:HG23	1:C:1032:ILE:CD1	2.47	0.44
1:A:1095:ARG:HH22	1:A:1210:GLU:CG	2.21	0.44
1:B:1139:ARG:NH1	1:B:1140:ASN:OD1	2.51	0.44
1:B:1250:GLN:HB3	1:B:1255:MET:HB3	2.00	0.44
1:C:1135:ASP:O	1:C:1140:ASN:ND2	2.51	0.44
1:C:1004:GLU:OE2	1:C:1012:MET:HE3	2.18	0.43
1:C:1113:ILE:HD11	1:C:1240:MET:CE	2.47	0.43
1:B:1106:PRO:CB	1:B:1107:PRO:HD2	2.49	0.43
1:B:1175:PRO:HG2	5:B:182:HOH:O	2.18	0.43
1:B:1078:ILE:N	1:B:1078:ILE:CD1	2.82	0.43
1:C:1066:LEU:HB2	1:C:1078:ILE:HG22	1.99	0.43
1:A:1030:VAL:HG23	1:A:1032:ILE:CD1	2.48	0.43
1:B:1106:PRO:O	1:B:1107:PRO:C	2.60	0.43
1:A:1053:VAL:CG1	1:A:1156:MET:HE3	2.49	0.43
1:C:1007:GLN:HA	1:C:1012:MET:HA	2.00	0.43
1:A:1019:LYS:HE3	1:A:1027:GLU:CG	2.49	0.43
1:B:1036:ASN:OD1	1:B:1037:GLU:N	2.52	0.43
1:B:1113:ILE:HG23	1:B:1266:ILE:HG12	2.00	0.43
1:B:1034:THR:HG22	1:B:1076:LEU:CD2	2.49	0.42
1:B:1201:VAL:O	1:B:1205:ILE:HG13	2.18	0.42
1:A:1084:ARG:HH11	1:A:1084:ARG:HG2	1.83	0.42
1:A:1236:ASN:HB2	5:A:227:HOH:O	2.18	0.42
1:B:1081:LEU:HD13	1:B:1083:THR:HG23	2.00	0.42
1:A:1156:MET:O	1:A:1157:THR:CB	2.67	0.42
1:B:1108:SER:OG	1:B:1111:LYS:HG2	2.19	0.42
1:A:1004:GLU:OE2	1:A:1012:MET:HE3	2.19	0.42
1:A:1259:PHE:O	1:A:1263:ILE:HG13	2.20	0.42
1:B:1004:GLU:OE2	1:B:1012:MET:HE3	2.19	0.42
1:C:1095:ARG:HH22	1:C:1210:GLU:HG2	1.84	0.42
1:A:1108:SER:OG	1:A:1111:LYS:HG2	2.20	0.42
1:A:1139:ARG:HG3	1:A:1139:ARG:NH1	2.35	0.41
1:C:1259:PHE:O	1:C:1263:ILE:HG13	2.20	0.41
1:A:1139:ARG:HH12	1:A:1140:ASN:ND2	2.19	0.41
1:C:1092:ARG:NE	1:C:1095:ARG:HE	2.18	0.41
1:B:1007:GLN:NE2	1:B:1011:GLY:HA2	2.34	0.41
1:A:991:GLU:CD	1:B:1226:MET:HE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:LEU:HD11	1:A:1240:MET:HE3	2.01	0.41
1:A:1135:ASP:O	1:A:1140:ASN:ND2	2.52	0.41
1:B:1019:LYS:HE3	1:B:1027:GLU:CG	2.50	0.41
1:A:986:VAL:CG2	1:B:1172:GLY:O	2.60	0.41
1:A:1073:GLN:HB3	1:A:1074:PRO:HD2	1.80	0.41
1:C:1084:ARG:HG2	1:C:1084:ARG:HH11	1.85	0.41
1:C:1243:GLU:HA	1:C:1243:GLU:OE2	2.21	0.41
1:B:1243:GLU:OE2	1:B:1243:GLU:HA	2.21	0.41
1:C:1036:ASN:OD1	1:C:1037:GLU:N	2.54	0.40
1:C:1109:LEU:HD11	1:C:1240:MET:HE3	2.04	0.40
1:C:1131:PHE:HE2	1:C:1156:MET:HG2	1.86	0.40
1:A:1171:LYS:NZ	5:A:249:HOH:O	2.54	0.40
1:B:1133:HIS:O	1:B:1134:ARG:HB2	2.21	0.40
1:C:1037:GLU:HG3	1:C:1038:ALA:N	2.36	0.40
1:C:1096:PRO:C	1:C:1097:GLU:OE2	2.64	0.40
1:B:1285:ASN:OD1	1:B:1286:LYS:HD3	2.21	0.40
1:C:1250:GLN:HG3	1:C:1255:MET:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1223:ARG:NH1	3:A:305:SO4:O3[1_545]	1.79	0.41

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/308 (92%)	273 (96%)	11 (4%)	1 (0%)	30	28
1	B	281/308 (91%)	268 (95%)	11 (4%)	2 (1%)	18	15
1	C	285/308 (92%)	273 (96%)	9 (3%)	3 (1%)	11	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	851/924 (92%)	814 (96%)	31 (4%)	6 (1%)	18	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1074	PRO
1	B	1074	PRO
1	B	1107	PRO
1	C	1074	PRO
1	C	985	ASP
1	C	1096	PRO

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	253/268 (94%)	239 (94%)	14 (6%)	19	18
1	B	250/268 (93%)	238 (95%)	12 (5%)	23	23
1	C	253/268 (94%)	238 (94%)	15 (6%)	18	16
All	All	756/804 (94%)	715 (95%)	41 (5%)	20	18

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	994	VAL
1	A	997	GLU
1	A	1003	ARG
1	A	1048	LEU
1	A	1074	PRO
1	A	1078	ILE
1	A	1081	LEU
1	A	1093	SER
1	A	1104	LEU
1	A	1109	LEU

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Mol	Chain	Res	Type
1	A	1157	THR
1	A	1191	THR
1	A	1222	LEU
1	A	1268	GLU
1	B	985	ASP
1	B	997	GLU
1	B	1003	ARG
1	B	1048	LEU
1	B	1074	PRO
1	B	1081	LEU
1	B	1107	PRO
1	B	1109	LEU
1	B	1191	THR
1	B	1222	LEU
1	B	1255	MET
1	B	1268	GLU
1	C	994	VAL
1	C	997	GLU
1	C	1003	ARG
1	C	1048	LEU
1	C	1053	VAL
1	C	1074	PRO
1	C	1081	LEU
1	C	1103	VAL
1	C	1109	LEU
1	C	1157	THR
1	C	1167	ARG
1	C	1191	THR
1	C	1222	LEU
1	C	1255	MET
1	C	1268	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1071	GLN
1	A	1127	ASN
1	A	1214	GLN
1	A	1236	ASN
1	B	1007	GLN
1	B	1071	GLN
1	B	1214	GLN

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Mol	Chain	Res	Type
1	B	1236	ASN
1	C	1007	GLN
1	C	1071	GLN
1	C	1127	ASN
1	C	1214	GLN
1	C	1236	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
4	ANP	A	301	2	33,33,33	2.28	13 (39%)	45,52,52	2.66	14 (31%)
3	SO4	C	306	-	4,4,4	0.50	0	6,6,6	0.14	0
3	SO4	A	305	-	4,4,4	0.43	0	6,6,6	0.16	0
4	ANP	B	302	-	33,33,33	2.09	8 (24%)	45,52,52	2.44	16 (35%)
4	ANP	C	303	-	33,33,33	2.07	7 (21%)	45,52,52	2.45	16 (35%)
3	SO4	B	307	-	4,4,4	0.29	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	C	303	-	-	5/18/38/38	0/3/3/3
4	ANP	A	301	2	-	6/18/38/38	0/3/3/3
4	ANP	B	302	-	-	4/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	ANP	PB-O3A	6.16	1.66	1.59
4	C	303	ANP	PB-O3A	5.96	1.66	1.59
4	A	301	ANP	PB-O1B	5.47	1.54	1.46
4	C	303	ANP	PB-O2B	-5.29	1.42	1.56
4	A	301	ANP	PB-O3A	4.74	1.65	1.59
4	A	301	ANP	PB-O2B	-4.66	1.44	1.56
4	A	301	ANP	PG-O1G	4.34	1.52	1.46
4	B	302	ANP	PB-O2B	-4.24	1.45	1.56
4	B	302	ANP	PG-O1G	4.15	1.52	1.46
4	C	303	ANP	PG-O1G	3.63	1.51	1.46
4	B	302	ANP	PG-N3B	3.44	1.72	1.63
4	B	302	ANP	PB-O1B	2.76	1.50	1.46
4	B	302	ANP	C2-N1	2.69	1.38	1.33
4	A	301	ANP	PG-N3B	2.64	1.70	1.63
4	C	303	ANP	PG-N3B	2.63	1.70	1.63
4	B	302	ANP	C4-N9	-2.57	1.32	1.37
4	A	301	ANP	C5-C6	2.52	1.48	1.41
4	C	303	ANP	C2-N1	2.46	1.38	1.33
4	A	301	ANP	PG-O2G	-2.46	1.50	1.56
4	C	303	ANP	PB-O1B	2.41	1.49	1.46
4	A	301	ANP	C5-N7	-2.36	1.34	1.39
4	A	301	ANP	C1'-N9	2.34	1.52	1.46
4	B	302	ANP	C5-N7	-2.33	1.34	1.39
4	A	301	ANP	C2'-C1'	-2.21	1.46	1.53
4	A	301	ANP	C5'-C4'	2.18	1.58	1.51
4	C	303	ANP	PG-O2G	-2.11	1.51	1.56
4	A	301	ANP	C2-N1	2.02	1.37	1.33
4	A	301	ANP	PA-O3A	2.01	1.61	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	ANP	O1B-PB-N3B	-8.76	98.88	111.77
4	A	301	ANP	C5-C4-N3	-7.03	117.03	126.72
4	C	303	ANP	C5-C4-N3	-6.79	117.37	126.72
4	B	302	ANP	C5-C4-N3	-6.32	118.01	126.72
4	B	302	ANP	O1B-PB-N3B	-6.14	102.73	111.77
4	C	303	ANP	N3-C4-N9	5.84	137.10	127.17
4	A	301	ANP	N3-C4-N9	5.70	136.86	127.17
4	B	302	ANP	N3-C4-N9	5.39	136.33	127.17
4	A	301	ANP	O4'-C1'-N9	5.18	118.05	108.09
4	C	303	ANP	O1B-PB-N3B	-4.93	104.51	111.77
4	C	303	ANP	O4'-C1'-N9	4.61	116.94	108.09
4	C	303	ANP	O1G-PG-N3B	-4.50	105.14	111.77
4	A	301	ANP	C2-N3-C4	4.43	122.66	111.83
4	B	302	ANP	O4'-C1'-N9	4.40	116.54	108.09
4	B	302	ANP	O1G-PG-N3B	-4.32	105.40	111.77
4	C	303	ANP	C4'-O4'-C1'	4.32	119.00	109.47
4	B	302	ANP	C2-N3-C4	4.10	121.84	111.83
4	A	301	ANP	O1G-PG-N3B	-4.08	105.75	111.77
4	C	303	ANP	C2-N3-C4	4.06	121.75	111.83
4	A	301	ANP	C4'-O4'-C1'	4.03	118.37	109.47
4	B	302	ANP	C4'-O4'-C1'	3.95	118.19	109.47
4	B	302	ANP	O3A-PB-N3B	3.30	115.74	106.59
4	B	302	ANP	N3-C2-N1	-3.29	123.61	128.58
4	C	303	ANP	O3A-PB-N3B	3.27	115.67	106.59
4	A	301	ANP	N3-C2-N1	-3.07	123.94	128.58
4	B	302	ANP	O4'-C4'-C3'	-3.03	99.14	105.15
4	C	303	ANP	N3-C2-N1	-2.98	124.07	128.58
4	C	303	ANP	O4'-C1'-C2'	-2.85	100.51	106.62
4	B	302	ANP	C4-N9-C8	2.83	108.71	105.74
4	A	301	ANP	O3A-PB-N3B	2.81	114.39	106.59
4	A	301	ANP	O4'-C4'-C3'	-2.66	99.88	105.15
4	C	303	ANP	C6-C5-C4	2.63	120.77	117.18
4	C	303	ANP	O4'-C4'-C3'	-2.56	100.07	105.15
4	C	303	ANP	C3'-C2'-C1'	2.52	106.23	101.46
4	B	302	ANP	O4'-C1'-C2'	-2.44	101.40	106.62
4	C	303	ANP	C4-N9-C8	2.41	108.27	105.74
4	A	301	ANP	C3'-C2'-C1'	2.40	106.00	101.46
4	B	302	ANP	C6-C5-C4	2.40	120.45	117.18
4	A	301	ANP	C6-C5-C4	2.39	120.45	117.18
4	B	302	ANP	N9-C8-N7	-2.32	110.64	113.94
4	A	301	ANP	O4'-C1'-C2'	-2.32	101.66	106.62
4	B	302	ANP	C3'-C2'-C1'	2.16	105.56	101.46
4	C	303	ANP	N9-C8-N7	-2.16	110.86	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	ANP	N9-C8-N7	-2.09	110.97	113.94
4	B	302	ANP	O2'-C2'-C3'	2.06	118.42	111.82
4	C	303	ANP	O2'-C2'-C3'	2.00	118.24	111.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	ANP	PB-N3B-PG-O1G
4	A	301	ANP	PG-N3B-PB-O1B
4	A	301	ANP	PA-O3A-PB-O1B
4	A	301	ANP	PA-O3A-PB-O2B
4	B	302	ANP	PB-N3B-PG-O1G
4	C	303	ANP	PB-N3B-PG-O1G
4	C	303	ANP	O4'-C4'-C5'-O5'
4	C	303	ANP	C3'-C4'-C5'-O5'
4	B	302	ANP	C3'-C4'-C5'-O5'
4	B	302	ANP	PB-O3A-PA-O2A
4	C	303	ANP	PB-O3A-PA-O2A
4	A	301	ANP	PB-O3A-PA-O2A
4	C	303	ANP	PG-N3B-PB-O1B
4	A	301	ANP	PB-O3A-PA-O1A
4	B	302	ANP	O4'-C4'-C5'-O5'

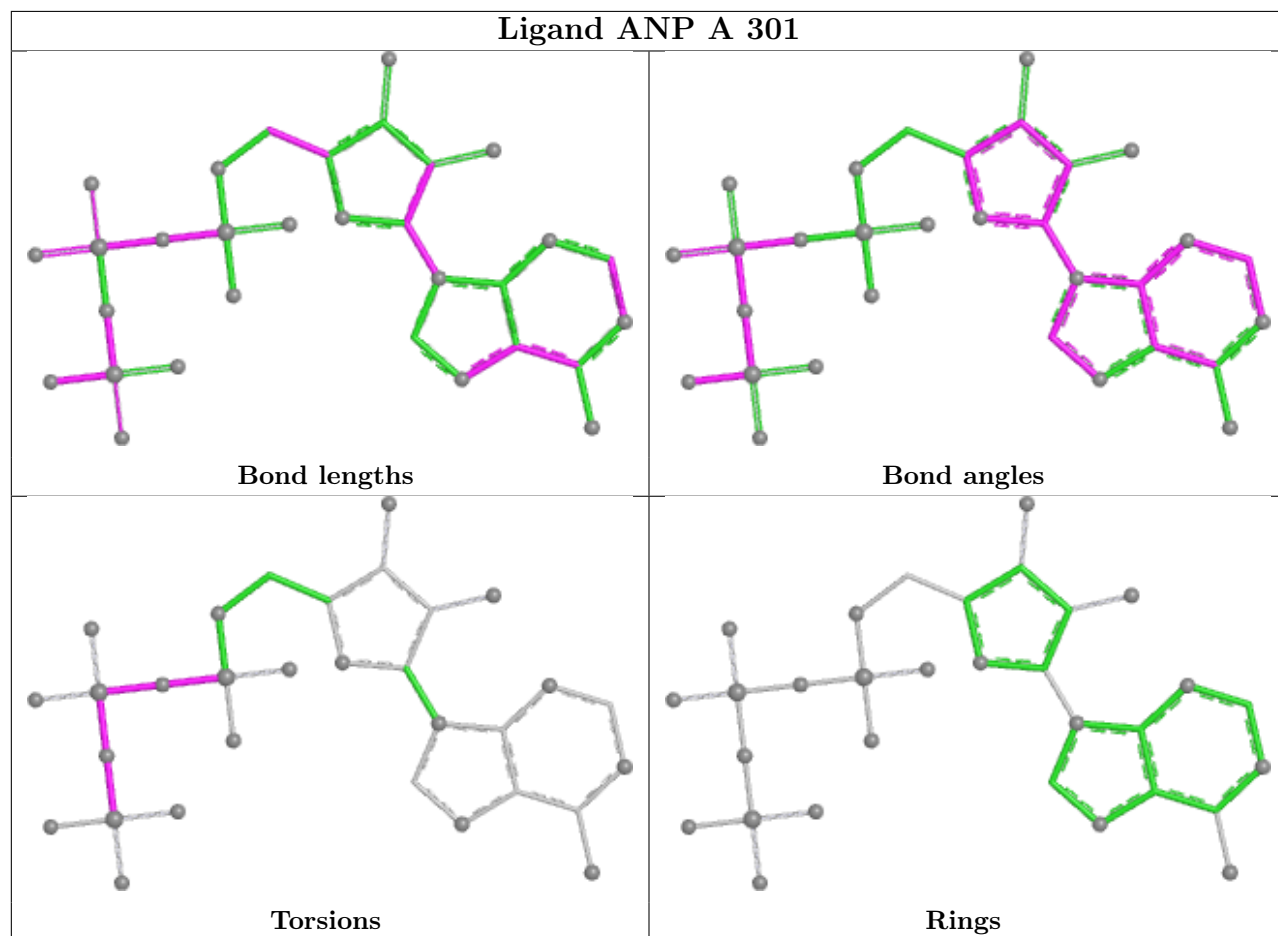
There are no ring outliers.

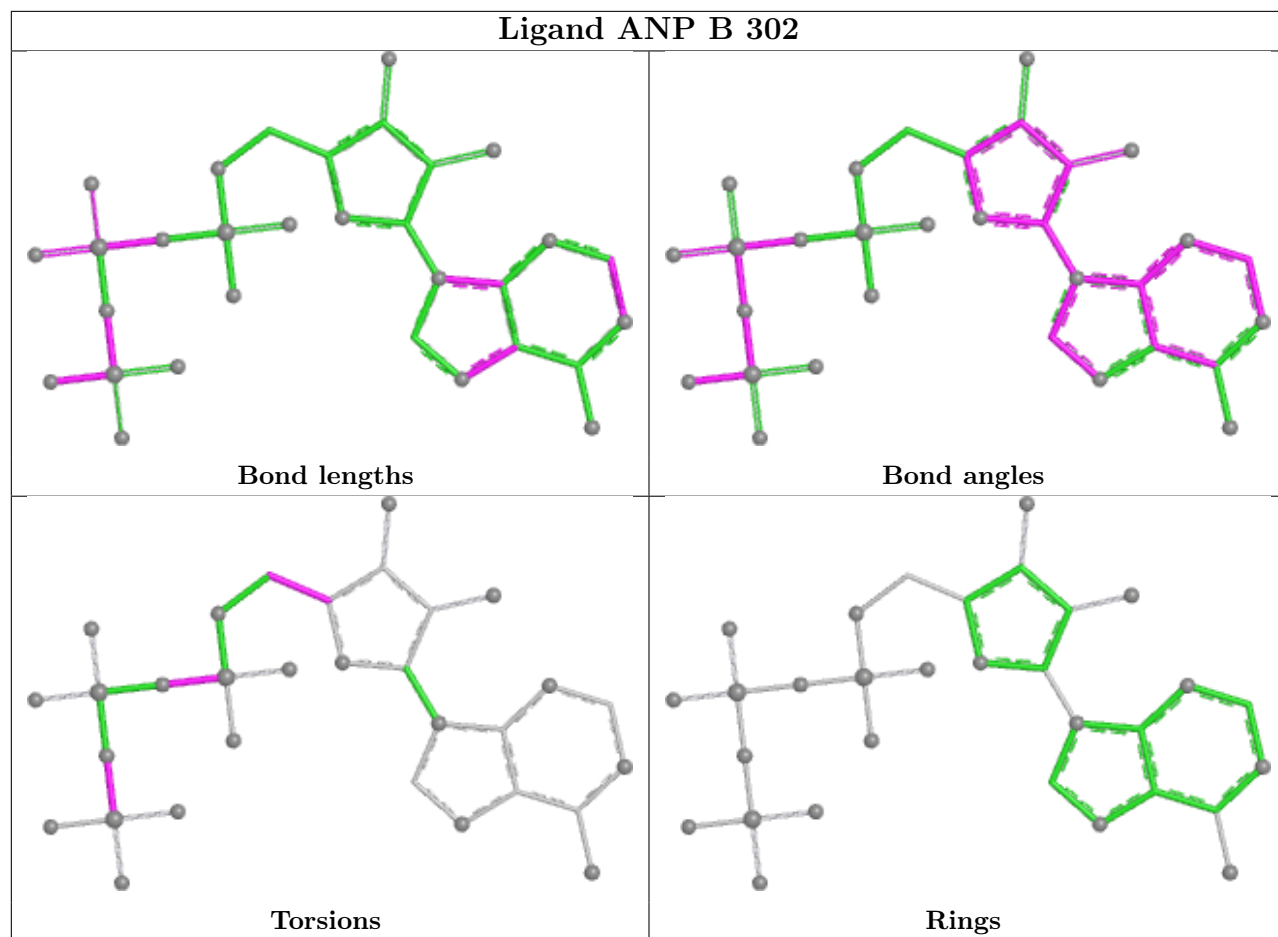
4 monomers are involved in 4 short contacts:

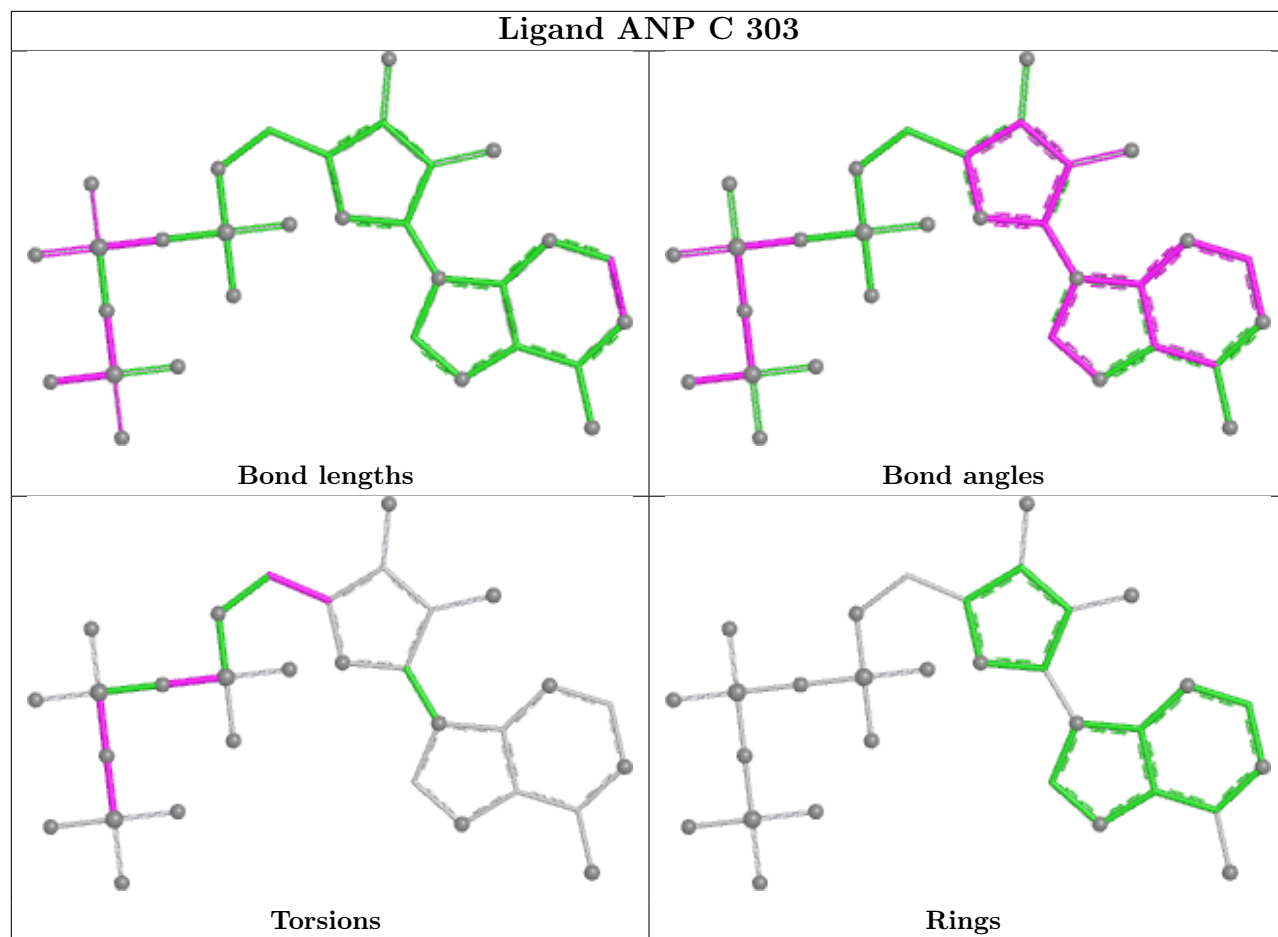
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	306	SO4	1	0
3	A	305	SO4	0	1
4	B	302	ANP	1	0
4	C	303	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	291/308 (94%)	-1.32	0 100 100	24, 42, 66, 84	0
1	B	287/308 (93%)	-1.36	0 100 100	24, 40, 65, 85	0
1	C	291/308 (94%)	-1.36	0 100 100	22, 39, 66, 83	0
All	All	869/924 (94%)	-1.35	0 100 100	22, 41, 66, 85	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	304	1/1	0.98	0.04	54,54,54,54	0
3	SO4	B	307	5/5	0.98	0.04	19,19,19,19	5
3	SO4	C	306	5/5	0.99	0.04	20,20,20,20	5
4	ANP	A	301	31/31	0.99	0.03	39,53,71,72	0
4	ANP	B	302	31/31	0.99	0.03	28,46,76,79	0

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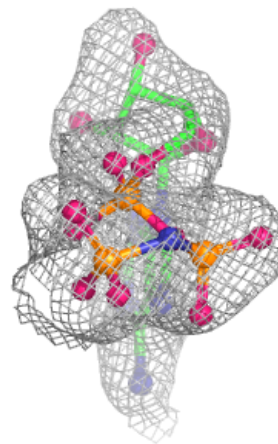
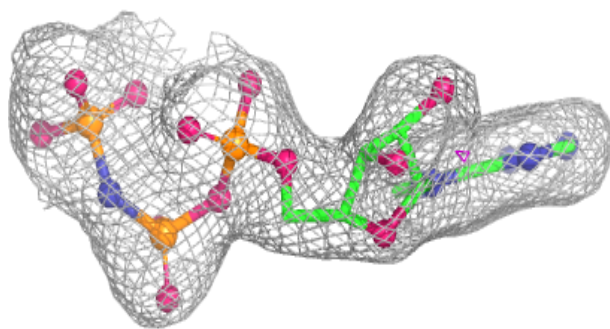
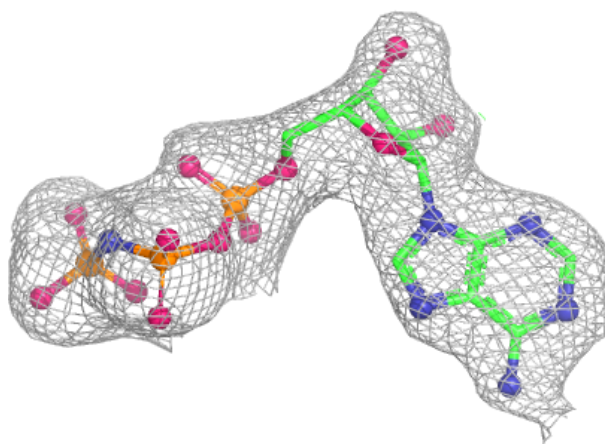
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ANP	C	303	31/31	0.99	0.03	45,54,72,74	0
3	SO4	A	305	5/5	1.00	0.07	20,20,20,20	5

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.

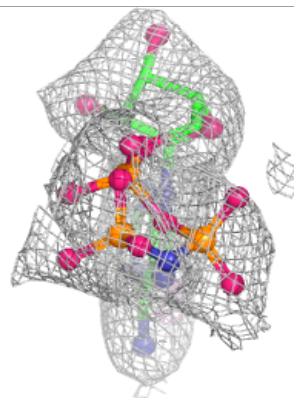
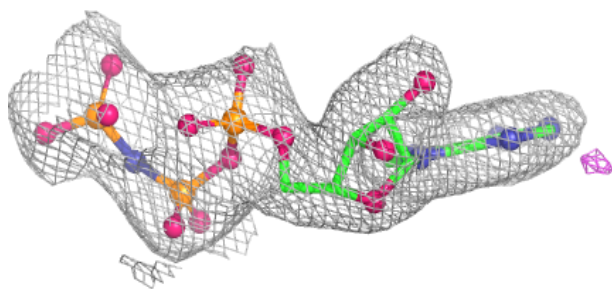
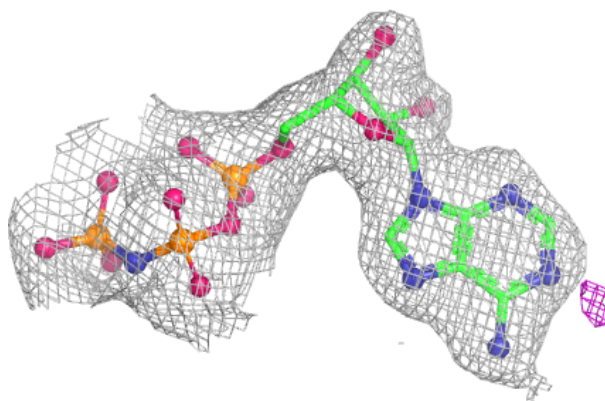
Electron density around ANP A 301:

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

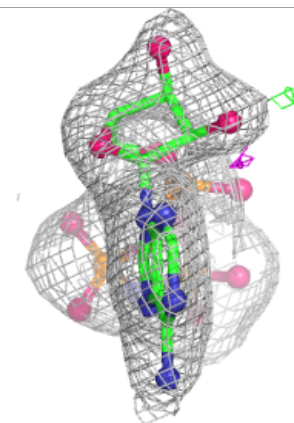
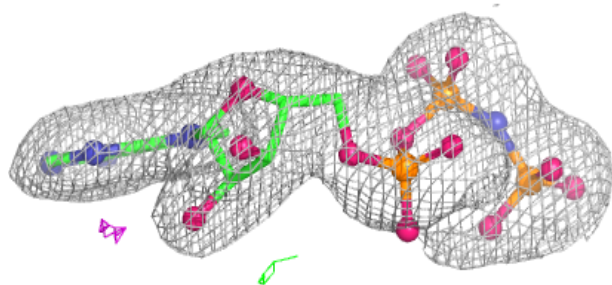
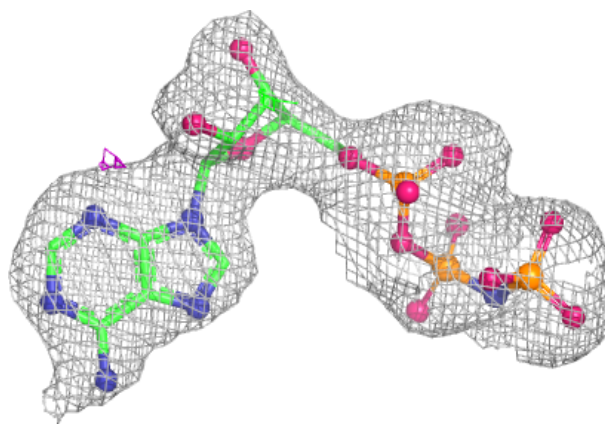


Electron density around ANP B 302:

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

**Electron density around ANP C 303:**

$2mF_o-DF_c$ (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.