



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:08 AM UTC

PDB ID : 2OID / pdb_00002oid
Title : Crystal structure of IRAK4 kinase domain complexed with AMPPNP
Authors : Kuglstatter, A.; Villasenor, A.G.; Browner, M.F.
Deposited on : 2007-01-10
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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

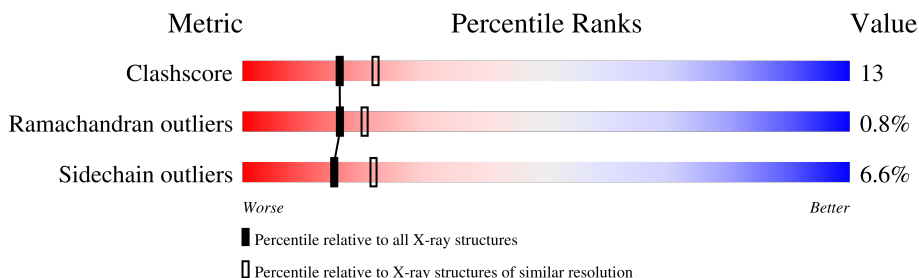
1 Overall quality at a glance

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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8921 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	266	2105	1321	356	412	3	13	0	0	0
1	B	274	2171	1364	368	424	2	13	0	0	0
1	C	259	2052	1286	344	405	3	14	0	0	0
1	D	277	2190	1370	369	434	3	14	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	TPO	THR	modified residue	UNP Q9NWZ3
A	345	TPO	THR	modified residue	UNP Q9NWZ3
A	346	SEP	SER	modified residue	UNP Q9NWZ3
B	342	TPO	THR	modified residue	UNP Q9NWZ3
B	345	TPO	THR	modified residue	UNP Q9NWZ3
B	346	SEP	SER	modified residue	UNP Q9NWZ3
C	342	TPO	THR	modified residue	UNP Q9NWZ3
C	345	TPO	THR	modified residue	UNP Q9NWZ3
C	346	SEP	SER	modified residue	UNP Q9NWZ3
D	342	TPO	THR	modified residue	UNP Q9NWZ3
D	345	TPO	THR	modified residue	UNP Q9NWZ3
D	346	SEP	SER	modified residue	UNP Q9NWZ3

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

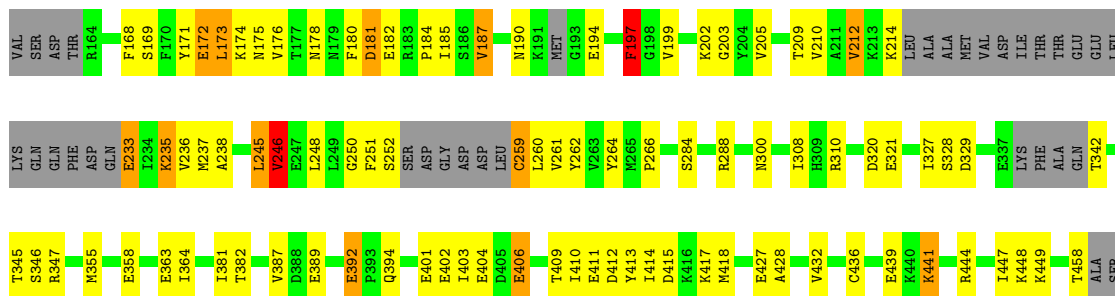
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

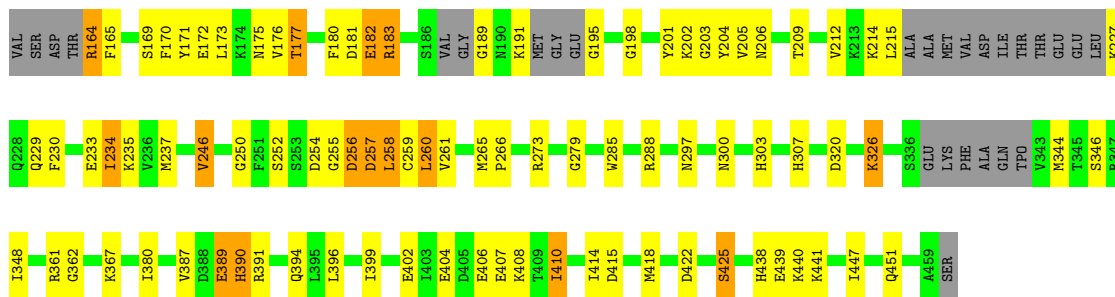
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A: 



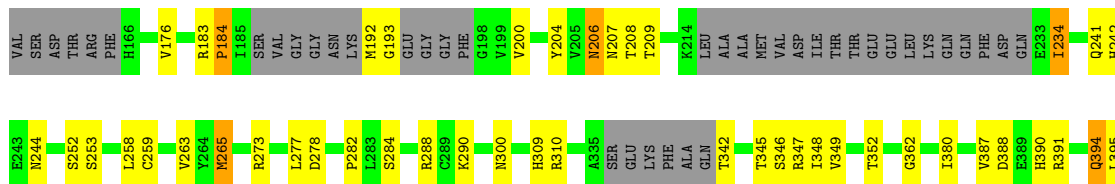
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B: 



- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.12Å 138.97Å 89.20Å 90.00° 126.43° 90.00°	Depositor
Resolution (Å)	49.94 – 2.30	Depositor
% Data completeness (in resolution range)	99.3 (49.94-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP, 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	A	0.76	1/2106 (0.0%)	0.94	3/2833 (0.1%)
1	B	0.76	1/2184 (0.0%)	0.94	2/2938 (0.1%)
1	C	0.64	0/2051	0.88	0/2762
1	D	0.63	0/2191	0.86	0/2948
All	All	0.70	2/8532 (0.0%)	0.91	5/11481 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	VAL	CA-CB	6.26	1.60	1.54
1	B	246	VAL	CA-CB	5.57	1.59	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	N-CA-C	7.88	120.39	107.23
1	B	234	ILE	N-CA-C	6.45	116.61	110.42
1	A	441	LYS	N-CA-C	5.83	118.38	111.33
1	A	381	ILE	N-CA-C	5.18	115.39	110.42
1	A	355	MET	N-CA-C	5.09	117.86	109.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2105	0	2077	73	2
1	B	2171	0	2138	81	3
1	C	2052	0	2024	39	0
1	D	2190	0	2148	36	1
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	4	0
2	D	31	0	13	3	0
3	A	89	0	0	7	0
3	B	83	0	0	2	1
3	C	56	0	0	1	0
3	D	51	0	0	2	0
All	All	8921	0	8439	226	4

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 13.

All (226) 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:B:170:PHE:HA	1:B:173:LEU:HD12	1.34	1.09
1:B:233:GLU:O	1:B:237:MET:HG2	1.59	1.02
1:B:265:MET:HE1	1:B:320:ASP:HB3	1.49	0.94
1:D:195:GLY:HA3	2:D:4:ANP:O2G	1.70	0.92
1:A:169:SER:O	1:A:172:GLU:HG2	1.74	0.87
1:B:265:MET:CE	1:B:320:ASP:HB3	2.03	0.87
1:B:391:ARG:HA	1:C:390:HIS:O	1.77	0.84
1:D:176:VAL:CG1	1:D:204:TYR:H	1.91	0.84
1:B:170:PHE:HA	1:B:173:LEU:CD1	2.08	0.83
1:A:169:SER:N	1:A:172:GLU:OE2	2.10	0.81
1:B:173:LEU:HD11	1:B:252:SER:HB2	1.63	0.78
1:D:194:GLU:HG3	1:D:195:GLY:N	1.99	0.77
1:B:181:ASP:OD1	1:B:183:ARG:HB2	1.83	0.77
1:D:246:VAL:HG12	1:D:326:LYS:HB3	1.67	0.77
1:A:181:ASP:HB3	1:A:190:ASN:HD22	1.51	0.76
1:A:178:ASN:HB3	1:A:190:ASN:ND2	2.02	0.75
1:A:329:ASP:HB2	3:A:2096:HOH:O	1.87	0.74
1:A:410:ILE:HD11	1:A:427:GLU:HG2	1.71	0.72
1:B:176:VAL:O	1:B:204:TYR:HD2	1.72	0.72
1:A:237:MET:HE3	1:A:262:TYR:OH	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:HIS:HE1	1:B:440:LYS:HD2	1.55	0.71
1:B:177:THR:HG23	1:B:180:PHE:H	1.56	0.71
1:B:257:ASP:O	1:B:258:LEU:HD23	1.90	0.71
1:A:266:PRO:HG2	1:A:321:GLU:HG3	1.73	0.71
1:B:170:PHE:CA	1:B:173:LEU:HD12	2.16	0.70
2:A:1:ANP:O1A	3:A:2096:HOH:O	2.09	0.70
1:A:250:GLY:O	1:A:261:VAL:N	2.26	0.68
1:C:388:ASP:O	1:C:394:GLN:HG3	1.93	0.68
1:C:265:MET:HE2	1:C:265:MET:HA	1.76	0.68
1:A:172:GLU:O	1:A:176:VAL:HG13	1.93	0.68
1:B:173:LEU:HD11	1:B:252:SER:CB	2.24	0.67
1:B:173:LEU:O	1:B:176:VAL:HG22	1.95	0.67
1:C:206:ASN:C	1:C:208:THR:H	2.03	0.66
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.77	0.66
1:B:256:ASP:O	1:B:257:ASP:HB2	1.96	0.65
1:B:390:HIS:O	1:C:391:ARG:HA	1.96	0.65
1:B:170:PHE:N	1:B:254:ASP:OD2	2.29	0.64
1:A:402:GLU:OE2	1:A:413:TYR:OH	2.12	0.64
1:B:177:THR:HG21	1:B:180:PHE:CD1	2.33	0.64
1:C:388:ASP:O	1:C:394:GLN:CG	2.46	0.64
1:A:403:ILE:HD13	1:A:410:ILE:HG22	1.79	0.63
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.79	0.63
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.81	0.63
1:B:438:HIS:CE1	1:B:440:LYS:HD2	2.35	0.62
1:A:169:SER:O	1:A:173:LEU:HD22	2.00	0.61
1:A:197:PHE:HB2	3:A:3003:HOH:O	2.01	0.60
1:A:246:VAL:CG1	1:A:328:SER:HB3	2.31	0.60
1:A:392:GLU:HG2	3:D:2081:HOH:O	2.00	0.60
1:B:198:GLY:HA3	1:B:214:LYS:O	2.02	0.60
1:A:264:TYR:HE2	3:A:2064:HOH:O	1.85	0.60
1:A:212:VAL:HG13	1:A:261:VAL:HG22	1.84	0.59
1:B:169:SER:H	1:B:172:GLU:CD	2.10	0.59
1:B:396:LEU:O	1:B:399:ILE:HB	2.02	0.59
1:C:200:VAL:HG21	2:C:3:ANP:H5'1	1.84	0.59
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.84	0.59
1:A:389:GLU:HA	1:A:394:GLN:NE2	2.16	0.59
1:B:173:LEU:O	1:B:177:THR:HG22	2.02	0.59
1:D:174:LYS:HD3	1:D:179:ASN:HA	1.84	0.59
1:A:321:GLU:H	1:A:321:GLU:CD	2.12	0.58
1:A:411:GLU:HA	1:A:414:ILE:HD12	1.85	0.57
1:B:265:MET:HE3	1:B:320:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASN:HB3	1:A:190:ASN:HD21	1.68	0.57
1:C:387:VAL:HA	1:C:394:GLN:O	2.03	0.57
1:B:266:PRO:HD2	1:B:320:ASP:HA	1.87	0.57
1:B:389:GLU:C	1:B:391:ARG:H	2.11	0.57
1:C:391:ARG:HD3	3:C:2111:HOH:O	2.05	0.57
1:A:251:PHE:HB3	1:A:259:CYS:O	2.05	0.56
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.87	0.56
1:A:252:SER:H	1:A:259:CYS:HB3	1.71	0.56
1:C:242:HIS:CD2	1:C:244:ASN:H	2.24	0.56
1:A:173:LEU:CD2	1:A:252:SER:OG	2.54	0.56
1:C:193:GLY:HA3	2:C:3:ANP:H4'	1.87	0.56
1:D:200:VAL:HG21	2:D:4:ANP:H5'1	1.87	0.55
1:D:452:GLN:NE2	1:D:456:GLU:OE1	2.40	0.55
1:A:246:VAL:HG11	1:A:328:SER:HB3	1.88	0.54
1:A:214:LYS:HD2	1:A:214:LYS:N	2.23	0.54
1:D:391:ARG:HD3	3:D:2057:HOH:O	2.08	0.54
1:B:230:PHE:CG	1:B:258:LEU:HD22	2.42	0.54
1:A:173:LEU:HD23	1:A:252:SER:OG	2.08	0.54
1:B:164:ARG:HG2	1:B:165:PHE:H	1.72	0.53
1:D:284:SER:O	1:D:288:ARG:HG3	2.08	0.53
1:A:436:CYS:O	1:A:444:ARG:HD3	2.08	0.53
1:B:164:ARG:HD3	1:B:164:ARG:N	2.24	0.53
1:A:168:PHE:HB3	1:A:173:LEU:HD21	1.91	0.53
1:A:237:MET:CE	1:A:262:TYR:OH	2.56	0.53
1:A:233:GLU:O	1:A:236:VAL:HB	2.09	0.52
1:D:232:GLN:HE21	1:D:236:VAL:HG23	1.75	0.52
1:D:311:ASP:HB2	1:D:332:LEU:HD12	1.92	0.52
1:C:192:MET:HG2	1:C:200:VAL:O	2.11	0.51
1:D:176:VAL:HG11	1:D:204:TYR:H	1.72	0.51
1:B:439:GLU:CD	1:B:439:GLU:H	2.19	0.51
1:B:230:PHE:CD2	1:B:258:LEU:HB3	2.46	0.50
1:A:173:LEU:O	1:A:176:VAL:HG22	2.12	0.50
1:B:183:ARG:HB3	1:B:189:GLY:HA3	1.92	0.50
1:A:203:GLY:O	1:A:209:THR:HA	2.12	0.50
1:D:176:VAL:HG21	1:D:205:VAL:HG22	1.94	0.49
1:B:202:LYS:HE2	1:B:209:THR:HG21	1.94	0.49
1:D:387:VAL:HA	1:D:394:GLN:O	2.13	0.49
1:A:389:GLU:HA	1:A:394:GLN:HE21	1.77	0.49
1:A:176:VAL:HG11	1:A:205:VAL:HG22	1.95	0.49
1:B:172:GLU:O	1:B:176:VAL:HG13	2.13	0.49
1:D:306:HIS:HB3	1:D:336:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:PRO:HB3	1:D:449:LYS:HG2	1.95	0.48
1:A:417:LYS:HD3	1:D:276:CYS:HB2	1.94	0.48
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.95	0.48
1:B:387:VAL:HA	1:B:394:GLN:O	2.12	0.48
1:C:200:VAL:CG2	2:C:3:ANP:H5'1	2.43	0.48
1:B:176:VAL:HG11	1:B:204:TYR:O	2.14	0.48
1:B:348:ILE:HG12	1:B:362:GLY:HA2	1.96	0.48
1:D:265:MET:HE2	1:D:265:MET:HA	1.96	0.48
1:D:342:TPO:O1P	1:D:441:LYS:NZ	2.46	0.48
1:A:210:VAL:C	1:A:264:TYR:HB2	2.39	0.47
1:B:265:MET:HE1	1:B:326:LYS:HE3	1.96	0.47
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.95	0.47
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.97	0.47
1:C:409:THR:HG23	1:C:411:GLU:H	1.79	0.47
1:A:197:PHE:CB	3:A:3003:HOH:O	2.62	0.47
1:A:409:THR:HG23	1:A:412:ASP:H	1.78	0.47
1:A:264:TYR:CE2	3:A:2064:HOH:O	2.56	0.47
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.97	0.47
1:B:169:SER:O	1:B:173:LEU:HD12	2.14	0.47
1:C:193:GLY:CA	2:C:3:ANP:H4'	2.44	0.47
1:B:389:GLU:HA	1:B:394:GLN:NE2	2.30	0.47
1:C:176:VAL:HB	1:C:204:TYR:H	1.79	0.47
1:A:404:GLU:C	1:A:406:GLU:H	2.23	0.46
1:B:234:ILE:HD11	1:B:260:LEU:HD21	1.96	0.46
1:A:169:SER:O	1:A:172:GLU:CG	2.55	0.46
1:A:194:GLU:HB3	1:A:199:VAL:HG13	1.97	0.46
1:A:387:VAL:HA	1:A:394:GLN:O	2.15	0.46
1:A:171:TYR:CD1	1:A:171:TYR:C	2.94	0.46
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.97	0.46
1:D:391:ARG:HG2	1:D:392:GLU:N	2.31	0.46
1:B:182:GLU:HA	1:B:191:LYS:HB2	1.97	0.46
1:C:263:VAL:HG12	1:C:265:MET:HE3	1.98	0.46
1:C:410:ILE:HD13	1:C:430:TYR:CD1	2.51	0.46
1:C:452:GLN:O	1:C:456:GLU:HG3	2.16	0.46
1:B:195:GLY:N	1:B:198:GLY:O	2.49	0.46
1:B:265:MET:HE3	1:B:320:ASP:CB	2.47	0.45
1:B:265:MET:HE3	1:B:320:ASP:CA	2.46	0.45
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.98	0.45
1:C:388:ASP:CG	1:C:391:ARG:HB2	2.41	0.45
1:C:277:LEU:O	1:C:278:ASP:HB2	2.17	0.45
1:A:428:ALA:O	1:A:432:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PHE:CG	1:B:255:GLY:HA3	2.52	0.45
1:A:259:CYS:C	1:A:260:LEU:HG	2.41	0.45
1:A:382:THR:HG22	1:A:413:TYR:HB3	1.99	0.45
1:B:171:TYR:CD1	1:B:172:GLU:N	2.85	0.45
1:B:297:ASN:OD1	1:B:451:GLN:NE2	2.49	0.45
1:C:192:MET:CE	1:C:200:VAL:HG12	2.47	0.45
1:D:245:LEU:HD23	1:D:327:ILE:HB	1.98	0.45
1:D:342:TPO:HG21	1:D:363:GLU:OE1	2.17	0.45
1:B:246:VAL:HG21	3:B:2090:HOH:O	2.17	0.44
1:B:410:ILE:HD12	1:B:410:ILE:HA	1.86	0.44
1:A:184:PRO:O	1:A:187:VAL:HG12	2.17	0.44
1:B:279:GLY:HA2	1:C:282:PRO:HG2	1.99	0.44
1:A:284:SER:O	1:A:288:ARG:HG3	2.17	0.44
1:B:176:VAL:O	1:B:204:TYR:CD2	2.62	0.44
1:B:177:THR:O	1:B:177:THR:OG1	2.33	0.44
1:B:203:GLY:HA3	1:B:212:VAL:HG23	1.99	0.44
1:D:288:ARG:HB3	1:D:380:ILE:CG2	2.48	0.44
1:A:235:LYS:HA	1:A:238:ALA:HB3	2.00	0.44
1:A:401:GLU:OE2	3:A:2141:HOH:O	2.21	0.44
1:B:257:ASP:C	1:B:258:LEU:HG	2.42	0.44
1:B:285:TRP:HE1	1:B:425:SER:HB3	1.82	0.43
1:C:288:ARG:HB3	1:C:380:ILE:HG23	2.00	0.43
1:A:251:PHE:CB	1:A:259:CYS:O	2.65	0.43
1:A:363:GLU:OE2	1:A:441:LYS:HE2	2.17	0.43
1:A:410:ILE:HD11	1:A:427:GLU:CG	2.44	0.43
1:B:169:SER:N	1:B:172:GLU:CD	2.76	0.43
1:D:277:LEU:O	1:D:278:ASP:HB2	2.17	0.43
1:B:171:TYR:O	1:B:172:GLU:C	2.62	0.43
1:B:404:GLU:C	1:B:406:GLU:H	2.27	0.43
1:D:174:LYS:HG2	1:D:180:PHE:CE1	2.52	0.43
1:B:173:LEU:CD1	1:B:252:SER:CB	2.95	0.43
1:B:265:MET:CE	1:B:320:ASP:CB	2.88	0.43
1:C:348:ILE:HG12	1:C:362:GLY:HA2	2.01	0.43
1:A:345:TPO:O2P	1:A:347:ARG:CZ	2.67	0.43
1:A:248:LEU:HD12	1:A:261:VAL:O	2.18	0.43
1:A:178:ASN:CB	1:A:190:ASN:HD21	2.31	0.42
1:A:308:ILE:HG22	1:A:310:ARG:HG2	2.01	0.42
1:C:192:MET:HE3	1:C:200:VAL:HG12	2.01	0.42
1:A:173:LEU:HD21	1:A:252:SER:OG	2.19	0.42
1:D:185:ILE:H	1:D:185:ILE:HG12	1.63	0.42
1:B:410:ILE:O	1:B:414:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:H	1:B:182:GLU:HG2	1.60	0.42
1:B:256:ASP:O	1:B:257:ASP:CB	2.64	0.42
1:C:388:ASP:O	1:C:394:GLN:HG2	2.18	0.42
1:B:176:VAL:HB	1:B:204:TYR:H	1.84	0.42
1:C:288:ARG:HB3	1:C:380:ILE:CG2	2.50	0.42
1:B:407:GLU:O	1:B:408:LYS:HG3	2.19	0.42
1:B:402:GLU:O	1:B:407:GLU:HG2	2.19	0.42
1:B:422:ASP:OD1	1:B:425:SER:HB2	2.18	0.42
1:D:288:ARG:HB3	1:D:380:ILE:HG23	2.00	0.42
1:A:168:PHE:O	1:A:252:SER:HA	2.20	0.42
1:A:245:LEU:HD12	1:A:327:ILE:HB	2.02	0.42
1:B:205:VAL:HG12	1:B:206:ASN:HD22	1.85	0.42
1:D:270:LEU:HD13	1:D:291:ILE:HG21	2.02	0.42
1:A:358:GLU:HG3	1:A:441:LYS:HD3	2.02	0.41
1:A:233:GLU:OE2	1:A:233:GLU:C	2.63	0.41
1:A:411:GLU:HA	1:A:414:ILE:CD1	2.50	0.41
1:B:288:ARG:HB3	1:B:380:ILE:CG2	2.50	0.41
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.01	0.41
1:D:234:ILE:HG12	1:D:260:LEU:HD21	2.01	0.41
1:D:316:ASN:OD1	2:D:4:ANP:O2B	2.38	0.41
1:B:273:ARG:HA	1:B:273:ARG:NE	2.35	0.41
1:C:183:ARG:HB3	1:C:184:PRO:HD2	2.02	0.41
1:C:309:HIS:O	1:C:310:ARG:HB2	2.21	0.41
1:D:204:TYR:CZ	1:D:207:ASN:HA	2.55	0.41
1:C:284:SER:O	1:C:288:ARG:HG3	2.20	0.41
1:C:234:ILE:H	1:C:234:ILE:HG13	1.54	0.41
1:C:395:LEU:O	1:C:398:ASP:HB2	2.21	0.41
1:A:174:LYS:HG3	1:A:180:PHE:CE1	2.56	0.41
1:A:185:ILE:HD13	1:A:202:LYS:HD2	2.02	0.41
1:B:367:LYS:HD2	1:B:441:LYS:O	2.20	0.41
1:B:288:ARG:HB3	1:B:380:ILE:HG23	2.03	0.40
1:B:303:HIS:HD2	1:B:307:HIS:O	2.04	0.40
1:C:273:ARG:HA	1:C:273:ARG:NE	2.36	0.40
1:C:345:TPO:O2P	1:C:347:ARG:HB2	2.21	0.40
1:B:182:GLU:HG2	3:B:2068:HOH:O	2.21	0.40
1:D:243:GLU:O	1:D:326:LYS:NZ	2.52	0.40
1:B:182:GLU:HA	1:B:201:TYR:HE1	1.86	0.40
1:D:176:VAL:CG1	1:D:204:TYR:N	2.73	0.40
1:D:332:LEU:HD22	1:D:349:VAL:HG21	2.03	0.40
1:A:308:ILE:HD13	1:A:364:ILE:HG22	2.04	0.40
1:A:320:ASP:OD2	1:A:320:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:THR:HG23	1:C:411:GLU:N	2.36	0.40

All (4) 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)
3:B:2108:HOH:O	3:B:2108:HOH:O[2_555]	1.85	0.35
1:A:175:ASN:ND2	1:B:176:VAL:CG1[2_555]	1.89	0.31
1:A:176:VAL:CG1	1:B:175:ASN:ND2[2_555]	2.15	0.05
1:B:361:ARG:NH1	1:D:355:MET:O[4_546]	2.17	0.03

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	254/301 (84%)	242 (95%)	9 (4%)	3 (1%)	10	12
1	B	262/301 (87%)	245 (94%)	15 (6%)	2 (1%)	16	20
1	C	247/301 (82%)	228 (92%)	17 (7%)	2 (1%)	16	20
1	D	266/301 (88%)	255 (96%)	10 (4%)	1 (0%)	30	38
All	All	1029/1204 (86%)	970 (94%)	51 (5%)	8 (1%)	16	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	A	197	PHE
1	B	257	ASP
1	C	207	ASN
1	B	390	HIS
1	D	329	ASP

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Mol	Chain	Res	Type
1	A	181	ASP
1	C	184	PRO

5.3.2 Protein sidechains [i](#)

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	229/259 (88%)	213 (93%)	16 (7%)	14	19
1	B	238/259 (92%)	222 (93%)	16 (7%)	15	21
1	C	225/259 (87%)	211 (94%)	14 (6%)	16	24
1	D	239/259 (92%)	224 (94%)	15 (6%)	16	23
All	All	931/1036 (90%)	870 (93%)	61 (7%)	15	21

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
1	A	173	LEU
1	A	182	GLU
1	A	187	VAL
1	A	197	PHE
1	A	212	VAL
1	A	233	GLU
1	A	235	LYS
1	A	245	LEU
1	A	246	VAL
1	A	259	CYS
1	A	392	GLU
1	A	439	GLU
1	A	448	LYS
1	A	449	LYS
1	A	458	THR
1	B	164	ARG
1	B	177	THR
1	B	182	GLU

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Mol	Chain	Res	Type
1	B	183	ARG
1	B	215	LEU
1	B	227	LYS
1	B	229	GLN
1	B	235	LYS
1	B	256	ASP
1	B	260	LEU
1	B	261	VAL
1	B	326	LYS
1	B	344	MET
1	B	389	GLU
1	B	410	ILE
1	B	425	SER
1	C	206	ASN
1	C	209	THR
1	C	234	ILE
1	C	241	GLN
1	C	253	SER
1	C	258	LEU
1	C	265	MET
1	C	290	LYS
1	C	349	VAL
1	C	352	THR
1	C	394	GLN
1	C	397	LEU
1	C	411	GLU
1	C	448	LYS
1	D	164	ARG
1	D	175	ASN
1	D	178	ASN
1	D	185	ILE
1	D	187	VAL
1	D	194	GLU
1	D	197	PHE
1	D	208	THR
1	D	209	THR
1	D	246	VAL
1	D	329	ASP
1	D	343	VAL
1	D	344	MET
1	D	389	GLU
1	D	392	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	190	ASN
1	A	286	HIS
1	A	293	GLN
1	A	305	ASN
1	A	390	HIS
1	A	394	GLN
1	A	455	GLN
1	B	166	HIS
1	B	190	ASN
1	B	206	ASN
1	B	207	ASN
1	B	394	GLN
1	C	166	HIS
1	C	175	ASN
1	C	242	HIS
1	C	244	ASN
1	C	394	GLN
1	D	166	HIS
1	D	175	ASN
1	D	190	ASN
1	D	206	ASN
1	D	207	ASN
1	D	232	GLN
1	D	390	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	C	342	1	8,10,11	0.83	0	10,14,16	1.09	1 (10%)
1	SEP	D	346	1	8,9,10	1.65	1 (12%)	7,12,14	1.62	1 (14%)
1	TPO	B	345	1	8,10,11	0.92	0	10,14,16	1.00	0
1	TPO	D	342	1	8,10,11	0.78	0	10,14,16	1.03	0
1	SEP	B	346	1	8,9,10	1.67	1 (12%)	7,12,14	1.15	0
1	SEP	C	346	1	8,9,10	1.63	1 (12%)	7,12,14	1.51	1 (14%)
1	TPO	D	345	1	8,10,11	0.82	0	10,14,16	1.08	0
1	SEP	A	346	1	8,9,10	1.67	1 (12%)	7,12,14	1.29	1 (14%)
1	TPO	C	345	1	8,10,11	0.88	0	10,14,16	0.88	0
1	TPO	A	345	1	8,10,11	0.98	0	10,14,16	0.82	0
1	TPO	A	342	1	8,10,11	0.79	0	10,14,16	1.02	1 (10%)

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
1	TPO	C	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	TPO	B	345	1	-	5/9/11/13	-
1	TPO	D	342	1	-	0/9/11/13	-
1	SEP	B	346	1	-	5/6/8/10	-
1	SEP	C	346	1	-	4/6/8/10	-
1	TPO	D	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	1/6/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	A	342	1	-	0/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	346	SEP	P-O1P	3.69	1.61	1.50
1	A	346	SEP	P-O1P	3.63	1.61	1.50
1	B	346	SEP	P-O1P	3.62	1.61	1.50
1	C	346	SEP	P-O1P	3.54	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	3.60	111.65	108.14
1	C	346	SEP	OG-CB-CA	3.46	111.52	108.14
1	A	346	SEP	OG-CB-CA	2.51	110.58	108.14
1	C	342	TPO	O3P-P-O2P	2.19	116.01	107.80
1	A	342	TPO	O3P-P-O2P	2.17	115.92	107.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
1	B	346	SEP	CB-OG-P-O2P
1	B	346	SEP	CB-OG-P-O3P
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	346	SEP	N-CA-CB-OG
1	C	346	SEP	C-CA-CB-OG
1	C	346	SEP	CB-OG-P-O1P
1	C	346	SEP	CB-OG-P-O2P
1	D	345	TPO	N-CA-CB-OG1
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	C-CA-CB-OG
1	B	346	SEP	CB-OG-P-O1P
1	A	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	CB-OG-P-O1P
1	B	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	CB-OG1-P-O3P
1	B	345	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	342	TPO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	345	TPO	1	0
1	A	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	A	1	-	33,33,33	2.09	8 (24%)	45,52,52	2.11	11 (24%)
2	ANP	C	3	-	33,33,33	2.12	10 (30%)	45,52,52	2.05	11 (24%)
2	ANP	B	2	-	33,33,33	2.11	9 (27%)	45,52,52	2.09	16 (35%)
2	ANP	D	4	-	33,33,33	2.13	10 (30%)	45,52,52	1.88	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	1	-	-	1/18/38/38	0/3/3/3
2	ANP	C	3	-	-	6/18/38/38	0/3/3/3
2	ANP	B	2	-	-	4/18/38/38	0/3/3/3
2	ANP	D	4	-	-	7/18/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	ANP	C5-C4	5.19	1.48	1.39
2	D	4	ANP	PB-N3B	4.99	1.76	1.63
2	B	2	ANP	C5-C4	4.93	1.47	1.39
2	A	1	ANP	PG-N3B	4.91	1.76	1.63
2	D	4	ANP	C5-C4	4.88	1.47	1.39
2	A	1	ANP	C5-C4	4.87	1.47	1.39
2	B	2	ANP	PG-N3B	4.78	1.75	1.63
2	C	3	ANP	PG-N3B	4.75	1.75	1.63
2	D	4	ANP	PG-N3B	4.73	1.75	1.63
2	B	2	ANP	PB-N3B	4.61	1.75	1.63
2	C	3	ANP	PB-N3B	4.56	1.75	1.63
2	A	1	ANP	PB-N3B	4.47	1.75	1.63
2	A	1	ANP	PB-O1B	4.21	1.52	1.46
2	B	2	ANP	PG-O1G	4.10	1.52	1.46
2	C	3	ANP	PB-O1B	4.08	1.52	1.46
2	D	4	ANP	PG-O1G	3.85	1.52	1.46
2	C	3	ANP	PG-O1G	3.83	1.52	1.46
2	B	2	ANP	PB-O1B	3.75	1.51	1.46
2	D	4	ANP	PB-O1B	3.66	1.51	1.46
2	A	1	ANP	PG-O1G	3.57	1.51	1.46
2	A	1	ANP	PB-O3A	3.18	1.63	1.59
2	C	3	ANP	PB-O3A	2.98	1.62	1.59
2	B	2	ANP	PB-O3A	2.94	1.62	1.59
2	D	4	ANP	PB-O3A	2.88	1.62	1.59
2	D	4	ANP	PA-O3A	2.75	1.62	1.59
2	A	1	ANP	C8-N7	2.66	1.36	1.31
2	A	1	ANP	PA-O3A	2.54	1.62	1.59
2	B	2	ANP	C8-N7	2.54	1.36	1.31
2	B	2	ANP	PA-O3A	2.42	1.62	1.59
2	D	4	ANP	C5-N7	-2.38	1.34	1.39
2	C	3	ANP	C5-N7	-2.37	1.34	1.39
2	C	3	ANP	PA-O3A	2.36	1.62	1.59
2	D	4	ANP	C8-N7	2.29	1.36	1.31
2	D	4	ANP	PB-O2B	-2.21	1.50	1.56
2	C	3	ANP	C8-N7	2.11	1.35	1.31
2	B	2	ANP	C4-N9	-2.09	1.33	1.37
2	C	3	ANP	PB-O2B	-2.01	1.51	1.56

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ANP	C5-C4-N3	-6.22	118.16	126.72
2	C	3	ANP	C5-C4-N3	-5.94	118.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	ANP	C5-C4-N3	-5.93	118.55	126.72
2	B	2	ANP	C5-C4-N3	-5.00	119.84	126.72
2	C	3	ANP	N3-C4-N9	4.86	135.44	127.17
2	A	1	ANP	N3-C4-N9	4.81	135.34	127.17
2	C	3	ANP	O1G-PG-N3B	-4.69	104.87	111.77
2	A	1	ANP	O1G-PG-N3B	-4.66	104.91	111.77
2	D	4	ANP	N3-C4-N9	4.45	134.73	127.17
2	A	1	ANP	O2B-PB-O1B	4.22	118.91	109.87
2	B	2	ANP	C2'-C1'-N9	-4.14	103.03	113.30
2	A	1	ANP	N3-C2-N1	-4.12	122.35	128.58
2	B	2	ANP	N3-C4-N9	4.06	134.07	127.17
2	B	2	ANP	N3-C2-N1	-4.03	122.49	128.58
2	C	3	ANP	N3-C2-N1	-3.98	122.56	128.58
2	D	4	ANP	O1G-PG-N3B	-3.90	106.03	111.77
2	D	4	ANP	C4-C5-N7	-3.86	106.17	110.58
2	D	4	ANP	N3-C2-N1	-3.82	122.80	128.58
2	C	3	ANP	O2B-PB-O1B	3.77	117.94	109.87
2	B	2	ANP	C4-C5-N7	-3.66	106.40	110.58
2	B	2	ANP	C4-N9-C8	3.61	109.53	105.74
2	B	2	ANP	O2B-PB-O1B	3.57	117.53	109.87
2	A	1	ANP	C2-N3-C4	3.45	120.25	111.83
2	A	1	ANP	C4-C5-N7	-3.43	106.67	110.58
2	C	3	ANP	C4-C5-N7	-3.41	106.68	110.58
2	B	2	ANP	O1G-PG-N3B	-3.27	106.96	111.77
2	C	3	ANP	C2-N3-C4	3.26	119.78	111.83
2	D	4	ANP	C2-N3-C4	3.18	119.60	111.83
2	A	1	ANP	O2G-PG-O3G	3.11	115.95	107.59
2	B	2	ANP	C5-N7-C8	2.89	107.99	103.45
2	B	2	ANP	C2-N3-C4	2.86	118.83	111.83
2	B	2	ANP	N9-C8-N7	-2.79	109.98	113.94
2	A	1	ANP	C5-N7-C8	2.69	107.68	103.45
2	D	4	ANP	C5-N7-C8	2.66	107.63	103.45
2	C	3	ANP	C5-N7-C8	2.63	107.59	103.45
2	D	4	ANP	O2B-PB-O1B	2.62	115.48	109.87
2	C	3	ANP	O2G-PG-O3G	2.60	114.59	107.59
2	C	3	ANP	O1B-PB-N3B	-2.46	108.14	111.77
2	B	2	ANP	O2G-PG-O3G	2.45	114.18	107.59
2	B	2	ANP	O1B-PB-N3B	-2.40	108.24	111.77
2	C	3	ANP	C4-N9-C8	2.37	108.22	105.74
2	A	1	ANP	C4-N9-C8	2.32	108.17	105.74
2	B	2	ANP	O4'-C1'-N9	2.26	112.43	108.09
2	B	2	ANP	C2-N1-C6	2.22	122.37	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	ANP	O2G-PG-O3G	2.22	113.54	107.59
2	B	2	ANP	O3'-C3'-C4'	2.20	117.39	111.08
2	D	4	ANP	C4-N9-C8	2.16	108.01	105.74
2	A	1	ANP	N9-C8-N7	-2.08	110.99	113.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ANP	PB-N3B-PG-O1G
2	B	2	ANP	PB-N3B-PG-O1G
2	C	3	ANP	PB-N3B-PG-O1G
2	D	4	ANP	PB-N3B-PG-O1G
2	D	4	ANP	PG-N3B-PB-O1B
2	D	4	ANP	PA-O3A-PB-O1B
2	C	3	ANP	O4'-C4'-C5'-O5'
2	D	4	ANP	O4'-C4'-C5'-O5'
2	C	3	ANP	C3'-C4'-C5'-O5'
2	B	2	ANP	PB-O3A-PA-O1A
2	D	4	ANP	C3'-C4'-C5'-O5'
2	D	4	ANP	PB-O3A-PA-O5'
2	C	3	ANP	C5'-O5'-PA-O1A
2	B	2	ANP	PB-O3A-PA-O2A
2	C	3	ANP	PG-N3B-PB-O1B
2	C	3	ANP	PB-O3A-PA-O5'
2	D	4	ANP	PA-O3A-PB-O2B
2	B	2	ANP	PA-O3A-PB-O1B

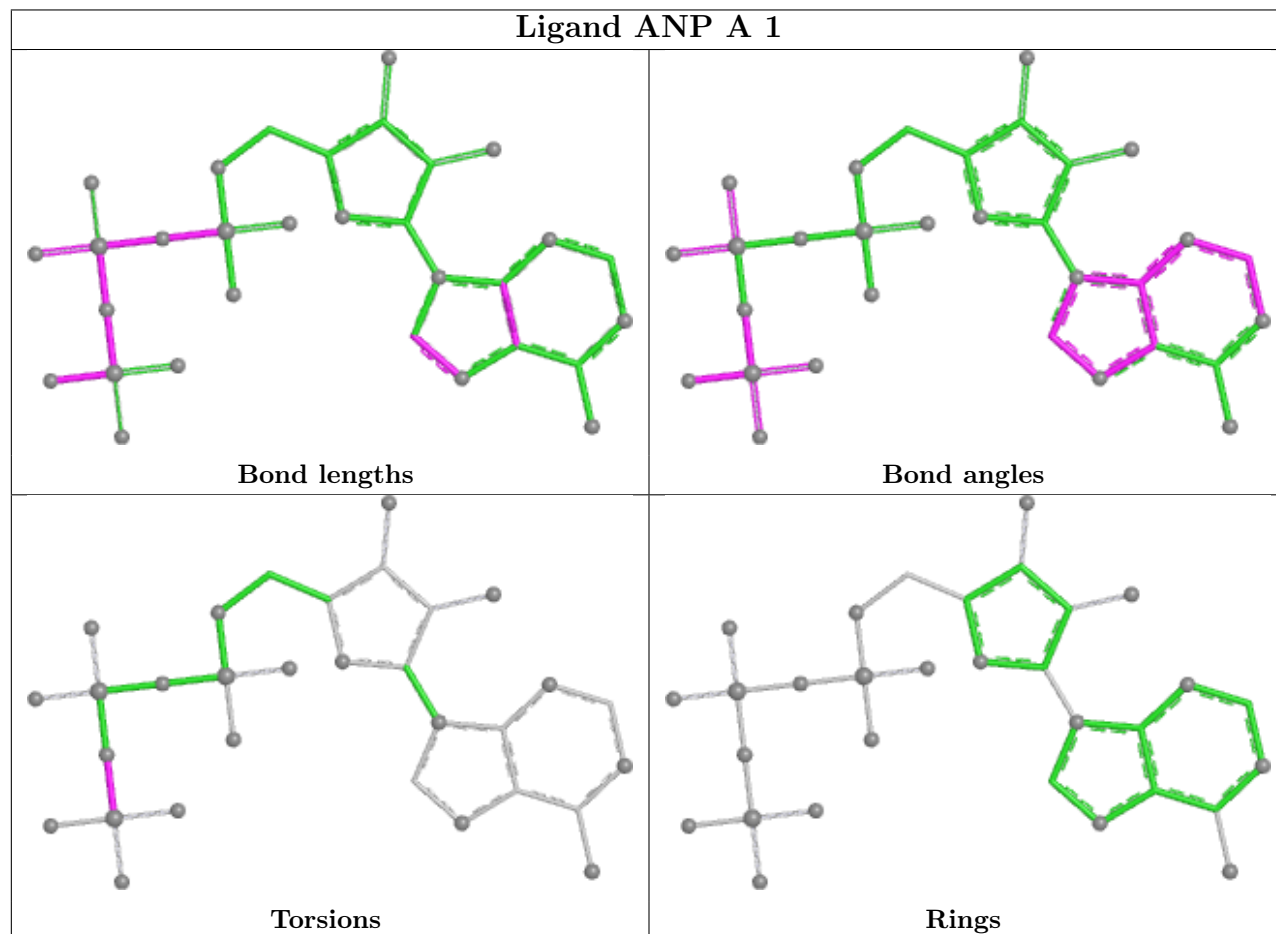
There are no ring outliers.

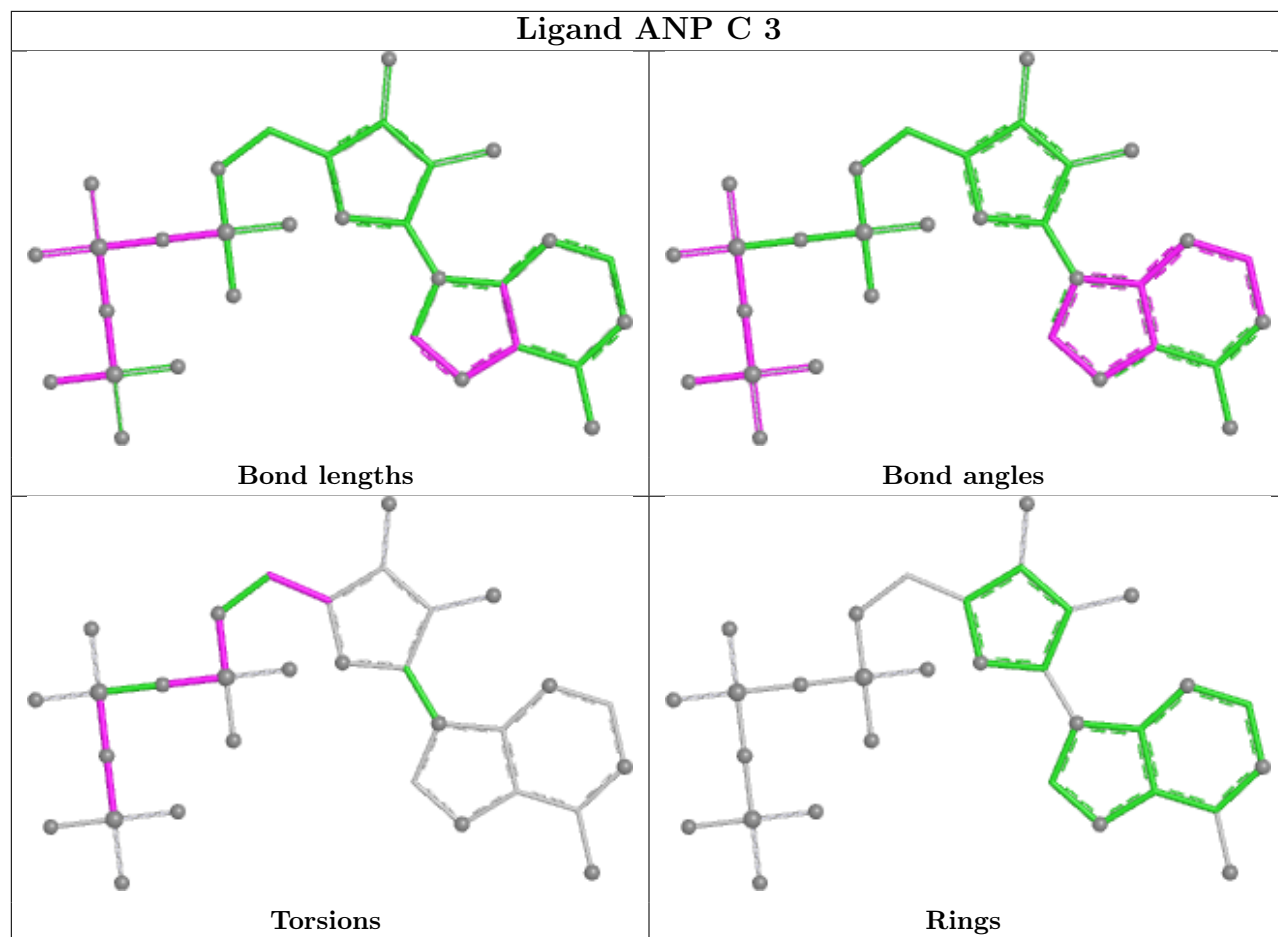
3 monomers are involved in 8 short contacts:

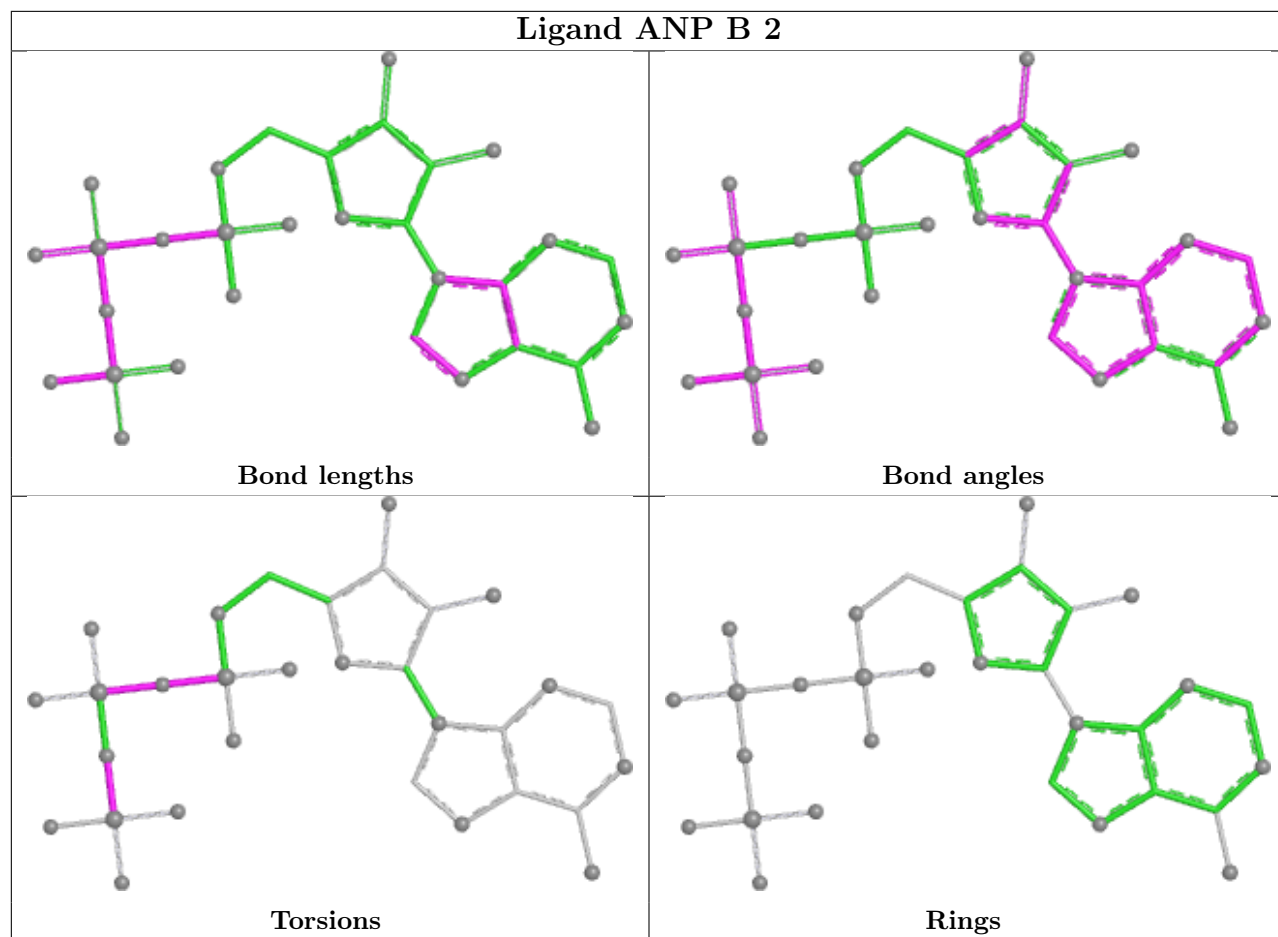
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ANP	1	0
2	C	3	ANP	4	0
2	D	4	ANP	3	0

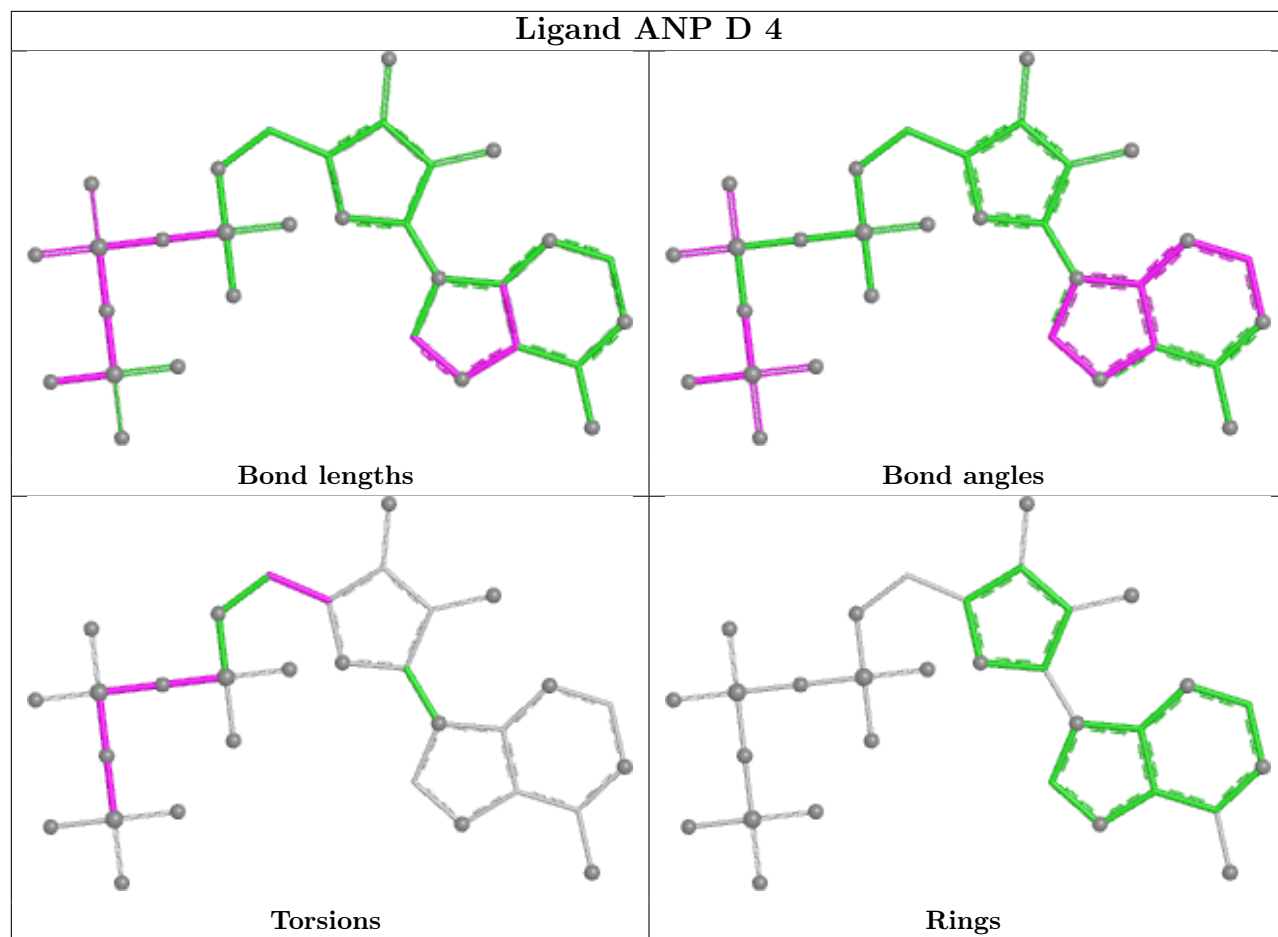
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.