



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:20 PM UTC

PDB ID : 1QOR / pdb_00001qor
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI QUINONE OXIDOREDUCTASE COMPLEXED WITH NADPH
Authors : Thorn, J.M.; Barton, J.D.; Dixon, N.E.; Ollis, D.L.; Edwards, K.J.
Deposited on : 1995-02-14
Resolution : 2.20 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)	:	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

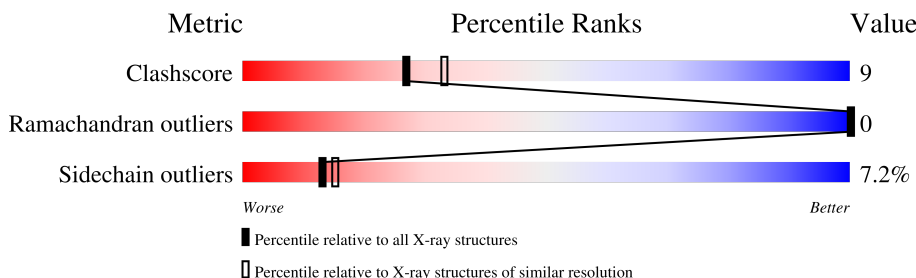
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	327	 75% 22% ..
1	B	327	 76% 21% ..

2 Entry composition [i](#)

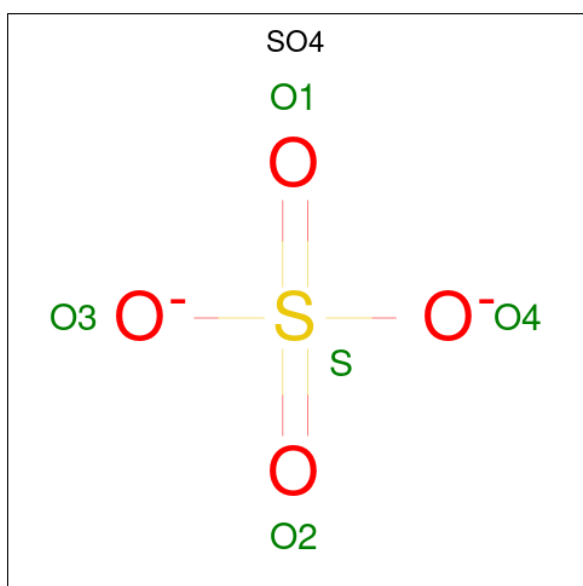
There are 4 unique types of molecules in this entry. The entry contains 5394 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 QUINONE OXIDOREDUCTASE.

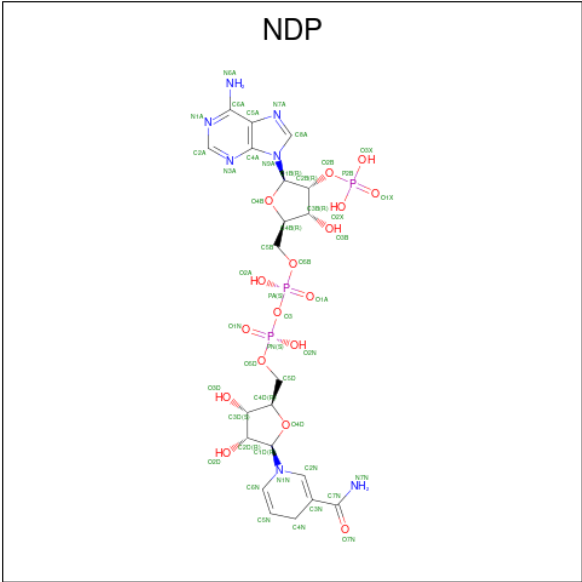
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2428	1548	415	462	3			
1	B	326	Total	C	N	O	S	0	0	0
			2428	1547	419	459	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

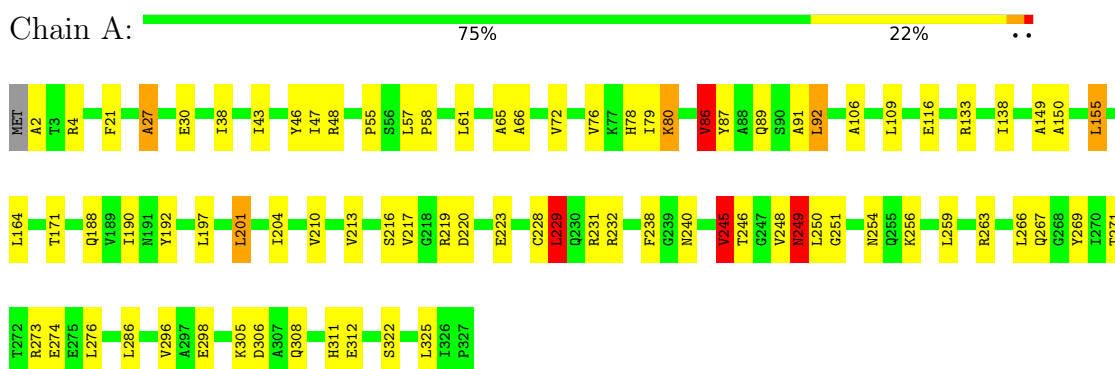
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	B	202	Total	O	0	0
			202	202		

3 Residue-property plots

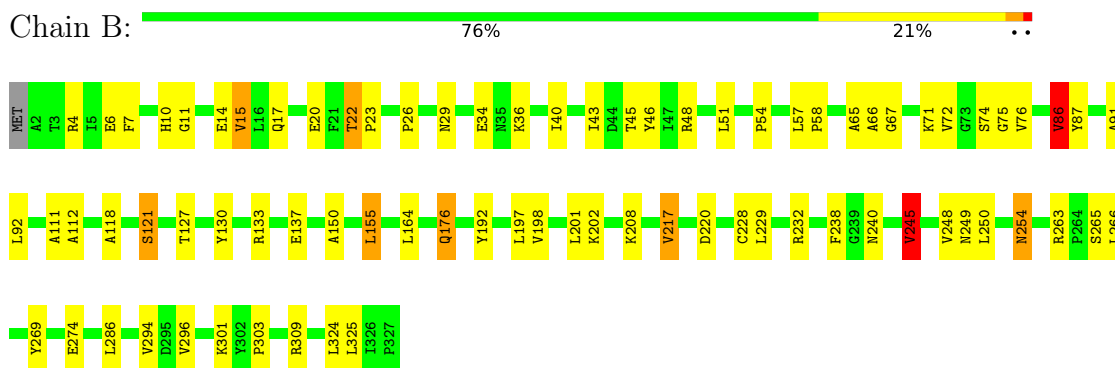
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: QUINONE OXIDOREDUCTASE



• Molecule 1: QUINONE OXIDOREDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.44Å 104.06Å 77.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.140 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5394	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, SO4

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	0.90	2/2472 (0.1%)	1.14	10/3355 (0.3%)
1	B	0.89	2/2472 (0.1%)	1.17	16/3355 (0.5%)
All	All	0.89	4/4944 (0.1%)	1.15	26/6710 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	VAL	CA-CB	5.93	1.60	1.53
1	B	45	THR	CA-CB	5.71	1.62	1.53
1	A	296	VAL	CA-CB	5.67	1.61	1.54
1	B	217	VAL	CA-CB	5.58	1.61	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLY	N-CA-C	-10.48	102.37	113.58
1	B	86	VAL	CB-CA-C	-7.83	98.65	110.55
1	A	86	VAL	CB-CA-C	-7.51	99.14	110.55
1	A	219	ARG	N-CA-C	6.30	118.67	111.11
1	B	220	ASP	N-CA-C	6.23	118.88	111.71
1	A	27	ALA	N-CA-C	-6.10	102.91	110.41
1	B	121	SER	N-CA-C	5.94	123.28	113.89
1	B	111	ALA	N-CA-C	5.61	118.12	111.33
1	B	22	THR	CA-C-N	5.60	125.78	119.90
1	B	22	THR	C-N-CA	5.60	125.78	119.90
1	A	322	SER	N-CA-C	5.60	118.11	110.55
1	A	91	ALA	N-CA-C	-5.59	103.10	110.43
1	A	249	ASN	N-CA-C	-5.57	99.65	108.73
1	A	197	LEU	N-CA-C	5.53	117.74	111.11
1	A	220	ASP	N-CA-C	5.30	117.80	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	VAL	CB-CA-C	5.24	117.90	111.25
1	A	229	LEU	N-CA-C	5.23	118.00	109.59
1	B	91	ALA	N-CA-C	-5.18	103.69	110.53
1	B	74	SER	CA-C-N	-5.15	117.84	123.30
1	B	74	SER	C-N-CA	-5.15	117.84	123.30
1	B	51	LEU	N-CA-C	-5.12	105.69	111.28
1	B	208	LYS	N-CA-C	5.11	117.75	111.82
1	B	229	LEU	N-CA-C	5.09	118.11	109.76
1	A	149	ALA	N-CA-C	5.05	119.07	113.01
1	B	34	GLU	N-CA-C	-5.04	100.29	108.41
1	B	303	PRO	N-CA-C	-5.04	103.37	111.38

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	2428	0	2422	55	0
1	B	2428	0	2417	44	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	48	0	26	2	0
3	B	48	0	26	3	0
4	A	230	0	0	6	0
4	B	202	0	0	4	0
All	All	5394	0	4891	91	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 9.

All (91) 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:A:298:GLU:HG3	4:A:570:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PHE:O	3:A:350:NDP:H2N	1.88	0.72
1:A:249:ASN:HD22	1:A:251:GLY:H	1.38	0.72
1:A:269:TYR:CZ	1:B:232:ARG:HD3	2.28	0.68
1:A:150:ALA:HA	1:A:155:LEU:HD13	1.76	0.67
1:B:7:PHE:HB2	1:B:15:VAL:HG13	1.77	0.65
1:A:213:VAL:HG23	1:A:229:LEU:HD13	1.79	0.63
1:A:249:ASN:ND2	1:A:251:GLY:H	1.97	0.61
1:B:150:ALA:HA	1:B:155:LEU:HD13	1.82	0.61
1:A:232:ARG:HD3	1:B:269:TYR:CZ	2.36	0.60
1:B:238:PHE:O	3:B:350:NDP:H2N	2.01	0.60
1:A:80:LYS:HB3	1:A:80:LYS:NZ	2.15	0.60
1:A:273:ARG:NH2	1:A:276:LEU:HD23	2.18	0.59
1:A:66:ALA:HB2	1:A:86:VAL:HG13	1.85	0.59
1:A:273:ARG:HH21	1:A:276:LEU:HD23	1.67	0.58
1:A:201:LEU:O	1:A:201:LEU:HG	2.03	0.58
1:A:116:GLU:HG3	4:A:395:HOH:O	2.04	0.58
1:A:256:LYS:HB3	1:A:259:LEU:HD11	1.87	0.56
1:B:121:SER:HB3	1:B:294:VAL:HG11	1.87	0.56
1:A:308:GLN:O	1:A:312:GLU:HG3	2.05	0.56
1:A:38:ILE:HB	1:A:325:LEU:HB2	1.88	0.56
1:B:254:ASN:C	1:B:254:ASN:HD22	2.16	0.52
1:B:127:THR:HG21	3:B:350:NDP:H41N	1.92	0.52
1:A:72:VAL:CG1	1:A:76:VAL:HB	2.40	0.51
1:A:249:ASN:HD22	1:A:249:ASN:C	2.19	0.51
1:A:231:ARG:HG2	1:A:231:ARG:HH11	1.76	0.50
1:A:240:ASN:HD21	1:A:263:ARG:HH21	1.60	0.50
1:B:201:LEU:HD22	1:B:228:CYS:HB3	1.93	0.50
1:A:201:LEU:HD22	1:A:228:CYS:HB3	1.93	0.50
1:A:86:VAL:HG22	1:A:109:LEU:HG	1.94	0.49
1:A:254:ASN:HD21	1:B:265:SER:HB3	1.77	0.49
1:B:72:VAL:CG1	1:B:76:VAL:HB	2.42	0.49
1:B:198:VAL:HG12	1:B:202:LYS:HE3	1.94	0.48
1:A:48:ARG:HH21	1:A:311:HIS:HD2	1.59	0.48
1:B:65:ALA:HB3	1:B:87:TYR:CZ	2.49	0.48
1:A:43:ILE:HA	1:A:46:TYR:CD2	2.49	0.48
1:B:86:VAL:CG1	1:B:118:ALA:HB1	2.44	0.47
1:A:245:VAL:HG22	1:B:250:LEU:HG	1.95	0.47
1:A:240:ASN:ND2	1:A:263:ARG:HH21	2.13	0.47
1:A:57:LEU:HA	1:A:58:PRO:C	2.41	0.46
1:B:296:VAL:HG12	4:B:444:HOH:O	2.15	0.46
1:A:89:GLN:HG2	4:A:499:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG22	1:B:249:ASN:ND2	2.29	0.46
1:B:274:GLU:H	1:B:274:GLU:CD	2.23	0.46
1:A:254:ASN:ND2	1:B:265:SER:HB3	2.30	0.46
1:A:48:ARG:HH21	1:A:311:HIS:CD2	2.34	0.46
1:B:36:LYS:HG2	1:B:67:GLY:HA2	1.97	0.45
1:B:296:VAL:HG13	1:B:301:LYS:CE	2.46	0.45
1:A:188:GLN:NE2	1:A:204:ILE:HG23	2.32	0.45
1:B:11:GLY:O	1:B:48:ARG:HD2	2.17	0.45
1:B:127:THR:CG2	3:B:350:NDP:H41N	2.47	0.45
1:B:22:THR:HA	1:B:23:PRO:HD3	1.76	0.44
1:B:26:PRO:CD	1:B:71:LYS:HG3	2.47	0.44
1:B:66:ALA:HB2	1:B:86:VAL:HG13	1.99	0.44
1:A:2:ALA:HB3	1:A:21:PHE:CE1	2.53	0.44
1:B:112:ALA:HA	4:B:504:HOH:O	2.18	0.44
1:A:27:ALA:HB3	1:A:30:GLU:HG3	2.00	0.44
1:B:296:VAL:HG11	1:B:324:LEU:HD12	1.99	0.44
1:A:171:THR:HA	1:A:190:ILE:O	2.18	0.44
1:A:305:LYS:HD2	1:A:306:ASP:OD1	2.18	0.44
1:B:254:ASN:C	1:B:254:ASN:ND2	2.76	0.44
1:B:4:ARG:NH1	1:B:6:GLU:OE1	2.51	0.43
1:A:232:ARG:HD2	4:A:474:HOH:O	2.18	0.43
1:A:78:HIS:CD2	1:A:79:ILE:HG13	2.53	0.43
1:A:250:LEU:HG	1:B:245:VAL:HG22	1.99	0.43
1:A:274:GLU:H	1:A:274:GLU:CD	2.27	0.43
1:B:309:ARG:NH2	4:B:471:HOH:O	2.46	0.43
1:A:4:ARG:HD3	4:A:352:HOH:O	2.18	0.43
1:A:55:PRO:HD2	4:A:377:HOH:O	2.19	0.43
1:B:176:GLN:NE2	4:B:534:HOH:O	2.51	0.43
1:B:86:VAL:HG13	1:B:118:ALA:HB1	2.01	0.42
1:B:296:VAL:HG13	1:B:301:LYS:HE2	2.02	0.42
1:B:133:ARG:NH2	1:B:137:GLU:HG2	2.35	0.42
1:B:57:LEU:HA	1:B:58:PRO:C	2.45	0.42
1:A:267:GLN:O	1:A:271:THR:HG22	2.20	0.42
1:A:269:TYR:CE2	1:B:232:ARG:HD3	2.54	0.42
1:A:80:LYS:HB3	1:A:80:LYS:HZ2	1.82	0.42
1:A:106:ALA:O	1:A:273:ARG:NH2	2.45	0.41
1:B:40:ILE:HD11	1:B:325:LEU:HG	2.02	0.41
1:B:10:HIS:CE1	1:B:54:PRO:HD2	2.56	0.41
1:B:240:ASN:ND2	1:B:263:ARG:HH21	2.18	0.41
1:A:267:GLN:H	1:A:267:GLN:CD	2.29	0.41
1:A:72:VAL:HG13	1:A:76:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:HD21	1:B:263:ARG:HH21	1.69	0.41
1:A:47:ILE:HD13	1:A:92:LEU:HD11	2.02	0.41
1:A:133:ARG:NH2	1:A:138:ILE:O	2.53	0.41
1:B:43:ILE:HA	1:B:46:TYR:CD2	2.55	0.40
1:A:216:SER:HB2	3:A:350:NDP:H4D	2.02	0.40
1:A:256:LYS:HB3	1:A:259:LEU:CD1	2.49	0.40
1:A:65:ALA:HB3	1:A:87:TYR:CZ	2.56	0.40
1:B:29:ASN:OD1	1:B:29:ASN:N	2.48	0.40

There are no symmetry-related clashes.

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	324/327 (99%)	316 (98%)	8 (2%)	0	100	100
1	B	324/327 (99%)	312 (96%)	12 (4%)	0	100	100
All	All	648/654 (99%)	628 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	244/258 (95%)	227 (93%)	17 (7%)	14	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	242/258 (94%)	224 (93%)	18 (7%)	13	14
All	All	486/516 (94%)	451 (93%)	35 (7%)	13	15

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	80	LYS
1	A	86	VAL
1	A	92	LEU
1	A	155	LEU
1	A	164	LEU
1	A	192	TYR
1	A	201	LEU
1	A	210	VAL
1	A	217	VAL
1	A	223	GLU
1	A	229	LEU
1	A	245	VAL
1	A	248	VAL
1	A	249	ASN
1	A	266	LEU
1	A	286	LEU
1	B	14	GLU
1	B	15	VAL
1	B	17	GLN
1	B	20	GLU
1	B	86	VAL
1	B	92	LEU
1	B	130	TYR
1	B	155	LEU
1	B	164	LEU
1	B	176	GLN
1	B	192	TYR
1	B	197	LEU
1	B	217	VAL
1	B	245	VAL
1	B	248	VAL
1	B	254	ASN
1	B	266	LEU
1	B	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	143	GLN
1	A	179	GLN
1	A	240	ASN
1	A	249	ASN
1	A	254	ASN
1	A	255	GLN
1	A	311	HIS
1	B	10	HIS
1	B	35	ASN
1	B	143	GLN
1	B	240	ASN
1	B	254	ASN
1	B	308	GLN

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](#)

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
3	NDP	A	350	-	51,52,52	1.67	8 (15%)	71,80,80	2.12	18 (25%)
3	NDP	B	350	-	51,52,52	1.80	11 (21%)	71,80,80	2.11	23 (32%)
2	SO4	A	328	-	4,4,4	1.13	0	6,6,6	1.69	2 (33%)
2	SO4	B	328	-	4,4,4	0.75	0	6,6,6	1.75	2 (33%)

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
3	NDP	A	350	-	-	6/34/77/77	0/5/5/5
3	NDP	B	350	-	-	5/34/77/77	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	350	NDP	C4N-C3N	-5.86	1.38	1.50
3	B	350	NDP	P2B-O2B	4.92	1.68	1.59
3	B	350	NDP	PN-O3	4.56	1.64	1.59
3	B	350	NDP	C4N-C3N	-4.39	1.41	1.50
3	B	350	NDP	PA-O3	4.29	1.64	1.59
3	A	350	NDP	P2B-O2B	4.23	1.66	1.59
3	A	350	NDP	C5A-N7A	-3.93	1.31	1.39
3	B	350	NDP	C7N-C3N	3.60	1.56	1.48
3	B	350	NDP	C5A-N7A	-3.33	1.33	1.39
3	A	350	NDP	C4N-C5N	-3.27	1.40	1.49
3	A	350	NDP	O4D-C1D	2.95	1.48	1.42
3	B	350	NDP	C4N-C5N	-2.67	1.42	1.49
3	A	350	NDP	C2B-C1B	2.61	1.59	1.53
3	B	350	NDP	C6N-C5N	2.43	1.40	1.33
3	B	350	NDP	C8A-N7A	2.24	1.36	1.31
3	A	350	NDP	C8A-N9A	-2.20	1.33	1.37
3	B	350	NDP	P2B-O2X	-2.18	1.46	1.54
3	B	350	NDP	C4A-N9A	-2.09	1.33	1.37
3	A	350	NDP	P2B-O2X	-2.02	1.47	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	350	NDP	C2B-C1B-N9A	-5.94	103.98	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	350	NDP	N3A-C4A-N9A	5.79	137.01	127.17
3	A	350	NDP	C2B-C1B-N9A	-5.58	104.57	113.75
3	A	350	NDP	O4B-C1B-N9A	5.57	118.78	108.09
3	B	350	NDP	O4D-C1D-N1N	-5.55	97.50	108.08
3	A	350	NDP	C5A-C4A-N3A	-5.46	119.20	126.72
3	A	350	NDP	N3A-C2A-N1A	-5.15	120.79	128.58
3	B	350	NDP	C1D-N1N-C2N	-4.81	113.22	121.14
3	B	350	NDP	N3A-C4A-N9A	4.59	134.98	127.17
3	B	350	NDP	C5A-C4A-N3A	-4.48	120.55	126.72
3	B	350	NDP	N3A-C2A-N1A	-4.03	122.48	128.58
3	A	350	NDP	O4D-C1D-N1N	-3.97	100.51	108.08
3	A	350	NDP	C6A-C5A-C4A	3.78	122.34	117.18
3	A	350	NDP	C6A-C5A-N7A	-3.61	125.13	132.09
3	B	350	NDP	O4B-C4B-C5B	-3.48	98.17	109.33
3	B	350	NDP	O7N-C7N-C3N	-3.47	114.37	120.90
3	B	350	NDP	C6A-C5A-N7A	-3.31	125.70	132.09
3	A	350	NDP	C4A-N9A-C8A	3.30	109.21	105.74
3	A	350	NDP	C3N-C2N-N1N	-3.27	118.40	123.20
3	A	350	NDP	C2D-C1D-N1N	3.17	121.10	113.31
3	B	350	NDP	O4B-C4B-C3B	-3.16	98.88	105.15
3	B	350	NDP	C6N-N1N-C2N	3.01	122.54	119.32
3	A	350	NDP	C2A-N3A-C4A	2.95	119.04	111.83
3	A	350	NDP	N9A-C8A-N7A	-2.90	109.82	113.94
3	A	350	NDP	O3B-C3B-C2B	2.87	119.22	111.19
3	B	350	NDP	C4A-C5A-N7A	2.82	113.81	110.58
3	B	350	NDP	C3N-C2N-N1N	-2.81	119.08	123.20
2	B	328	SO4	O2-S-O1	-2.74	89.75	109.06
3	A	350	NDP	O3-PA-O1A	-2.71	102.54	110.70
2	A	328	SO4	O4-S-O3	-2.69	93.69	108.54
3	A	350	NDP	O4D-C1D-C2D	-2.65	100.94	106.62
2	B	328	SO4	O4-S-O2	2.62	123.24	109.56
3	A	350	NDP	C2A-N1A-C6A	2.62	123.03	118.73
3	B	350	NDP	C2A-N3A-C4A	2.58	118.14	111.83
3	B	350	NDP	O2N-PN-O1N	2.45	123.85	112.44
3	B	350	NDP	C6A-C5A-C4A	2.42	120.49	117.18
3	B	350	NDP	O3X-P2B-O1X	2.39	120.16	110.83
3	B	350	NDP	C4A-N9A-C1B	-2.33	121.18	126.63
3	A	350	NDP	O4B-C4B-C5B	-2.31	101.93	109.33
3	B	350	NDP	O4B-C1B-N9A	2.31	112.52	108.09
3	B	350	NDP	O3X-P2B-O2B	-2.26	97.04	105.85
2	A	328	SO4	O3-S-O2	2.20	121.07	109.56
3	B	350	NDP	C4A-N9A-C8A	2.15	108.00	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	350	NDP	O4B-C1B-C2B	-2.09	102.99	106.59
3	B	350	NDP	N9A-C8A-N7A	-2.01	111.09	113.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

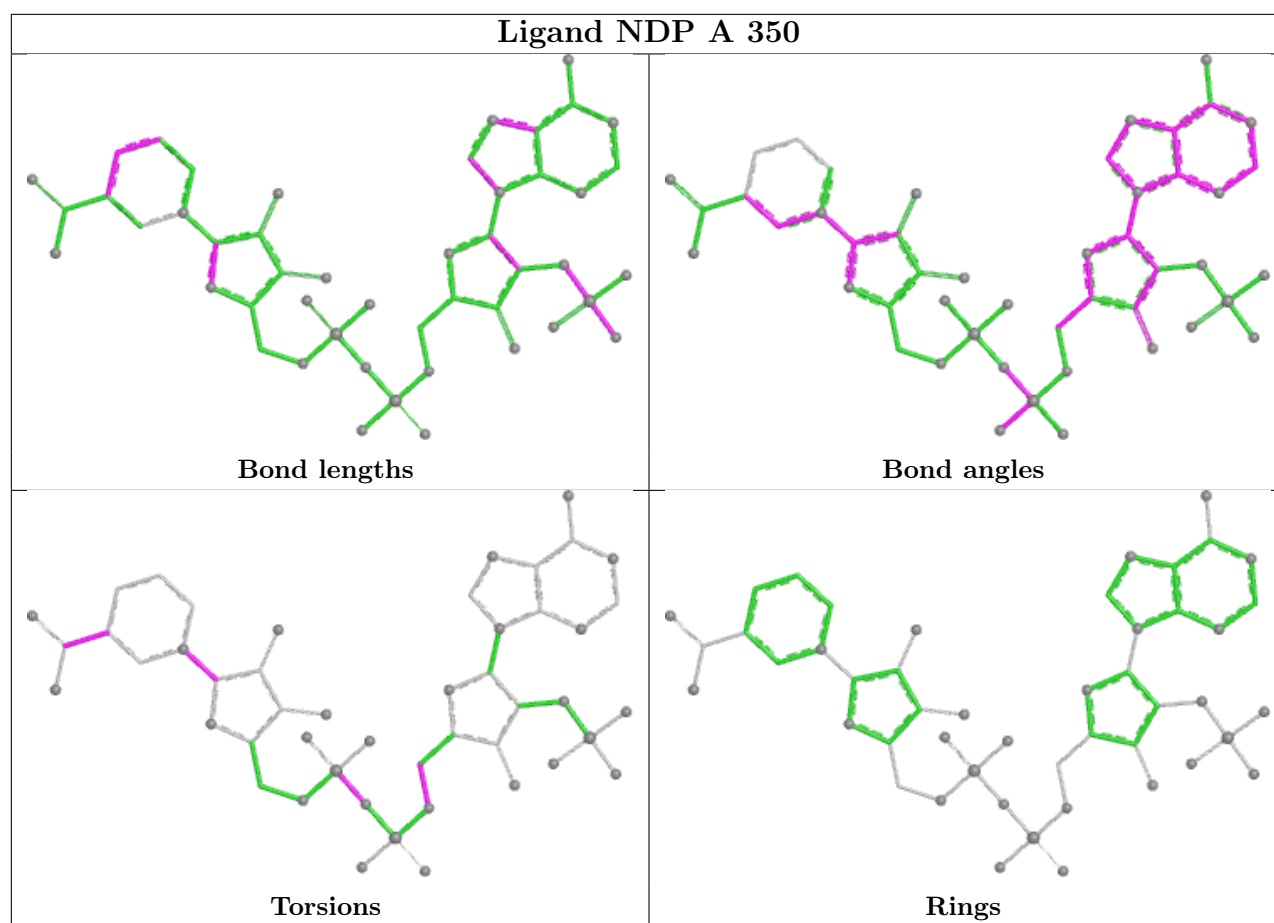
Mol	Chain	Res	Type	Atoms
3	B	350	NDP	C4B-C5B-O5B-PA
3	A	350	NDP	PA-O3-PN-O1N
3	A	350	NDP	C4B-C5B-O5B-PA
3	A	350	NDP	O4D-C1D-N1N-C2N
3	B	350	NDP	O4D-C1D-N1N-C2N
3	A	350	NDP	C2N-C3N-C7N-N7N
3	B	350	NDP	C2N-C3N-C7N-N7N
3	B	350	NDP	C2D-C1D-N1N-C2N
3	A	350	NDP	C2D-C1D-N1N-C2N
3	A	350	NDP	PA-O3-PN-O2N
3	B	350	NDP	PA-O3-PN-O2N

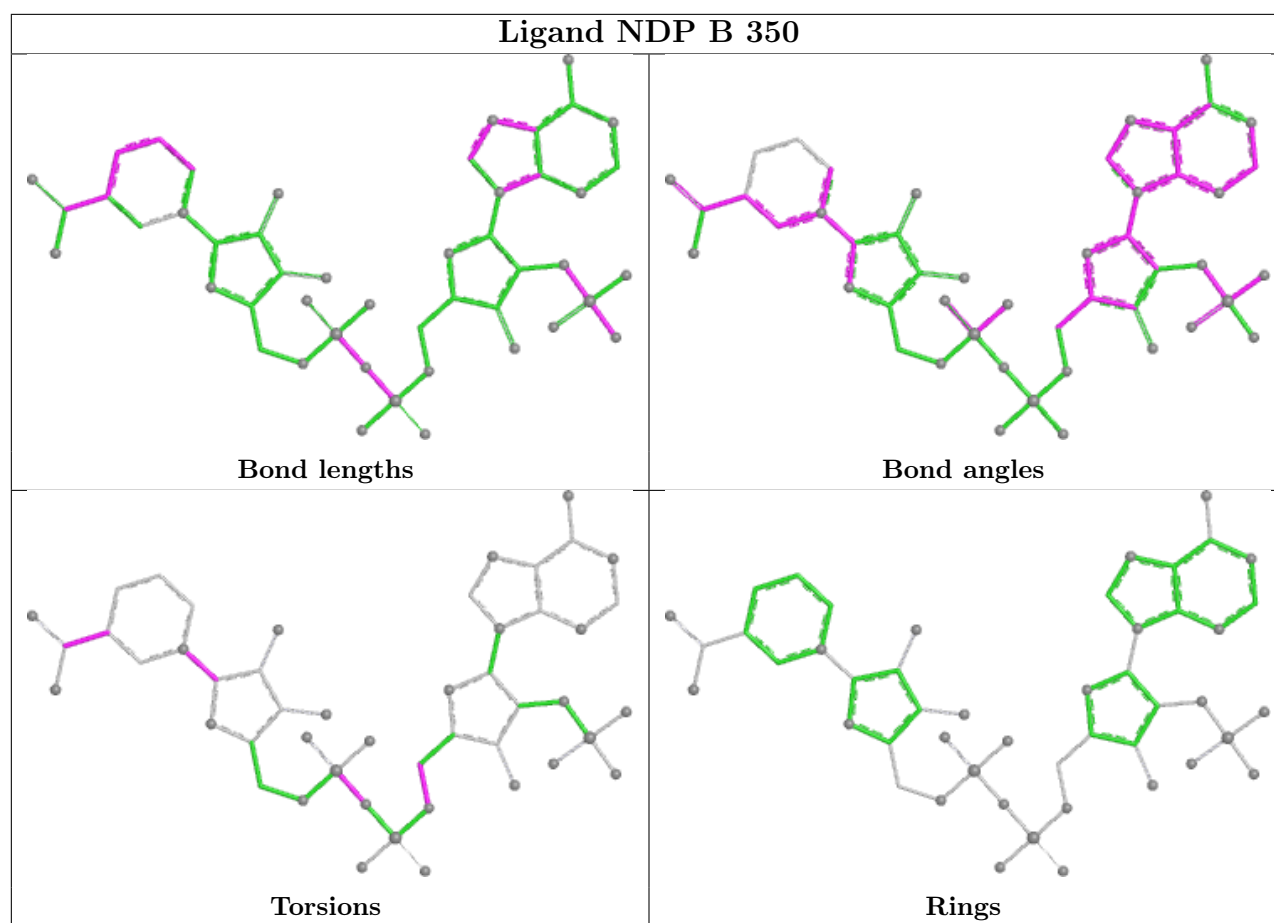
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	350	NDP	2	0
3	B	350	NDP	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.