



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:33 PM UTC

PDB ID : 1Q5M / pdb_00001q5m
Title : Binary complex of rabbit 20alpha-hydroxysteroid dehydrogenase with NADPH
Authors : Couture, J.F.; Legrand, P.; Cantin, L.; Labrie, F.; Luu-The, V.; Breton, R.
Deposited on : 2003-08-08
Resolution : 1.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

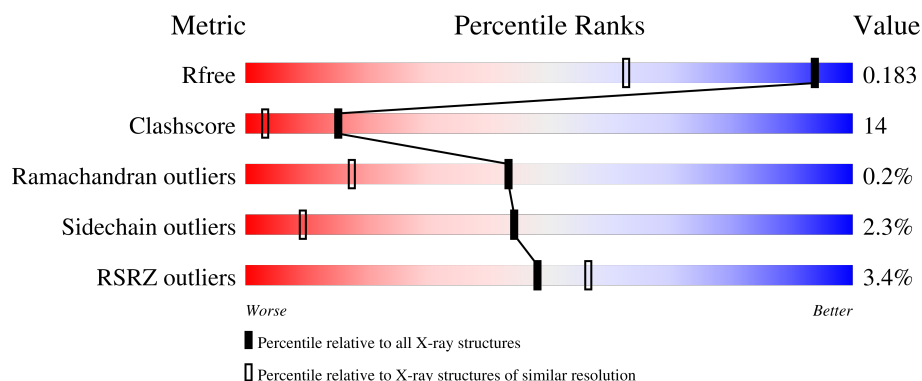
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

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 $\leq 5\%$. 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	322	5% 75% 21% .
1	B	322	2% 77% 19% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6032 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 Prostaglandin-E2 9-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	7	0
			2598	1671	438	479	10			
1	B	322	Total	C	N	O	S	0	5	0
			2595	1672	436	477	10			

- 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		

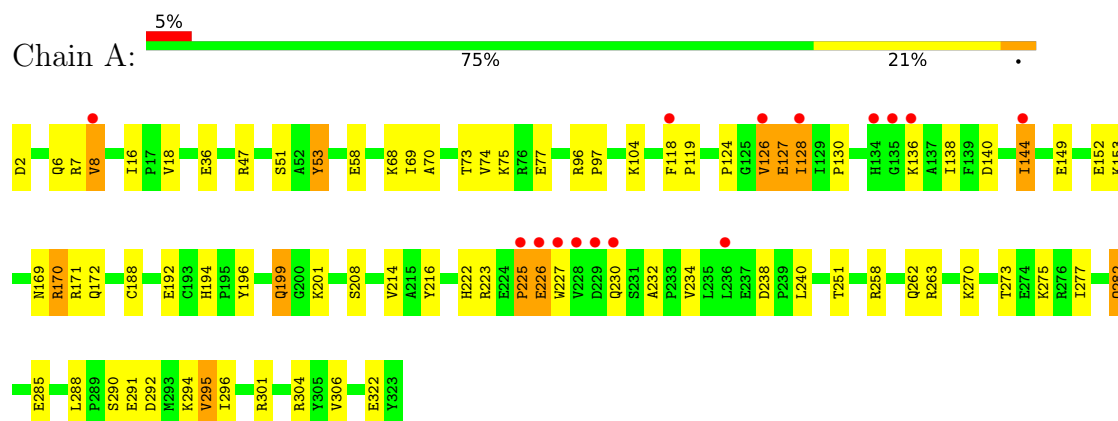
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	333	Total	O	4	0
			333	333		
4	B	400	Total	O	22	0
			400	400		

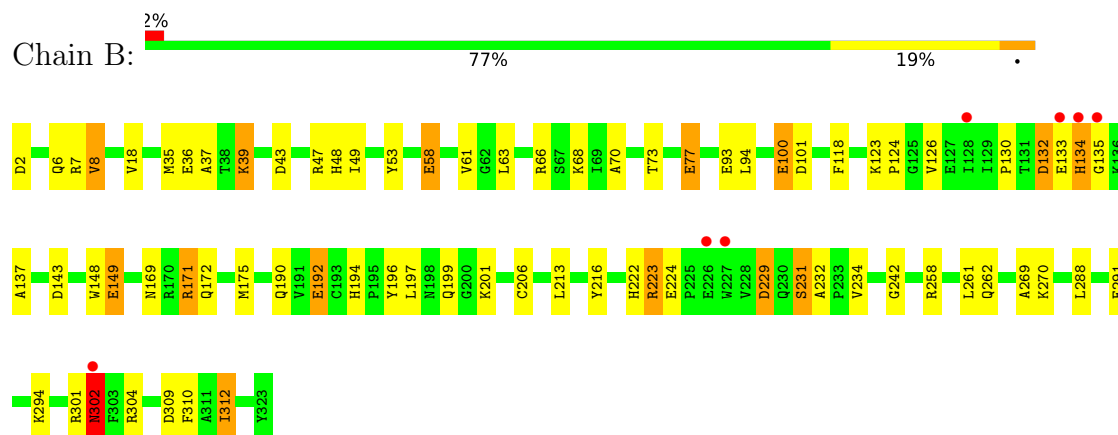
3 Residue-property plots

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: Prostaglandin-E2 9-reductase



• Molecule 1: Prostaglandin-E2 9-reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.54Å 85.27Å 66.15Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	57.74 – 1.32 57.74 – 1.32	Depositor EDS
% Data completeness (in resolution range)	96.4 (57.74-1.32) 96.4 (57.74-1.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.148 , 0.177 0.157 , 0.183	Depositor DCC
R_{free} test set	5499 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.82	32/2700 (1.2%)	1.48	23/3653 (0.6%)
1	B	1.81	40/2683 (1.5%)	1.47	10/3632 (0.3%)
All	All	1.82	72/5383 (1.3%)	1.47	33/7285 (0.5%)

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	A	0	1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	VAL	CA-CB	17.04	1.76	1.54
1	A	138	ILE	CA-CB	11.93	1.68	1.54
1	B	35	MET	SD-CE	-10.68	1.52	1.79
1	B	8	VAL	CA-CB	9.27	1.66	1.54
1	B	77	GLU	CD-OE2	9.06	1.42	1.25
1	A	51	SER	CA-CB	-8.42	1.42	1.53
1	B	234	VAL	CA-CB	8.07	1.62	1.53
1	A	70	ALA	CA-CB	-7.79	1.40	1.53
1	B	242	GLY	N-CA	-7.72	1.36	1.45
1	B	94	LEU	N-CA	-7.65	1.35	1.46
1	B	6	GLN	CB-CG	-7.32	1.30	1.52
1	B	39	LYS	CE-NZ	7.03	1.70	1.49
1	A	6	GLN	CB-CG	-7.00	1.31	1.52
1	A	69	ILE	C-O	6.87	1.32	1.24
1	A	208	SER	N-CA	6.74	1.55	1.46
1	B	312	ILE	CA-C	-6.64	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	HIS	CA-CB	-6.50	1.44	1.53
1	A	69	ILE	CA-C	-6.47	1.43	1.52
1	A	124	PRO	CB-CG	-6.31	1.18	1.49
1	A	234	VAL	CA-CB	-6.31	1.46	1.53
1	B	58	GLU	N-CA	-6.22	1.38	1.46
1	B	224	GLU	CA-C	-6.13	1.46	1.52
1	A	291	GLU	CD-OE2	6.13	1.36	1.25
1	B	291	GLU	CD-OE2	6.09	1.36	1.25
1	B	100	GLU	CD-OE1	6.05	1.36	1.25
1	B	100	GLU	CG-CD	5.96	1.67	1.52
1	B	301	ARG	CB-CG	-5.94	1.34	1.52
1	A	16	ILE	CA-C	5.92	1.56	1.52
1	A	214	VAL	CA-CB	5.90	1.61	1.54
1	B	93	GLU	CD-OE2	5.84	1.36	1.25
1	A	188	CYS	CA-C	-5.83	1.45	1.52
1	A	126	VAL	CA-CB	5.76	1.62	1.54
1	A	74	VAL	CA-CB	5.70	1.63	1.54
1	B	37	ALA	CA-C	-5.67	1.45	1.52
1	B	6	GLN	CA-CB	-5.59	1.44	1.53
1	B	302	ASN	CB-CG	5.58	1.66	1.52
1	B	213	LEU	C-O	5.55	1.30	1.24
1	A	6	GLN	CA-CB	-5.53	1.44	1.53
1	A	306	VAL	CA-CB	-5.52	1.47	1.53
1	A	296	ILE	CA-C	5.50	1.59	1.52
1	A	73	THR	C-O	-5.49	1.17	1.24
1	A	263	ARG	CZ-NH2	-5.49	1.26	1.33
1	B	261	LEU	CA-C	-5.47	1.45	1.52
1	A	199	GLN	CD-OE1	5.47	1.33	1.23
1	B	49	ILE	N-CA	5.45	1.53	1.46
1	A	277	ILE	CA-CB	5.43	1.60	1.54
1	A	128	ILE	CA-CB	-5.39	1.47	1.54
1	A	240	LEU	CA-C	5.39	1.59	1.52
1	B	73	THR	N-CA	-5.38	1.39	1.46
1	B	269	ALA	C-O	5.35	1.30	1.23
1	B	130	PRO	CA-C	-5.35	1.45	1.52
1	B	137	ALA	C-O	5.32	1.30	1.23
1	B	310	PHE	CA-CB	5.32	1.62	1.53
1	B	70	ALA	CA-CB	-5.30	1.44	1.53
1	B	192	GLU	CA-C	-5.30	1.45	1.52
1	B	304	ARG	CD-NE	-5.30	1.38	1.46
1	B	232	ALA	CA-CB	-5.28	1.45	1.53
1	B	231	SER	C-O	-5.26	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	TYR	CD1-CE1	5.24	1.54	1.38
1	A	47	ARG	C-O	5.23	1.30	1.24
1	B	171	ARG	C-O	-5.22	1.18	1.24
1	A	225	PRO	C-O	-5.17	1.17	1.23
1	A	7	ARG	CD-NE	-5.15	1.39	1.46
1	B	47	ARG	C-O	5.14	1.30	1.24
1	B	148	TRP	CA-C	-5.14	1.46	1.52
1	B	61	VAL	CA-C	-5.14	1.46	1.52
1	A	140	ASP	CA-C	-5.13	1.46	1.52
1	A	118	PHE	CB-CG	-5.09	1.39	1.50
1	B	68	LYS	CD-CE	-5.09	1.37	1.52
1	B	206	CYS	CA-CB	5.01	1.61	1.53
1	B	43	ASP	N-CA	5.01	1.52	1.46
1	A	304	ARG	N-CA	-5.01	1.40	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	TYR	CE1-CZ-CE2	7.87	136.03	120.30
1	B	118	PHE	O-C-N	-6.81	116.68	121.65
1	A	171	ARG	CA-C-O	6.78	127.74	120.55
1	A	251	THR	O-C-N	-6.52	116.46	121.55
1	B	301	ARG	NH1-CZ-NH2	6.52	127.78	119.30
1	A	170	ARG	CD-NE-CZ	6.46	133.45	124.40
1	A	232	ALA	O-C-N	6.28	127.77	121.30
1	A	118	PHE	CB-CA-C	-6.25	100.29	109.97
1	A	238	ASP	O-C-N	-6.11	115.50	121.18
1	A	138	ILE	N-CA-C	6.07	117.52	108.23
1	A	126	VAL	N-CA-C	6.04	118.64	111.09
1	B	223	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	A	232	ALA	CA-C-O	-5.97	113.96	120.17
1	A	53	TYR	CZ-CE2-CD2	-5.81	109.14	119.60
1	B	126	VAL	N-CA-C	-5.76	104.72	111.00
1	B	312	ILE	O-C-N	-5.61	116.56	122.67
1	B	301	ARG	CG-CD-NE	-5.59	99.71	112.00
1	A	170	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	301	ARG	NE-CZ-NH2	-5.34	114.40	119.20
1	A	223	ARG	CA-C-N	-5.30	113.44	120.65
1	A	223	ARG	C-N-CA	-5.30	113.44	120.65
1	B	100	GLU	CG-CD-OE1	5.25	130.48	118.40
1	A	294	LYS	O-C-N	-5.22	116.58	122.12
1	A	170	ARG	NE-CZ-NH1	5.18	126.68	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	TYR	CE1-CZ-CE2	5.16	130.62	120.30
1	A	295	VAL	CA-CB-CG2	5.16	119.17	110.40
1	A	127[A]	GLU	O-C-N	5.15	129.08	123.01
1	A	127[B]	GLU	O-C-N	5.15	129.08	123.01
1	A	130	PRO	N-CD-CG	5.11	110.86	103.20
1	B	132	ASP	O-C-N	5.09	128.52	122.20
1	A	118	PHE	CB-CG-CD2	5.04	129.27	120.70
1	A	126	VAL	CG1-CB-CG2	5.02	121.85	110.80
1	B	143	ASP	N-CA-CB	-5.00	102.00	109.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	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	2598	0	2598	64	0
1	B	2595	0	2605	78	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	48	0	26	4	0
3	B	48	0	26	5	0
4	A	333	0	0	23	2
4	B	400	0	0	38	2
All	All	6032	0	5255	144	2

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 14.

All (144) 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:8:VAL:CA	1:A:8:VAL:CB	1.76	1.60
1:B:39:LYS:CE	1:B:39:LYS:NZ	1.70	1.52
1:B:302:ASN:HB2	4:B:1374:HOH:O	1.38	1.21
1:A:53:TYR:OH	4:A:1199:HOH:O	1.63	1.17
3:B:1004:NDP:O2N	4:B:1360:HOH:O	1.67	1.11
1:B:149[A]:GLU:HG3	4:B:1210:HOH:O	1.53	1.06
1:A:8:VAL:HG23	1:A:18:VAL:HG12	1.35	1.03
1:A:77:GLU:OE1	4:A:1112:HOH:O	1.77	1.01
3:A:1003:NDP:O2N	4:A:1300:HOH:O	1.80	0.99
1:A:8:VAL:HG23	1:A:18:VAL:CG1	1.95	0.96
1:B:8:VAL:HG23	1:B:18:VAL:HG12	1.45	0.96
1:A:258:ARG:HE	1:A:262:GLN:HE21	1.03	0.94
1:B:309[B]:ASP:OD1	4:B:1173:HOH:O	1.85	0.94
1:B:123[A]:LYS:HD2	4:B:1351:HOH:O	1.67	0.93
1:B:223:ARG:HD3	4:B:1328:HOH:O	1.69	0.93
1:B:258:ARG:HE	1:B:262:GLN:HE21	1.03	0.92
1:B:197:LEU:HD12	1:B:302:ASN:ND2	1.85	0.92
1:B:294:LYS:HG3	4:B:1030:HOH:O	1.69	0.91
1:A:262:GLN:HE22	1:A:288:LEU:H	1.14	0.90
1:B:8:VAL:HG23	1:B:18:VAL:CG1	2.02	0.89
1:B:2:ASP:N	4:B:1348:HOH:O	2.06	0.88
1:B:39:LYS:NZ	1:B:39:LYS:CD	2.35	0.88
1:A:8:VAL:CG2	1:A:18:VAL:HG12	2.04	0.87
1:B:134:HIS:CG	1:B:135:GLY:N	2.42	0.86
1:B:18:VAL:HG11	4:B:1321:HOH:O	1.75	0.86
1:B:100:GLU:HG2	4:B:1263:HOH:O	1.74	0.86
1:B:262:GLN:HE22	1:B:288:LEU:H	1.21	0.85
1:A:2:ASP:N	4:A:1174:HOH:O	2.11	0.83
1:B:149[B]:GLU:HG3	4:B:1210:HOH:O	1.78	0.83
1:B:123[B]:LYS:HD2	1:B:124:PRO:HD2	1.61	0.81
1:A:149[B]:GLU:OE1	1:A:153:LYS:HE3	1.84	0.78
1:B:132:ASP:O	1:B:134:HIS:O	2.02	0.77
1:B:149[A]:GLU:OE2	4:B:1308:HOH:O	2.01	0.76
1:A:282[A]:GLN:NE2	1:A:285:GLU:OE2	2.19	0.75
1:A:8:VAL:CA	1:A:8:VAL:CG2	2.65	0.74
1:B:77:GLU:HG3	4:B:1205:HOH:O	1.89	0.73
1:B:134:HIS:CG	1:B:135:GLY:H	2.05	0.73
1:B:149[B]:GLU:OE1	4:B:1210:HOH:O	2.06	0.73
1:B:8:VAL:CG2	1:B:18:VAL:HG12	2.18	0.72
1:B:201:LYS:HE3	4:B:1380:HOH:O	1.90	0.72
1:B:197:LEU:CD1	1:B:302:ASN:ND2	2.55	0.70
1:B:312:ILE:HD11	4:B:1173:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:CA	1:A:8:VAL:CG1	2.68	0.69
1:A:8:VAL:CB	1:A:8:VAL:N	2.55	0.69
1:B:123[A]:LYS:CD	4:B:1351:HOH:O	2.34	0.67
1:A:8:VAL:CB	1:A:8:VAL:C	2.68	0.67
1:B:194:HIS:HD2	1:B:196:TYR:H	1.44	0.65
1:A:194:HIS:HD2	1:A:196:TYR:H	1.44	0.65
1:A:136:LYS:HD2	4:A:1187:HOH:O	1.97	0.64
1:B:101[B]:ASP:OD1	4:B:1153:HOH:O	2.07	0.64
1:A:77:GLU:HG3	4:A:1066:HOH:O	1.97	0.63
1:A:136:LYS:CD	4:A:1325:HOH:O	2.47	0.63
1:A:292:ASP:HA	1:A:295:VAL:HG22	1.80	0.62
1:A:136:LYS:HD2	4:A:1325:HOH:O	2.00	0.61
1:A:128:ILE:HD13	4:A:1286:HOH:O	2.00	0.61
1:B:229:ASP:OD1	1:B:231:SER:OG	2.19	0.61
1:B:192:GLU:OE2	1:B:194:HIS:HE1	1.83	0.60
1:A:77:GLU:CG	4:A:1066:HOH:O	2.49	0.59
1:A:192:GLU:OE2	1:A:194:HIS:HE1	1.85	0.59
1:B:302:ASN:ND2	4:B:1342:HOH:O	2.23	0.59
1:A:169:ASN:H	1:A:172:GLN:HE21	1.49	0.58
1:A:77:GLU:H	1:A:77:GLU:CD	2.11	0.57
1:A:149[A]:GLU:OE2	1:A:152:GLU:OE1	2.22	0.57
1:A:262:GLN:NE2	1:A:288:LEU:H	1.94	0.57
1:B:169:ASN:H	1:B:172:GLN:HE21	1.51	0.56
1:A:201[A]:LYS:HE3	1:A:322:GLU:OE1	2.05	0.56
1:B:63[A]:LEU:HD23	1:B:66:ARG:NH2	2.21	0.55
1:B:309[B]:ASP:CG	4:B:1173:HOH:O	2.42	0.55
1:B:302:ASN:CB	4:B:1374:HOH:O	2.17	0.54
1:B:100:GLU:OE2	4:B:1263:HOH:O	2.18	0.54
1:A:227:TRP:HE3	4:A:1104:HOH:O	1.91	0.54
1:A:270:LYS:O	3:A:1003:NDP:H8A	2.09	0.53
1:B:262:GLN:NE2	1:B:288:LEU:H	1.99	0.52
1:A:75:LYS:HE3	4:A:1066:HOH:O	2.09	0.52
1:A:282[A]:GLN:OE1	4:A:1055:HOH:O	2.18	0.52
1:B:216:TYR:CE1	3:B:1004:NDP:H41N	2.44	0.52
1:A:275:LYS:HE2	4:A:1328:HOH:O	2.10	0.51
1:A:225:PRO:O	1:A:226:GLU:CG	2.59	0.51
1:B:63[A]:LEU:HD23	1:B:66:ARG:HH22	1.76	0.51
1:A:58:GLU:HG3	4:A:1108:HOH:O	2.11	0.51
1:A:75:LYS:HB3	1:A:77:GLU:OE2	2.10	0.51
1:A:36:GLU:HG2	4:A:1210:HOH:O	2.11	0.50
1:A:225:PRO:O	1:A:226:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LYS:O	3:B:1004:NDP:H8A	2.12	0.49
1:A:273:THR:HG21	1:A:275:LYS:HE3	1.93	0.49
1:B:302:ASN:CB	4:B:1342:HOH:O	2.61	0.49
1:A:128:ILE:CD1	4:A:1286:HOH:O	2.58	0.49
1:B:197:LEU:HD12	1:B:302:ASN:HD22	1.75	0.48
1:A:77:GLU:CD	4:A:1066:HOH:O	2.55	0.48
1:A:169:ASN:H	1:A:172:GLN:NE2	2.12	0.48
1:B:309[A]:ASP:OD1	1:B:312:ILE:CD1	2.62	0.48
1:B:100:GLU:CG	4:B:1263:HOH:O	2.45	0.48
1:A:222:HIS:HE1	4:A:1300:HOH:O	1.97	0.48
1:B:132:ASP:O	1:B:134:HIS:C	2.57	0.47
1:B:134:HIS:ND1	1:B:135:GLY:N	2.58	0.47
1:B:222:HIS:HE1	4:B:1360:HOH:O	1.98	0.47
1:B:216:TYR:CZ	3:B:1004:NDP:H41N	2.49	0.47
1:B:149[B]:GLU:OE2	4:B:1308:HOH:O	2.21	0.46
1:B:194:HIS:HD2	1:B:196:TYR:N	2.12	0.46
1:B:309[A]:ASP:OD1	1:B:312:ILE:HD12	2.15	0.46
1:B:63[B]:LEU:HG	1:B:66:ARG:NH2	2.29	0.46
1:B:123[B]:LYS:HD3	4:B:1351:HOH:O	2.15	0.46
1:A:149[B]:GLU:OE2	1:A:152:GLU:HB2	2.15	0.46
1:A:136:LYS:CD	4:A:1187:HOH:O	2.62	0.46
1:B:63[A]:LEU:CD2	1:B:66:ARG:HH22	2.29	0.46
1:A:226:GLU:HG2	1:A:227:TRP:CD1	2.51	0.45
1:A:136:LYS:HD3	4:A:1325:HOH:O	2.14	0.44
1:B:169:ASN:H	1:B:172:GLN:NE2	2.16	0.44
1:B:7:ARG:CZ	4:B:1280:HOH:O	2.66	0.44
1:B:123[A]:LYS:CE	4:B:1351:HOH:O	2.63	0.44
1:B:294:LYS:HD3	4:B:1239:HOH:O	2.17	0.44
1:A:216:TYR:CE1	3:A:1003:NDP:H41N	2.52	0.44
1:B:100:GLU:CD	4:B:1263:HOH:O	2.61	0.43
1:A:77:GLU:OE2	4:A:1066:HOH:O	2.20	0.43
1:B:190:GLN:OE1	3:B:1004:NDP:H2N	2.19	0.43
1:A:96:ARG:HB3	1:A:97:PRO:HD3	2.00	0.42
1:B:77:GLU:CG	4:B:1205:HOH:O	2.56	0.42
1:A:149[B]:GLU:OE2	1:A:152:GLU:OE1	2.38	0.42
1:B:302:ASN:HB2	4:B:1342:HOH:O	2.17	0.42
1:B:175:MET:HE3	4:B:1343:HOH:O	2.18	0.42
1:B:294:LYS:CE	4:B:1030:HOH:O	2.68	0.42
1:A:216:TYR:CZ	3:A:1003:NDP:H41N	2.55	0.42
1:A:258:ARG:HE	1:A:262:GLN:NE2	1.89	0.42
1:A:225:PRO:O	1:A:226:GLU:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLU:HG3	4:B:1242:HOH:O	2.19	0.41
1:A:119:PRO:O	1:A:144:ILE:HD11	2.21	0.41
1:B:258:ARG:HE	1:B:262:GLN:NE2	1.89	0.41
1:A:68:LYS:NZ	4:A:1329:HOH:O	2.53	0.41
1:B:149[B]:GLU:CD	4:B:1210:HOH:O	2.57	0.41
1:B:36:GLU:HG2	4:B:1337:HOH:O	2.20	0.41
1:A:225:PRO:O	1:A:226:GLU:HG2	2.21	0.40
1:B:171:ARG:O	1:B:175:MET:HG3	2.22	0.40

All (2) 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)
4:A:1294:HOH:O	4:B:1353:HOH:O[1_455]	2.02	0.18
4:A:1091:HOH:O	4:B:1006:HOH:O[2_646]	2.06	0.14

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	327/322 (102%)	318 (97%)	9 (3%)	0	100	100
1	B	325/322 (101%)	317 (98%)	7 (2%)	1 (0%)	36	15
All	All	652/644 (101%)	635 (97%)	16 (2%)	1 (0%)	43	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	HIS

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	287/280 (102%)	277 (96%)	10 (4%)	32 3
1	B	285/280 (102%)	279 (98%)	6 (2%)	47 11
All	All	572/560 (102%)	556 (97%)	16 (3%)	44 6

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	126	VAL
1	A	144	ILE
1	A	199	GLN
1	A	226	GLU
1	A	230	GLN
1	A	282[A]	GLN
1	A	282[B]	GLN
1	A	290[A]	SER
1	A	290[B]	SER
1	B	133	GLU
1	B	149[A]	GLU
1	B	149[B]	GLU
1	B	199	GLN
1	B	229	ASP
1	B	302	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	194	HIS
1	A	250	GLN
1	A	262	GLN
1	A	287	GLN
1	B	105	ASN

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Mol	Chain	Res	Type
1	B	172	GLN
1	B	178	ASN
1	B	194	HIS
1	B	262	GLN
1	B	316	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](#)

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	SO4	B	1002	-	4,4,4	0.76	0	6,6,6	0.66	0
3	NDP	B	1004	-	51,52,52	1.67	9 (17%)	71,80,80	1.65	11 (15%)
3	NDP	A	1003	-	51,52,52	1.69	10 (19%)	71,80,80	1.63	12 (16%)
2	SO4	A	1001	-	4,4,4	0.80	0	6,6,6	1.18	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
3	NDP	B	1004	-	-	4/34/77/77	0/5/5/5
3	NDP	A	1003	-	-	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	B	1004	NDP	C4N-C3N	-6.16	1.38	1.50
3	A	1003	NDP	C4N-C3N	-5.66	1.39	1.50
3	A	1003	NDP	PN-O1N	-3.86	1.37	1.50
3	B	1004	NDP	PA-O3	3.70	1.63	1.59
3	A	1003	NDP	PA-O2A	-3.33	1.39	1.55
3	A	1003	NDP	C4N-C5N	-3.29	1.40	1.49
3	A	1003	NDP	C6N-N1N	3.22	1.45	1.37
3	B	1004	NDP	PN-O1N	-3.06	1.40	1.50
3	B	1004	NDP	C2A-N1A	2.75	1.38	1.33
3	B	1004	NDP	C3D-C4D	-2.55	1.46	1.53
3	A	1003	NDP	C3D-C4D	-2.55	1.46	1.53
3	A	1003	NDP	C2A-N3A	2.44	1.38	1.33
3	A	1003	NDP	PN-O3	-2.38	1.56	1.59
3	A	1003	NDP	C5A-C4A	-2.32	1.34	1.39
3	B	1004	NDP	C1D-N1N	2.26	1.52	1.46
3	B	1004	NDP	PA-O2A	-2.22	1.45	1.55
3	B	1004	NDP	PN-O3	-2.16	1.57	1.59
3	A	1003	NDP	C2A-N1A	-2.14	1.30	1.33
3	B	1004	NDP	C6N-C5N	2.13	1.39	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	NDP	C5A-C4A-N9A	5.70	112.02	105.81
3	A	1003	NDP	C5A-C4A-N9A	5.26	111.54	105.81
3	B	1004	NDP	C4A-N9A-C8A	-4.34	101.18	105.74
3	A	1003	NDP	C6A-C5A-C4A	3.88	122.48	117.18
3	B	1004	NDP	C6A-C5A-C4A	3.88	122.47	117.18
3	A	1003	NDP	C6N-N1N-C2N	-3.85	115.20	119.32
3	B	1004	NDP	O7N-C7N-C3N	-3.71	113.91	120.90
3	A	1003	NDP	O7N-C7N-C3N	-3.61	114.11	120.90
3	B	1004	NDP	C3N-C2N-N1N	-3.38	118.25	123.20
3	B	1004	NDP	C4A-C5A-N7A	-3.31	106.80	110.58
3	A	1003	NDP	O4B-C4B-C3B	3.31	111.72	105.15
3	A	1003	NDP	C5A-C4A-N3A	-3.04	122.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	NDP	C2B-C1B-N9A	3.04	118.75	113.75
3	B	1004	NDP	C3N-C7N-N7N	3.03	123.05	117.67
3	A	1003	NDP	O4B-C1B-N9A	-2.68	102.94	108.09
3	B	1004	NDP	N3A-C2A-N1A	-2.44	124.89	128.58
3	A	1003	NDP	C4A-N9A-C8A	-2.41	103.21	105.74
3	B	1004	NDP	N3A-C4A-N9A	-2.29	123.27	127.17
3	A	1003	NDP	O2N-PN-O1N	2.19	122.66	112.44
3	A	1003	NDP	C4A-N9A-C1B	2.17	131.71	126.63
3	B	1004	NDP	O2N-PN-O1N	2.16	122.48	112.44
3	B	1004	NDP	O2N-PN-O3	-2.15	101.47	107.27
3	A	1003	NDP	C4B-O4B-C1B	-2.05	104.94	109.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	NDP	O4D-C1D-N1N-C2N
3	B	1004	NDP	O4D-C1D-N1N-C2N
3	A	1003	NDP	PA-O3-PN-O5D
3	B	1004	NDP	PA-O3-PN-O5D
3	B	1004	NDP	C4D-C5D-O5D-PN
3	A	1003	NDP	C4D-C5D-O5D-PN
3	B	1004	NDP	PA-O3-PN-O2N
3	A	1003	NDP	C2B-O2B-P2B-O2X
3	A	1003	NDP	PA-O3-PN-O2N

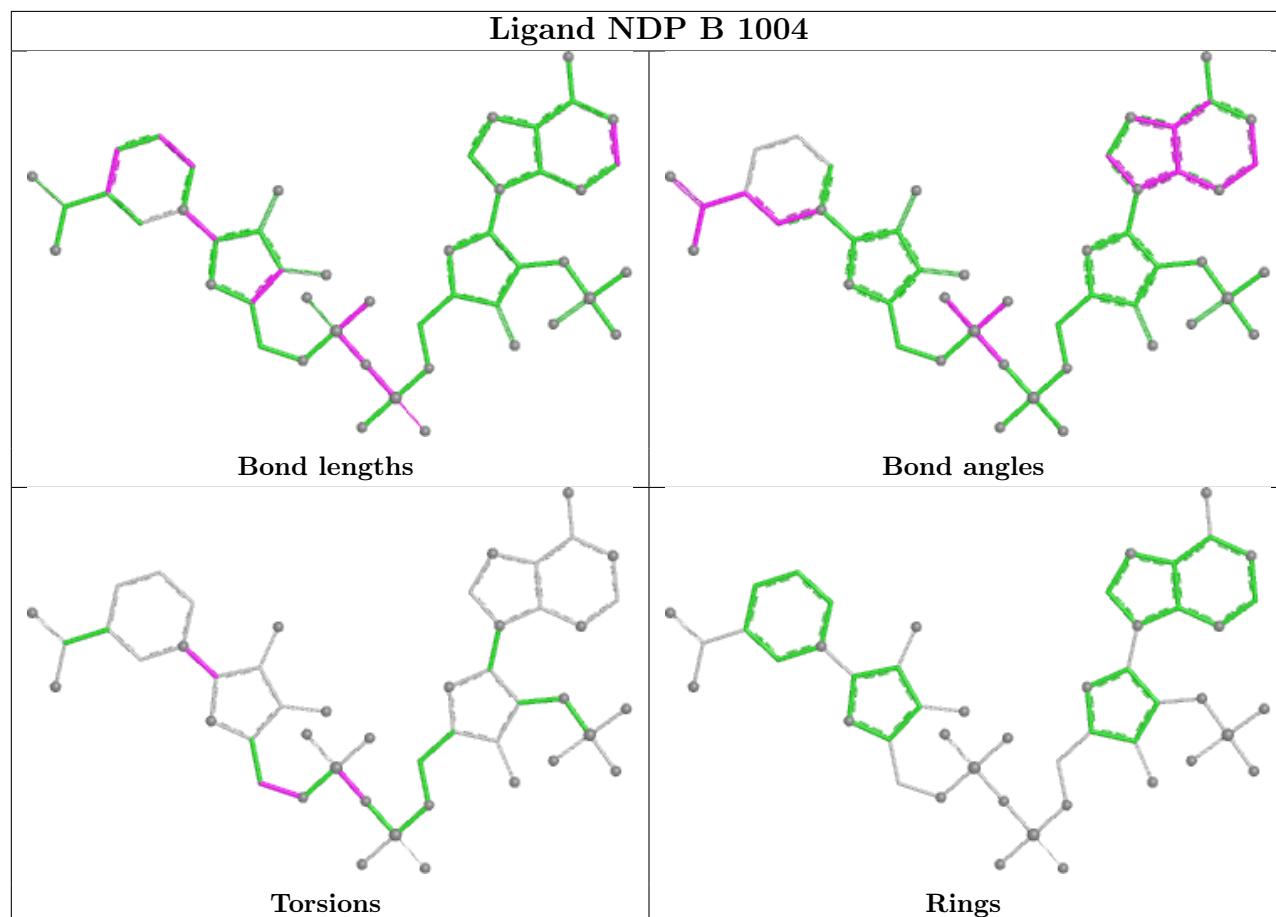
There are no ring outliers.

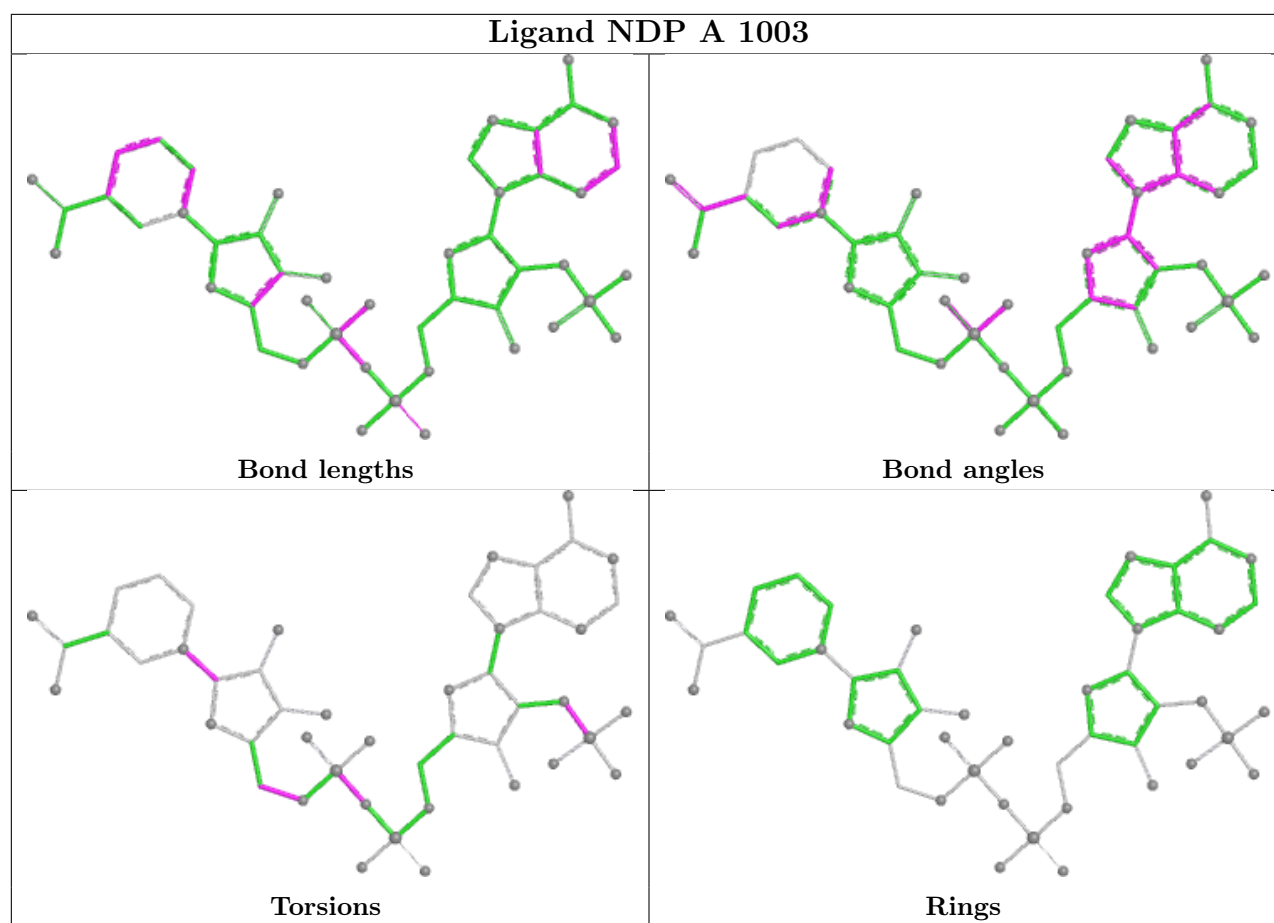
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1004	NDP	5	0
3	A	1003	NDP	4	0

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/322 (100%)	0.43	15 (4%) 36 45	12, 15, 25, 50	7 (2%)
1	B	322/322 (100%)	0.21	7 (2%) 62 69	12, 15, 26, 49	5 (1%)
All	All	644/644 (100%)	0.32	22 (3%) 48 56	12, 15, 25, 50	12 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	TRP	9.5
1	B	227	TRP	6.8
1	B	134	HIS	4.4
1	B	135	GLY	4.4
1	A	228	VAL	3.7
1	A	230	GLN	3.5
1	A	225	PRO	3.4
1	B	302	ASN	3.3
1	A	226	GLU	3.0
1	A	135	GLY	3.0
1	A	229	ASP	3.0
1	B	133	GLU	3.0
1	A	126	VAL	2.9
1	A	136	LYS	2.5
1	A	144	ILE	2.5
1	A	118	PHE	2.4
1	A	128	ILE	2.4
1	A	8	VAL	2.3
1	B	128	ILE	2.2
1	A	134	HIS	2.2
1	A	236	LEU	2.1
1	B	226	GLU	2.0

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](#)

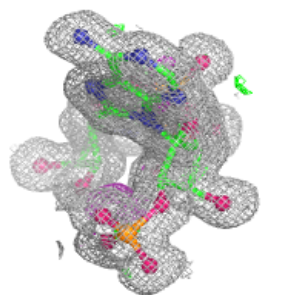
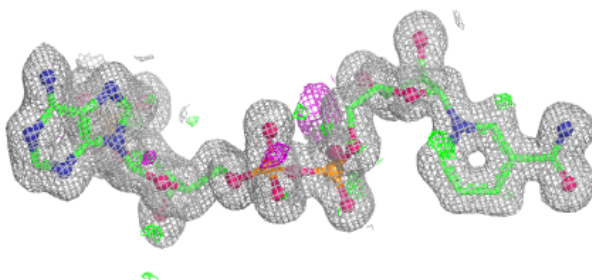
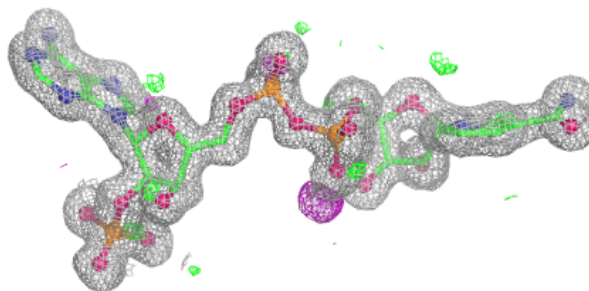
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1001	5/5	0.97	0.06	15,19,26,27	0
2	SO4	B	1002	5/5	0.97	0.07	19,20,22,29	0
3	NDP	A	1003	48/48	0.98	0.05	12,13,16,19	0
3	NDP	B	1004	48/48	0.99	0.04	11,13,15,18	0

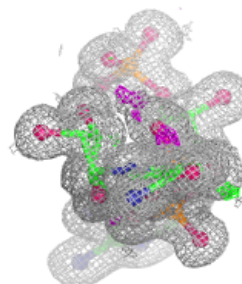
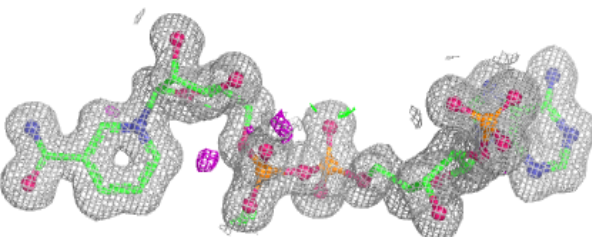
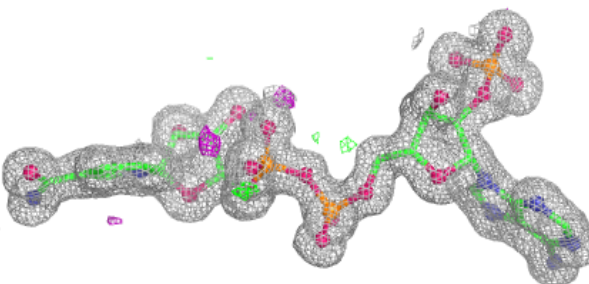
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP A 1003:

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

**Electron density around NDP B 1004:**

$2mF_o-DF_c$ (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.