



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:42 am BST

PDB ID : 1OHK
Title : HUMAN DIHYDROFOLATE REDUCTASE, ORTHORHOMBIC (P21 21 21)
CRYSTAL FORM
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.
Deposited on : 1997-09-17
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

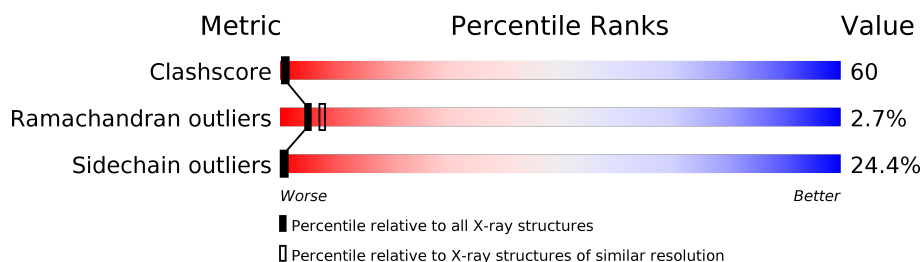
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on 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	186	<div> <div style="width: 16%; background-color: green;"></div> <div style="width: 41%; background-color: yellow;"></div> <div style="width: 32%; background-color: orange;"></div> <div style="width: 11%; background-color: red;"></div> </div> <div>16% 41% 32% 11%</div>

2 Entry composition [i](#)

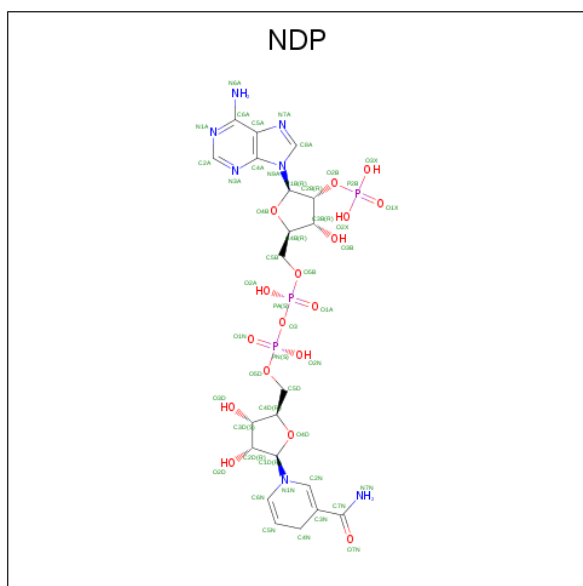
There are 4 unique types of molecules in this entry. The entry contains 1638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

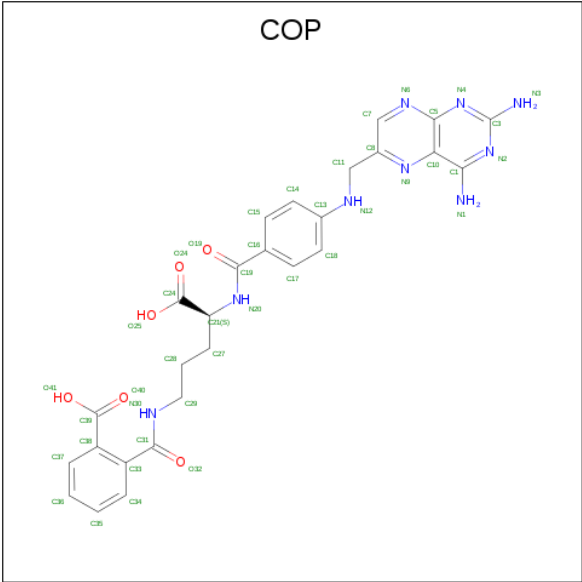
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1502	963	253	279	7	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is N-(4-CARBOXY-4-{4-[(2,4-DIAMINO-PTERIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-BUTYL)-PHTHALAMIC ACID (three-letter code: COP) (formula: $C_{27}H_{27}N_9O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			70	47	11	12		

- Molecule 4 is water.

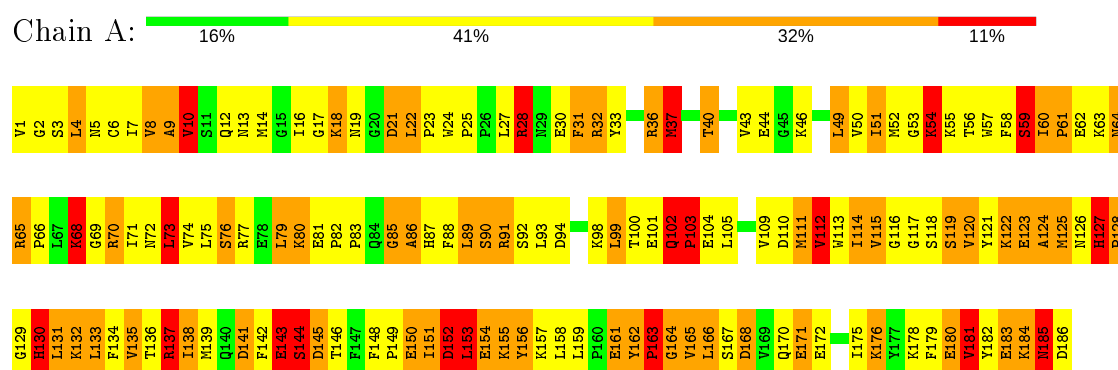
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: DIHYDROFOLATE REDUCTASE



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	36.90 Å 69.19 Å 69.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	94.7 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1638	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: COP, 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	1.19	2/1537 (0.1%)	2.79	135/2073 (6.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CD-OE1	-5.74	1.19	1.25
1	A	112	VAL	N-CA	-5.36	1.35	1.46

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH2	-16.87	111.87	120.30
1	A	28	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	A	137	ARG	NE-CZ-NH2	-14.92	112.84	120.30
1	A	44	GLU	O-C-N	14.46	147.78	123.20
1	A	36	ARG	CD-NE-CZ	14.26	143.57	123.60
1	A	137	ARG	NE-CZ-NH1	13.03	126.81	120.30
1	A	168	ASP	CB-CG-OD1	-12.43	107.12	118.30
1	A	168	ASP	CB-CG-OD2	12.21	129.29	118.30
1	A	70	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	65	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	91	ARG	CD-NE-CZ	-10.02	109.58	123.60
1	A	76	SER	O-C-N	9.67	138.17	122.70
1	A	145	ASP	CB-CG-OD2	9.62	126.96	118.30
1	A	64	ASN	OD1-CG-ND2	9.43	143.58	121.90
1	A	123	GLU	CA-CB-CG	9.40	134.07	113.40
1	A	130	HIS	CA-CB-CG	-9.39	97.64	113.60
1	A	164	GLY	C-N-CA	-9.39	98.24	121.70
1	A	22	LEU	CA-CB-CG	9.33	136.77	115.30
1	A	54	LYS	CB-CG-CD	9.24	135.63	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	GLY	CA-C-N	-9.14	97.09	117.20
1	A	164	GLY	O-C-N	9.12	137.29	122.70
1	A	143	GLU	CA-CB-CG	9.10	133.41	113.40
1	A	10	VAL	CB-CA-C	9.03	128.56	111.40
1	A	33	TYR	CB-CG-CD2	-9.01	115.59	121.00
1	A	145	ASP	CB-CG-OD1	8.96	126.36	118.30
1	A	64	ASN	CB-CG-OD1	-8.85	103.91	121.60
1	A	73	LEU	CB-CA-C	8.82	126.97	110.20
1	A	172	GLU	O-C-N	8.82	136.81	122.70
1	A	137	ARG	CD-NE-CZ	8.79	135.90	123.60
1	A	145	ASP	OD1-CG-OD2	-8.75	106.68	123.30
1	A	81	GLU	OE1-CD-OE2	-8.61	112.97	123.30
1	A	58	PHE	C-N-CA	7.92	141.50	121.70
1	A	59	SER	CB-CA-C	-7.88	95.13	110.10
1	A	89	LEU	O-C-N	7.79	135.16	122.70
1	A	44	GLU	CA-C-O	-7.71	103.91	120.10
1	A	176	LYS	CA-CB-CG	7.64	130.20	113.40
1	A	88	PHE	O-C-N	7.58	134.83	122.70
1	A	44	GLU	C-N-CA	-7.51	106.54	122.30
1	A	62	GLU	C-N-CA	7.50	140.46	121.70
1	A	8	VAL	CA-CB-CG1	7.46	122.09	110.90
1	A	153	LEU	CB-CG-CD2	-7.29	98.60	111.00
1	A	43	VAL	CB-CA-C	7.07	124.83	111.40
1	A	60	ILE	CB-CG1-CD1	7.01	133.52	113.90
1	A	18	LYS	CB-CA-C	-6.99	96.42	110.40
1	A	88	PHE	N-CA-CB	6.96	123.12	110.60
1	A	36	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	A	37	MET	CG-SD-CE	-6.78	89.35	100.20
1	A	94	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	A	150	GLU	CG-CD-OE1	-6.75	104.80	118.30
1	A	30	GLU	OE1-CD-OE2	-6.74	115.22	123.30
1	A	162	TYR	CB-CG-CD2	6.69	125.01	121.00
1	A	162	TYR	N-CA-CB	6.66	122.59	110.60
1	A	185	ASN	O-C-N	6.66	133.35	122.70
1	A	126	ASN	CB-CA-C	6.60	123.60	110.40
1	A	10	VAL	CA-CB-CG1	6.59	120.79	110.90
1	A	181	VAL	CG1-CB-CG2	6.55	121.39	110.90
1	A	44	GLU	OE1-CD-OE2	6.52	131.12	123.30
1	A	172	GLU	OE1-CD-OE2	6.51	131.12	123.30
1	A	28	ARG	CA-C-O	-6.49	106.47	120.10
1	A	51	ILE	O-C-N	6.49	133.09	122.70
1	A	183	GLU	O-C-N	6.43	132.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ALA	N-CA-CB	6.42	119.08	110.10
1	A	36	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	158	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	49	LEU	CB-CA-C	6.37	122.30	110.20
1	A	172	GLU	CG-CD-OE2	-6.36	105.58	118.30
1	A	44	GLU	CB-CA-C	-6.35	97.70	110.40
1	A	70	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	A	70	ARG	N-CA-CB	-6.29	99.28	110.60
1	A	123	GLU	C-N-CA	6.28	137.40	121.70
1	A	111	MET	CG-SD-CE	6.27	110.23	100.20
1	A	21	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	81	GLU	CA-CB-CG	6.26	127.17	113.40
1	A	32	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	156	TYR	O-C-N	6.17	132.57	122.70
1	A	185	ASN	N-CA-CB	6.12	121.61	110.60
1	A	116	GLY	C-N-CA	6.10	135.10	122.30
1	A	183	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	A	119	SER	CB-CA-C	6.08	121.65	110.10
1	A	36	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	A	62	GLU	O-C-N	-6.06	113.00	122.70
1	A	158	LEU	CB-CG-CD1	6.05	121.28	111.00
1	A	125	MET	CA-CB-CG	5.97	123.46	113.30
1	A	81	GLU	CG-CD-OE1	5.94	130.18	118.30
1	A	180	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	A	158	LEU	N-CA-CB	5.93	122.26	110.40
1	A	167	SER	N-CA-CB	5.92	119.38	110.50
1	A	158	LEU	CB-CG-CD2	-5.89	100.98	111.00
1	A	80	LYS	N-CA-CB	5.88	121.18	110.60
1	A	86	ALA	N-CA-CB	5.86	118.30	110.10
1	A	144	SER	C-N-CA	5.86	136.34	121.70
1	A	4	LEU	CB-CA-C	5.85	121.32	110.20
1	A	80	LYS	O-C-N	5.84	132.04	122.70
1	A	150	GLU	CG-CD-OE2	5.78	129.86	118.30
1	A	115	VAL	N-CA-CB	-5.73	98.89	111.50
1	A	152	ASP	CA-C-O	-5.73	108.07	120.10
1	A	119	SER	N-CA-CB	-5.71	101.94	110.50
1	A	135	VAL	CA-CB-CG2	5.69	119.43	110.90
1	A	103	PRO	N-CA-C	5.68	126.88	112.10
1	A	8	VAL	CA-C-O	-5.67	108.18	120.10
1	A	18	LYS	CA-C-O	-5.63	108.28	120.10
1	A	68	LYS	CB-CG-CD	5.63	126.23	111.60
1	A	54	LYS	CG-CD-CE	5.61	128.73	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	GLU	C-N-CA	5.60	135.71	121.70
1	A	181	VAL	CB-CA-C	5.59	122.03	111.40
1	A	114	ILE	O-C-N	5.58	131.62	122.70
1	A	94	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	134	PHE	CB-CA-C	5.55	121.50	110.40
1	A	161	GLU	CA-C-O	-5.54	108.47	120.10
1	A	19	ASN	N-CA-CB	5.53	120.54	110.60
1	A	165	VAL	CB-CA-C	5.51	121.87	111.40
1	A	65	ARG	CG-CD-NE	5.48	123.32	111.80
1	A	127	HIS	CA-CB-CG	5.47	122.91	113.60
1	A	12	GLN	CG-CD-OE1	-5.46	110.68	121.60
1	A	6	CYS	N-CA-CB	5.43	120.37	110.60
1	A	120	VAL	CA-CB-CG2	5.42	119.03	110.90
1	A	69	GLY	N-CA-C	5.40	126.61	113.10
1	A	98	LYS	N-CA-CB	5.38	120.28	110.60
1	A	85	GLY	C-N-CA	5.29	134.93	121.70
1	A	138	ILE	N-CA-C	-5.29	96.73	111.00
1	A	132	LYS	CA-C-O	5.24	131.10	120.10
1	A	102	GLN	N-CA-CB	5.22	119.99	110.60
1	A	186	ASP	CA-CB-CG	5.21	124.86	113.40
1	A	183	GLU	CB-CA-C	-5.20	99.99	110.40
1	A	68	LYS	O-C-N	-5.19	114.37	123.20
1	A	49	LEU	C-N-CA	5.18	134.65	121.70
1	A	141	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	161	GLU	O-C-N	5.17	130.96	122.70
1	A	88	PHE	CA-C-N	-5.14	105.88	117.20
1	A	156	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	58	PHE	CA-C-N	5.07	128.35	117.20
1	A	130	HIS	O-C-N	5.05	130.78	122.70
1	A	168	ASP	CA-CB-CG	-5.05	102.30	113.40
1	A	62	GLU	CA-C-O	5.03	130.67	120.10
1	A	123	GLU	N-CA-CB	5.01	119.62	110.60

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	1502	0	1510	190	3
2	A	48	0	25	16	0
3	A	70	0	33	8	0
4	A	18	0	0	1	5
All	All	1638	0	1568	190	5

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 60.

All (190) 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:28:ARG:HD3	3:A:188[A]:COP:O40	1.15	1.32
1:A:102:GLN:NE2	1:A:102:GLN:HA	1.36	1.25
1:A:102:GLN:CA	1:A:102:GLN:HE21	1.38	1.19
1:A:166:LEU:HD12	1:A:166:LEU:H	1.04	1.10
1:A:54:LYS:N	2:A:187:NDP:H52A	1.65	1.10
1:A:100:THR:HG23	1:A:109:VAL:HG11	1.42	0.99
1:A:36:ARG:HH22	1:A:165:VAL:HG22	1.25	0.99
1:A:28:ARG:CD	3:A:188[A]:COP:O40	2.10	0.98
1:A:49:LEU:HD12	1:A:71:ILE:HB	1.45	0.95
1:A:53:GLY:C	2:A:187:NDP:H52A	1.88	0.94
1:A:54:LYS:N	2:A:187:NDP:C5B	2.30	0.93
1:A:72:ASN:H	1:A:87:HIS:CD2	1.86	0.93
1:A:99:LEU:HD23	1:A:105:LEU:HD12	1.51	0.92
1:A:93:LEU:HD23	1:A:123:GLU:HB3	1.52	0.92
1:A:54:LYS:H	2:A:187:NDP:C4B	1.85	0.90
1:A:53:GLY:HA3	2:A:187:NDP:H51A	1.52	0.89
1:A:166:LEU:CD1	1:A:166:LEU:H	1.85	0.89
1:A:162:TYR:CG	1:A:163:PRO:HD2	2.07	0.89
1:A:166:LEU:N	1:A:166:LEU:HD12	1.88	0.88
1:A:54:LYS:H	2:A:187:NDP:C5B	1.87	0.88
1:A:72:ASN:H	1:A:87:HIS:HD2	0.95	0.87
1:A:124:ALA:O	1:A:127:HIS:HB2	1.75	0.87
1:A:56:THR:O	1:A:59:SER:OG	1.93	0.86
1:A:127:HIS:O	1:A:184:LYS:NZ	2.08	0.85
1:A:53:GLY:HA3	2:A:187:NDP:C5B	2.05	0.85
1:A:75:LEU:HD23	1:A:90:SER:O	1.76	0.84
1:A:51:ILE:CG2	1:A:75:LEU:HD11	2.08	0.83
1:A:37:MET:HA	1:A:37:MET:CE	2.10	0.81
1:A:135:VAL:HG11	1:A:137:ARG:HE	1.45	0.81
1:A:36:ARG:NH2	1:A:164:GLY:O	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HB3	1:A:123:GLU:OE1	1.80	0.81
1:A:146:THR:HG21	2:A:187:NDP:H4D	1.63	0.79
1:A:162:TYR:CD1	1:A:163:PRO:HD2	2.18	0.79
1:A:184:LYS:O	1:A:184:LYS:HG3	1.83	0.78
1:A:93:LEU:HB3	1:A:123:GLU:CD	2.04	0.78
1:A:31:PHE:HB3	3:A:188[B]:COP:H291	1.67	0.77
1:A:40:THR:O	1:A:40:THR:HG22	1.82	0.77
1:A:102:GLN:NE2	1:A:103:PRO:HD2	2.00	0.77
1:A:51:ILE:HG21	1:A:75:LEU:HD11	1.67	0.77
1:A:171:GLU:HG2	1:A:175:ILE:O	1.86	0.76
1:A:51:ILE:CD1	1:A:112:VAL:HG23	2.16	0.75
1:A:99:LEU:HD23	1:A:105:LEU:CD1	2.15	0.75
1:A:102:GLN:CD	1:A:103:PRO:HD2	2.07	0.75
1:A:128:PRO:O	1:A:128:PRO:HG2	1.85	0.75
1:A:51:ILE:O	1:A:115:VAL:HG22	1.86	0.74
1:A:2:GLY:HA3	1:A:111:MET:HG2	1.69	0.74
1:A:102:GLN:HE21	1:A:102:GLN:HA	0.62	0.74
1:A:53:GLY:CA	2:A:187:NDP:C5B	2.65	0.74
1:A:31:PHE:HB3	3:A:188[A]:COP:H292	1.70	0.74
1:A:53:GLY:CA	2:A:187:NDP:H51A	2.18	0.73
1:A:17:GLY:HA3	1:A:146:THR:HG23	1.69	0.73
1:A:73:LEU:HD23	1:A:73:LEU:C	2.08	0.73
1:A:46:LYS:HB3	1:A:110:ASP:HB2	1.70	0.72
1:A:55:LYS:HZ2	1:A:55:LYS:HB3	1.54	0.72
1:A:17:GLY:CA	1:A:146:THR:HG23	2.19	0.72
1:A:102:GLN:CG	1:A:103:PRO:HD2	2.20	0.71
1:A:102:GLN:HG3	1:A:103:PRO:CD	2.20	0.71
1:A:72:ASN:N	1:A:87:HIS:HD2	1.80	0.71
1:A:129:GLY:O	1:A:184:LYS:HE3	1.91	0.70
1:A:132:LYS:NZ	1:A:162:TYR:OH	2.16	0.70
1:A:36:ARG:CZ	1:A:164:GLY:O	2.38	0.70
1:A:50:VAL:HG11	1:A:70:ARG:HD2	1.74	0.70
1:A:17:GLY:O	1:A:144:SER:HB3	1.93	0.68
1:A:168:ASP:OD1	1:A:168:ASP:N	2.16	0.68
1:A:105:LEU:O	1:A:109:VAL:HB	1.94	0.68
1:A:37:MET:HA	1:A:37:MET:HE2	1.76	0.67
1:A:54:LYS:HB3	2:A:187:NDP:H4B	1.77	0.67
1:A:37:MET:HA	1:A:37:MET:HE3	1.75	0.67
1:A:115:VAL:O	1:A:121:TYR:OH	2.11	0.67
1:A:53:GLY:CA	2:A:187:NDP:H52A	2.25	0.66
1:A:51:ILE:CG2	1:A:75:LEU:CD1	2.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:O	1:A:170:GLN:NE2	2.27	0.66
1:A:55:LYS:HZ2	1:A:55:LYS:CB	2.06	0.66
1:A:28:ARG:HB2	3:A:188[A]:COP:C39	2.25	0.66
1:A:28:ARG:HD3	3:A:188[A]:COP:C39	2.26	0.63
1:A:162:TYR:CG	1:A:163:PRO:CD	2.81	0.63
1:A:27:LEU:HD21	1:A:175:ILE:HD13	1.80	0.63
1:A:128:PRO:O	1:A:128:PRO:CG	2.47	0.62
1:A:162:TYR:CD2	1:A:163:PRO:HD2	2.34	0.62
1:A:135:VAL:HG11	1:A:137:ARG:NE	2.14	0.62
1:A:17:GLY:HA3	1:A:146:THR:CG2	2.29	0.62
1:A:135:VAL:HG12	1:A:135:VAL:O	1.99	0.61
1:A:36:ARG:NH1	1:A:164:GLY:O	2.34	0.61
1:A:57:TRP:CZ2	1:A:86:ALA:HB2	2.36	0.61
1:A:119:SER:HA	1:A:122:LYS:CB	2.30	0.61
1:A:32:ARG:HG2	3:A:188[A]:COP:O41	2.01	0.60
1:A:36:ARG:NH2	1:A:165:VAL:HG22	2.08	0.59
1:A:18:LYS:HA	1:A:145:ASP:OD1	2.02	0.59
1:A:93:LEU:CD2	1:A:123:GLU:HB3	2.30	0.59
1:A:54:LYS:N	2:A:187:NDP:C4B	2.60	0.58
1:A:68:LYS:HG3	1:A:68:LYS:O	2.03	0.58
1:A:52:MET:HB3	1:A:115:VAL:HG21	1.87	0.57
1:A:119:SER:HA	1:A:122:LYS:HB2	1.85	0.57
1:A:40:THR:O	1:A:40:THR:CG2	2.50	0.57
1:A:57:TRP:O	1:A:60:ILE:HB	2.04	0.57
1:A:13:ASN:HB3	1:A:141:ASP:OD1	2.04	0.57
1:A:151:ILE:O	1:A:153:LEU:N	2.38	0.57
1:A:133:LEU:HB2	1:A:182:TYR:HB2	1.87	0.57
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.87	0.56
1:A:18:LYS:HD3	1:A:143:GLU:O	2.05	0.56
1:A:83:PRO:O	1:A:86:ALA:HB3	2.06	0.56
1:A:102:GLN:CA	1:A:102:GLN:NE2	2.19	0.56
1:A:102:GLN:HG3	1:A:103:PRO:HG2	1.89	0.55
1:A:13:ASN:ND2	1:A:142:PHE:O	2.35	0.55
1:A:131:LEU:HB3	1:A:184:LYS:HG2	1.89	0.55
1:A:57:TRP:CH2	1:A:86:ALA:HB2	2.41	0.55
1:A:60:ILE:HG22	1:A:65:ARG:CG	2.37	0.55
1:A:3:SER:HB3	1:A:130:HIS:O	2.07	0.54
1:A:180:GLU:OE1	1:A:182:TYR:OH	2.15	0.54
1:A:130:HIS:ND1	1:A:185:ASN:OD1	2.39	0.53
1:A:102:GLN:CG	1:A:103:PRO:CD	2.84	0.53
1:A:102:GLN:HG3	1:A:103:PRO:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HE2	1:A:180:GLU:OE2	2.08	0.53
1:A:31:PHE:HB3	3:A:188[B]:COP:C29	2.28	0.52
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.35	0.52
1:A:49:LEU:HD12	1:A:71:ILE:CB	2.29	0.52
1:A:82:PRO:HB3	1:A:89:LEU:HB2	1.91	0.52
1:A:46:LYS:CB	1:A:110:ASP:HB2	2.39	0.51
1:A:102:GLN:HG3	1:A:103:PRO:HD2	1.84	0.51
1:A:50:VAL:HG22	1:A:71:ILE:O	2.11	0.50
1:A:72:ASN:HD22	1:A:72:ASN:N	2.10	0.50
1:A:119:SER:O	1:A:123:GLU:N	2.45	0.50
1:A:100:THR:CG2	1:A:109:VAL:HG11	2.29	0.49
1:A:10:VAL:O	1:A:138:ILE:HB	2.12	0.49
1:A:23:PRO:HB2	1:A:24:TRP:CE3	2.47	0.49
1:A:17:GLY:HA2	1:A:23:PRO:HD3	1.95	0.49
1:A:119:SER:HA	1:A:122:LYS:HB3	1.93	0.49
1:A:131:LEU:HB2	1:A:184:LYS:HE2	1.94	0.48
1:A:159:LEU:HD12	1:A:181:VAL:HG22	1.95	0.48
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.48	0.48
1:A:117:GLY:HA3	2:A:187:NDP:O2A	2.14	0.48
1:A:50:VAL:HG11	1:A:70:ARG:CD	2.42	0.48
1:A:79:LEU:O	1:A:91:ARG:NH2	2.44	0.47
1:A:93:LEU:HD23	1:A:123:GLU:CB	2.36	0.47
1:A:8:VAL:HG11	1:A:148:PHE:CE1	2.49	0.47
1:A:156:TYR:HA	1:A:183:GLU:O	2.13	0.47
1:A:185:ASN:HD22	1:A:185:ASN:C	2.18	0.47
1:A:60:ILE:HG22	1:A:65:ARG:HG3	1.97	0.47
1:A:16:ILE:O	2:A:187:NDP:H2N	2.15	0.47
1:A:61:PRO:O	1:A:65:ARG:HG3	2.15	0.47
1:A:152:ASP:OD2	1:A:155:LYS:NZ	2.38	0.46
1:A:60:ILE:CG2	1:A:65:ARG:HG2	2.46	0.46
1:A:55:LYS:HG2	1:A:55:LYS:HZ3	1.39	0.46
1:A:37:MET:CA	1:A:37:MET:HE3	2.45	0.46
1:A:115:VAL:C	1:A:121:TYR:OH	2.54	0.45
1:A:74:VAL:O	1:A:89:LEU:HD12	2.16	0.45
1:A:8:VAL:HG21	1:A:148:PHE:CD1	2.51	0.45
1:A:4:LEU:HD12	1:A:4:LEU:HA	1.75	0.45
1:A:171:GLU:HG3	1:A:176:LYS:HD3	1.99	0.45
1:A:114:ILE:CG2	1:A:120:VAL:HG12	2.46	0.45
1:A:23:PRO:O	1:A:142:PHE:HB3	2.17	0.45
1:A:89:LEU:HD21	1:A:91:ARG:CZ	2.46	0.45
1:A:10:VAL:HG12	1:A:137:ARG:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:O	1:A:40:THR:HB	2.16	0.44
1:A:66:PRO:HB3	1:A:85:GLY:O	2.17	0.44
1:A:17:GLY:CA	1:A:146:THR:CG2	2.91	0.44
1:A:76:SER:CB	1:A:79:LEU:HD12	2.48	0.44
1:A:80:LYS:HB2	1:A:80:LYS:HE2	1.65	0.44
1:A:168:ASP:C	1:A:168:ASP:OD1	2.53	0.44
1:A:89:LEU:HD21	1:A:91:ARG:NH2	2.34	0.43
1:A:51:ILE:HD11	1:A:112:VAL:HG23	1.97	0.43
1:A:28:ARG:O	1:A:32:ARG:HG3	2.18	0.43
1:A:135:VAL:CG1	1:A:137:ARG:HD3	2.48	0.43
1:A:2:GLY:HA3	1:A:111:MET:CG	2.46	0.43
1:A:104:GLU:OE1	1:A:104:GLU:N	2.51	0.43
1:A:168:ASP:OD1	1:A:168:ASP:O	2.36	0.43
1:A:125:MET:C	1:A:127:HIS:H	2.21	0.43
1:A:75:LEU:HA	1:A:90:SER:O	2.19	0.43
1:A:79:LEU:HD13	1:A:83:PRO:HD3	2.01	0.43
1:A:145:ASP:OD1	1:A:146:THR:HG22	2.19	0.42
1:A:52:MET:HB3	1:A:115:VAL:CG2	2.48	0.42
1:A:102:GLN:HA	1:A:103:PRO:HD2	1.71	0.42
1:A:5:ASN:HB3	1:A:113:TRP:CZ3	2.55	0.42
1:A:93:LEU:CD2	1:A:123:GLU:CB	2.96	0.42
1:A:135:VAL:CG1	1:A:137:ARG:HE	2.25	0.42
1:A:77:ARG:H	2:A:187:NDP:P2B	2.43	0.42
1:A:63:LYS:HG2	1:A:64:ASN:OD1	2.20	0.42
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.69	0.41
1:A:118:SER:O	1:A:122:LYS:HB2	2.20	0.41
1:A:122:LYS:HA	1:A:122:LYS:HD2	1.58	0.41
1:A:152:ASP:OD1	1:A:154:GLU:HG3	2.21	0.41
1:A:166:LEU:HD13	1:A:179:PHE:CE2	2.56	0.41
1:A:9:ALA:HA	1:A:136:THR:HB	2.03	0.41
1:A:156:TYR:CD2	1:A:184:LYS:HB3	2.56	0.41
1:A:51:ILE:HG22	1:A:75:LEU:CD1	2.51	0.41
1:A:132:LYS:HA	1:A:182:TYR:O	2.22	0.40
1:A:182:TYR:HE2	4:A:202:HOH:O	2.04	0.40
1:A:60:ILE:HG21	1:A:65:ARG:HG2	2.02	0.40
1:A:175:ILE:HG22	1:A:176:LYS:N	2.36	0.40

All (5) 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:195:HOH:O	4:A:201:HOH:O[2_555]	1.65	0.55
1:A:157:LYS:NZ	4:A:194:HOH:O[2_554]	1.68	0.52
4:A:196:HOH:O	4:A:202:HOH:O[2_555]	1.76	0.44
1:A:157:LYS:CD	4:A:194:HOH:O[2_554]	1.96	0.24
1:A:157:LYS:CE	4:A:194:HOH:O[2_554]	1.99	0.21

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	184/186 (99%)	161 (88%)	18 (10%)	5 (3%)	5 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ALA
1	A	152	ASP
1	A	40	THR
1	A	103	PRO
1	A	163	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	168/168 (100%)	127 (76%)	41 (24%)	0 1

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

Mol	Chain	Res	Type
1	A	1	VAL
1	A	7	ILE
1	A	10	VAL
1	A	14	MET
1	A	21	ASP
1	A	28	ARG
1	A	31	PHE
1	A	37	MET
1	A	54	LYS
1	A	59	SER
1	A	61	PRO
1	A	68	LYS
1	A	73	LEU
1	A	79	LEU
1	A	90	SER
1	A	92	SER
1	A	99	LEU
1	A	101	GLU
1	A	102	GLN
1	A	112	VAL
1	A	122	LYS
1	A	127	HIS
1	A	128	PRO
1	A	130	HIS
1	A	131	LEU
1	A	133	LEU
1	A	137	ARG
1	A	139	MET
1	A	143	GLU
1	A	144	SER
1	A	150	GLU
1	A	151	ILE
1	A	153	LEU
1	A	155	LYS
1	A	161	GLU
1	A	163	PRO
1	A	166	LEU
1	A	171	GLU
1	A	181	VAL
1	A	184	LYS
1	A	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	102	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 carbohydrates 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	COP	A	188[C]	-	40,45,45	1.77	7 (17%)	51,62,62	3.84	26 (50%)
2	NDP	A	187	-	45,52,52	2.88	14 (31%)	53,80,80	2.36	19 (35%)
3	COP	A	188[B]	-	40,45,45	1.76	7 (17%)	51,62,62	4.03	27 (52%)
3	COP	A	188[A]	-	40,45,45	2.16	8 (20%)	51,62,62	3.82	25 (49%)

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	COP	A	188[C]	-	-	11/24/32/32	0/4/4/4
2	NDP	A	187	-	-	13/30/77/77	0/5/5/5
3	COP	A	188[B]	-	-	11/24/32/32	0/4/4/4
3	COP	A	188[A]	-	-	11/24/32/32	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-10.02	1.22	1.45
2	A	187	NDP	P2B-O2B	8.58	1.75	1.59
2	A	187	NDP	O3B-C3B	-8.15	1.23	1.43
3	A	188[A]	COP	C29-N30	6.75	1.61	1.46
3	A	188[A]	COP	C31-N30	5.81	1.46	1.33
3	A	188[A]	COP	C38-C39	5.27	1.52	1.47
3	A	188[C]	COP	C5-N6	-5.12	1.30	1.37
3	A	188[B]	COP	C5-N6	-5.12	1.30	1.37
3	A	188[A]	COP	C5-N6	-5.12	1.30	1.37
3	A	188[C]	COP	C29-N30	4.92	1.57	1.46
3	A	188[B]	COP	C29-N30	4.91	1.57	1.46
3	A	188[C]	COP	C31-N30	4.44	1.43	1.33
3	A	188[B]	COP	C31-N30	4.41	1.43	1.33
3	A	188[C]	COP	C3-N2	-3.67	1.28	1.35
3	A	188[B]	COP	C3-N2	-3.67	1.28	1.35
3	A	188[A]	COP	C3-N2	-3.67	1.28	1.35
2	A	187	NDP	C5A-C4A	-3.38	1.32	1.40
2	A	187	NDP	C6A-C5A	3.30	1.55	1.43
2	A	187	NDP	C3B-C4B	3.10	1.60	1.53
2	A	187	NDP	C1D-N1N	2.98	1.54	1.46
2	A	187	NDP	PN-O1N	-2.97	1.40	1.50
2	A	187	NDP	O4D-C1D	2.90	1.48	1.42
2	A	187	NDP	O4B-C1B	2.67	1.44	1.41
2	A	187	NDP	PA-O2A	-2.61	1.43	1.55
2	A	187	NDP	P2B-O3X	-2.31	1.45	1.54
3	A	188[C]	COP	C11-C8	2.25	1.55	1.51
3	A	188[B]	COP	C11-C8	2.25	1.55	1.51
3	A	188[A]	COP	C11-C8	2.25	1.55	1.51
2	A	187	NDP	O4D-C4D	2.23	1.50	1.45
3	A	188[C]	COP	C10-N9	-2.10	1.33	1.37
3	A	188[B]	COP	C10-N9	-2.10	1.33	1.37
3	A	188[A]	COP	C10-N9	-2.10	1.33	1.37
3	A	188[C]	COP	C1-N2	-2.10	1.30	1.33
3	A	188[B]	COP	C1-N2	-2.10	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[A]	COP	C1-N2	-2.10	1.30	1.33
2	A	187	NDP	C4N-C3N	2.00	1.53	1.49

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[C]	COP	C21-N20-C19	18.27	145.90	122.34
3	A	188[B]	COP	C21-N20-C19	18.27	145.90	122.34
3	A	188[A]	COP	C21-N20-C19	18.27	145.90	122.34
3	A	188[B]	COP	C27-C28-C29	-9.41	83.84	112.05
3	A	188[C]	COP	C1-C10-N9	-7.27	114.72	120.33
3	A	188[B]	COP	C1-C10-N9	-7.27	114.72	120.33
3	A	188[A]	COP	C1-C10-N9	-7.27	114.72	120.33
3	A	188[C]	COP	N6-C5-N4	6.82	123.61	115.82
3	A	188[B]	COP	N6-C5-N4	6.82	123.61	115.82
3	A	188[A]	COP	N6-C5-N4	6.82	123.61	115.82
3	A	188[C]	COP	C16-C19-N20	6.72	129.95	117.06
3	A	188[B]	COP	C16-C19-N20	6.72	129.95	117.06
3	A	188[A]	COP	C16-C19-N20	6.72	129.95	117.06
3	A	188[C]	COP	C10-C1-N1	-5.63	111.79	120.35
3	A	188[B]	COP	C10-C1-N1	-5.63	111.79	120.35
3	A	188[A]	COP	C10-C1-N1	-5.63	111.79	120.35
2	A	187	NDP	O3B-C3B-C4B	-5.38	95.50	111.05
2	A	187	NDP	C1B-N9A-C4A	-4.74	118.32	126.64
2	A	187	NDP	O3X-P2B-O2X	4.68	125.52	107.64
2	A	187	NDP	C2D-C1D-N1N	4.68	125.02	113.30
3	A	188[C]	COP	C11-N12-C13	-4.52	110.52	122.15
3	A	188[B]	COP	C11-N12-C13	-4.52	110.52	122.15
3	A	188[A]	COP	C11-N12-C13	-4.52	110.52	122.15
3	A	188[C]	COP	N1-C1-N2	4.47	129.22	117.07
3	A	188[B]	COP	N1-C1-N2	4.47	129.22	117.07
3	A	188[A]	COP	N1-C1-N2	4.47	129.22	117.07
2	A	187	NDP	O4B-C4B-C5B	-4.31	95.18	109.37
2	A	187	NDP	O2B-C2B-C1B	-4.07	95.44	110.10
3	A	188[C]	COP	O19-C19-C16	-4.05	113.71	120.94
3	A	188[B]	COP	O19-C19-C16	-4.05	113.71	120.94
3	A	188[A]	COP	O19-C19-C16	-4.05	113.71	120.94
3	A	188[B]	COP	O32-C31-C33	-3.92	113.85	121.01
3	A	188[C]	COP	N4-C3-N2	-3.91	122.01	127.22
3	A	188[B]	COP	N4-C3-N2	-3.91	122.01	127.22
3	A	188[A]	COP	N4-C3-N2	-3.91	122.01	127.22
3	A	188[C]	COP	O32-C31-C33	-3.86	113.95	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	C1D-N1N-C2N	-3.81	114.77	121.11
3	A	188[C]	COP	C29-N30-C31	3.65	130.41	122.08
3	A	188[B]	COP	C29-N30-C31	3.65	130.41	122.08
3	A	188[C]	COP	C5-C10-N9	3.62	126.77	122.41
3	A	188[B]	COP	C5-C10-N9	3.62	126.77	122.41
3	A	188[A]	COP	C5-C10-N9	3.62	126.77	122.41
3	A	188[A]	COP	C37-C38-C33	3.49	121.99	118.03
2	A	187	NDP	O5B-C5B-C4B	-3.48	97.00	108.99
3	A	188[C]	COP	N3-C3-N4	3.44	123.40	117.79
3	A	188[B]	COP	N3-C3-N4	3.44	123.40	117.79
3	A	188[A]	COP	N3-C3-N4	3.44	123.40	117.79
3	A	188[A]	COP	C34-C33-C38	-3.43	115.79	119.74
3	A	188[C]	COP	C27-C28-C29	3.36	122.13	112.05
3	A	188[A]	COP	C37-C38-C39	-3.34	115.23	120.20
3	A	188[C]	COP	O19-C19-N20	-3.32	116.34	122.45
3	A	188[B]	COP	O19-C19-N20	-3.32	116.34	122.45
3	A	188[A]	COP	O19-C19-N20	-3.32	116.34	122.45
2	A	187	NDP	O4B-C1B-C2B	-3.29	100.89	106.59
3	A	188[B]	COP	C28-C29-N30	3.21	121.40	112.21
3	A	188[C]	COP	C28-C29-N30	3.21	121.37	112.21
2	A	187	NDP	O2B-P2B-O1X	-3.20	97.05	109.39
3	A	188[C]	COP	C10-C1-N2	-3.09	118.98	121.01
3	A	188[B]	COP	C10-C1-N2	-3.09	118.98	121.01
3	A	188[A]	COP	C10-C1-N2	-3.09	118.98	121.01
2	A	187	NDP	N6A-C6A-N1A	3.07	124.94	118.57
2	A	187	NDP	O2D-C2D-C1D	-2.99	100.02	110.02
2	A	187	NDP	O2B-C2B-C3B	-2.96	100.94	111.68
3	A	188[C]	COP	C8-N9-C10	-2.84	113.45	118.04
3	A	188[B]	COP	C8-N9-C10	-2.84	113.45	118.04
3	A	188[A]	COP	C8-N9-C10	-2.84	113.45	118.04
2	A	187	NDP	O2N-PN-O1N	2.83	126.24	112.24
2	A	187	NDP	C2D-C3D-C4D	-2.81	97.18	102.64
3	A	188[C]	COP	C3-N4-C5	2.67	118.40	115.36
3	A	188[B]	COP	C3-N4-C5	2.67	118.40	115.36
3	A	188[A]	COP	C3-N4-C5	2.67	118.40	115.36
3	A	188[C]	COP	C11-C8-C7	2.61	126.09	121.55
3	A	188[B]	COP	C11-C8-C7	2.61	126.09	121.55
3	A	188[A]	COP	C11-C8-C7	2.61	126.09	121.55
2	A	187	NDP	O3D-C3D-C4D	-2.53	103.74	111.05
3	A	188[C]	COP	C3-N2-C1	2.44	123.69	116.72
3	A	188[B]	COP	C3-N2-C1	2.44	123.69	116.72
3	A	188[A]	COP	C3-N2-C1	2.44	123.69	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	C4A-C5A-N7A	2.32	111.82	109.40
3	A	188[C]	COP	C11-C8-N9	-2.23	112.70	116.66
3	A	188[B]	COP	C11-C8-N9	-2.23	112.70	116.66
3	A	188[A]	COP	C11-C8-N9	-2.23	112.70	116.66
3	A	188[C]	COP	C8-C11-N12	2.20	117.94	113.07
3	A	188[B]	COP	C8-C11-N12	2.20	117.94	113.07
3	A	188[A]	COP	C8-C11-N12	2.20	117.94	113.07
3	A	188[C]	COP	C14-C15-C16	2.20	123.34	120.78
3	A	188[B]	COP	C14-C15-C16	2.20	123.34	120.78
3	A	188[A]	COP	C14-C15-C16	2.20	123.34	120.78
2	A	187	NDP	N3A-C2A-N1A	2.19	132.09	128.68
3	A	188[A]	COP	C33-C31-N30	2.11	121.50	117.36
2	A	187	NDP	O4D-C4D-C3D	-2.10	100.95	105.11
3	A	188[C]	COP	C10-C5-N4	-2.05	118.39	121.71
3	A	188[B]	COP	C10-C5-N4	-2.05	118.39	121.71
3	A	188[A]	COP	C10-C5-N4	-2.05	118.39	121.71
3	A	188[B]	COP	C37-C38-C39	-2.04	117.16	120.20
3	A	188[B]	COP	C33-C31-N30	2.03	121.35	117.36
3	A	188[C]	COP	C37-C38-C39	-2.02	117.19	120.20

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	188[C]	COP	C24-C21-C27-C28
3	A	188[C]	COP	N20-C21-C27-C28
3	A	188[C]	COP	C24-C21-N20-C19
3	A	188[C]	COP	C33-C31-N30-C29
3	A	188[B]	COP	C24-C21-C27-C28
3	A	188[B]	COP	C24-C21-N20-C19
3	A	188[B]	COP	C33-C31-N30-C29
3	A	188[A]	COP	C24-C21-C27-C28
3	A	188[A]	COP	N20-C21-C27-C28
3	A	188[A]	COP	C24-C21-N20-C19
3	A	188[A]	COP	C33-C31-N30-C29
3	A	188[B]	COP	O32-C31-N30-C29
3	A	188[A]	COP	O32-C31-N30-C29
3	A	188[C]	COP	C28-C29-N30-C31
3	A	188[B]	COP	C28-C29-N30-C31
3	A	188[C]	COP	O32-C31-N30-C29
3	A	188[B]	COP	C27-C28-C29-N30
3	A	188[B]	COP	N20-C21-C27-C28

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Mol	Chain	Res	Type	Atoms
3	A	188[C]	COP	C27-C28-C29-N30
2	A	187	NDP	O4B-C4B-C5B-O5B
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	188[A]	COP	C27-C28-C29-N30
2	A	187	NDP	C1B-C2B-O2B-P2B
2	A	187	NDP	C3B-C2B-O2B-P2B
3	A	188[C]	COP	C21-C27-C28-C29
3	A	188[C]	COP	C27-C21-N20-C19
3	A	188[B]	COP	C27-C21-N20-C19
3	A	188[A]	COP	C27-C21-N20-C19
3	A	188[C]	COP	C16-C19-N20-C21
3	A	188[B]	COP	C16-C19-N20-C21
3	A	188[A]	COP	C16-C19-N20-C21
3	A	188[B]	COP	C21-C27-C28-C29
3	A	188[C]	COP	O19-C19-N20-C21
3	A	188[B]	COP	O19-C19-N20-C21
3	A	188[A]	COP	O19-C19-N20-C21
2	A	187	NDP	C3B-C4B-C5B-O5B
2	A	187	NDP	O4D-C1D-N1N-C2N
3	A	188[A]	COP	O32-C31-C33-C34
2	A	187	NDP	C2D-C1D-N1N-C2N
3	A	188[A]	COP	N30-C31-C33-C34
2	A	187	NDP	O4D-C1D-N1N-C6N
2	A	187	NDP	C5B-O5B-PA-O3
2	A	187	NDP	C2B-O2B-P2B-O3X
2	A	187	NDP	PN-O3-PA-O2A
2	A	187	NDP	C2N-C3N-C7N-N7N

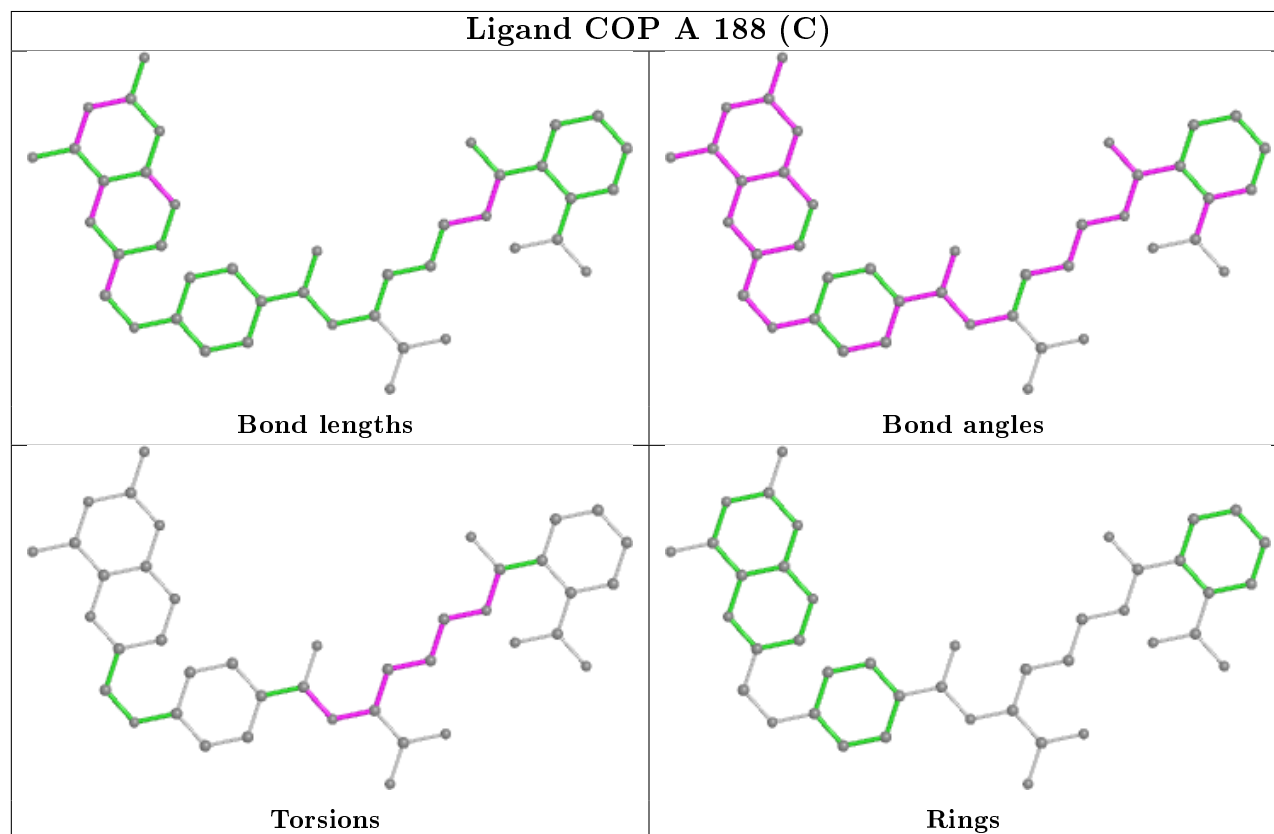
There are no ring outliers.

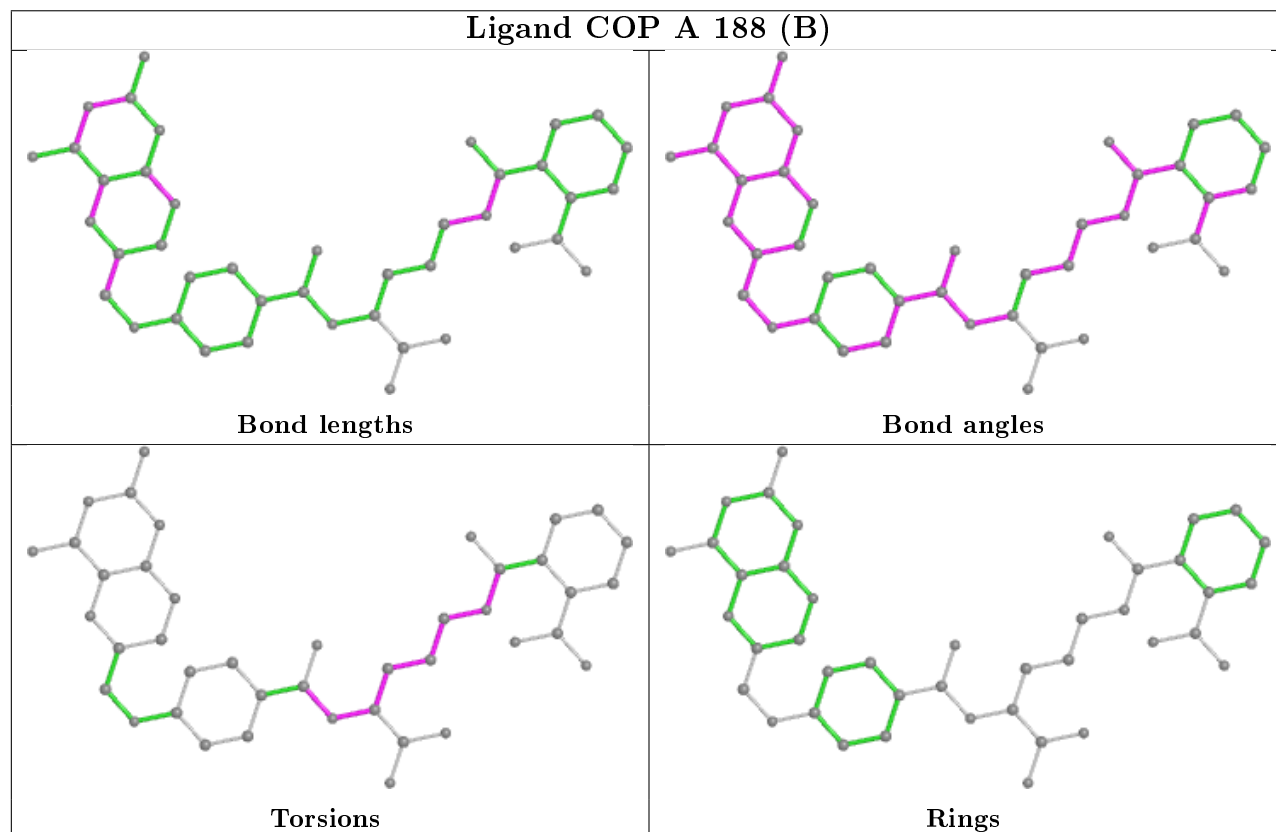
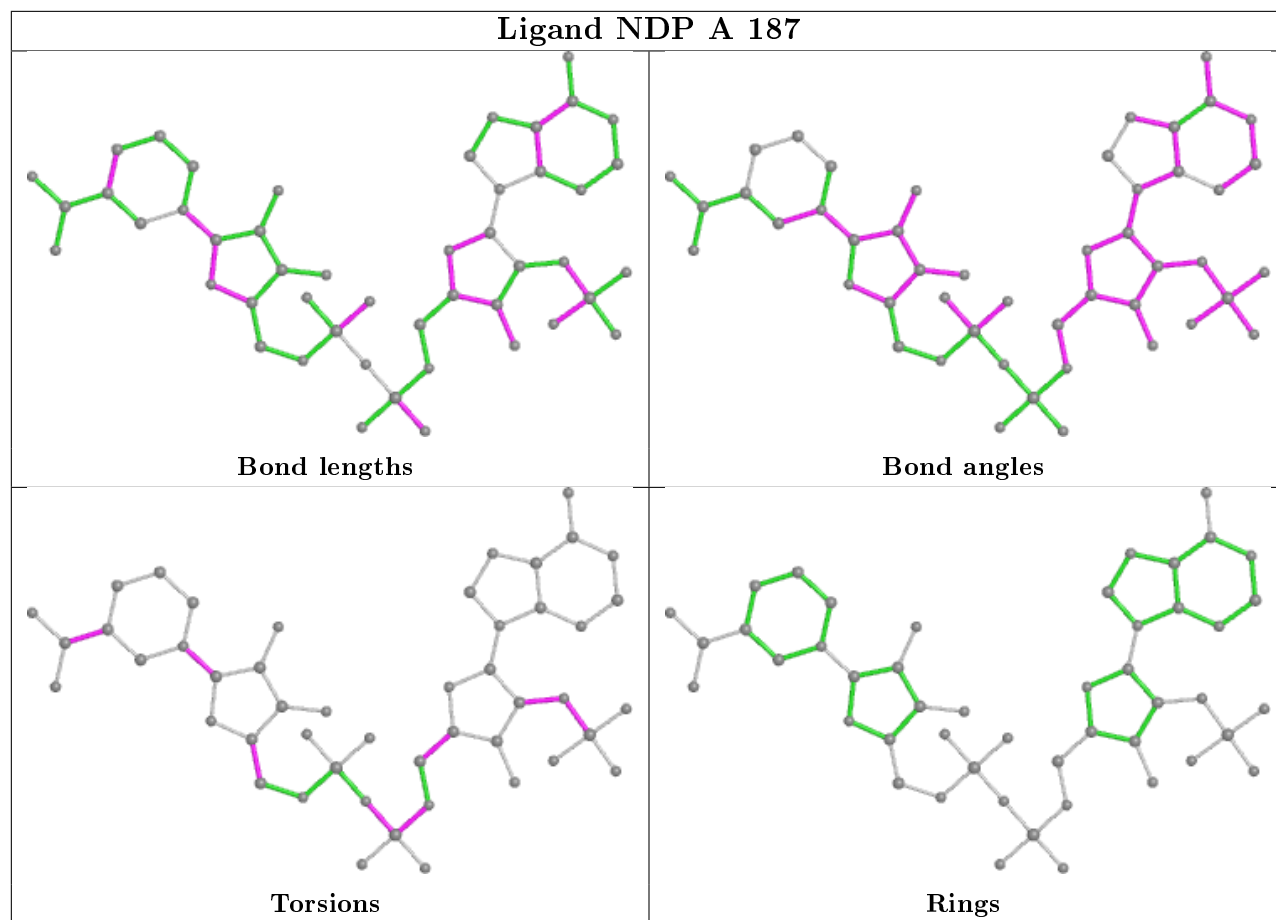
3 monomers are involved in 24 short contacts:

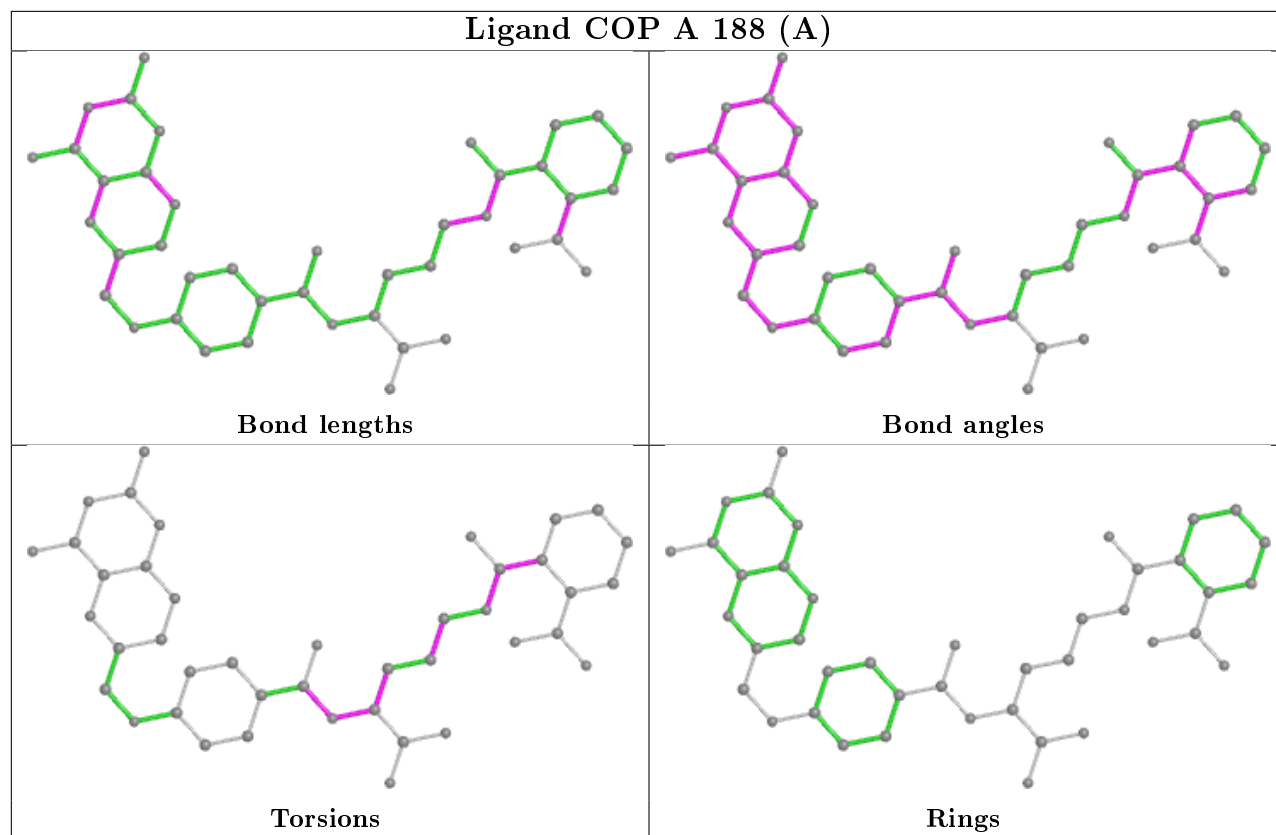
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	16	0
3	A	188[B]	COP	2	0
3	A	188[A]	COP	6	0

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.