



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 1OHK / pdb_00001ohk
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 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

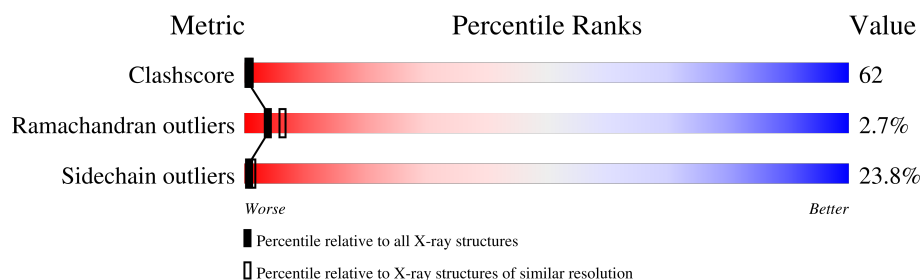
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	186	

2 Entry composition [i](#)

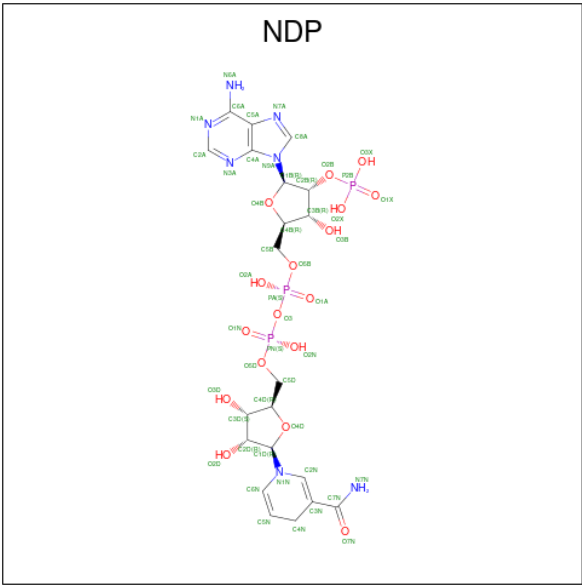
There are 4 unique types of molecules in this entry. The entry contains 1638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

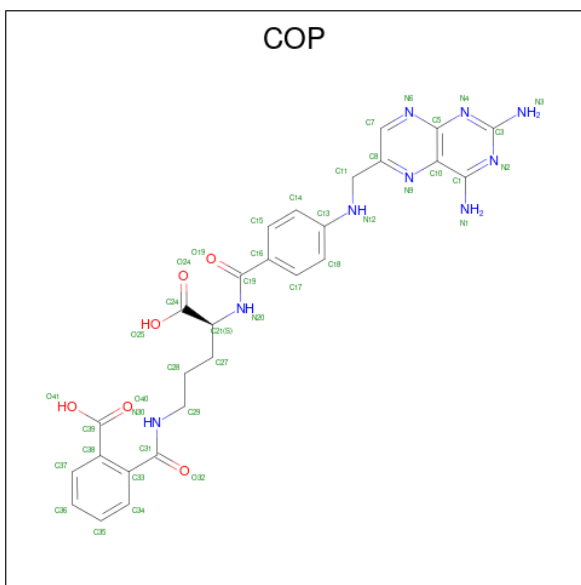
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1502	963	253	279	7	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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 (CCD ID: COP) (formula: C₂₇H₂₇N₉O₆).



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

- Molecule 4 is water.

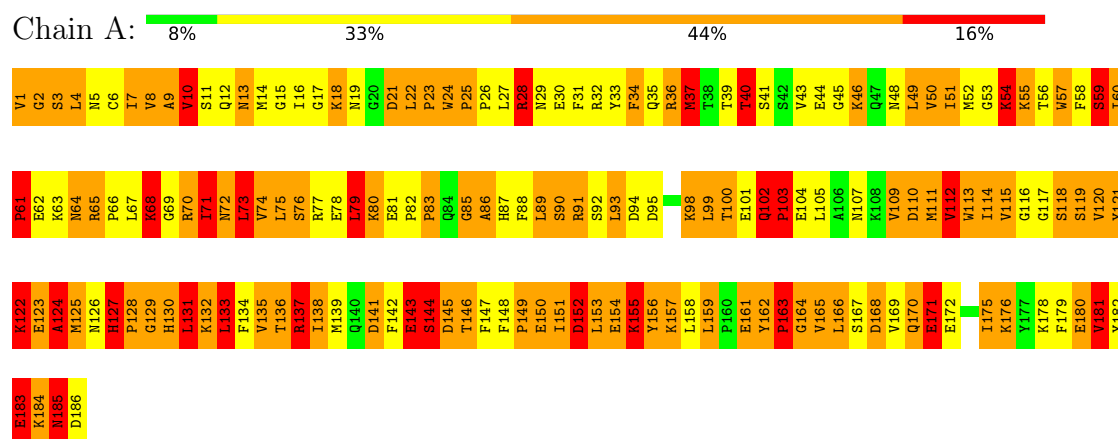
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0

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: 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	36.90Å 69.19Å 69.95Å 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 (i)

5.1 Standard geometry (i)

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

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	1.51	10/1537 (0.7%)	3.62	298/2073 (14.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	VAL	N-CA	-9.10	1.35	1.46
1	A	111	MET	C-N	-8.60	1.22	1.33
1	A	103	PRO	C-N	-7.03	1.23	1.33
1	A	111	MET	CA-C	-7.02	1.44	1.52
1	A	2	GLY	N-CA	6.94	1.51	1.44
1	A	3	SER	N-CA	6.89	1.53	1.45
1	A	110	ASP	CA-C	6.63	1.57	1.52
1	A	60	ILE	CA-CB	5.42	1.61	1.54
1	A	136	THR	CA-CB	5.26	1.59	1.52
1	A	48	ASN	N-CA	5.13	1.51	1.45

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLU	O-C-N	21.02	147.78	123.19
1	A	64	ASN	OD1-CG-ND2	20.98	143.58	122.60
1	A	164	GLY	CA-C-N	-17.81	98.24	122.99
1	A	164	GLY	C-N-CA	-17.81	98.24	122.99
1	A	130	HIS	CA-CB-CG	-16.16	97.64	113.80
1	A	44	GLU	CA-C-O	-15.21	103.91	120.80
1	A	58	PHE	CA-C-N	14.94	141.50	120.29
1	A	58	PHE	C-N-CA	14.94	141.50	120.29
1	A	62	GLU	CA-C-N	14.75	140.46	120.54
1	A	62	GLU	C-N-CA	14.75	140.46	120.54
1	A	36	ARG	CD-NE-CZ	13.69	143.57	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	CA-C-O	-13.29	106.47	120.55
1	A	76	SER	O-C-N	13.12	138.17	123.48
1	A	164	GLY	O-C-N	12.79	137.29	122.33
1	A	24	TRP	O-C-N	12.38	129.63	121.71
1	A	8	VAL	CA-C-O	-12.35	108.18	121.28
1	A	186	ASP	CA-CB-CG	12.26	124.86	112.60
1	A	44	GLU	CA-C-N	-12.25	106.54	123.08
1	A	44	GLU	C-N-CA	-12.25	106.54	123.08
1	A	141	ASP	CA-CB-CG	11.71	124.31	112.60
1	A	10	VAL	CB-CA-C	11.52	128.56	110.82
1	A	30	GLU	CA-C-N	11.23	135.71	120.44
1	A	30	GLU	C-N-CA	11.23	135.71	120.44
1	A	48	ASN	CA-CB-CG	11.14	123.74	112.60
1	A	121	TYR	N-CA-C	-10.60	99.81	111.36
1	A	19	ASN	CA-CB-CG	10.59	123.19	112.60
1	A	91	ARG	CD-NE-CZ	-10.59	109.58	124.40
1	A	54	LYS	CB-CG-CD	10.58	135.63	111.30
1	A	172	GLU	O-C-N	10.45	136.81	123.23
1	A	168	ASP	CA-CB-CG	-10.30	102.30	112.60
1	A	88	PHE	O-C-N	10.16	134.83	123.25
1	A	161	GLU	CA-C-O	-10.11	108.47	120.60
1	A	123	GLU	CA-CB-CG	9.99	134.07	114.10
1	A	132	LYS	CA-C-O	9.95	131.10	120.36
1	A	185	ASN	CA-CB-CG	-9.93	102.67	112.60
1	A	170	GLN	OE1-CD-NE2	9.89	132.49	122.60
1	A	26	PRO	CB-CA-C	9.84	123.36	111.46
1	A	89	LEU	O-C-N	9.75	135.16	123.27
1	A	135	VAL	N-CA-C	9.68	121.93	107.51
1	A	143	GLU	CA-CB-CG	9.66	133.41	114.10
1	A	59	SER	CA-C-O	9.58	130.58	120.42
1	A	73	LEU	CB-CA-C	9.54	126.97	109.70
1	A	79	LEU	CA-C-O	-9.48	112.06	122.01
1	A	83	PRO	CA-C-O	-9.47	110.65	121.36
1	A	60	ILE	CB-CG1-CD1	9.39	133.52	113.80
1	A	85	GLY	CA-C-N	9.39	134.93	121.50
1	A	85	GLY	C-N-CA	9.39	134.93	121.50
1	A	62	GLU	CA-C-O	9.29	130.67	120.63
1	A	59	SER	CB-CA-C	-9.25	95.13	110.85
1	A	154	GLU	N-CA-C	-9.18	101.60	113.17
1	A	145	ASP	CA-CB-CG	9.17	121.77	112.60
1	A	127	HIS	CA-CB-CG	9.11	122.91	113.80
1	A	51	ILE	O-C-N	9.06	133.09	123.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLY	CA-C-N	9.02	132.53	121.71
1	A	15	GLY	C-N-CA	9.02	132.53	121.71
1	A	1	VAL	CA-C-N	-8.98	114.28	121.82
1	A	1	VAL	C-N-CA	-8.98	114.28	121.82
1	A	29	ASN	CA-CB-CG	-8.89	103.71	112.60
1	A	123	GLU	CB-CG-CD	8.79	127.55	112.60
1	A	152	ASP	CA-C-O	-8.70	108.07	120.51
1	A	49	LEU	CA-C-N	8.69	134.65	123.10
1	A	49	LEU	C-N-CA	8.69	134.65	123.10
1	A	70	ARG	CA-C-O	-8.67	109.88	120.54
1	A	62	GLU	O-C-N	-8.60	113.00	122.12
1	A	172	GLU	CA-C-O	-8.57	111.44	120.70
1	A	18	LYS	CA-C-O	-8.55	108.28	120.51
1	A	100	THR	CA-C-O	8.53	130.02	120.90
1	A	64	ASN	CB-CG-OD1	-8.45	103.91	120.80
1	A	175	ILE	CA-C-O	-8.43	112.48	121.93
1	A	72	ASN	CA-C-O	-8.43	110.99	120.43
1	A	123	GLU	CA-C-N	8.30	137.40	121.54
1	A	123	GLU	C-N-CA	8.30	137.40	121.54
1	A	124	ALA	CA-C-N	8.29	133.26	120.82
1	A	124	ALA	C-N-CA	8.29	133.26	120.82
1	A	43	VAL	CB-CA-C	8.29	124.83	111.32
1	A	22	LEU	CA-C-O	8.26	126.43	119.66
1	A	137	ARG	CD-NE-CZ	8.22	135.90	124.40
1	A	28	ARG	NE-CZ-NH2	-8.15	111.87	119.20
1	A	144	SER	CA-C-N	8.13	136.34	122.36
1	A	144	SER	C-N-CA	8.13	136.34	122.36
1	A	94	ASP	CA-C-O	-8.10	112.36	120.70
1	A	109	VAL	N-CA-CB	-8.08	101.19	110.49
1	A	176	LYS	CA-CB-CG	8.05	130.20	114.10
1	A	76	SER	CA-C-O	-8.03	112.06	120.89
1	A	120	VAL	N-CA-C	-8.01	103.05	110.82
1	A	125	MET	CA-C-O	8.00	129.88	120.92
1	A	153	LEU	N-CA-C	8.00	122.41	113.21
1	A	78	GLU	N-CA-C	7.99	123.95	114.04
1	A	138	ILE	N-CA-C	-7.98	96.73	108.54
1	A	183	GLU	O-C-N	7.96	132.99	122.96
1	A	48	ASN	N-CA-C	-7.90	98.77	110.46
1	A	165	VAL	CB-CA-C	7.90	121.87	110.33
1	A	57	TRP	CA-C-N	7.72	131.40	120.28
1	A	57	TRP	C-N-CA	7.72	131.40	120.28
1	A	180	GLU	CA-C-O	-7.71	111.79	120.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	SER	N-CA-C	7.71	119.37	110.97
1	A	95	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	181	VAL	CB-CA-C	7.65	122.03	110.62
1	A	14	MET	CA-C-N	7.62	128.94	121.62
1	A	14	MET	C-N-CA	7.62	128.94	121.62
1	A	7	ILE	CB-CA-C	7.61	120.70	110.42
1	A	54	LYS	CG-CD-CE	7.58	128.73	111.30
1	A	2	GLY	CA-C-O	-7.56	113.48	121.57
1	A	116	GLY	CA-C-N	7.45	135.10	121.70
1	A	116	GLY	C-N-CA	7.45	135.10	121.70
1	A	138	ILE	CB-CA-C	7.44	119.79	111.08
1	A	162	TYR	CA-C-O	7.44	128.87	120.46
1	A	126	ASN	CA-CB-CG	-7.43	105.17	112.60
1	A	80	LYS	O-C-N	7.42	132.04	122.10
1	A	11	SER	N-CA-C	-7.36	98.32	110.17
1	A	169	VAL	CA-C-N	7.33	133.57	122.65
1	A	169	VAL	C-N-CA	7.33	133.57	122.65
1	A	69	GLY	N-CA-C	7.30	126.61	114.48
1	A	158	LEU	N-CA-CB	7.19	122.26	110.39
1	A	149	PRO	CB-CA-C	7.17	120.14	111.46
1	A	51	ILE	CA-C-O	-7.16	112.91	120.57
1	A	116	GLY	O-C-N	-7.15	115.60	123.10
1	A	72	ASN	CA-CB-CG	-7.14	105.46	112.60
1	A	167	SER	CA-C-O	-7.11	111.22	119.05
1	A	74	VAL	N-CA-C	7.09	118.10	108.17
1	A	121	TYR	CA-C-O	-7.07	112.93	120.42
1	A	137	ARG	NE-CZ-NH2	-7.07	112.84	119.20
1	A	2	GLY	N-CA-C	-7.07	100.82	111.14
1	A	156	TYR	O-C-N	7.06	132.57	123.11
1	A	18	LYS	CB-CA-C	-7.04	96.42	110.42
1	A	85	GLY	CA-C-O	7.04	126.80	119.27
1	A	44	GLU	CB-CA-C	-7.01	97.70	109.48
1	A	103	PRO	N-CA-C	7.00	126.88	112.47
1	A	28	ARG	N-CA-C	6.99	118.90	111.28
1	A	68	LYS	O-C-N	-6.92	114.37	122.95
1	A	98	LYS	N-CA-CB	6.91	120.28	110.12
1	A	28	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	A	8	VAL	CA-CB-CG1	6.88	122.09	110.40
1	A	26	PRO	CA-C-N	6.87	134.02	123.23
1	A	26	PRO	C-N-CA	6.87	134.02	123.23
1	A	88	PHE	N-CA-CB	6.87	123.12	111.66
1	A	58	PHE	N-CA-C	6.78	119.50	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	VAL	CA-C-N	6.77	133.77	122.87
1	A	181	VAL	C-N-CA	6.77	133.77	122.87
1	A	145	ASP	OD1-CG-OD2	-6.76	106.68	122.90
1	A	50	VAL	O-C-N	-6.75	116.05	123.20
1	A	71	ILE	N-CA-CB	6.74	117.88	110.53
1	A	162	TYR	N-CA-CB	6.74	122.59	110.72
1	A	150	GLU	CA-C-N	6.73	131.52	122.90
1	A	150	GLU	C-N-CA	6.73	131.52	122.90
1	A	68	LYS	CG-CD-CE	6.70	126.71	111.30
1	A	49	LEU	N-CA-C	-6.68	98.08	109.24
1	A	114	ILE	O-C-N	6.67	131.62	122.88
1	A	120	VAL	N-CA-CB	6.67	120.13	110.52
1	A	134	PHE	CA-CB-CG	6.64	120.44	113.80
1	A	126	ASN	CB-CA-C	6.62	123.60	110.42
1	A	113	TRP	CA-C-O	6.58	127.69	120.71
1	A	137	ARG	CA-C-O	6.57	127.76	120.92
1	A	70	ARG	N-CA-CB	-6.55	99.28	111.13
1	A	49	LEU	CB-CA-C	6.54	122.30	109.35
1	A	81	GLU	CA-CB-CG	6.53	127.17	114.10
1	A	69	GLY	O-C-N	-6.53	115.36	122.41
1	A	129	GLY	CA-C-O	6.50	128.46	121.83
1	A	2	GLY	CA-C-N	-6.50	111.43	122.67
1	A	2	GLY	C-N-CA	-6.50	111.43	122.67
1	A	68	LYS	CB-CG-CD	6.49	126.23	111.30
1	A	76	SER	CA-CB-OG	-6.47	98.16	111.10
1	A	86	ALA	CA-C-N	6.45	131.64	120.68
1	A	86	ALA	C-N-CA	6.45	131.64	120.68
1	A	103	PRO	CB-CA-C	6.42	122.16	111.56
1	A	123	GLU	N-CA-CB	6.39	119.62	110.16
1	A	71	ILE	N-CA-C	-6.37	100.48	108.89
1	A	146	THR	CB-CA-C	6.33	120.78	109.38
1	A	161	GLU	O-C-N	6.31	130.96	123.33
1	A	80	LYS	N-CA-CB	6.28	121.18	110.51
1	A	93	LEU	CA-C-O	-6.25	113.03	120.10
1	A	122	LYS	CA-C-O	-6.23	113.95	120.55
1	A	185	ASN	N-CA-CB	6.19	121.61	111.58
1	A	102	GLN	O-C-N	6.17	128.41	121.32
1	A	10	VAL	CA-CB-CG1	6.11	120.79	110.40
1	A	130	HIS	O-C-N	6.11	130.78	122.48
1	A	80	LYS	N-CA-C	-6.10	105.74	113.43
1	A	171	GLU	CA-C-O	6.10	126.92	120.33
1	A	115	VAL	N-CA-CB	-6.07	98.89	111.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	PHE	CB-CA-C	6.07	121.50	111.31
1	A	68	LYS	CA-C-N	6.06	131.72	120.87
1	A	68	LYS	C-N-CA	6.06	131.72	120.87
1	A	157	LYS	CA-C-O	-6.04	114.09	120.80
1	A	118	SER	CA-C-O	-6.04	114.66	121.00
1	A	64	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	102	GLN	CG-CD-NE2	-6.03	107.36	116.40
1	A	25	PRO	N-CA-C	-6.02	103.36	110.70
1	A	172	GLU	CB-CG-CD	-6.00	102.40	112.60
1	A	185	ASN	O-C-N	6.00	133.35	122.44
1	A	25	PRO	N-CA-CB	5.98	108.88	103.08
1	A	107	ASN	O-C-N	5.97	129.61	122.27
1	A	141	ASP	O-C-N	5.96	129.95	123.10
1	A	93	LEU	O-C-N	5.95	129.19	122.22
1	A	34	PHE	N-CA-C	-5.95	104.71	111.07
1	A	72	ASN	CA-C-N	-5.94	113.59	122.74
1	A	72	ASN	C-N-CA	-5.94	113.59	122.74
1	A	131	LEU	O-C-N	5.94	130.37	123.30
1	A	167	SER	N-CA-CB	5.94	119.38	110.65
1	A	19	ASN	CB-CG-ND2	-5.94	107.50	116.40
1	A	37	MET	CA-C-O	5.92	128.43	120.13
1	A	150	GLU	CG-CD-OE1	-5.91	104.80	118.40
1	A	83	PRO	O-C-N	5.90	130.39	122.89
1	A	61	PRO	N-CA-CB	-5.85	97.11	103.25
1	A	41	SER	CA-C-O	5.85	127.39	120.66
1	A	22	LEU	CA-CB-CG	5.85	136.77	116.30
1	A	136	THR	CA-C-N	5.78	130.90	122.41
1	A	136	THR	C-N-CA	5.78	130.90	122.41
1	A	51	ILE	N-CA-CB	5.75	117.89	110.99
1	A	136	THR	N-CA-CB	5.72	118.87	110.35
1	A	67	LEU	CA-C-O	-5.72	115.23	120.95
1	A	33	TYR	CA-C-O	5.70	126.58	120.70
1	A	136	THR	CA-CB-OG1	5.69	118.14	109.60
1	A	18	LYS	CA-CB-CG	-5.66	102.77	114.10
1	A	94	ASP	N-CA-C	-5.66	105.03	111.14
1	A	98	LYS	O-C-N	5.62	128.08	122.12
1	A	170	GLN	O-C-N	-5.62	116.61	123.19
1	A	69	GLY	CA-C-N	5.60	131.80	121.94
1	A	69	GLY	C-N-CA	5.60	131.80	121.94
1	A	144	SER	CA-C-O	-5.58	115.09	121.40
1	A	119	SER	CB-CA-C	5.58	121.65	109.99
1	A	172	GLU	CG-CD-OE2	-5.58	105.58	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	CA-C-O	5.57	128.26	122.24
1	A	55	LYS	N-CA-C	5.57	119.55	112.87
1	A	34	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	155	LYS	CG-CD-CE	5.56	124.08	111.30
1	A	159	LEU	CA-C-O	-5.55	114.25	119.80
1	A	50	VAL	CA-C-N	5.53	129.90	122.93
1	A	50	VAL	C-N-CA	5.53	129.90	122.93
1	A	95	ASP	N-CA-CB	5.53	118.82	110.30
1	A	4	LEU	CA-C-N	-5.52	114.92	122.93
1	A	4	LEU	C-N-CA	-5.52	114.92	122.93
1	A	23	PRO	CA-C-O	-5.52	110.55	120.60
1	A	133	LEU	O-C-N	5.50	129.60	123.05
1	A	71	ILE	CB-CA-C	-5.49	104.01	111.15
1	A	6	CYS	N-CA-CB	5.48	120.37	110.83
1	A	4	LEU	CB-CA-C	5.48	121.32	110.42
1	A	35	GLN	CA-C-O	-5.44	115.11	120.82
1	A	13	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	147	PHE	N-CA-C	5.43	117.67	109.41
1	A	39	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	19	ASN	N-CA-CB	5.43	120.54	111.53
1	A	24	TRP	CA-C-O	-5.42	115.51	120.50
1	A	147	PHE	O-C-N	5.42	130.37	122.94
1	A	146	THR	CA-C-O	5.42	126.45	120.71
1	A	70	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	102	GLN	N-CA-CB	5.41	119.99	110.37
1	A	86	ALA	N-CA-CB	5.39	118.30	109.95
1	A	110	ASP	CB-CA-C	5.37	119.38	111.65
1	A	126	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	A	152	ASP	N-CA-CB	5.35	119.53	110.49
1	A	113	TRP	O-C-N	-5.35	116.42	123.21
1	A	121	TYR	N-CA-CB	5.33	118.05	110.16
1	A	50	VAL	N-CA-CB	-5.33	104.71	111.64
1	A	135	VAL	CA-CB-CG2	5.31	119.43	110.40
1	A	137	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	A	36	ARG	N-CA-C	5.29	122.06	110.80
1	A	7	ILE	CA-CB-CG2	5.28	119.48	110.50
1	A	147	PHE	CA-C-O	-5.28	115.45	121.58
1	A	107	ASN	CB-CA-C	-5.28	100.53	110.67
1	A	156	TYR	CA-C-O	-5.27	115.29	121.46
1	A	118	SER	CA-CB-OG	-5.27	100.57	111.10
1	A	37	MET	CG-SD-CE	-5.25	89.35	100.90
1	A	10	VAL	CA-C-O	5.23	128.23	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	PRO	N-CA-C	-5.23	102.90	110.80
1	A	139	MET	CA-C-N	5.21	130.72	121.80
1	A	139	MET	C-N-CA	5.21	130.72	121.80
1	A	12	GLN	CB-CG-CD	-5.21	103.74	112.60
1	A	143	GLU	CB-CG-CD	5.21	121.45	112.60
1	A	75	LEU	O-C-N	5.20	129.40	123.27
1	A	119	SER	N-CA-CB	-5.19	101.94	110.40
1	A	46	LYS	N-CA-C	5.18	117.93	109.59
1	A	102	GLN	CA-C-N	5.18	126.31	119.84
1	A	102	GLN	C-N-CA	5.18	126.31	119.84
1	A	28	ARG	N-CA-CB	5.17	117.72	110.12
1	A	181	VAL	CA-C-O	-5.17	114.62	120.67
1	A	4	LEU	N-CA-C	-5.17	99.78	110.80
1	A	78	GLU	CB-CG-CD	-5.17	103.81	112.60
1	A	81	GLU	N-CA-C	-5.16	102.20	110.10
1	A	143	GLU	N-CA-C	-5.15	102.66	110.28
1	A	65	ARG	CG-CD-NE	5.14	123.32	112.00
1	A	81	GLU	CG-CD-OE1	5.12	130.18	118.40
1	A	2	GLY	O-C-N	5.12	128.06	123.60
1	A	4	LEU	CA-C-O	5.12	127.83	120.51
1	A	58	PHE	CA-C-O	-5.09	114.35	120.10
1	A	120	VAL	CA-CB-CG2	5.08	119.03	110.40
1	A	74	VAL	CA-C-O	5.07	125.85	120.48
1	A	115	VAL	N-CA-C	-5.07	105.61	113.16
1	A	12	GLN	CG-CD-OE1	-5.06	110.68	120.80
1	A	36	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	36	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	A	35	GLN	CA-C-N	5.05	131.18	121.54
1	A	35	GLN	C-N-CA	5.05	131.18	121.54
1	A	144	SER	N-CA-C	-5.04	101.63	109.24
1	A	8	VAL	O-C-N	5.03	128.73	123.00
1	A	81	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	141	ASP	N-CA-CB	5.01	118.80	110.63
1	A	45	GLY	O-C-N	5.01	127.97	122.56
1	A	9	ALA	N-CA-CB	5.00	119.08	110.68

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	1511	196	3
2	A	48	0	25	18	0
3	A	70	0	33	8	0
4	A	18	0	0	1	5
All	All	1638	0	1569	196	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 62.

All (196) 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:HE21	1:A:102:GLN:CA	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:37:MET:HA	1:A:37:MET:HE2	1.29	1.09
1:A:102:GLN:NE2	1:A:102:GLN:HA	1.36	1.06
1:A:36:ARG:HH22	1:A:165:VAL:HG22	1.25	0.99
1:A:100:THR:HG23	1:A:109:VAL:HG11	1.42	0.99
1:A:28:ARG:CD	3:A:188[A]:COP:O40	2.10	0.98
1:A:53:GLY:C	2:A:187:NDP:H52A	1.88	0.98
1:A:49:LEU:HD12	1:A:71:ILE:HB	1.45	0.95
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:H	1:A:166:LEU:CD1	1.85	0.89
1:A:162:TYR:CG	1:A:163:PRO:HD2	2.07	0.89
1:A:166:LEU:HD12	1:A:166:LEU:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:LEU:HB3	1:A:123:GLU:CD	2.04	0.82
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
1:A:93:LEU:HB3	1:A:123:GLU:OE1	1.80	0.81
1:A:102:GLN:CD	1:A:103:PRO:HD2	2.07	0.80
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:73:LEU:C	1:A:73:LEU:HD23	2.08	0.79
1:A:37:MET:HA	1:A:37:MET:CE	2.10	0.78
1:A:184:LYS:O	1:A:184:LYS:HG3	1.83	0.78
1:A:31:PHE:HB3	3:A:188[B]:COP:H291	1.67	0.77
1:A:40:THR:HG22	1:A:40:THR:O	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: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: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:36:ARG:CZ	1:A:164:GLY:O	2.38	0.70
1:A:132:LYS:NZ	1:A:162:TYR:OH	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:N	1:A:168:ASP:OD1	2.16	0.68
1:A:105:LEU:O	1:A:109:VAL:HB	1.94	0.68
1:A:54:LYS:HB3	2:A:187:NDP:H4B	1.77	0.67
1:A:115:VAL:O	1:A:121:TYR:OH	2.11	0.67
1:A:53:GLY:C	2:A:187:NDP:C5B	2.68	0.66
1:A:51:ILE:CG2	1:A:75:LEU:CD1	2.72	0.66
1:A:53:GLY:CA	2:A:187:NDP:H52A	2.25	0.66
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:27:LEU:HD21	1:A:175:ILE:HD13	1.80	0.63
1:A:162:TYR:CG	1:A:163:PRO:CD	2.81	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:17:GLY:HA3	1:A:146:THR:CG2	2.29	0.62
1:A:135:VAL:HG11	1:A:137:ARG:NE	2.14	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:37:MET:HE2	1:A:37:MET:CA	2.11	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:O	1:A:68:LYS:HG3	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: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:13:ASN:ND2	1:A:142:PHE:O	2.35	0.55
1:A:102:GLN:HG3	1:A:103:PRO:HG2	1.89	0.55
1:A:57:TRP:CH2	1:A:86:ALA:HB2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HB3	1:A:184:LYS:HG2	1.89	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
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:49:LEU:HD12	1:A:71:ILE:CB	2.29	0.52
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.35	0.52
1:A:82:PRO:HB3	1:A:89:LEU:HB2	1.91	0.52
1:A:185:ASN:HD22	1:A:185:ASN:C	2.18	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:115:VAL:C	1:A:121:TYR:OH	2.54	0.50
1:A:72:ASN:N	1:A:72:ASN:HD22	2.10	0.50
1:A:119:SER:O	1:A:123:GLU:N	2.45	0.50
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:100:THR:CG2	1:A:109:VAL:HG11	2.29	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:40:THR:O	1:A:40:THR:CG2	2.50	0.48
1:A:117:GLY:HA3	2:A:187:NDP:O2A	2.14	0.48
1:A:168:ASP:OD1	1:A:168:ASP:C	2.53	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:125:MET:C	1:A:127:HIS:H	2.21	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: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:60:ILE:CG2	1:A:65:ARG:HG2	2.46	0.46
1:A:55:LYS:HZ3	1:A:55:LYS:HG2	1.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG21	1:A:148:PHE:CD1	2.51	0.45
1:A:74:VAL:O	1:A:89:LEU:HD12	2.16	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:23:PRO:O	1:A:142:PHE:HB3	2.17	0.45
1:A:114:ILE:CG2	1:A:120:VAL:HG12	2.46	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
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:89:LEU:HD21	1:A:91:ARG:NH2	2.34	0.43
1:A:28:ARG:O	1:A:32:ARG:HG3	2.18	0.43
1:A:51:ILE:HD11	1:A:112:VAL:HG23	1.97	0.43
1:A:152:ASP:OD1	1:A:152:ASP:C	2.61	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:73:LEU:C	1:A:73:LEU:CD2	2.87	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: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:5:ASN:HB3	1:A:113:TRP:CZ3	2.55	0.42
1:A:102:GLN:HA	1:A:103:PRO:HD2	1.71	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:34:PHE:CD1	1:A:34:PHE:C	2.96	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:21:ASP:O	2:A:187:NDP:O3D	2.38	0.41
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.69	0.41
1:A:118:SER:O	1:A:122:LYS:HB2	2.20	0.41
1:A:152:ASP:OD2	1:A:155:LYS:NZ	2.38	0.41
1:A:104:GLU:H	1:A:104:GLU:CD	2.28	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:9:ALA:HA	1:A:136:THR:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD13	1:A:179:PHE:CE2	2.56	0.41
1:A:51:ILE:HG22	1:A:75:LEU:CD1	2.51	0.41
1:A:156:TYR:CD2	1:A:184:LYS:HB3	2.56	0.41
1:A:132:LYS:HA	1:A:182:TYR:O	2.22	0.40
1:A:60:ILE:HG21	1:A:65:ARG:HG2	2.02	0.40
1:A:164:GLY:C	1:A:165:VAL:CG2	2.95	0.40
1:A:182:TYR:HE2	4:A:202:HOH:O	2.04	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

5.3.1 Protein backbone

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%)	4 6

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	163	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	168/168 (100%)	128 (76%)	40 (24%)	1 1

All (40) 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	21	ASP
1	A	28	ARG
1	A	37	MET
1	A	40	THR
1	A	54	LYS
1	A	59	SER
1	A	61	PRO
1	A	68	LYS
1	A	71	ILE
1	A	73	LEU
1	A	79	LEU
1	A	90	SER
1	A	92	SER
1	A	98	LYS
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	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	LEU
1	A	137	ARG
1	A	143	GLU
1	A	144	SER
1	A	150	GLU
1	A	151	ILE
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	183	GLU
1	A	184	LYS
1	A	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	87	HIS
1	A	102	GLN
1	A	140	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	COP	A	188[B]	-	45,45,45	1.90	12 (26%)	60,62,62	4.14	31 (51%)
3	COP	A	188[C]	-	45,45,45	1.90	12 (26%)	60,62,62	3.96	31 (51%)
3	COP	A	188[A]	-	45,45,45	2.14	11 (24%)	60,62,62	3.13	27 (45%)
2	NDP	A	187	-	51,52,52	2.92	17 (33%)	71,80,80	2.37	27 (38%)

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[B]	-	-	10/32/32/32	0/4/4/4
3	COP	A	188[C]	-	-	11/32/32/32	0/4/4/4
3	COP	A	188[A]	-	-	10/32/32/32	0/4/4/4
2	NDP	A	187	-	-	14/34/77/77	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-10.07	1.22	1.45
2	A	187	NDP	P2B-O2B	9.12	1.75	1.59
2	A	187	NDP	O3B-C3B	-7.74	1.23	1.43
3	A	188[A]	COP	C29-N30	6.86	1.61	1.46
3	A	188[A]	COP	C31-N30	5.79	1.46	1.33
3	A	188[A]	COP	O40-C39	5.51	1.38	1.22
2	A	187	NDP	C5A-C6A	5.23	1.55	1.41
3	A	188[C]	COP	C29-N30	5.00	1.57	1.46
3	A	188[B]	COP	C29-N30	4.99	1.57	1.46
3	A	188[A]	COP	C5-N6	-4.98	1.30	1.37
3	A	188[B]	COP	C5-N6	-4.98	1.30	1.37
3	A	188[C]	COP	C5-N6	-4.98	1.30	1.37
3	A	188[C]	COP	C31-N30	4.43	1.43	1.33
3	A	188[B]	COP	C31-N30	4.40	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	C5A-N7A	4.15	1.46	1.39
3	A	188[B]	COP	O41-C39	-3.99	1.18	1.30
2	A	187	NDP	C5A-C4A	-3.98	1.32	1.39
3	A	188[C]	COP	O41-C39	-3.97	1.18	1.30
3	A	188[A]	COP	C3-N2	-3.77	1.28	1.35
3	A	188[B]	COP	C3-N2	-3.77	1.28	1.35
3	A	188[C]	COP	C3-N2	-3.77	1.28	1.35
2	A	187	NDP	C4A-N9A	-3.66	1.30	1.37
3	A	188[C]	COP	O40-C39	3.51	1.32	1.22
3	A	188[B]	COP	O40-C39	3.50	1.32	1.22
2	A	187	NDP	PN-O3	3.28	1.63	1.59
2	A	187	NDP	C3B-C4B	3.13	1.60	1.53
2	A	187	NDP	C1D-N1N	3.07	1.54	1.46
2	A	187	NDP	PN-O1N	-3.01	1.40	1.50
2	A	187	NDP	O4D-C1D	2.98	1.48	1.42
2	A	187	NDP	PA-O2A	-2.65	1.43	1.55
3	A	188[A]	COP	O25-C24	-2.47	1.22	1.30
3	A	188[B]	COP	O25-C24	-2.47	1.22	1.30
3	A	188[C]	COP	O25-C24	-2.47	1.22	1.30
2	A	187	NDP	P2B-O3X	-2.39	1.45	1.54
3	A	188[B]	COP	C35-C36	-2.28	1.33	1.38
3	A	188[C]	COP	C35-C36	-2.25	1.33	1.38
2	A	187	NDP	O4D-C4D	2.24	1.50	1.45
3	A	188[A]	COP	C17-C18	2.21	1.42	1.38
3	A	188[B]	COP	C17-C18	2.21	1.42	1.38
3	A	188[C]	COP	C17-C18	2.21	1.42	1.38
3	A	188[A]	COP	C1-N2	-2.16	1.30	1.33
3	A	188[B]	COP	C1-N2	-2.16	1.30	1.33
3	A	188[C]	COP	C1-N2	-2.16	1.30	1.33
3	A	188[A]	COP	O41-C39	-2.16	1.24	1.30
3	A	188[A]	COP	C11-C8	2.11	1.55	1.50
3	A	188[B]	COP	C11-C8	2.11	1.55	1.50
3	A	188[C]	COP	C11-C8	2.11	1.55	1.50
3	A	188[A]	COP	C10-N9	-2.05	1.33	1.37
3	A	188[B]	COP	C10-N9	-2.05	1.33	1.37
3	A	188[C]	COP	C10-N9	-2.05	1.33	1.37
2	A	187	NDP	C4N-C3N	2.04	1.53	1.50
2	A	187	NDP	P2B-O2X	-2.03	1.47	1.54

All (116) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[B]	COP	O41-C39-O40	-16.19	88.54	123.35
3	A	188[C]	COP	O41-C39-O40	-16.16	88.61	123.35
3	A	188[A]	COP	C21-N20-C19	10.15	145.90	121.56
3	A	188[B]	COP	C21-N20-C19	10.15	145.90	121.56
3	A	188[C]	COP	C21-N20-C19	10.15	145.90	121.56
3	A	188[B]	COP	C27-C28-C29	-9.78	83.84	112.07
3	A	188[B]	COP	O41-C39-C38	9.64	142.69	115.28
3	A	188[C]	COP	O41-C39-C38	9.62	142.63	115.28
3	A	188[A]	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[C]	COP	C1-C10-N9	-7.27	114.72	120.33
3	A	188[A]	COP	N6-C5-N4	7.19	123.61	115.77
3	A	188[B]	COP	N6-C5-N4	7.19	123.61	115.77
3	A	188[C]	COP	N6-C5-N4	7.19	123.61	115.77
3	A	188[A]	COP	C16-C19-N20	6.96	129.95	117.04
3	A	188[B]	COP	C16-C19-N20	6.96	129.95	117.04
3	A	188[C]	COP	C16-C19-N20	6.96	129.95	117.04
3	A	188[A]	COP	C10-C1-N1	-5.59	111.79	120.31
3	A	188[B]	COP	C10-C1-N1	-5.59	111.79	120.31
3	A	188[C]	COP	C10-C1-N1	-5.59	111.79	120.31
2	A	187	NDP	O3B-C3B-C4B	-5.42	95.50	111.08
3	A	188[A]	COP	C27-C21-C24	-5.31	97.76	110.35
3	A	188[B]	COP	C27-C21-C24	-5.31	97.76	110.35
3	A	188[C]	COP	C27-C21-C24	-5.31	97.76	110.35
2	A	187	NDP	C4A-N9A-C8A	5.12	111.11	105.74
3	A	188[A]	COP	O40-C39-C38	-5.09	109.81	121.97
3	A	188[A]	COP	C24-C21-N20	4.83	121.77	110.57
3	A	188[B]	COP	C24-C21-N20	4.83	121.77	110.57
3	A	188[C]	COP	C24-C21-N20	4.83	121.77	110.57
2	A	187	NDP	C4B-O4B-C1B	4.79	120.05	109.47
2	A	187	NDP	C2D-C1D-N1N	4.76	125.02	113.31
2	A	187	NDP	O3X-P2B-O2X	4.72	125.52	107.80
3	A	188[A]	COP	N1-C1-N2	4.50	129.22	117.11
3	A	188[B]	COP	N1-C1-N2	4.50	129.22	117.11
3	A	188[C]	COP	N1-C1-N2	4.50	129.22	117.11
2	A	187	NDP	O4B-C4B-C5B	-4.42	95.18	109.33
2	A	187	NDP	O2B-C2B-C1B	-4.16	95.44	110.05
3	A	188[A]	COP	N4-C3-N2	-4.09	122.01	127.21
3	A	188[B]	COP	N4-C3-N2	-4.09	122.01	127.21
3	A	188[C]	COP	N4-C3-N2	-4.09	122.01	127.21
3	A	188[A]	COP	C5-C10-N9	3.96	126.77	122.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[B]	COP	C5-C10-N9	3.96	126.77	122.35
3	A	188[C]	COP	C5-C10-N9	3.96	126.77	122.35
3	A	188[B]	COP	O32-C31-C33	-3.92	113.85	121.03
2	A	187	NDP	C1D-N1N-C2N	-3.87	114.77	121.14
3	A	188[C]	COP	O32-C31-C33	-3.86	113.95	121.03
3	A	188[C]	COP	C29-N30-C31	3.67	130.41	122.11
3	A	188[B]	COP	C29-N30-C31	3.67	130.41	122.11
2	A	187	NDP	P2B-O2B-C2B	3.64	133.15	123.43
3	A	188[A]	COP	O19-C19-C16	-3.63	113.71	120.90
3	A	188[B]	COP	O19-C19-C16	-3.63	113.71	120.90
3	A	188[C]	COP	O19-C19-C16	-3.63	113.71	120.90
2	A	187	NDP	O2A-PA-O3	3.61	117.03	107.27
3	A	188[A]	COP	N3-C3-N4	3.60	123.40	117.79
3	A	188[B]	COP	N3-C3-N4	3.60	123.40	117.79
3	A	188[C]	COP	N3-C3-N4	3.60	123.40	117.79
2	A	187	NDP	C4A-N9A-C1B	-3.56	118.32	126.63
3	A	188[A]	COP	C11-N12-C13	-3.54	110.52	121.87
3	A	188[B]	COP	C11-N12-C13	-3.54	110.52	121.87
3	A	188[C]	COP	C11-N12-C13	-3.54	110.52	121.87
2	A	187	NDP	O5B-C5B-C4B	-3.52	97.00	108.99
3	A	188[C]	COP	C27-C28-C29	3.49	122.13	112.07
2	A	187	NDP	O2B-P2B-O1X	-3.45	97.05	109.33
3	A	188[A]	COP	C8-N9-C10	-3.34	113.45	118.17
3	A	188[B]	COP	C8-N9-C10	-3.34	113.45	118.17
3	A	188[C]	COP	C8-N9-C10	-3.34	113.45	118.17
2	A	187	NDP	O4B-C1B-C2B	-3.31	100.89	106.59
3	A	188[B]	COP	C28-C29-N30	3.28	121.40	112.20
3	A	188[C]	COP	C28-C29-N30	3.27	121.37	112.20
3	A	188[A]	COP	O19-C19-N20	-3.22	116.34	122.47
3	A	188[B]	COP	O19-C19-N20	-3.22	116.34	122.47
3	A	188[C]	COP	O19-C19-N20	-3.22	116.34	122.47
3	A	188[A]	COP	C34-C33-C38	-3.09	115.79	119.26
2	A	187	NDP	O2B-C2B-C3B	-2.99	100.94	111.68
2	A	187	NDP	O3-PA-O1A	-2.98	101.74	110.70
2	A	187	NDP	O2N-PN-O1N	2.97	126.24	112.44
2	A	187	NDP	N6A-C6A-N1A	2.95	124.94	118.38
2	A	187	NDP	O2D-C2D-C1D	-2.93	100.02	110.10
3	A	188[B]	COP	O40-C39-C38	2.83	128.73	121.97
3	A	188[C]	COP	O40-C39-C38	2.83	128.72	121.97
3	A	188[A]	COP	O41-C39-O40	2.82	129.41	123.35
2	A	187	NDP	C2D-C3D-C4D	-2.81	97.18	102.61
3	A	188[A]	COP	C3-N4-C5	2.71	118.40	115.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[B]	COP	C3-N4-C5	2.71	118.40	115.48
3	A	188[C]	COP	C3-N4-C5	2.71	118.40	115.48
2	A	187	NDP	O2N-PN-O3	-2.64	100.14	107.27
3	A	188[A]	COP	C11-C8-C7	2.62	126.09	121.38
3	A	188[B]	COP	C11-C8-C7	2.62	126.09	121.38
3	A	188[C]	COP	C11-C8-C7	2.62	126.09	121.38
2	A	187	NDP	O3D-C3D-C4D	-2.56	103.74	111.08
3	A	188[A]	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[C]	COP	C3-N2-C1	2.44	123.69	116.72
3	A	188[A]	COP	C37-C38-C33	2.43	121.99	119.26
3	A	188[A]	COP	C14-C15-C16	2.38	123.34	120.80
3	A	188[B]	COP	C14-C15-C16	2.38	123.34	120.80
3	A	188[C]	COP	C14-C15-C16	2.38	123.34	120.80
3	A	188[C]	COP	C37-C38-C33	-2.32	116.65	119.26
2	A	187	NDP	N3A-C2A-N1A	2.32	132.09	128.58
3	A	188[B]	COP	C37-C38-C33	-2.28	116.70	119.26
2	A	187	NDP	C5A-C6A-N6A	-2.27	117.67	123.29
3	A	188[A]	COP	C8-C11-N12	2.19	117.94	113.13
3	A	188[B]	COP	C8-C11-N12	2.19	117.94	113.13
3	A	188[C]	COP	C8-C11-N12	2.19	117.94	113.13
3	A	188[A]	COP	C10-C5-N4	-2.17	118.39	121.74
3	A	188[B]	COP	C10-C5-N4	-2.17	118.39	121.74
3	A	188[C]	COP	C10-C5-N4	-2.17	118.39	121.74
2	A	187	NDP	O2X-P2B-O2B	-2.16	97.41	105.85
3	A	188[A]	COP	C33-C31-N30	2.15	121.50	117.32
2	A	187	NDP	C5A-N7A-C8A	-2.12	100.11	103.45
2	A	187	NDP	O4D-C4D-C3D	-2.12	100.95	105.15
3	A	188[A]	COP	C11-C8-N9	-2.08	112.70	116.64
3	A	188[B]	COP	C11-C8-N9	-2.08	112.70	116.64
3	A	188[C]	COP	C11-C8-N9	-2.08	112.70	116.64
3	A	188[B]	COP	C33-C31-N30	2.07	121.35	117.32
3	A	188[C]	COP	C33-C31-N30	2.02	121.25	117.32

There are no chirality outliers.

All (45) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

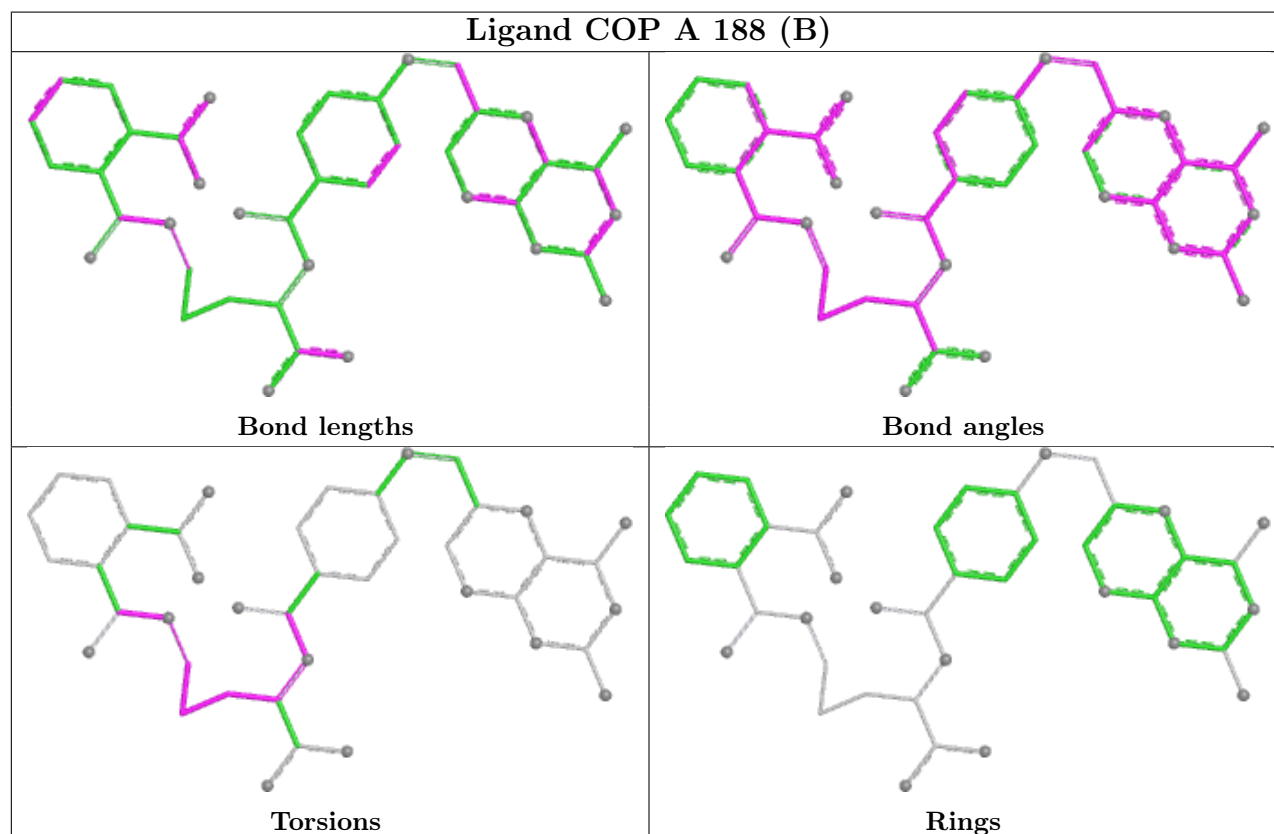
Mol	Chain	Res	Type	Atoms
3	A	188[C]	COP	C33-C31-N30-C29
3	A	188[A]	COP	O32-C31-N30-C29
3	A	188[B]	COP	O32-C31-N30-C29
3	A	188[B]	COP	C28-C29-N30-C31
3	A	188[C]	COP	C28-C29-N30-C31
3	A	188[C]	COP	O32-C31-N30-C29
3	A	188[B]	COP	N20-C21-C27-C28
3	A	188[B]	COP	C27-C28-C29-N30
3	A	188[C]	COP	C27-C28-C29-N30
3	A	188[A]	COP	C27-C28-C29-N30
3	A	188[B]	COP	C24-C21-C27-C28
3	A	188[C]	COP	C24-C21-C27-C28
2	A	187	NDP	O4B-C4B-C5B-O5B
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C1B-C2B-O2B-P2B
2	A	187	NDP	C3B-C2B-O2B-P2B
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	188[C]	COP	C21-C27-C28-C29
3	A	188[A]	COP	C24-C21-C27-C28
2	A	187	NDP	C3B-C4B-C5B-O5B
3	A	188[A]	COP	C24-C21-N20-C19
3	A	188[B]	COP	C24-C21-N20-C19
3	A	188[C]	COP	C24-C21-N20-C19
3	A	188[A]	COP	C16-C19-N20-C21
3	A	188[B]	COP	C16-C19-N20-C21
3	A	188[C]	COP	C16-C19-N20-C21
3	A	188[A]	COP	O19-C19-N20-C21
3	A	188[B]	COP	O19-C19-N20-C21
3	A	188[C]	COP	O19-C19-N20-C21
2	A	187	NDP	C5B-O5B-PA-O3
3	A	188[B]	COP	C21-C27-C28-C29
3	A	188[A]	COP	O32-C31-C33-C34
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2N-C3N-C7N-N7N
3	A	188[A]	COP	N30-C31-C33-C34
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	PN-O3-PA-O2A
2	A	187	NDP	O4D-C1D-N1N-C6N
3	A	188[C]	COP	O32-C31-C33-C34
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N

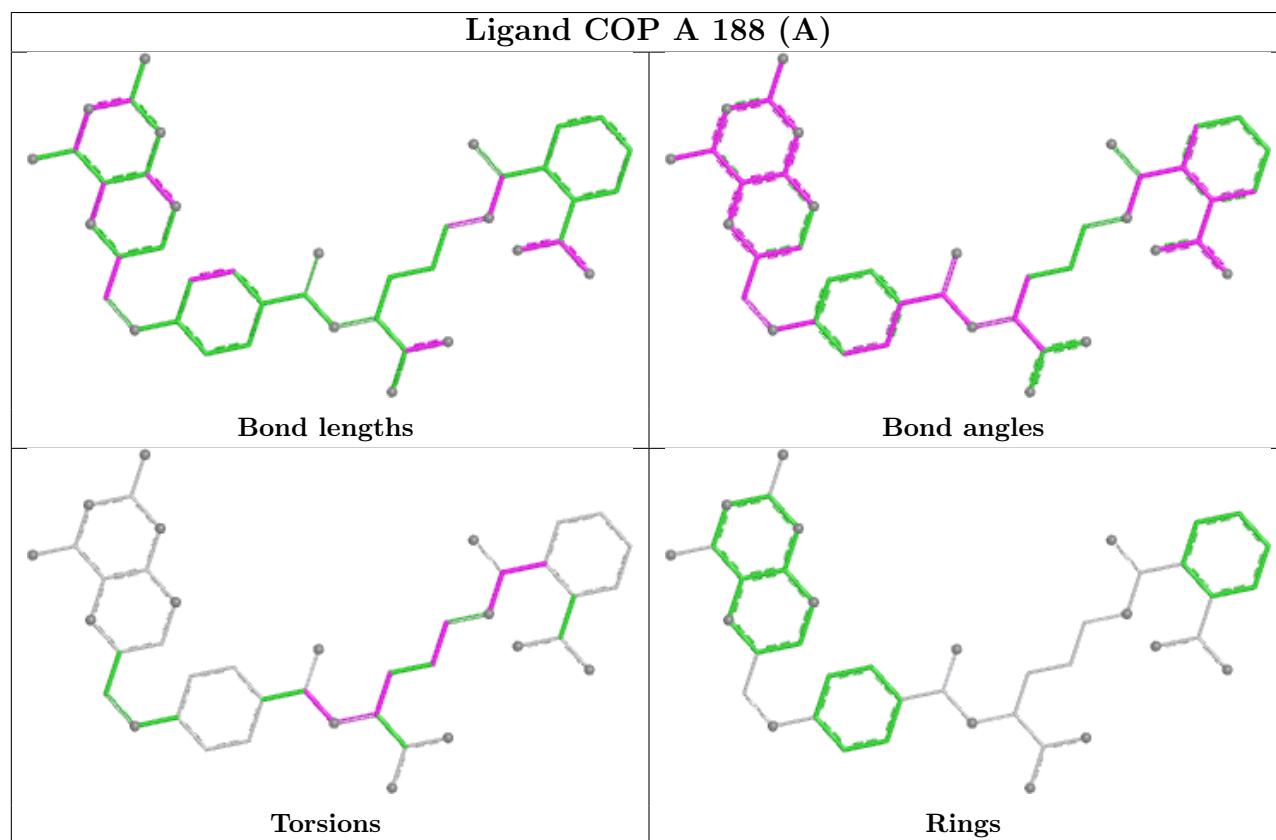
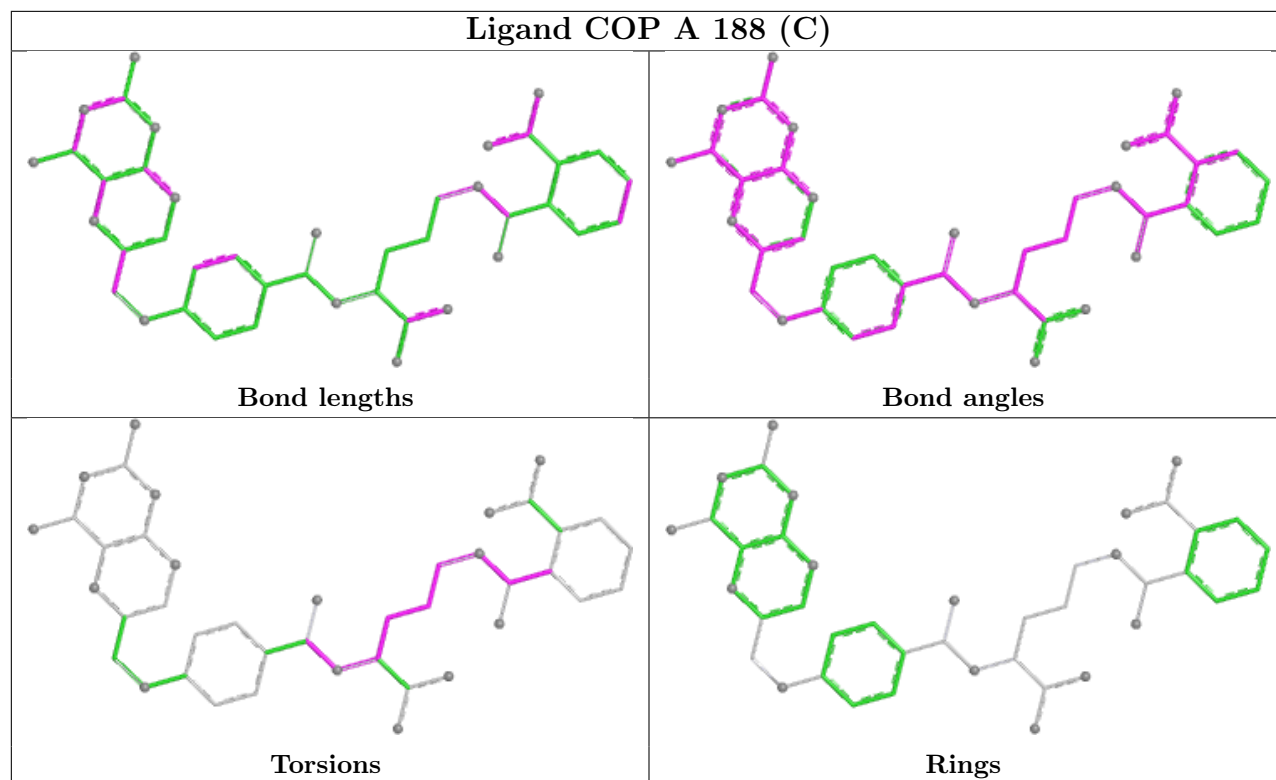
There are no ring outliers.

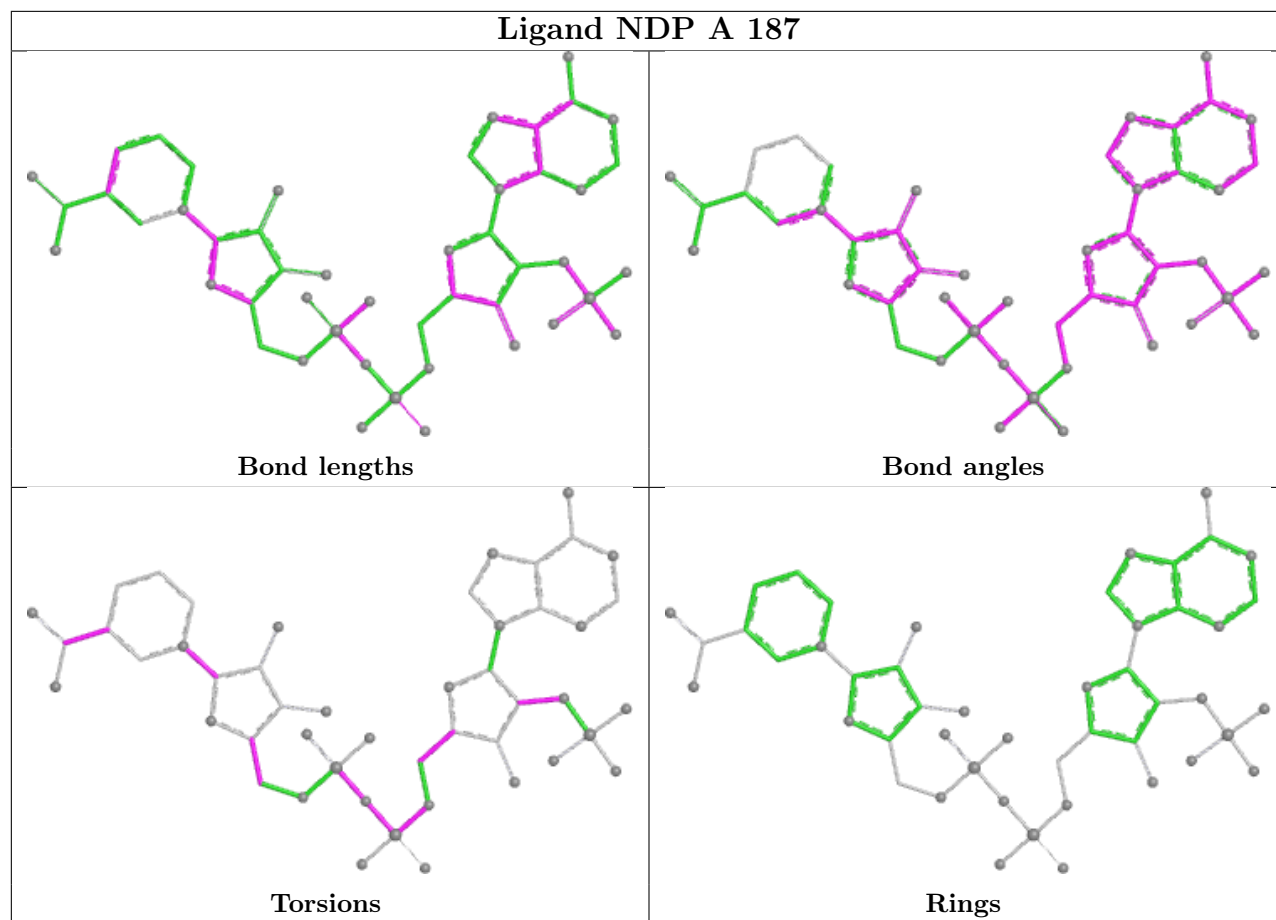
3 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	188[B]	COP	2	0
3	A	188[A]	COP	6	0
2	A	187	NDP	18	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.