



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:00 PM UTC

PDB ID : 2DHF / pdb_00002dhf
Title : CRYSTAL STRUCTURES OF RECOMBINANT HUMAN DIHYDROFOLATE REDUCTASE COMPLEXED WITH FOLATE AND 5-DEAZOFOLATE
Authors : Davies /II, J.F.; Kraut, J.
Deposited on : 1989-10-25
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

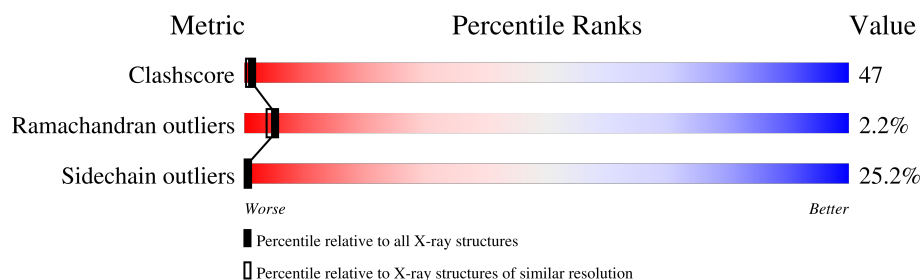
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

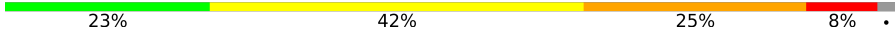
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	
1	B	186	

2 Entry composition [i](#)

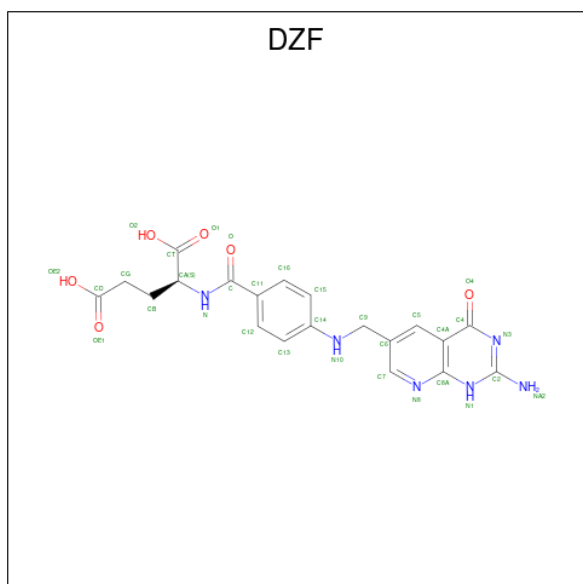
There are 3 unique types of molecules in this entry. The entry contains 3123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	182	Total	C	N	O	S	0	0	0
			1476	949	249	271	7			
1	B	182	Total	C	N	O	S	0	0	0
			1472	947	249	269	7			

- Molecule 2 is 5-DEAZAFOLIC ACID (CCD ID: DZF) (formula: $C_{20}H_{20}N_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	20	6	6		
2	B	1	Total	C	N	O	0	0
			32	20	6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	59	Total 59	O 59	0	0

3 Residue-property plots

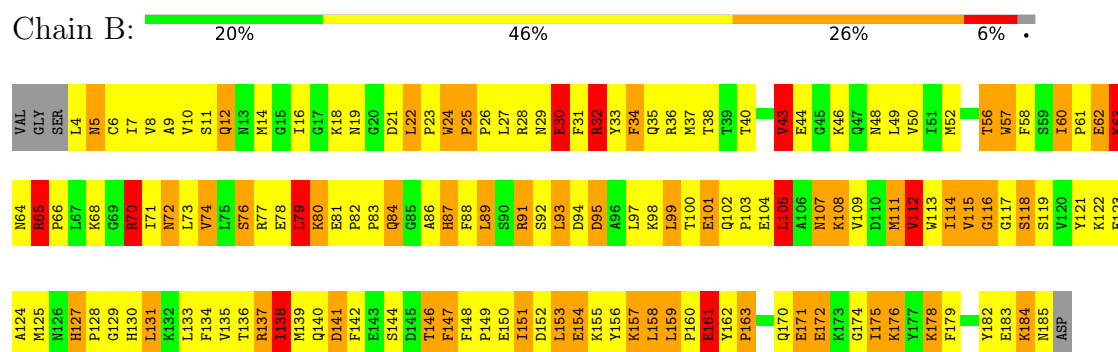
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• 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 1	Depositor
Cell constants a, b, c, α , β , γ	36.10Å 38.50Å 76.80Å 93.90° 91.40° 111.50°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: DZF

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	1.45	6/1511 (0.4%)	2.24	76/2039 (3.7%)
1	B	1.55	12/1507 (0.8%)	2.41	102/2034 (5.0%)
All	All	1.50	18/3018 (0.6%)	2.33	178/4073 (4.4%)

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	1	4
1	B	0	5
All	All	1	9

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	ARG	CD-NE	-8.21	1.34	1.46
1	B	142	PHE	N-CA	6.89	1.54	1.46
1	B	138	ILE	N-CA	6.44	1.53	1.46
1	B	9	ALA	CA-C	6.35	1.60	1.52
1	B	93	LEU	N-CA	5.85	1.53	1.46
1	B	109	VAL	N-CA	-5.70	1.39	1.46
1	B	151	ILE	CA-CB	5.54	1.60	1.53
1	B	116	GLY	N-CA	5.49	1.50	1.45
1	A	37	MET	C-O	5.45	1.30	1.24
1	B	6	CYS	CA-C	5.44	1.59	1.52
1	B	30	GLU	CA-CB	-5.36	1.44	1.53
1	B	176	LYS	N-CA	5.29	1.52	1.46
1	A	151	ILE	CA-C	5.21	1.58	1.53
1	A	11	SER	N-CA	5.16	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	LEU	N-CA	5.14	1.52	1.46
1	A	38	THR	CA-CB	5.10	1.62	1.53
1	B	92	SER	N-CA	5.08	1.52	1.46
1	A	65	ARG	CA-C	5.06	1.58	1.52

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ARG	CD-NE-CZ	17.07	148.30	124.40
1	B	29	ASN	CA-CB-CG	13.42	126.02	112.60
1	B	141	ASP	CA-CB-CG	10.46	123.06	112.60
1	A	95	ASP	CA-CB-CG	10.42	123.02	112.60
1	A	31	PHE	CA-CB-CG	-9.14	104.66	113.80
1	B	30	GLU	CA-CB-CG	9.06	132.22	114.10
1	B	65	ARG	O-C-N	9.06	129.45	121.39
1	B	63	LYS	CA-C-O	8.85	128.20	119.08
1	B	129	GLY	CA-C-N	8.56	134.75	122.85
1	B	129	GLY	C-N-CA	8.56	134.75	122.85
1	B	174	GLY	CA-C-O	8.56	128.52	119.02
1	A	102	GLN	N-CA-C	-8.49	99.04	109.83
1	B	87	HIS	CA-CB-CG	-8.21	105.59	113.80
1	A	64	ASN	OD1-CG-ND2	8.17	130.77	122.60
1	A	65	ARG	NE-CZ-NH2	-8.09	111.92	119.20
1	B	71	ILE	N-CA-C	-7.98	97.08	108.58
1	B	185	ASN	OD1-CG-ND2	7.92	130.52	122.60
1	B	144	SER	N-CA-CB	-7.84	98.56	111.66
1	B	99	LEU	CA-C-O	7.79	128.93	120.20
1	B	64	ASN	CA-CB-CG	7.64	120.24	112.60
1	B	93	LEU	CB-CA-C	7.60	123.40	110.79
1	A	67	LEU	CB-CA-C	7.46	122.85	109.64
1	B	22	LEU	O-C-N	7.42	129.69	121.53
1	B	64	ASN	N-CA-C	-7.41	102.23	112.30
1	A	65	ARG	N-CA-C	-7.37	99.00	109.24
1	A	104	GLU	N-CA-C	-7.36	103.34	111.36
1	B	182	TYR	N-CA-CB	7.33	122.50	110.69
1	A	22	LEU	N-CA-C	-7.30	100.37	109.64
1	A	60	ILE	O-C-N	7.28	129.40	121.10
1	B	25	PRO	N-CA-C	-7.27	101.83	110.70
1	B	58	PHE	CA-CB-CG	-7.19	106.61	113.80
1	B	26	PRO	CB-CA-C	7.16	117.91	111.40
1	A	13	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	22	LEU	CB-CA-C	7.09	120.72	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	LEU	CB-CA-C	7.04	121.94	110.88
1	B	118	SER	CA-C-N	7.04	130.02	120.38
1	B	118	SER	C-N-CA	7.04	130.02	120.38
1	B	179	PHE	CA-CB-CG	6.98	120.78	113.80
1	B	140	GLN	OE1-CD-NE2	6.97	129.57	122.60
1	B	135	VAL	N-CA-C	6.85	117.99	107.99
1	B	44	GLU	CA-CB-CG	6.84	127.78	114.10
1	A	94	ASP	CA-CB-CG	-6.82	105.78	112.60
1	A	155	LYS	N-CA-C	6.79	121.89	112.45
1	A	30	GLU	O-C-N	6.79	129.89	122.15
1	B	108	LYS	CA-C-N	6.78	132.02	123.14
1	B	108	LYS	C-N-CA	6.78	132.02	123.14
1	A	154	GLU	CB-CG-CD	6.71	124.00	112.60
1	A	161	GLU	CA-CB-CG	6.68	127.46	114.10
1	A	94	ASP	O-C-N	6.62	128.91	122.03
1	A	38	THR	CA-CB-OG1	-6.58	99.72	109.60
1	A	154	GLU	N-CA-C	-6.58	104.19	111.36
1	B	161	GLU	CB-CG-CD	6.58	123.78	112.60
1	B	72	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	83	PRO	N-CA-C	-6.57	100.77	111.21
1	B	11	SER	N-CA-C	-6.54	102.07	110.19
1	B	70	ARG	NE-CZ-NH2	6.44	124.99	119.20
1	A	179	PHE	O-C-N	6.36	130.45	123.13
1	B	137	ARG	O-C-N	6.35	130.61	123.05
1	A	62	GLU	CB-CG-CD	6.35	123.39	112.60
1	A	141	ASP	CA-CB-CG	-6.34	106.26	112.60
1	B	105	LEU	CA-C-N	6.34	129.63	120.38
1	B	105	LEU	C-N-CA	6.34	129.63	120.38
1	A	153	LEU	CB-CA-C	6.34	122.56	109.95
1	A	62	GLU	CA-CB-CG	6.33	126.75	114.10
1	B	79	LEU	O-C-N	6.27	130.92	122.59
1	B	56	THR	CA-CB-OG1	-6.26	100.21	109.60
1	A	185	ASN	CA-CB-CG	6.25	118.85	112.60
1	B	24	TRP	O-C-N	6.21	126.89	120.99
1	A	84	GLN	CB-CA-C	-6.18	98.12	110.42
1	B	172	GLU	CA-CB-CG	6.08	126.25	114.10
1	B	50	VAL	CA-C-N	6.07	130.71	123.19
1	B	50	VAL	C-N-CA	6.07	130.71	123.19
1	A	71	ILE	N-CA-C	-6.06	98.97	108.23
1	B	95	ASP	CA-CB-CG	6.03	118.62	112.60
1	B	48	ASN	O-C-N	6.00	129.78	123.06
1	B	65	ARG	N-CA-CB	5.99	120.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	112	VAL	O-C-N	5.97	129.45	123.18
1	A	142	PHE	O-C-N	5.96	130.06	123.33
1	B	185	ASN	CA-C-O	5.96	130.93	120.80
1	B	60	ILE	O-C-N	5.95	127.88	121.10
1	B	154	GLU	CA-CB-CG	5.92	125.94	114.10
1	B	19	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	102	GLN	O-C-N	5.89	128.03	121.43
1	B	35	GLN	CA-C-N	5.88	128.42	120.65
1	B	35	GLN	C-N-CA	5.88	128.42	120.65
1	B	30	GLU	CB-CA-C	5.88	121.46	110.70
1	B	176	LYS	CA-C-O	5.88	126.94	120.71
1	A	63	LYS	N-CA-C	5.87	119.50	112.93
1	A	71	ILE	O-C-N	5.86	130.09	122.94
1	A	168	ASP	N-CA-CB	5.86	118.74	110.36
1	B	109	VAL	N-CA-C	5.85	116.31	108.11
1	B	100	THR	CB-CA-C	5.83	121.86	110.67
1	A	15	GLY	N-CA-C	-5.77	104.29	112.37
1	B	134	PHE	CA-C-O	-5.76	114.14	120.70
1	B	138	ILE	CB-CA-C	5.75	118.56	111.25
1	B	84	GLN	CA-C-N	5.75	131.34	122.20
1	B	84	GLN	C-N-CA	5.75	131.34	122.20
1	B	70	ARG	O-C-N	5.69	130.55	123.15
1	B	44	GLU	N-CA-CB	5.68	118.76	109.95
1	B	9	ALA	CB-CA-C	-5.68	99.42	109.70
1	A	72	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	110	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	142	PHE	N-CA-C	-5.66	99.43	109.06
1	A	111	MET	CA-C-N	5.66	130.14	122.90
1	A	111	MET	C-N-CA	5.66	130.14	122.90
1	A	181	VAL	CA-CB-CG2	5.64	119.99	110.40
1	A	80	LYS	N-CA-CB	5.63	119.23	110.44
1	A	79	LEU	CB-CA-C	5.60	118.24	109.84
1	B	100	THR	CA-CB-OG1	-5.60	101.20	109.60
1	B	114	ILE	N-CA-CB	-5.58	104.68	111.21
1	A	65	ARG	CA-C-O	-5.57	115.20	119.32
1	A	30	GLU	N-CA-C	-5.56	105.30	111.36
1	B	116	GLY	CA-C-N	5.55	131.69	121.70
1	B	116	GLY	C-N-CA	5.55	131.69	121.70
1	A	67	LEU	N-CA-C	-5.55	103.03	110.24
1	B	142	PHE	CB-CA-C	5.53	120.61	109.38
1	A	145	ASP	CB-CA-C	5.52	118.35	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PRO	CB-CA-C	-5.51	102.47	111.56
1	A	61	PRO	N-CA-C	-5.51	101.13	112.47
1	A	64	ASN	CA-C-O	5.50	124.74	119.08
1	B	7	ILE	O-C-N	5.48	128.68	123.03
1	B	57	TRP	CA-C-N	5.48	128.07	120.29
1	B	57	TRP	C-N-CA	5.48	128.07	120.29
1	A	22	LEU	N-CA-CB	-5.48	101.38	109.98
1	B	118	SER	N-CA-CB	5.44	118.97	109.72
1	B	147	PHE	CA-C-O	5.43	127.25	121.11
1	B	34	PHE	CA-C-O	5.42	126.29	120.55
1	B	171	GLU	CB-CA-C	-5.41	98.96	109.68
1	B	185	ASN	CB-CA-C	5.40	120.37	110.10
1	A	184	LYS	CA-C-O	-5.40	115.50	121.33
1	A	146	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	71	ILE	N-CA-CB	5.37	117.13	111.00
1	A	60	ILE	CB-CA-C	-5.37	101.59	111.36
1	B	43	VAL	N-CA-C	5.37	117.29	108.97
1	A	27	LEU	CB-CA-C	5.37	119.54	110.79
1	A	138	ILE	O-C-N	5.36	130.04	122.59
1	A	9	ALA	CA-C-O	-5.35	114.38	120.32
1	B	74	VAL	CA-C-N	5.35	129.53	122.42
1	B	74	VAL	C-N-CA	5.35	129.53	122.42
1	B	65	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	A	172	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	29	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	169	VAL	CB-CA-C	5.29	119.94	111.32
1	A	7	ILE	N-CA-CB	5.28	119.01	111.82
1	A	76	SER	CA-CB-OG	-5.28	100.54	111.10
1	A	128	PRO	CA-C-O	-5.26	115.42	121.36
1	B	5	ASN	OD1-CG-ND2	5.23	127.83	122.60
1	B	9	ALA	CA-C-O	-5.22	114.52	120.32
1	B	74	VAL	N-CA-C	5.22	115.47	108.17
1	A	64	ASN	CB-CG-ND2	-5.21	108.59	116.40
1	B	185	ASN	CA-CB-CG	-5.20	107.40	112.60
1	B	76	SER	N-CA-CB	5.18	119.14	110.59
1	A	185	ASN	N-CA-CB	5.18	119.30	110.50
1	A	120	VAL	N-CA-C	-5.17	105.36	111.00
1	B	99	LEU	CB-CA-C	5.17	120.49	110.46
1	B	94	ASP	CB-CA-C	5.17	119.14	110.92
1	A	154	GLU	CA-CB-CG	5.16	124.42	114.10
1	B	65	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	B	5	ASN	CA-CB-CG	-5.15	107.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ILE	CA-C-N	-5.12	115.50	122.93
1	B	175	ILE	C-N-CA	-5.12	115.50	122.93
1	B	141	ASP	CA-C-N	-5.11	113.58	122.37
1	B	141	ASP	C-N-CA	-5.11	113.58	122.37
1	B	93	LEU	N-CA-C	-5.11	105.71	111.28
1	A	25	PRO	N-CA-C	-5.10	104.48	110.70
1	A	161	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	115	VAL	N-CA-C	5.08	117.06	112.29
1	A	64	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	185	ASN	CB-CA-C	5.05	119.70	110.10
1	A	116	GLY	CA-C-N	5.05	130.79	121.70
1	A	116	GLY	C-N-CA	5.05	130.79	121.70
1	A	101	GLU	CA-CB-CG	5.04	124.19	114.10
1	B	127	HIS	CA-CB-CG	-5.04	108.76	113.80
1	A	55	LYS	N-CA-C	5.04	116.77	111.28
1	B	121	TYR	CA-C-N	5.02	127.31	120.54
1	B	121	TYR	C-N-CA	5.02	127.31	120.54
1	B	86	ALA	CA-C-O	-5.02	116.09	121.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	LEU	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	65	ARG	Sidechain
1	B	91	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	1476	0	1487	147	1
1	B	1472	0	1483	140	1
2	A	32	0	18	0	0
2	B	32	0	17	4	0
3	A	52	0	0	6	0
3	B	59	0	0	17	0
All	All	3123	0	3005	282	1

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 47.

All (282) 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:171:GLU:OE2	1:A:176:LYS:HE2	1.38	1.22
1:B:80:LYS:NZ	1:B:80:LYS:HA	1.56	1.19
1:B:80:LYS:NZ	1:B:80:LYS:CA	2.10	1.15
1:B:80:LYS:HA	1:B:80:LYS:HZ2	1.08	1.13
1:B:80:LYS:HE3	1:B:80:LYS:C	1.74	1.12
1:B:80:LYS:CA	1:B:80:LYS:HZ2	1.63	1.11
1:A:156:TYR:C	1:A:157:LYS:HD3	1.76	1.09
1:A:14:MET:HE2	1:A:14:MET:HA	1.31	1.09
1:A:66:PRO:O	1:A:68:LYS:HD2	1.51	1.09
1:B:130:HIS:HE1	1:B:183:GLU:OE1	1.35	1.07
1:B:76:SER:O	1:B:91:ARG:HD3	1.59	1.01
1:A:64:ASN:N	1:A:64:ASN:HD22	1.58	1.01
1:B:107:ASN:HB3	3:B:493:HOH:O	1.58	1.01
1:B:80:LYS:C	1:B:80:LYS:CE	2.35	1.00
1:A:77:ARG:HA	1:A:91:ARG:HD2	1.44	0.99
1:A:156:TYR:O	1:A:157:LYS:HD3	1.65	0.96
1:B:130:HIS:CE1	1:B:183:GLU:OE1	2.19	0.96
1:B:104:GLU:HA	3:B:468:HOH:O	1.66	0.94
1:A:153:LEU:O	1:A:153:LEU:CD1	2.15	0.94
1:A:153:LEU:O	1:A:153:LEU:HD13	1.67	0.94
1:B:146:THR:HG21	3:B:408:HOH:O	1.65	0.93
1:A:64:ASN:N	1:A:64:ASN:ND2	2.11	0.92
1:B:23:PRO:HG2	1:B:24:TRP:CZ3	2.05	0.92
1:B:146:THR:HG23	3:B:421:HOH:O	1.70	0.91
1:B:81:GLU:HB3	1:B:82:PRO:HD2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD12	3:B:428:HOH:O	1.70	0.90
1:B:80:LYS:HE3	1:B:80:LYS:O	1.72	0.89
1:A:160:PRO:HG2	1:A:161:GLU:OE2	1.71	0.89
1:A:14:MET:HE2	1:A:14:MET:CA	2.05	0.85
1:A:54:LYS:HG3	1:A:79:LEU:HD11	1.60	0.84
1:A:171:GLU:OE2	1:A:176:LYS:CE	2.25	0.84
1:B:139:MET:HG2	3:B:501:HOH:O	1.78	0.84
1:B:24:TRP:HB2	1:B:25:PRO:HD2	1.60	0.83
1:B:99:LEU:HD11	1:B:105:LEU:CD2	2.07	0.83
1:B:99:LEU:HD11	1:B:105:LEU:HD21	1.60	0.82
1:A:95:ASP:HA	1:A:98:LYS:HZ3	1.42	0.82
1:B:80:LYS:NZ	1:B:80:LYS:C	2.36	0.81
1:B:104:GLU:HG2	3:B:468:HOH:O	1.80	0.80
1:A:14:MET:HA	1:A:14:MET:CE	2.10	0.80
1:B:99:LEU:CD1	1:B:105:LEU:CD2	2.60	0.79
1:A:98:LYS:O	1:A:101:GLU:CB	2.31	0.78
1:A:94:ASP:O	1:A:98:LYS:HD3	1.83	0.78
1:B:80:LYS:HA	1:B:80:LYS:HZ1	1.46	0.78
1:B:89:LEU:HD21	1:B:91:ARG:NH2	1.99	0.77
1:B:118:SER:HB2	3:B:440:HOH:O	1.84	0.77
1:B:80:LYS:CE	1:B:80:LYS:O	2.32	0.77
1:A:64:ASN:HD22	1:A:64:ASN:H	1.31	0.76
1:B:154:GLU:CD	3:B:487:HOH:O	2.28	0.75
1:B:78:GLU:O	1:B:79:LEU:C	2.27	0.75
1:B:99:LEU:O	1:B:105:LEU:HD23	1.85	0.75
1:B:76:SER:O	1:B:91:ARG:CD	2.34	0.75
1:A:171:GLU:HG3	1:A:176:LYS:HD3	1.69	0.75
1:A:98:LYS:O	1:A:101:GLU:HB2	1.86	0.75
1:A:80:LYS:HA	1:A:80:LYS:HE2	1.69	0.75
1:B:81:GLU:CB	1:B:82:PRO:HD2	2.16	0.75
1:A:68:LYS:N	1:A:70:ARG:HH11	1.86	0.74
1:A:54:LYS:HG3	1:A:79:LEU:CD1	2.18	0.73
1:A:66:PRO:O	1:A:68:LYS:CD	2.33	0.73
1:A:6:CYS:HB2	1:A:133:LEU:HD23	1.70	0.72
1:A:84:GLN:CG	1:A:85:GLY:N	2.49	0.72
1:A:153:LEU:O	1:A:153:LEU:HD12	1.88	0.72
1:A:40:THR:O	1:A:111:MET:HE3	1.90	0.72
1:A:68:LYS:H	1:A:70:ARG:HH11	1.34	0.71
1:B:89:LEU:HD21	1:B:91:ARG:HH22	1.53	0.71
1:B:114:ILE:HD13	1:B:124:ALA:CB	2.18	0.71
1:A:154:GLU:OE1	1:A:155:LYS:HD3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HE2	1:A:80:LYS:O	1.91	0.70
1:A:152:ASP:OD1	1:A:154:GLU:N	2.25	0.70
1:B:136:THR:HG22	1:B:138:ILE:CD1	2.22	0.69
1:B:23:PRO:HG2	1:B:24:TRP:CE3	2.27	0.69
1:B:81:GLU:HB3	1:B:82:PRO:CD	2.22	0.69
1:A:76:SER:O	1:A:91:ARG:HD3	1.93	0.69
1:B:62:GLU:CG	1:B:62:GLU:O	2.39	0.69
1:B:79:LEU:HD13	1:B:83:PRO:HD3	1.74	0.69
1:B:159:LEU:HD21	1:B:183:GLU:HB3	1.73	0.68
1:B:40:THR:O	1:B:111:MET:CE	2.42	0.68
1:B:79:LEU:CD1	1:B:83:PRO:HD3	2.24	0.67
1:B:80:LYS:C	1:B:80:LYS:HZ1	2.03	0.67
1:A:18:LYS:HD2	1:A:143:GLU:O	1.95	0.67
1:A:61:PRO:HB2	1:A:64:ASN:HD21	1.58	0.67
1:B:114:ILE:HD13	1:B:124:ALA:HB2	1.76	0.67
1:A:139:MET:HE2	1:A:177:TYR:HA	1.77	0.66
1:B:40:THR:O	1:B:111:MET:HE1	1.96	0.66
1:A:14:MET:HE2	1:A:14:MET:N	2.12	0.65
1:A:137:ARG:O	1:A:177:TYR:HA	1.97	0.65
1:B:76:SER:HB3	1:B:79:LEU:HB2	1.79	0.65
1:A:171:GLU:HG3	1:A:176:LYS:CD	2.27	0.64
1:A:80:LYS:O	1:A:80:LYS:CE	2.45	0.64
1:B:80:LYS:CA	1:B:80:LYS:CE	2.76	0.64
1:B:62:GLU:O	1:B:62:GLU:HG2	1.98	0.63
1:A:71:ILE:CD1	1:A:71:ILE:N	2.62	0.63
1:A:80:LYS:HE2	1:A:80:LYS:CA	2.28	0.63
1:A:18:LYS:HA	1:A:145:ASP:OD1	1.98	0.62
1:A:171:GLU:HA	1:A:175:ILE:O	1.99	0.62
1:A:183:GLU:HG2	1:A:184:LYS:N	2.13	0.62
1:B:61:PRO:O	1:B:63:LYS:N	2.30	0.61
1:A:68:LYS:H	1:A:70:ARG:NH1	1.99	0.61
1:A:170:GLN:O	1:A:176:LYS:HA	2.01	0.61
1:A:139:MET:CE	1:A:177:TYR:HA	2.30	0.61
1:B:151:ILE:O	1:B:153:LEU:HD22	2.00	0.61
1:A:61:PRO:O	1:A:64:ASN:ND2	2.34	0.61
1:A:84:GLN:C	1:A:86:ALA:H	2.08	0.61
1:A:83:PRO:O	1:A:84:GLN:O	2.19	0.61
1:B:99:LEU:CD1	1:B:105:LEU:HD23	2.30	0.61
1:A:95:ASP:HA	1:A:98:LYS:NZ	2.13	0.61
1:B:24:TRP:HB2	1:B:25:PRO:CD	2.29	0.61
1:B:81:GLU:CB	1:B:82:PRO:CD	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:N	1:A:71:ILE:HD13	2.15	0.60
1:A:104:GLU:OE1	1:A:104:GLU:HA	2.01	0.60
1:B:30:GLU:OE1	2:B:187:DZF:NA2	2.30	0.60
1:A:139:MET:CE	1:A:177:TYR:CA	2.79	0.60
1:A:36:ARG:HH12	1:A:164:GLY:C	2.10	0.60
1:A:80:LYS:HE2	1:A:80:LYS:C	2.26	0.60
1:B:139:MET:HB2	1:B:176:LYS:O	2.01	0.60
1:B:130:HIS:HE1	1:B:183:GLU:CD	2.07	0.60
1:A:63:LYS:CD	1:A:63:LYS:O	2.49	0.59
1:B:5:ASN:O	1:B:113:TRP:HA	2.02	0.59
1:A:11:SER:O	1:A:14:MET:HE2	2.03	0.59
1:B:98:LYS:O	1:B:101:GLU:HG2	2.02	0.59
1:B:171:GLU:HA	1:B:175:ILE:O	2.03	0.58
1:A:81:GLU:HB3	1:A:82:PRO:HD2	1.85	0.58
1:B:80:LYS:NZ	1:B:80:LYS:O	2.33	0.58
1:A:130:HIS:NE2	1:A:183:GLU:OE1	2.24	0.58
1:B:22:LEU:HD12	3:B:454:HOH:O	2.03	0.58
1:A:98:LYS:O	1:A:101:GLU:HB3	2.04	0.58
1:B:80:LYS:CA	1:B:80:LYS:HZ1	1.99	0.57
1:A:63:LYS:O	1:A:63:LYS:HD3	2.04	0.57
1:A:23:PRO:HD2	1:A:24:TRP:CE3	2.40	0.57
1:A:139:MET:HE3	1:A:176:LYS:C	2.30	0.57
1:A:157:LYS:HD3	1:A:157:LYS:N	2.12	0.57
1:A:161:GLU:OE2	1:A:161:GLU:N	2.38	0.56
1:B:176:LYS:NZ	3:B:445:HOH:O	2.38	0.56
1:B:93:LEU:HD23	1:B:123:GLU:HB3	1.88	0.56
1:B:73:LEU:HG	1:B:88:PHE:HB2	1.87	0.55
1:A:77:ARG:HG3	1:A:91:ARG:HB3	1.86	0.55
1:A:77:ARG:HA	1:A:91:ARG:CD	2.29	0.55
1:A:84:GLN:O	1:A:86:ALA:N	2.38	0.55
1:B:148:PHE:CD2	1:B:149:PRO:O	2.59	0.55
1:B:56:THR:O	1:B:57:TRP:C	2.50	0.55
1:A:14:MET:HE1	3:A:426:HOH:O	2.06	0.54
1:A:75:LEU:HA	1:A:90:SER:O	2.06	0.54
1:A:72:ASN:O	1:A:87:HIS:HB2	2.07	0.54
1:A:14:MET:CA	1:A:14:MET:CE	2.78	0.54
1:A:57:TRP:CE2	1:A:65:ARG:HD3	2.42	0.54
1:A:10:VAL:HG12	1:A:16:ILE:CG2	2.38	0.54
1:B:22:LEU:CD1	3:B:454:HOH:O	2.53	0.54
1:B:52:MET:HB3	1:B:115:VAL:CG2	2.38	0.54
1:A:160:PRO:HG2	1:A:161:GLU:CD	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PHE:O	1:B:38:THR:HG23	2.08	0.53
1:B:66:PRO:HB2	1:B:72:ASN:CG	2.33	0.53
1:A:26:PRO:HA	3:A:488:HOH:O	2.08	0.53
1:B:63:LYS:C	1:B:63:LYS:CD	2.82	0.53
1:B:72:ASN:O	1:B:87:HIS:HB2	2.09	0.53
1:A:84:GLN:HG2	1:A:85:GLY:N	1.93	0.52
1:A:29:ASN:HB2	1:A:172:GLU:OE1	2.10	0.52
1:A:158:LEU:HD23	1:A:181:VAL:O	2.09	0.51
1:B:61:PRO:HB2	1:B:63:LYS:HE3	1.92	0.51
1:A:43:VAL:HG11	1:A:46:LYS:HG3	1.92	0.51
1:A:6:CYS:HB2	1:A:133:LEU:CD2	2.40	0.51
1:A:84:GLN:O	1:A:84:GLN:HG2	1.76	0.51
1:B:4:LEU:HB3	1:B:131:LEU:HG	1.91	0.51
1:A:158:LEU:C	1:A:158:LEU:CD2	2.83	0.51
1:A:154:GLU:OE1	1:A:154:GLU:O	2.28	0.51
1:A:140:GLN:HG2	1:A:141:ASP:N	2.25	0.50
1:B:117:GLY:O	1:B:118:SER:C	2.52	0.50
1:A:13:ASN:ND2	3:A:411:HOH:O	2.44	0.50
1:A:183:GLU:HG2	1:A:184:LYS:H	1.77	0.50
1:B:104:GLU:CA	3:B:468:HOH:O	2.42	0.50
1:B:60:ILE:O	1:B:65:ARG:NH2	2.38	0.50
1:B:99:LEU:HD12	1:B:105:LEU:HD23	1.94	0.50
1:B:31:PHE:HB3	2:B:187:DZF:CD	2.42	0.50
1:A:47:GLN:O	1:A:109:VAL:HA	2.12	0.50
1:A:51:ILE:CG2	1:A:75:LEU:HD11	2.42	0.50
1:B:104:GLU:CG	3:B:468:HOH:O	2.48	0.49
1:B:152:ASP:OD1	1:B:154:GLU:CB	2.60	0.49
1:B:161:GLU:OE1	1:B:163:PRO:HD3	2.12	0.49
1:A:40:THR:O	1:A:111:MET:CE	2.58	0.49
1:B:114:ILE:HD13	1:B:124:ALA:HB1	1.94	0.49
1:B:8:VAL:HG11	1:B:148:PHE:CE1	2.47	0.49
1:A:10:VAL:HG12	1:A:16:ILE:HG22	1.94	0.49
1:A:14:MET:HE2	1:A:14:MET:H	1.76	0.49
1:B:66:PRO:HB2	1:B:72:ASN:ND2	2.27	0.49
1:B:153:LEU:HD13	1:B:153:LEU:HA	1.48	0.49
1:A:80:LYS:HE3	1:A:91:ARG:NH1	2.27	0.49
1:A:83:PRO:O	1:A:84:GLN:C	2.56	0.48
1:A:152:ASP:OD1	1:A:152:ASP:C	2.55	0.48
1:B:114:ILE:CD1	1:B:124:ALA:HB1	2.43	0.48
1:B:49:LEU:HD23	1:B:112:VAL:HG13	1.95	0.48
1:B:4:LEU:HD23	1:B:4:LEU:HA	1.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HE1	3:A:404:HOH:O	2.13	0.48
1:A:155:LYS:C	1:A:157:LYS:HE2	2.39	0.48
1:B:27:LEU:HD22	1:B:172:GLU:HG2	1.95	0.48
1:B:70:ARG:O	3:B:465:HOH:O	2.20	0.48
1:B:102:GLN:HB2	1:B:105:LEU:HB2	1.95	0.48
1:A:11:SER:O	1:A:14:MET:CE	2.61	0.47
1:A:153:LEU:CD1	1:A:153:LEU:C	2.76	0.47
1:A:66:PRO:O	1:A:67:LEU:C	2.57	0.47
1:A:107:ASN:C	1:A:107:ASN:OD1	2.56	0.47
1:B:46:LYS:NZ	3:B:469:HOH:O	2.46	0.47
1:A:52:MET:HB3	1:A:115:VAL:CG2	2.45	0.47
1:A:176:LYS:HZ2	1:A:176:LYS:HG2	1.69	0.47
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.50	0.47
1:B:99:LEU:HD12	1:B:105:LEU:CD2	2.42	0.47
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.62	0.47
1:B:80:LYS:HE3	1:B:81:GLU:N	2.26	0.47
1:A:119:SER:N	3:A:456:HOH:O	2.49	0.46
1:A:84:GLN:C	1:A:86:ALA:N	2.73	0.46
1:A:158:LEU:C	1:A:158:LEU:HD22	2.40	0.46
1:B:60:ILE:HG23	1:B:61:PRO:HD2	1.98	0.46
1:A:169:VAL:CG2	1:A:176:LYS:HG3	2.45	0.46
1:A:83:PRO:C	1:A:84:GLN:O	2.59	0.46
1:B:34:PHE:C	1:B:34:PHE:CD2	2.94	0.46
1:A:24:TRP:O	3:A:477:HOH:O	2.20	0.46
1:A:162:TYR:HA	1:A:163:PRO:HD2	1.69	0.46
1:A:96:ALA:O	1:A:100:THR:HG23	2.15	0.46
1:B:12:GLN:HB3	1:B:141:ASP:OD1	2.16	0.45
1:A:7:ILE:O	1:A:121:TYR:OH	2.32	0.45
1:A:80:LYS:HZ2	1:B:98:LYS:CE	2.30	0.45
1:B:22:LEU:HD11	1:B:31:PHE:CZ	2.51	0.45
1:A:33:TYR:O	1:A:37:MET:HG2	2.16	0.45
1:B:127:HIS:HA	1:B:128:PRO:HD3	1.81	0.45
1:B:152:ASP:OD1	1:B:154:GLU:HB2	2.16	0.45
1:A:46:LYS:NZ	1:A:106:ALA:O	2.49	0.45
1:A:68:LYS:N	1:A:70:ARG:NH1	2.57	0.45
1:B:122:LYS:NZ	3:B:440:HOH:O	2.26	0.45
1:A:94:ASP:C	1:A:98:LYS:HD3	2.40	0.45
1:B:24:TRP:CB	1:B:25:PRO:CD	2.94	0.45
1:B:40:THR:O	1:B:111:MET:HE3	2.17	0.45
1:A:5:ASN:OD1	1:A:132:LYS:HB2	2.17	0.45
1:A:107:ASN:OD1	1:A:107:ASN:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.65	0.45
1:A:183:GLU:CG	1:A:184:LYS:N	2.77	0.45
1:B:78:GLU:O	1:B:79:LEU:O	2.34	0.45
1:B:14:MET:O	1:B:147:PHE:HA	2.17	0.45
1:B:73:LEU:C	1:B:73:LEU:HD23	2.42	0.45
1:A:42:SER:N	1:A:110:ASP:OD2	2.49	0.44
1:A:172:GLU:N	1:A:175:ILE:O	2.44	0.44
1:B:61:PRO:C	1:B:63:LYS:H	2.24	0.44
1:A:154:GLU:OE1	1:A:154:GLU:C	2.59	0.44
1:B:33:TYR:O	1:B:37:MET:HG2	2.17	0.44
1:A:14:MET:CE	1:A:14:MET:N	2.80	0.44
1:A:138:ILE:O	1:A:138:ILE:HG22	2.18	0.44
1:A:166:LEU:N	1:A:166:LEU:HD23	2.33	0.44
1:B:63:LYS:C	1:B:63:LYS:HD2	2.43	0.44
1:B:157:LYS:HB2	1:B:157:LYS:HE3	1.61	0.43
1:A:87:HIS:ND1	1:B:104:GLU:CG	2.82	0.43
1:A:171:GLU:CG	1:A:176:LYS:CD	2.96	0.43
1:A:171:GLU:HB2	1:A:176:LYS:HD2	2.01	0.43
1:B:62:GLU:HA	1:B:65:ARG:HG3	2.00	0.43
1:A:67:LEU:HB3	1:A:70:ARG:CZ	2.49	0.43
1:A:80:LYS:NZ	1:B:98:LYS:CE	2.82	0.43
1:A:49:LEU:HD12	1:A:71:ILE:HB	2.01	0.43
1:A:156:TYR:C	1:A:157:LYS:CD	2.68	0.43
1:B:52:MET:HB2	1:B:56:THR:HB	2.01	0.43
1:B:89:LEU:HD21	1:B:91:ARG:CZ	2.48	0.43
1:B:37:MET:HB3	1:B:37:MET:HE3	1.81	0.43
1:A:139:MET:HE2	1:A:177:TYR:CA	2.43	0.42
1:B:52:MET:HA	1:B:116:GLY:O	2.19	0.42
1:B:57:TRP:O	1:B:65:ARG:HD3	2.19	0.42
1:B:162:TYR:HA	1:B:163:PRO:HD2	1.81	0.42
1:B:43:VAL:HB	1:B:46:LYS:HB2	2.00	0.42
1:A:23:PRO:HB2	1:A:142:PHE:HB3	2.02	0.42
1:B:36:ARG:HH21	1:B:36:ARG:HD3	1.54	0.42
1:A:80:LYS:NZ	1:B:98:LYS:HE2	2.34	0.42
1:B:16:ILE:CG2	1:B:148:PHE:HB2	2.50	0.42
1:A:183:GLU:CG	1:A:184:LYS:H	2.33	0.41
1:B:21:ASP:OD2	1:B:22:LEU:N	2.51	0.41
1:B:115:VAL:O	2:B:187:DZF:H7	2.19	0.41
1:B:170:GLN:O	1:B:176:LYS:HA	2.19	0.41
1:A:22:LEU:HA	1:A:23:PRO:HD3	1.86	0.41
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:HG2	1:B:87:HIS:O	2.19	0.41
1:B:178:LYS:HE3	1:B:178:LYS:HB3	1.79	0.41
1:A:43:VAL:CG1	1:A:46:LYS:HG3	2.50	0.41
1:B:125:MET:HE2	1:B:125:MET:HB3	1.80	0.41
1:A:169:VAL:HG23	1:A:176:LYS:HG3	2.02	0.41
1:B:31:PHE:HB3	2:B:187:DZF:CG	2.50	0.41
1:A:66:PRO:C	1:A:67:LEU:O	2.59	0.41
1:B:156:TYR:CZ	1:B:184:LYS:HD3	2.56	0.41
1:B:124:ALA:O	1:B:131:LEU:HD11	2.21	0.40
1:B:159:LEU:HA	1:B:160:PRO:HD2	1.82	0.40
1:B:10:VAL:HG12	1:B:16:ILE:HG22	2.03	0.40

All (1) 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)
1:A:141:ASP:OD1	1:B:32:ARG:NH1[1_554]	2.08	0.12

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	109/186 (59%)	99 (91%)	7 (6%)	3 (3%)	4	2
1	B	162/186 (87%)	150 (93%)	9 (6%)	3 (2%)	6	5
All	All	271/372 (73%)	249 (92%)	16 (6%)	6 (2%)	5	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	85	GLY

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Mol	Chain	Res	Type
1	B	62	GLU
1	A	62	GLU
1	B	79	LEU
1	B	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	165/168 (98%)	118 (72%)	47 (28%)	0	0
1	B	164/168 (98%)	128 (78%)	36 (22%)	1	1
All	All	329/336 (98%)	246 (75%)	83 (25%)	0	0

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	18	LYS
1	A	28	ARG
1	A	31	PHE
1	A	32	ARG
1	A	39	THR
1	A	41	SER
1	A	42	SER
1	A	44	GLU
1	A	46	LYS
1	A	47	GLN
1	A	49	LEU
1	A	54	LYS
1	A	55	LYS
1	A	60	ILE
1	A	63	LYS
1	A	64	ASN
1	A	68	LYS
1	A	71	ILE

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Mol	Chain	Res	Type
1	A	76	SER
1	A	80	LYS
1	A	84	GLN
1	A	90	SER
1	A	98	LYS
1	A	105	LEU
1	A	107	ASN
1	A	111	MET
1	A	114	ILE
1	A	118	SER
1	A	122	LYS
1	A	123	GLU
1	A	126	ASN
1	A	131	LEU
1	A	138	ILE
1	A	141	ASP
1	A	150	GLU
1	A	153	LEU
1	A	154	GLU
1	A	158	LEU
1	A	161	GLU
1	A	168	ASP
1	A	169	VAL
1	A	173	LYS
1	A	176	LYS
1	A	178	LYS
1	A	184	LYS
1	A	185	ASN
1	B	12	GLN
1	B	18	LYS
1	B	30	GLU
1	B	32	ARG
1	B	43	VAL
1	B	63	LYS
1	B	68	LYS
1	B	70	ARG
1	B	74	VAL
1	B	77	ARG
1	B	79	LEU
1	B	80	LYS
1	B	84	GLN
1	B	89	LEU

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Mol	Chain	Res	Type
1	B	95	ASP
1	B	101	GLU
1	B	103	PRO
1	B	105	LEU
1	B	107	ASN
1	B	108	LYS
1	B	111	MET
1	B	112	VAL
1	B	119	SER
1	B	131	LEU
1	B	133	LEU
1	B	138	ILE
1	B	146	THR
1	B	150	GLU
1	B	153	LEU
1	B	155	LYS
1	B	157	LYS
1	B	158	LEU
1	B	159	LEU
1	B	161	GLU
1	B	178	LYS
1	B	184	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	64	ASN
1	A	126	ASN
1	B	12	GLN
1	B	29	ASN
1	B	47	GLN
1	B	130	HIS

5.3.3 RNA ⓘ

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](#)

2 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	DZF	B	187	-	34,34,34	2.10	11 (32%)	45,47,47	2.45	19 (42%)
2	DZF	A	187	-	34,34,34	1.94	10 (29%)	45,47,47	2.12	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DZF	B	187	-	-	1/22/22/22	0/3/3/3
2	DZF	A	187	-	-	4/22/22/22	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	DZF	C4A-C8A	-5.64	1.35	1.42
2	A	187	DZF	C4A-C8A	-4.76	1.36	1.42
2	B	187	DZF	C2-N3	4.03	1.43	1.33
2	A	187	DZF	CA-N	4.03	1.54	1.45
2	A	187	DZF	C5-C6	-3.70	1.33	1.39
2	B	187	DZF	CB-CG	3.51	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	DZF	CG-CD	3.45	1.58	1.50
2	A	187	DZF	CG-CD	3.37	1.58	1.50
2	A	187	DZF	CB-CG	2.98	1.61	1.52
2	A	187	DZF	C2-N3	2.75	1.39	1.33
2	A	187	DZF	C2-NA2	-2.51	1.28	1.34
2	B	187	DZF	C15-C14	2.48	1.43	1.39
2	A	187	DZF	C13-C14	-2.46	1.35	1.39
2	B	187	DZF	C2-NA2	-2.45	1.28	1.34
2	A	187	DZF	OE2-CD	-2.43	1.22	1.30
2	B	187	DZF	C13-C14	-2.32	1.35	1.39
2	B	187	DZF	C5-C6	-2.32	1.35	1.39
2	B	187	DZF	C-N	-2.32	1.28	1.34
2	B	187	DZF	C7-C6	2.22	1.43	1.38
2	A	187	DZF	C8A-N8	-2.21	1.31	1.35
2	B	187	DZF	C8A-N8	2.18	1.38	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	DZF	C5-C4A-C8A	5.70	123.09	117.25
2	A	187	DZF	OE1-CD-CG	-5.67	105.09	123.09
2	A	187	DZF	C5-C4A-C8A	5.44	122.82	117.25
2	B	187	DZF	O-C-N	-5.22	112.55	122.47
2	B	187	DZF	NA2-C2-N1	4.48	126.20	116.77
2	B	187	DZF	CB-CA-N	4.29	119.40	110.91
2	B	187	DZF	OE1-CD-CG	-4.16	109.89	123.09
2	B	187	DZF	C11-C-N	4.09	124.62	117.04
2	A	187	DZF	C4A-C5-C6	-3.83	115.43	121.38
2	A	187	DZF	CB-CA-N	-3.81	103.36	110.91
2	B	187	DZF	CA-N-C	3.43	129.78	121.56
2	B	187	DZF	C4A-C5-C6	-3.38	116.13	121.38
2	A	187	DZF	OE2-CD-CG	3.35	124.58	114.00
2	B	187	DZF	C13-C12-C11	3.29	124.32	120.80
2	A	187	DZF	NA2-C2-N1	3.24	123.59	116.77
2	A	187	DZF	CB-CG-CD	-3.19	103.98	112.49
2	B	187	DZF	N1-C2-N3	-3.11	117.63	123.32
2	B	187	DZF	C6-C7-N8	3.10	128.60	123.99
2	A	187	DZF	O4-C4-C4A	2.93	126.05	121.33
2	B	187	DZF	C16-C11-C12	-2.85	114.95	118.57
2	A	187	DZF	C12-C13-C14	-2.71	117.18	120.30
2	A	187	DZF	OE2-CD-OE1	2.68	130.23	123.33
2	B	187	DZF	C7-N8-C8A	-2.55	111.19	116.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	DZF	C13-C12-C11	2.48	123.45	120.80
2	B	187	DZF	CB-CG-CD	-2.48	105.87	112.49
2	B	187	DZF	OE2-CD-CG	2.39	121.54	114.00
2	A	187	DZF	N1-C8A-N8	-2.34	112.88	116.38
2	B	187	DZF	O4-C4-C4A	2.32	125.06	121.33
2	B	187	DZF	C16-C11-C	2.08	127.34	120.60
2	B	187	DZF	C15-C14-N10	-2.08	116.27	120.96
2	A	187	DZF	C15-C14-C13	2.04	121.76	119.04
2	B	187	DZF	OE2-CD-OE1	2.02	128.53	123.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	DZF	N-CA-CB-CG
2	A	187	DZF	CT-CA-CB-CG
2	A	187	DZF	CA-CB-CG-CD
2	A	187	DZF	C6-C9-N10-C14
2	B	187	DZF	OE2-CD-CG-CB

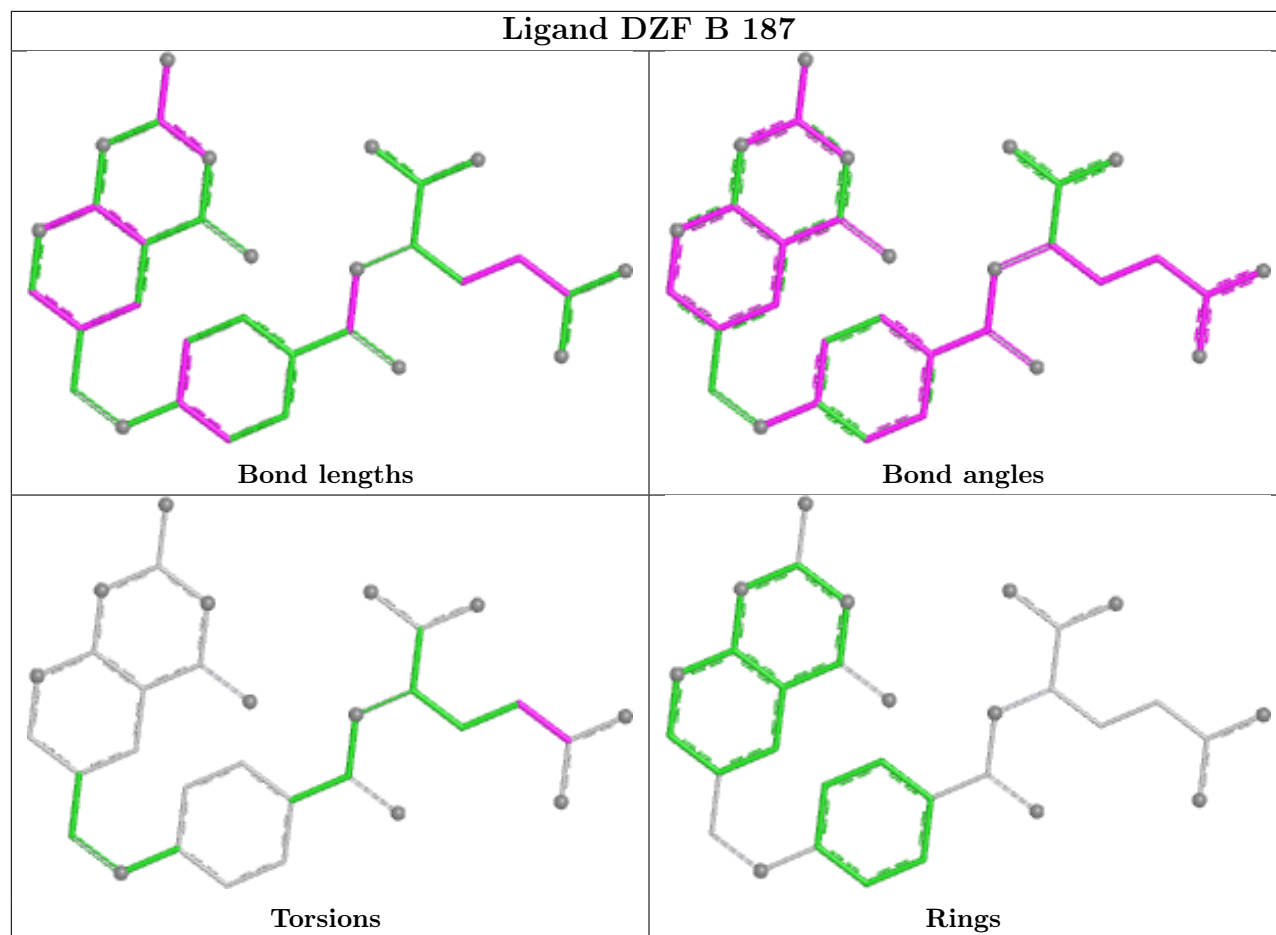
There are no ring outliers.

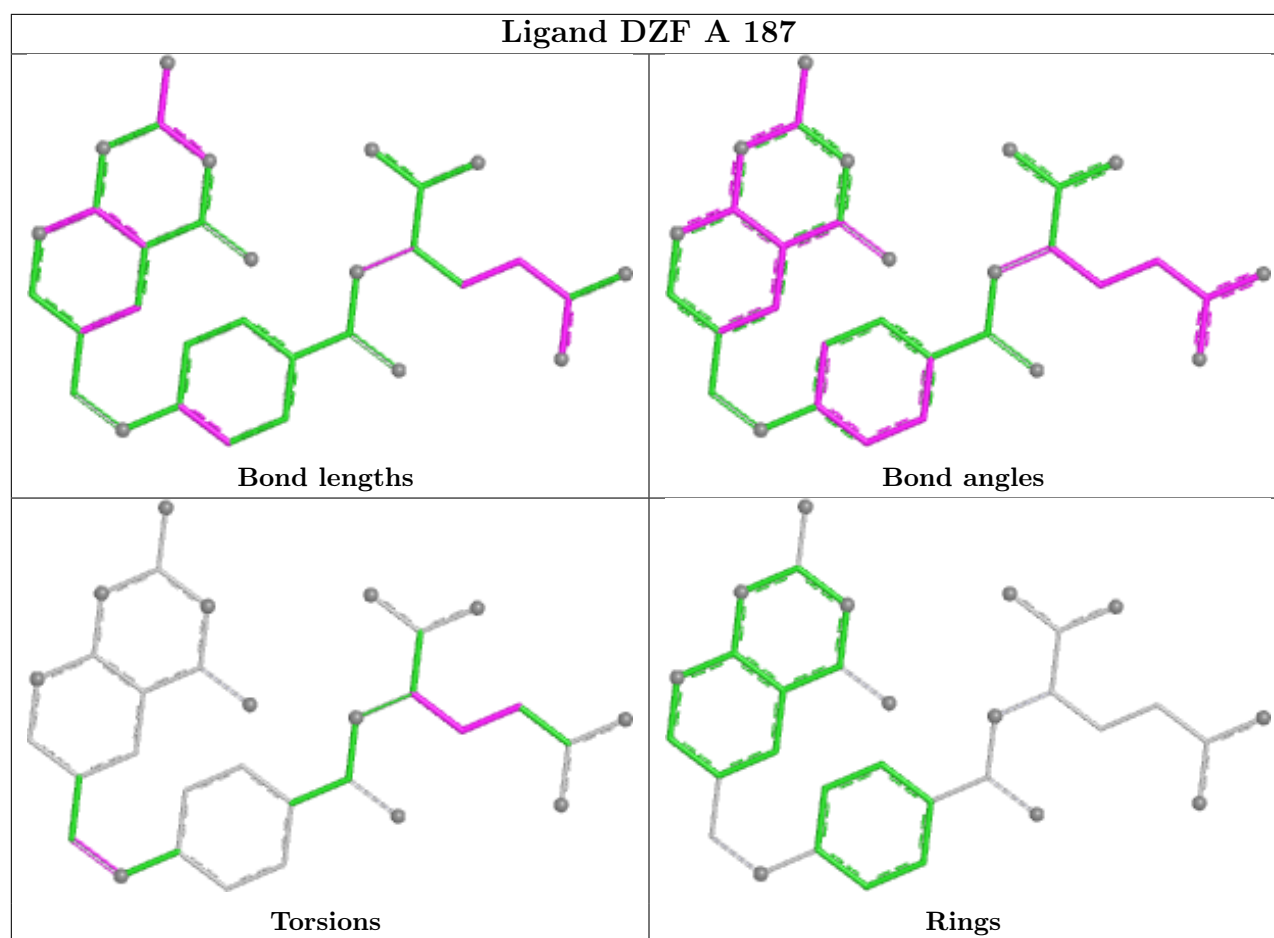
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	187	DZF	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.

Ligand DZF B 187





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.