



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:54 PM UTC

PDB ID : 1LCO / pdb_00001lco
Title : X-RAY STRUCTURE OF TWO COMPLEXES OF THE Y143F FLAVO-CYTOCHROME B2 MUTANT CRYSTALLIZED IN THE PRESENCE OF LACTATE OR PHENYL-LACTATE
Authors : Tegoni, M.; Cambillau, C.
Deposited on : 1995-03-30
Resolution : 2.90 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

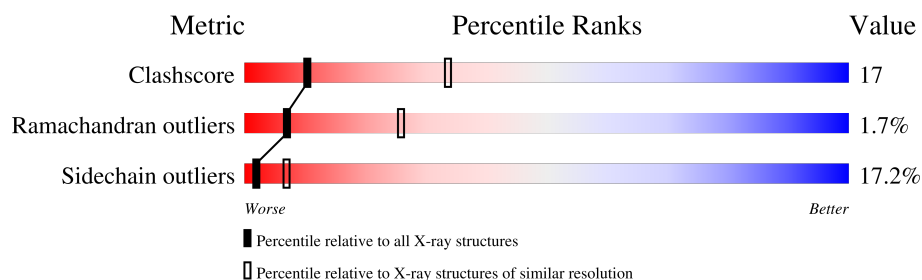
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	511	
1	B	511	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	A	570	X	-	-	-
3	FMN	B	570	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8915 atoms, of which 1840 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	480	Total	C	H	N	O	S	0	0	0
			4547	2384	811	631	707	14			
1	B	391	Total	C	H	N	O	S	0	0	0
			3732	1930	687	521	583	11			

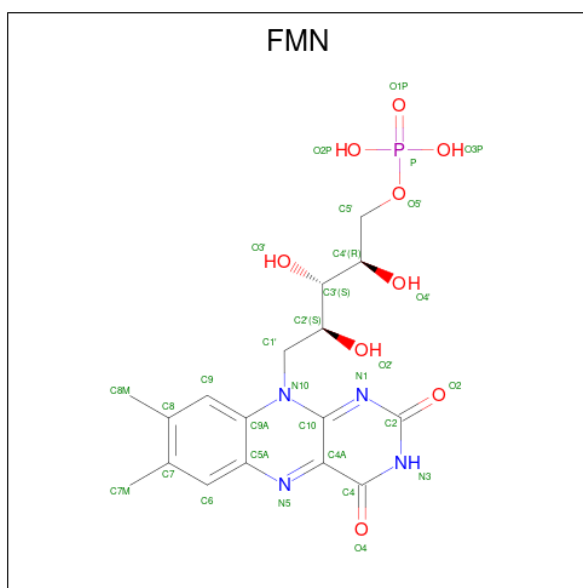
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	PHE	TYR	conflict	UNP P00175
B	143	PHE	TYR	conflict	UNP P00175

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

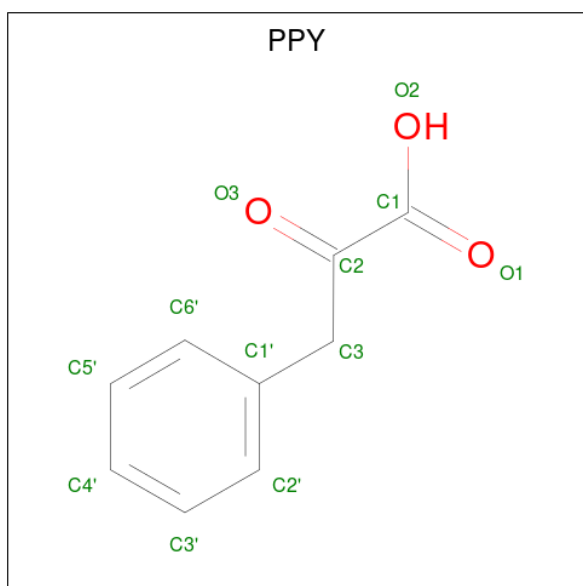


- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		
3	B	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		

- Molecule 4 is 3-PHENYLPYRUVIC ACID (CCD ID: PPY) (formula: $C_9H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 5 is water.

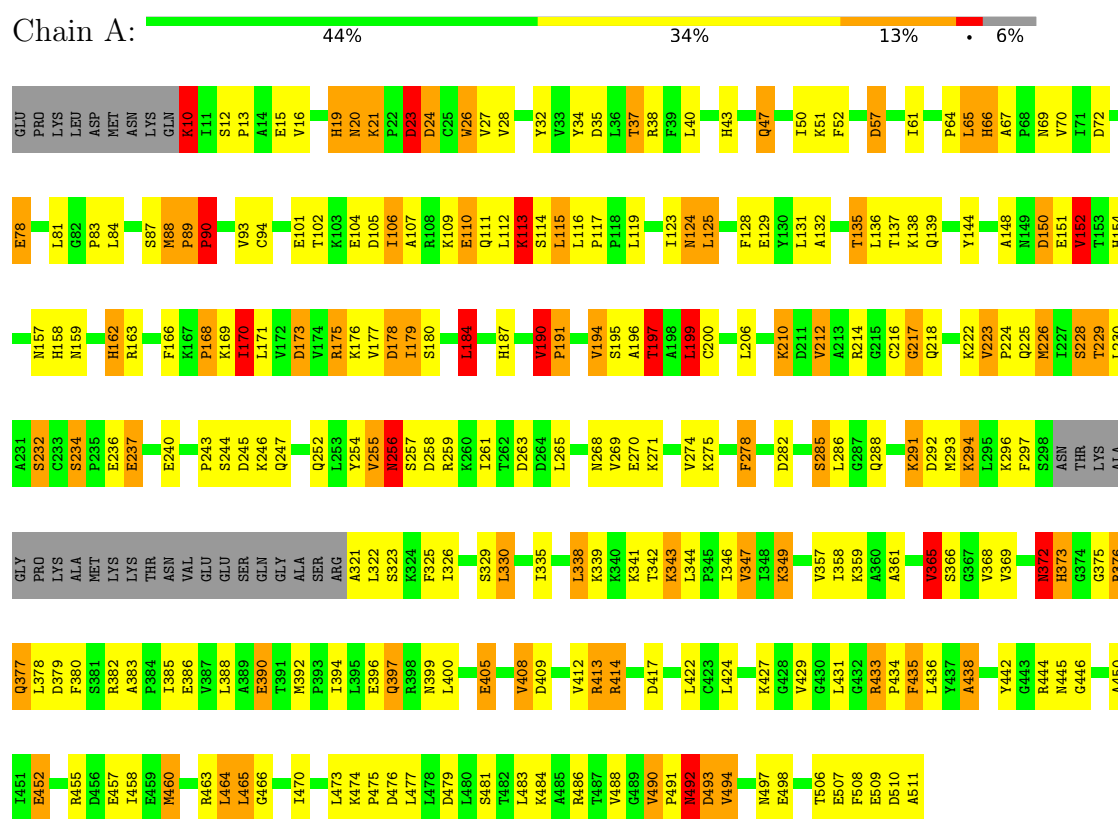
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	152	Total	H	O	0	0
			456	304	152		
5	B	13	Total	H	O	0	0
			39	26	13		

3 Residue-property plots

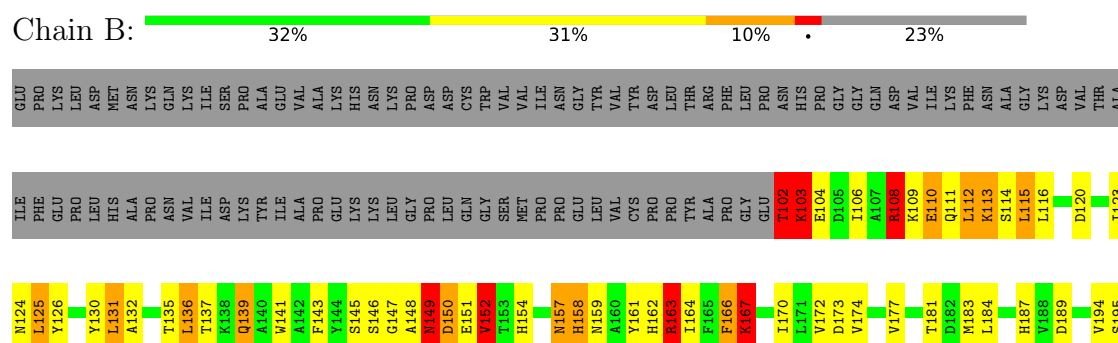
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

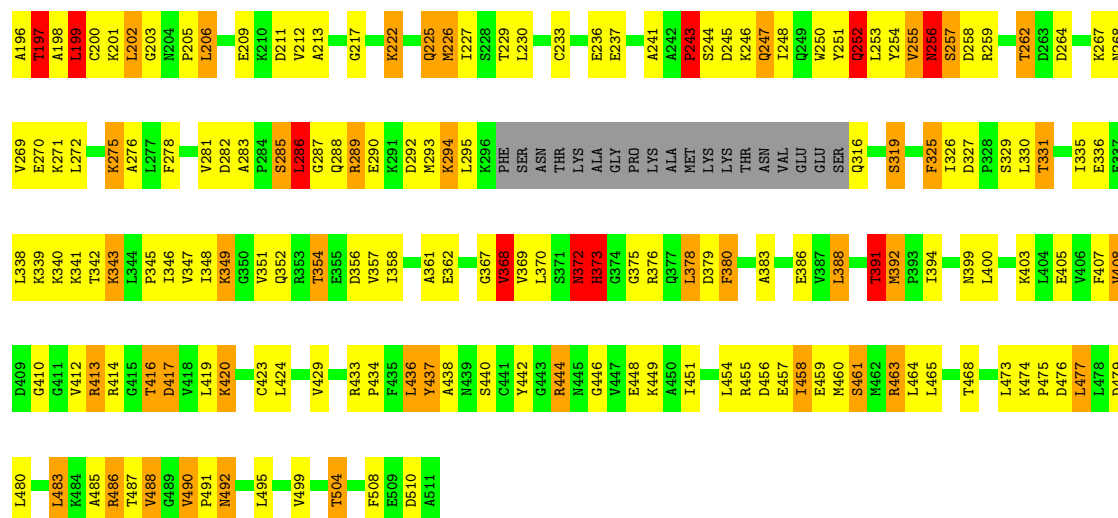
Note EDS was not executed.

• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.50Å 164.50Å 114.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FMN, HEM, PPY

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	1.25	14/3810 (0.4%)	2.24	182/5161 (3.5%)
1	B	1.26	11/3093 (0.4%)	2.19	144/4177 (3.4%)
All	All	1.25	25/6903 (0.4%)	2.22	326/9338 (3.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	HIS	CD2-NE2	-7.58	1.29	1.37
1	A	212	VAL	CA-CB	7.54	1.64	1.54
1	B	490	VAL	CA-CB	7.12	1.63	1.54
1	B	194	VAL	CA-CB	-6.83	1.45	1.54
1	A	158	HIS	CG-ND1	-6.83	1.30	1.38
1	B	158	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	154	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	373	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	154	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	19	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	158	HIS	CD2-NE2	-6.11	1.31	1.37
1	B	162	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	286	LEU	CB-CG	5.66	1.64	1.53
1	A	162	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	494	VAL	CA-CB	5.66	1.61	1.54
1	A	475	PRO	CA-CB	-5.39	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	HIS	CD2-NE2	-5.34	1.31	1.37
1	A	162	HIS	CG-ND1	-5.30	1.32	1.38
1	B	158	HIS	CG-ND1	-5.29	1.32	1.38
1	A	413	ARG	CZ-NH1	5.23	1.40	1.32
1	B	368	VAL	CA-CB	-5.21	1.47	1.54
1	A	191	PRO	CA-CB	-5.13	1.46	1.53
1	B	373	HIS	CG-ND1	-5.09	1.32	1.38
1	A	457	GLU	CA-CB	-5.08	1.45	1.53
1	A	187	HIS	CD2-NE2	-5.06	1.32	1.37

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CA-CB-CG	19.33	131.93	112.60
1	A	190	VAL	N-CA-CB	-13.59	97.09	111.64
1	A	379	ASP	CA-C-O	-13.33	104.00	119.60
1	B	372	ASN	CB-CG-ND2	12.09	134.53	116.40
1	B	149	ASN	CA-CB-CG	11.76	124.36	112.60
1	A	190	VAL	CB-CA-C	11.30	120.41	109.33
1	A	256	ASN	OD1-CG-ND2	-11.14	111.46	122.60
1	B	372	ASN	OD1-CG-ND2	-10.84	111.76	122.60
1	A	151	GLU	N-CA-C	10.26	125.37	112.86
1	A	124	ASN	OD1-CG-ND2	-10.24	112.36	122.60
1	A	357	VAL	N-CA-C	-10.20	99.89	111.00
1	A	117	PRO	O-C-N	-9.77	116.81	121.31
1	A	70	VAL	N-CA-C	9.67	120.48	110.62
1	B	417	ASP	CA-CB-CG	9.62	122.22	112.60
1	A	190	VAL	O-C-N	-9.38	115.78	121.69
1	A	435	PHE	CA-CB-CG	-9.37	104.43	113.80
1	B	256	ASN	OD1-CG-ND2	-9.17	113.43	122.60
1	B	486	ARG	N-CA-C	-9.14	92.57	108.20
1	A	497	ASN	OD1-CG-ND2	-9.09	113.51	122.60
1	A	223	VAL	N-CA-CB	-9.07	98.51	111.21
1	A	492	ASN	O-C-N	9.06	134.29	123.33
1	A	365	VAL	CA-C-O	-8.97	114.59	121.68
1	B	380	PHE	CA-CB-CG	-8.90	104.90	113.80
1	A	178	ASP	CA-CB-CG	8.81	121.42	112.60
1	B	159	ASN	CB-CG-ND2	8.65	129.38	116.40
1	A	256	ASN	CB-CG-ND2	8.61	129.31	116.40
1	A	372	ASN	OD1-CG-ND2	-8.55	114.05	122.60
1	A	124	ASN	CB-CG-ND2	8.48	129.12	116.40
1	B	212	VAL	N-CA-C	-8.47	102.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	THR	CA-C-O	-8.37	111.32	121.11
1	B	335	ILE	N-CA-C	-8.34	102.69	110.53
1	A	245	ASP	CA-CB-CG	8.19	120.78	112.60
1	A	417	ASP	CA-CB-CG	8.09	120.69	112.60
1	B	197	THR	N-CA-CB	-7.98	97.22	110.47
1	A	497	ASN	CB-CG-ND2	7.97	128.35	116.40
1	A	492	ASN	CA-CB-CG	7.96	120.56	112.60
1	A	176	LYS	N-CA-C	-7.96	96.77	109.59
1	B	474	LYS	O-C-N	-7.71	112.46	121.32
1	B	159	ASN	CA-CB-CG	7.68	120.28	112.60
1	A	226	MET	CG-SD-CE	-7.66	84.05	100.90
1	B	349	LYS	CG-CD-CE	-7.64	93.72	111.30
1	B	243	PRO	N-CA-C	7.63	123.83	113.98
1	B	327	ASP	CA-C-N	7.60	127.26	119.82
1	B	327	ASP	C-N-CA	7.60	127.26	119.82
1	A	254	TYR	O-C-N	-7.51	114.79	123.27
1	A	19	HIS	CB-CG-CD2	-7.50	121.45	131.20
1	A	24	ASP	CA-CB-CG	-7.47	105.13	112.60
1	A	115	LEU	N-CA-C	-7.43	103.68	112.89
1	B	247	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	A	365	VAL	N-CA-CB	-7.39	103.64	112.07
1	A	102	THR	CA-C-O	7.37	122.21	117.94
1	A	474	LYS	CA-C-O	-7.32	113.39	120.64
1	B	254	TYR	O-C-N	-7.29	114.71	123.16
1	A	481	SER	N-CA-C	7.24	121.21	112.38
1	B	154	HIS	CA-C-O	-7.20	113.20	120.90
1	B	373	HIS	CB-CG-CD2	-7.19	121.86	131.20
1	A	152	VAL	CA-C-O	-7.11	113.31	120.85
1	A	414	ARG	NE-CZ-NH1	7.11	128.61	121.50
1	A	43	HIS	CB-CG-CD2	-7.06	122.02	131.20
1	B	488	VAL	O-C-N	-7.04	115.21	123.03
1	B	444	ARG	CA-CB-CG	7.03	128.16	114.10
1	B	162	HIS	CA-CB-CG	-7.02	106.78	113.80
1	B	152	VAL	N-CA-C	-7.00	103.38	111.00
1	A	377	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	B	316	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	B	379	ASP	O-C-N	-6.98	112.49	122.41
1	B	264	ASP	N-CA-C	-6.98	103.29	111.03
1	B	463	ARG	N-CA-CB	-6.97	99.84	110.16
1	A	382	ARG	NE-CZ-NH2	-6.95	112.95	119.20
1	B	262	THR	CA-CB-OG1	-6.94	99.19	109.60
1	A	66	HIS	CB-CG-CD2	-6.93	122.18	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	PRO	CA-C-N	-6.93	110.45	122.37
1	A	491	PRO	C-N-CA	-6.93	110.45	122.37
1	A	465	LEU	N-CA-C	-6.92	103.96	112.88
1	B	147	GLY	O-C-N	-6.90	115.79	123.66
1	A	87	SER	N-CA-C	6.90	117.34	108.24
1	A	154	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	B	254	TYR	CA-C-O	-6.86	113.03	120.92
1	A	335	ILE	N-CA-C	-6.85	103.53	111.00
1	A	445	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	B	325	PHE	CA-CB-CG	6.83	120.63	113.80
1	A	93	VAL	N-CA-C	-6.81	98.05	107.99
1	A	43	HIS	ND1-CG-CD2	6.77	112.87	106.10
1	B	152	VAL	CA-C-O	-6.77	113.47	120.71
1	A	396	GLU	CA-C-O	-6.73	113.93	121.00
1	B	173	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	493	ASP	N-CA-C	6.68	125.03	110.80
1	A	217	GLY	O-C-N	-6.67	114.03	122.70
1	B	373	HIS	N-CA-C	6.67	120.99	112.86
1	A	94	CYS	CA-C-N	6.64	124.51	119.66
1	A	94	CYS	C-N-CA	6.64	124.51	119.66
1	A	170	ILE	N-CA-CB	-6.63	101.33	112.47
1	A	268	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	B	166	PHE	O-C-N	-6.62	114.94	122.68
1	A	23	ASP	CA-CB-CG	6.61	119.21	112.60
1	B	362	GLU	O-C-N	-6.59	115.13	122.12
1	A	466	GLY	O-C-N	-6.59	115.95	122.41
1	A	159	ASN	CB-CG-ND2	6.58	126.27	116.40
1	B	181	THR	N-CA-C	-6.58	99.66	108.74
1	B	352	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	422	LEU	O-C-N	-6.55	115.17	122.12
1	A	465	LEU	N-CA-CB	-6.52	100.62	110.73
1	A	507	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	197	THR	CB-CA-C	6.51	121.40	110.79
1	B	141	TRP	CG-CD2-CE3	6.50	140.40	133.90
1	B	375	GLY	O-C-N	6.50	128.49	122.57
1	A	386	GLU	CA-C-O	-6.48	114.02	120.70
1	A	37	THR	CA-CB-OG1	-6.43	99.96	109.60
1	A	184	LEU	N-CA-CB	-6.41	102.45	111.62
1	A	197	THR	N-CA-CB	-6.41	100.05	110.81
1	A	223	VAL	CA-C-N	6.40	126.35	119.76
1	A	223	VAL	C-N-CA	6.40	126.35	119.76
1	A	474	LYS	CA-C-N	6.40	126.15	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	LYS	C-N-CA	6.40	126.15	119.05
1	B	410	GLY	O-C-N	6.40	131.02	122.70
1	A	83	PRO	N-CA-C	6.37	121.18	111.19
1	A	61	ILE	N-CA-C	-6.36	104.55	110.53
1	A	492	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	A	179	ILE	N-CA-C	6.36	117.57	111.91
1	A	70	VAL	CB-CA-C	-6.35	103.57	112.14
1	A	110	GLU	CA-CB-CG	6.34	126.78	114.10
1	A	278	PHE	N-CA-C	-6.30	98.45	108.73
1	A	376	ARG	CD-NE-CZ	-6.30	115.58	124.40
1	B	256	ASN	CB-CG-ND2	6.29	125.83	116.40
1	A	106	ILE	CA-C-O	-6.28	113.49	120.46
1	A	162	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	B	379	ASP	CA-C-O	-6.26	111.73	119.18
1	B	391	THR	OG1-CB-CG2	-6.22	96.86	109.30
1	B	120	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	206	LEU	N-CA-C	6.20	117.70	111.07
1	A	409	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	417	ASP	N-CA-C	-6.16	104.49	111.14
1	B	464	LEU	O-C-N	-6.14	114.20	122.43
1	A	390	GLU	CA-C-O	-6.12	113.93	120.42
1	B	162	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	339	LYS	CB-CA-C	-6.07	100.71	110.79
1	B	289	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	B	199	LEU	N-CA-C	6.05	119.53	111.30
1	A	69	ASN	CB-CG-ND2	6.04	125.47	116.40
1	B	292	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	145	SER	CA-CB-OG	6.02	123.14	111.10
1	B	438	ALA	N-CA-C	-6.01	104.30	111.69
1	A	43	HIS	CA-C-N	6.00	125.48	119.24
1	A	43	HIS	C-N-CA	6.00	125.48	119.24
1	B	154	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	B	145	SER	N-CA-C	5.99	120.21	113.02
1	A	237	GLU	CB-CA-C	-5.98	100.69	110.85
1	A	24	ASP	O-C-N	5.96	130.59	123.33
1	B	449	LYS	CG-CD-CE	-5.95	97.61	111.30
1	A	438	ALA	N-CA-C	-5.95	104.71	111.14
1	A	20	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	B	492	ASN	CA-CB-CG	5.94	118.54	112.60
1	B	331	THR	N-CA-CB	-5.92	101.77	111.66
1	B	372	ASN	N-CA-CB	-5.92	102.95	111.54
1	A	498	GLU	N-CA-C	-5.92	104.91	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	GLN	N-CA-C	-5.91	104.76	111.14
1	B	212	VAL	CA-C-O	-5.91	114.49	121.05
1	A	19	HIS	CB-CG-ND1	5.89	131.53	122.70
1	B	226	MET	CG-SD-CE	-5.89	87.94	100.90
1	B	383	ALA	CA-C-N	5.88	125.36	119.24
1	B	383	ALA	C-N-CA	5.88	125.36	119.24
1	A	157	ASN	CB-CG-ND2	5.85	125.18	116.40
1	A	296	LYS	CA-CB-CG	-5.85	102.40	114.10
1	A	339	LYS	N-CA-CB	5.85	118.72	110.12
1	B	157	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	150	ASP	N-CA-C	5.83	123.22	110.80
1	A	168	PRO	CA-C-O	-5.83	114.69	121.34
1	A	379	ASP	CA-C-N	-5.83	111.49	122.27
1	A	379	ASP	C-N-CA	-5.83	111.49	122.27
1	A	78	GLU	CA-CB-CG	5.82	125.73	114.10
1	B	189	ASP	N-CA-C	5.81	117.62	111.28
1	B	510	ASP	CA-C-N	5.81	132.15	121.70
1	B	510	ASP	C-N-CA	5.81	132.15	121.70
1	A	240	GLU	CA-CB-CG	5.80	125.71	114.10
1	B	405	GLU	CA-CB-CG	-5.80	102.49	114.10
1	B	341	LYS	CA-CB-CG	5.79	125.69	114.10
1	A	479	ASP	O-C-N	-5.79	115.75	122.87
1	A	256	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	24	ASP	CA-C-O	5.77	130.05	122.44
1	B	368	VAL	N-CA-CB	-5.76	102.24	111.58
1	B	474	LYS	CA-C-N	5.75	125.45	119.64
1	B	474	LYS	C-N-CA	5.75	125.45	119.64
1	B	130	TYR	CA-C-O	-5.75	114.78	120.82
1	B	246	LYS	N-CA-C	5.75	120.13	113.18
1	B	226	MET	N-CA-C	-5.73	99.85	109.07
1	B	151	GLU	CA-C-N	-5.71	111.41	120.55
1	B	151	GLU	C-N-CA	-5.71	111.41	120.55
1	A	246	LYS	CA-CB-CG	-5.71	102.69	114.10
1	A	194	VAL	N-CA-CB	-5.70	104.51	111.00
1	B	264	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	382	ARG	CB-CG-CD	-5.69	98.22	111.30
1	A	116	LEU	CA-C-N	5.68	123.81	119.66
1	A	116	LEU	C-N-CA	5.68	123.81	119.66
1	B	461	SER	CA-CB-OG	-5.67	99.76	111.10
1	B	252	GLN	N-CA-C	-5.66	100.47	109.76
1	B	288	GLN	CA-CB-CG	5.66	125.41	114.10
1	B	292	ASP	CB-CA-C	-5.65	102.19	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	GLU	N-CA-C	-5.63	104.76	111.69
1	A	450	ALA	N-CA-C	-5.62	105.23	111.36
1	A	240	GLU	CB-CA-C	-5.62	101.46	110.79
1	B	159	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	433	ARG	CA-C-O	-5.62	113.22	118.73
1	A	379	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	43	HIS	CG-CD2-NE2	-5.61	101.59	107.20
1	A	476	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	362	GLU	CA-CB-CG	-5.61	102.88	114.10
1	A	187	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	297	PHE	N-CA-C	-5.60	105.05	112.94
1	B	195	SER	N-CA-C	-5.59	102.19	110.46
1	A	35	ASP	CA-C-O	5.58	126.34	120.54
1	A	285	SER	O-C-N	-5.58	115.97	123.23
1	B	348	ILE	CB-CG1-CD1	-5.58	102.09	113.80
1	A	259	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	A	47	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	B	189	ASP	O-C-N	5.55	128.00	122.12
1	B	454	LEU	N-CA-CB	-5.54	101.68	110.22
1	A	139	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	B	504	THR	CA-CB-OG1	-5.53	101.30	109.60
1	B	108	ARG	CA-C-O	-5.52	115.02	120.82
1	A	110	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	159	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	B	167	LYS	CA-C-N	5.50	125.45	119.78
1	B	167	LYS	C-N-CA	5.50	125.45	119.78
1	A	47	GLN	CA-CB-CG	5.49	125.09	114.10
1	B	354	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	397	GLN	CA-CB-CG	5.49	125.08	114.10
1	B	352	GLN	O-C-N	-5.48	114.64	122.04
1	B	369	VAL	CB-CA-C	-5.48	103.64	111.31
1	A	291	LYS	CG-CD-CE	5.48	123.89	111.30
1	A	180	SER	N-CA-C	-5.47	103.48	110.53
1	B	225	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	141	TRP	CB-CG-CD1	-5.46	118.71	126.90
1	B	286	LEU	CA-CB-CG	5.46	135.41	116.30
1	A	154	HIS	CA-C-O	-5.46	115.28	120.90
1	A	177	VAL	CA-C-O	-5.46	114.56	120.67
1	B	254	TYR	CA-C-N	-5.45	115.35	122.37
1	B	254	TYR	C-N-CA	-5.45	115.35	122.37
1	A	383	ALA	CA-C-N	5.44	125.78	119.47
1	A	383	ALA	C-N-CA	5.44	125.78	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	VAL	CA-C-O	-5.44	114.78	120.76
1	B	237	GLU	CA-C-N	5.40	127.45	120.70
1	B	237	GLU	C-N-CA	5.40	127.45	120.70
1	B	113	LYS	O-C-N	5.40	129.77	122.59
1	B	440	SER	CA-C-O	-5.39	113.77	119.97
1	B	115	LEU	N-CA-C	-5.39	107.08	113.97
1	B	408	VAL	O-C-N	-5.39	117.07	123.00
1	B	508	PHE	N-CA-C	-5.38	103.29	110.55
1	B	459	GLU	CB-CA-C	-5.37	102.45	110.88
1	B	437	TYR	N-CA-C	-5.37	106.73	113.28
1	A	484	LYS	O-C-N	-5.36	115.48	122.39
1	B	476	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	173	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	199	LEU	N-CA-C	5.35	122.19	110.80
1	B	163	ARG	CA-CB-CG	5.35	124.80	114.10
1	B	455	ARG	N-CA-C	-5.34	105.54	111.36
1	B	420	LYS	N-CA-C	-5.34	105.38	111.14
1	A	275	LYS	CA-CB-CG	-5.33	103.43	114.10
1	A	90	PRO	N-CA-C	5.31	123.42	112.47
1	A	228	SER	CA-C-O	-5.31	114.54	120.54
1	B	150	ASP	N-CA-CB	5.31	119.46	110.49
1	A	187	HIS	O-C-N	5.29	129.24	123.22
1	A	326	ILE	N-CA-C	-5.29	98.88	107.28
1	A	138	LYS	N-CA-C	5.28	117.72	111.33
1	A	111	GLN	CB-CG-CD	-5.28	103.63	112.60
1	B	196	ALA	N-CA-C	5.26	116.73	109.15
1	B	510	ASP	CA-C-O	5.26	126.00	119.79
1	B	114	SER	CA-C-N	-5.25	113.49	122.11
1	B	114	SER	C-N-CA	-5.25	113.49	122.11
1	B	463	ARG	CB-CA-C	5.25	119.78	110.85
1	A	52	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	69	ASN	N-CA-C	5.25	118.78	112.38
1	B	251	TYR	CB-CG-CD1	-5.25	112.93	120.80
1	B	245	ASP	N-CA-C	-5.25	105.74	111.82
1	B	463	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	B	110	GLU	CB-CG-CD	5.24	121.51	112.60
1	B	102	THR	N-CA-CB	-5.23	102.61	111.50
1	A	129	GLU	CB-CA-C	-5.23	102.64	110.90
1	B	172	VAL	N-CA-C	-5.23	100.59	108.12
1	B	444	ARG	CB-CG-CD	5.21	123.29	111.30
1	B	275	LYS	CA-CB-CG	-5.21	103.69	114.10
1	A	187	HIS	N-CA-C	-5.20	100.83	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	VAL	N-CA-C	-5.20	100.16	107.75
1	B	458	ILE	CA-C-O	-5.19	115.28	121.05
1	A	210	LYS	CA-CB-CG	-5.19	103.72	114.10
1	A	234	SER	CA-C-O	-5.18	115.08	120.88
1	A	225	GLN	CA-C-O	-5.17	114.63	120.32
1	A	89	PRO	CA-C-N	5.16	126.28	119.84
1	A	89	PRO	C-N-CA	5.16	126.28	119.84
1	A	405	GLU	CA-C-O	-5.15	114.72	120.54
1	A	26	TRP	N-CA-C	-5.15	101.76	109.95
1	A	88	MET	CA-C-N	5.15	125.68	120.38
1	A	88	MET	C-N-CA	5.15	125.68	120.38
1	A	10	LYS	CA-CB-CG	5.14	124.39	114.10
1	A	113	LYS	CA-CB-CG	5.14	124.38	114.10
1	A	225	GLN	CG-CD-NE2	5.13	124.10	116.40
1	A	43	HIS	ND1-CE1-NE2	5.13	113.53	108.40
1	A	229	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	463	ARG	N-CA-C	-5.12	105.39	110.97
1	B	483	LEU	CB-CA-C	-5.11	101.17	110.63
1	A	148	ALA	CB-CA-C	-5.11	101.51	109.84
1	B	146	SER	CA-CB-OG	5.11	121.31	111.10
1	B	335	ILE	CA-C-O	-5.10	115.38	121.05
1	A	413	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	A	377	GLN	N-CA-CB	-5.10	102.66	111.22
1	B	392	MET	CA-C-N	5.09	124.54	119.24
1	B	392	MET	C-N-CA	5.09	124.54	119.24
1	B	504	THR	N-CA-CB	-5.08	102.08	111.53
1	A	323	SER	O-C-N	-5.07	115.84	122.59
1	A	491	PRO	N-CA-C	-5.07	103.23	111.14
1	A	162	HIS	CB-CG-ND1	5.07	130.31	122.70
1	A	465	LEU	CB-CA-C	5.07	119.29	110.72
1	A	296	LYS	CB-CG-CD	5.06	122.94	111.30
1	A	240	GLU	CB-CG-CD	-5.06	104.00	112.60
1	A	212	VAL	N-CA-C	-5.05	104.67	111.44
1	A	135	THR	O-C-N	-5.05	115.24	122.41
1	A	34	TYR	CA-C-N	-5.05	116.28	122.84
1	A	34	TYR	C-N-CA	-5.05	116.28	122.84
1	A	57	ASP	N-CA-C	-5.04	100.30	108.41
1	B	259	ARG	N-CA-C	5.04	118.20	111.75
1	B	139	GLN	N-CA-CB	-5.01	102.75	110.12
1	B	163	ARG	N-CA-C	-5.01	107.16	113.28
1	A	347	VAL	CG1-CB-CG2	-5.01	99.77	110.80
1	B	316	GLN	CG-CD-NE2	5.01	123.92	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	GLU	CA-CB-CG	-5.01	104.08	114.10
1	A	349	LYS	CA-C-O	-5.01	114.81	120.32
1	A	507	GLU	N-CA-CB	-5.01	102.50	110.06

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ASP	Peptide
1	A	492	ASN	Mainchain

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	3736	811	3793	120	0
1	B	3045	687	3112	127	0
2	A	43	4	30	3	0
3	A	31	4	19	4	0
3	B	31	4	19	7	0
4	A	12	0	7	1	0
4	B	12	0	7	2	0
5	A	152	304	0	9	0
5	B	13	26	0	0	0
All	All	7075	1840	6987	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (236) 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:B:143:PHE:HA	1:B:289:ARG:HH22	1.45	0.79
1:B:290:GLU:HA	1:B:293:MET:HG3	1.64	0.79
1:A:226:MET:HE1	1:A:349:LYS:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HG	1:A:47:GLN:HB2	1.67	0.76
1:B:197:THR:HG21	1:B:436:LEU:HG	1.67	0.75
1:A:291:LYS:HD2	5:A:754:HOH:O	1.87	0.73
1:A:460:MET:HE2	1:B:285:SER:HB2	1.70	0.73
1:A:465:LEU:HD23	1:B:378:LEU:HD11	1.72	0.72
1:B:351:VAL:HG11	1:B:357:VAL:HG23	1.72	0.71
1:B:199:LEU:HD11	4:B:580:PPY:H3'	1.73	0.70
1:B:108:ARG:O	1:B:112:LEU:HD23	1.92	0.70
1:A:431:LEU:HD23	1:A:434:PRO:HG2	1.73	0.69
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.08	0.68
1:A:13:PRO:HB2	5:A:764:HOH:O	1.94	0.67
1:A:196:ALA:H	1:A:226:MET:HE2	1.59	0.66
1:A:16:VAL:HA	1:A:26:TRP:HE3	1.61	0.66
1:A:190:VAL:HG11	1:A:223:VAL:HG22	1.77	0.65
1:A:112:LEU:HG	1:A:135:THR:HB	1.78	0.65
1:B:197:THR:CG2	1:B:436:LEU:HG	2.27	0.64
1:B:269:VAL:HA	1:B:272:LEU:HD12	1.81	0.63
1:B:256:ASN:HD22	1:B:257:SER:N	1.95	0.63
1:A:361:ALA:HB1	1:A:400:LEU:HD22	1.81	0.63
1:A:132:ALA:HA	5:A:634:HOH:O	1.97	0.62
1:A:226:MET:HE3	1:A:252:GLN:HB2	1.82	0.62
1:B:226:MET:HE3	1:B:252:GLN:HB3	1.81	0.61
1:B:201:LYS:HE3	1:B:233:CYS:SG	2.40	0.61
1:B:461:SER:O	1:B:465:LEU:HD12	2.01	0.61
1:A:16:VAL:HA	1:A:26:TRP:CE3	2.35	0.61
1:B:157:ASN:HD21	1:B:372:ASN:HD21	1.48	0.61
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.83	0.60
1:A:385:ILE:HD11	1:A:424:LEU:HD12	1.84	0.60
1:A:256:ASN:HD22	1:A:257:SER:N	2.00	0.60
1:B:143:PHE:HA	1:B:289:ARG:NH2	2.16	0.59
1:B:416:THR:O	1:B:420:LYS:HG3	2.02	0.59
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.84	0.59
3:A:570:FMN:O4'	3:A:570:FMN:H1'2	2.02	0.59
1:A:162:HIS:HE1	5:A:670:HOH:O	1.86	0.58
1:A:490:VAL:HG22	1:A:492:ASN:ND2	2.19	0.58
1:A:270:GLU:OE1	1:A:343:LYS:HG3	2.04	0.58
1:B:347:VAL:HG13	1:B:367:GLY:C	2.29	0.58
1:A:508:PHE:CZ	1:B:131:LEU:HD12	2.39	0.58
1:A:218:GLN:NE2	1:A:444:ARG:HH11	2.01	0.58
1:A:144:TYR:O	1:A:433:ARG:HD3	2.04	0.57
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:HD22	1:B:126:TYR:H	1.53	0.57
1:B:400:LEU:HA	1:B:403:LYS:HD3	1.86	0.57
1:A:372:ASN:HD22	1:A:375:GLY:H	1.50	0.57
1:A:373:HIS:O	1:A:376:ARG:HG3	2.04	0.56
1:A:460:MET:HE3	1:B:286:LEU:O	2.06	0.56
1:A:234:SER:OG	1:A:237:GLU:HG3	2.06	0.56
1:A:511:ALA:H	1:B:115:LEU:HD13	1.71	0.56
1:B:108:ARG:HG2	1:B:135:THR:O	2.06	0.55
1:B:256:ASN:HA	1:B:325:PHE:O	2.07	0.55
1:A:285:SER:HA	1:A:321:ALA:O	2.06	0.55
1:B:148:ALA:N	1:B:376:ARG:HA	2.21	0.55
1:B:354:THR:HA	1:B:391:THR:HG22	1.89	0.55
1:A:218:GLN:HE22	1:A:444:ARG:HH11	1.54	0.55
1:A:358:ILE:HD11	1:A:394:ILE:HG21	1.89	0.55
1:A:490:VAL:HG22	1:A:492:ASN:HD22	1.72	0.55
1:A:270:GLU:HB3	1:A:343:LYS:NZ	2.21	0.54
1:B:424:LEU:HD21	1:B:480:LEU:HD11	1.87	0.54
1:A:244:SER:O	1:A:247:GLN:HG2	2.07	0.54
1:B:152:VAL:HG21	1:B:380:PHE:CE2	2.43	0.54
1:A:152:VAL:HG21	1:A:380:PHE:CE2	2.43	0.53
1:A:168:PRO:HG3	1:B:378:LEU:HD12	1.90	0.53
1:A:173:ASP:OD1	1:B:329:SER:HA	2.08	0.53
1:A:40:LEU:HD11	1:A:51:LYS:HG3	1.90	0.53
1:B:211:ASP:O	1:B:444:ARG:HB3	2.08	0.53
1:B:183:MET:CE	1:B:250:TRP:HH2	2.23	0.52
1:B:103:LYS:O	1:B:106:ILE:HG12	2.09	0.52
1:B:125:LEU:HG	1:B:434:PRO:HB3	1.92	0.52
1:A:460:MET:SD	1:A:460:MET:C	2.92	0.52
2:A:560:HEM:HBD1	4:A:580:PPY:H4'	1.91	0.51
1:B:199:LEU:HB2	1:B:202:LEU:HD12	1.90	0.51
1:B:403:LYS:HD2	1:B:403:LYS:N	2.25	0.51
1:A:282:ASP:O	1:A:377:GLN:HG2	2.10	0.51
1:B:109:LYS:O	1:B:113:LYS:HB3	2.11	0.51
1:B:111:GLN:HB3	1:B:135:THR:HG22	1.93	0.51
1:B:276:ALA:HA	1:B:345:PRO:HD2	1.91	0.51
1:A:24:ASP:HA	1:A:37:THR:OG1	2.10	0.51
1:A:256:ASN:ND2	1:A:258:ASP:H	2.09	0.51
1:A:460:MET:CE	1:B:285:SER:HB2	2.39	0.51
1:A:234:SER:HG	1:A:237:GLU:HG3	1.76	0.51
1:B:229:THR:OG1	1:B:253:LEU:HA	2.09	0.51
1:A:89:PRO:HD3	5:A:764:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ARG:HG3	1:B:457:GLU:OE1	2.11	0.50
1:A:392:MET:HG3	1:A:424:LEU:O	2.12	0.49
1:A:125:LEU:HG	1:A:434:PRO:HB3	1.92	0.49
1:B:198:ALA:HB1	4:B:580:PPY:H2'	1.94	0.49
1:A:109:LYS:HA	1:A:112:LEU:HD12	1.93	0.49
1:A:170:ILE:HD11	1:B:282:ASP:HA	1.94	0.49
1:A:66:HIS:HA	2:A:560:HEM:O2A	2.13	0.49
1:A:197:THR:HG23	1:A:436:LEU:HD21	1.93	0.49
1:B:349:LYS:NZ	3:B:570:FMN:H2'	2.28	0.49
1:B:124:ASN:HD21	1:B:126:TYR:HB2	1.78	0.49
1:B:339:LYS:HA	1:B:346:ILE:HD11	1.95	0.48
1:B:354:THR:OG1	1:B:391:THR:HG22	2.12	0.48
1:B:357:VAL:HG22	1:B:368:VAL:HG11	1.95	0.48
1:A:196:ALA:HB1	1:A:228:SER:HB2	1.95	0.48
1:A:105:ASP:O	1:A:109:LYS:HG3	2.13	0.48
1:A:110:GLU:HA	1:A:113:LYS:HG3	1.96	0.48
3:A:570:FMN:H1'2	3:A:570:FMN:H9	1.64	0.48
1:A:442:TYR:HB2	1:A:446:GLY:HA3	1.96	0.48
1:B:136:LEU:N	1:B:136:LEU:HD23	2.29	0.48
3:B:570:FMN:H9	3:B:570:FMN:O4'	2.14	0.48
1:A:270:GLU:HB3	1:A:343:LYS:HZ1	1.78	0.48
1:B:166:PHE:CE2	1:B:416:THR:HG22	2.48	0.48
1:B:349:LYS:HZ1	3:B:570:FMN:H2'	1.79	0.48
1:B:358:ILE:HD11	1:B:394:ILE:CG2	2.44	0.48
1:A:179:ILE:HD11	1:A:455:ARG:HG2	1.96	0.47
1:A:412:VAL:HG21	1:A:429:VAL:CG1	2.44	0.47
1:A:57:ASP:HB2	1:A:88:MET:HG3	1.96	0.47
1:A:175:ARG:HH11	1:A:175:ARG:HB2	1.79	0.47
1:A:113:LYS:O	1:A:115:LEU:N	2.45	0.47
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.45	0.47
1:B:149:ASN:HB3	1:B:290:GLU:OE2	2.14	0.47
1:A:163:ARG:NH1	1:A:486:ARG:HA	2.29	0.47
1:A:252:GLN:HA	1:A:278:PHE:O	2.14	0.47
1:B:183:MET:HE3	1:B:407:PHE:HE2	1.78	0.47
1:B:213:ALA:CA	1:B:225:GLN:HE22	2.28	0.47
1:B:423:CYS:O	1:B:475:PRO:HG3	2.15	0.47
1:A:508:PHE:CE1	1:B:131:LEU:HD12	2.50	0.47
1:B:164:ILE:HB	1:B:420:LYS:HD3	1.97	0.47
1:A:508:PHE:CE2	1:B:116:LEU:HD23	2.50	0.46
1:B:124:ASN:HD22	1:B:126:TYR:N	2.13	0.46
1:B:256:ASN:HD22	1:B:257:SER:H	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLU:HG3	1:A:455:ARG:NH2	2.31	0.46
1:B:278:PHE:HA	1:B:347:VAL:O	2.15	0.46
1:A:16:VAL:HG21	1:A:84:LEU:HD12	1.98	0.46
1:A:214:ARG:HA	1:A:243:PRO:HD3	1.97	0.46
1:A:171:LEU:HD21	1:B:281:VAL:HG11	1.97	0.46
1:A:107:ALA:HA	1:A:110:GLU:HG3	1.98	0.46
1:A:184:LEU:HD21	1:A:347:VAL:HG21	1.98	0.46
1:B:177:VAL:HG23	1:B:468:THR:HA	1.98	0.46
1:B:283:ALA:O	1:B:326:ILE:HG21	2.16	0.46
1:A:199:LEU:HD21	2:A:560:HEM:HAA2	1.97	0.45
1:B:109:LYS:NZ	1:B:112:LEU:HD11	2.31	0.45
1:B:252:GLN:HA	1:B:278:PHE:O	2.15	0.45
1:A:470:ILE:HA	1:A:473:LEU:HD12	1.96	0.45
1:A:113:LYS:C	1:A:115:LEU:H	2.24	0.45
1:A:270:GLU:HG2	1:A:344:LEU:HG	1.98	0.45
1:A:288:GLN:HG3	1:A:293:MET:SD	2.57	0.45
1:B:149:ASN:O	1:B:150:ASP:HB2	2.17	0.45
1:B:358:ILE:HD11	1:B:394:ILE:HG22	1.98	0.45
1:B:412:VAL:HG13	1:B:417:ASP:HB2	1.98	0.45
1:A:413:ARG:HA	1:A:413:ARG:HD3	1.84	0.45
1:B:166:PHE:HE2	1:B:416:THR:HG22	1.82	0.45
1:B:256:ASN:ND2	1:B:258:ASP:H	2.15	0.45
1:A:67:ALA:HA	1:A:232:SER:O	2.17	0.45
1:A:338:LEU:HD13	1:A:346:ILE:HD12	1.99	0.45
1:A:342:THR:HG21	1:A:346:ILE:HD11	1.98	0.45
1:A:508:PHE:HE2	1:B:116:LEU:HD23	1.82	0.45
1:B:109:LYS:HZ1	1:B:112:LEU:HD11	1.81	0.45
1:B:255:VAL:HG13	1:B:330:LEU:HD11	1.99	0.45
3:B:570:FMN:O4'	3:B:570:FMN:H1'2	2.17	0.45
1:A:10:LYS:HB3	5:A:761:HOH:O	2.17	0.45
1:A:107:ALA:O	1:A:110:GLU:HG3	2.17	0.45
1:A:255:VAL:HG11	1:A:330:LEU:HD21	1.99	0.45
1:B:256:ASN:HD22	1:B:258:ASP:H	1.64	0.45
1:B:419:LEU:HD21	1:B:458:ILE:HG23	1.98	0.45
1:B:361:ALA:CB	1:B:400:LEU:HD13	2.48	0.44
1:B:448:GLU:O	1:B:451:ILE:HB	2.17	0.44
1:B:495:LEU:O	1:B:499:VAL:HG22	2.18	0.44
1:A:21:LYS:HB3	1:A:23:ASP:O	2.18	0.44
1:A:286:LEU:HA	1:A:377:GLN:HE22	1.82	0.44
1:A:510:ASP:N	1:B:115:LEU:HD22	2.33	0.44
1:B:241:ALA:O	1:B:243:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:NZ	3:A:570:FMN:H2'	2.33	0.44
1:A:216:CYS:O	1:A:222:LYS:HA	2.18	0.44
1:A:349:LYS:HA	1:A:369:VAL:HB	2.00	0.44
1:B:163:ARG:HD2	1:B:485:ALA:O	2.17	0.44
1:B:270:GLU:OE2	1:B:343:LYS:HB3	2.18	0.44
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.77	0.44
1:B:108:ARG:NH2	1:B:137:THR:HA	2.33	0.44
1:B:158:HIS:O	1:B:161:TYR:HB2	2.18	0.44
1:B:413:ARG:HH22	3:B:570:FMN:P	2.41	0.43
1:A:217:GLY:O	1:A:222:LYS:NZ	2.50	0.43
1:B:456:ASP:O	1:B:460:MET:HG3	2.18	0.43
3:B:570:FMN:H9	3:B:570:FMN:H1'2	1.55	0.43
1:A:123:ILE:HD12	1:B:294:LYS:HG2	2.00	0.43
1:B:166:PHE:HE2	1:B:416:THR:CG2	2.32	0.43
1:B:213:ALA:HA	1:B:225:GLN:HE22	1.83	0.43
1:B:203:GLY:O	1:B:205:PRO:HD3	2.18	0.43
1:A:349:LYS:HZ1	3:A:570:FMN:H2'	1.84	0.43
1:B:199:LEU:HD23	1:B:230:LEU:O	2.19	0.43
1:B:400:LEU:O	1:B:403:LYS:HB2	2.19	0.43
1:B:106:ILE:O	1:B:110:GLU:HG2	2.17	0.43
1:B:388:LEU:HD22	1:B:392:MET:CG	2.49	0.43
1:A:136:LEU:N	5:A:634:HOH:O	2.52	0.43
1:B:148:ALA:H	1:B:376:ARG:HA	1.83	0.43
1:B:213:ALA:HA	1:B:225:GLN:NE2	2.34	0.43
1:B:174:VAL:O	1:B:463:ARG:HD3	2.17	0.43
1:B:465:LEU:HD23	1:B:477:LEU:HG	2.00	0.42
1:A:12:SER:HA	1:A:13:PRO:HD2	1.79	0.42
1:A:196:ALA:CB	1:A:226:MET:HE2	2.49	0.42
1:B:132:ALA:HB2	1:B:437:TYR:HB3	2.01	0.42
1:B:278:PHE:CD2	1:B:347:VAL:HB	2.54	0.42
1:B:108:ARG:HH21	1:B:137:THR:HA	1.83	0.42
1:B:268:ASN:O	1:B:271:LYS:HB3	2.20	0.42
1:B:433:ARG:HB3	1:B:437:TYR:CE2	2.54	0.42
1:A:414:ARG:NH2	1:B:290:GLU:OE2	2.53	0.42
1:B:351:VAL:HG13	1:B:356:ASP:HB2	2.02	0.42
1:A:166:PHE:C	1:A:168:PRO:HD3	2.44	0.42
1:A:405:GLU:OE1	1:A:427:LYS:HG2	2.20	0.42
1:B:286:LEU:HD13	1:B:287:GLY:O	2.20	0.42
1:A:194:VAL:HG22	1:A:435:PHE:CD2	2.55	0.42
1:A:210:LYS:HE3	1:A:210:LYS:HB2	1.78	0.42
1:B:222:LYS:HD2	1:B:222:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:NH1	1:B:488:VAL:O	2.53	0.41
1:A:390:GLU:HB2	5:A:739:HOH:O	2.19	0.41
1:A:458:ILE:HD13	1:A:458:ILE:HG21	1.82	0.41
1:B:102:THR:HB	1:B:104:GLU:OE2	2.20	0.41
1:B:111:GLN:CB	1:B:135:THR:HG22	2.50	0.41
1:A:197:THR:HG22	1:A:200:CYS:SG	2.60	0.41
1:A:322:LEU:HB2	5:A:730:HOH:O	2.19	0.41
1:A:269:VAL:O	1:A:274:VAL:HG22	2.21	0.41
1:A:144:TYR:CD1	1:A:436:LEU:HD13	2.56	0.41
1:B:282:ASP:CG	1:B:373:HIS:HD1	2.29	0.41
1:A:128:PHE:CD1	1:A:438:ALA:HA	2.55	0.41
1:A:294:LYS:NZ	1:A:294:LYS:HB2	2.36	0.41
1:B:290:GLU:HA	1:B:293:MET:CG	2.43	0.41
1:B:336:GLU:O	1:B:339:LYS:HB2	2.21	0.41
1:A:24:ASP:H	1:A:37:THR:HG23	1.86	0.41
1:A:40:LEU:HD12	1:A:50:ILE:HB	2.03	0.41
1:A:372:ASN:ND2	1:A:375:GLY:H	2.19	0.41
1:B:167:LYS:HD2	1:B:479:ASP:HB2	2.03	0.41
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.93	0.40
1:A:223:VAL:HA	1:A:224:PRO:HD3	2.01	0.40
1:A:256:ASN:HD22	1:A:258:ASP:H	1.67	0.40
1:A:346:ILE:HB	1:A:365:VAL:HG22	2.03	0.40
1:B:123:ILE:HD13	1:B:123:ILE:HG21	1.81	0.40
1:A:13:PRO:O	1:A:16:VAL:HB	2.22	0.40
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.89	0.40
1:A:465:LEU:CD1	1:A:477:LEU:HG	2.52	0.40
1:B:183:MET:HE2	1:B:250:TRP:HH2	1.86	0.40
1:B:413:ARG:NH2	3:B:570:FMN:O1P	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/511 (93%)	428 (90%)	39 (8%)	9 (2%)	6	23
1	B	387/511 (76%)	348 (90%)	33 (8%)	6 (2%)	7	27
All	All	863/1022 (84%)	776 (90%)	72 (8%)	15 (2%)	7	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	A	104	GLU
1	A	114	SER
1	A	119	LEU
1	A	493	ASP
1	B	319	SER
1	B	103	LYS
1	A	65	LEU
1	A	90	PRO
1	A	199	LEU
1	B	340	LYS
1	A	23	ASP
1	A	464	LEU
1	B	399	ASN
1	B	200	CYS

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	412/440 (94%)	341 (83%)	71 (17%)	2	7
1	B	336/440 (76%)	278 (83%)	58 (17%)	2	7
All	All	748/880 (85%)	619 (83%)	129 (17%)	2	7

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS

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Mol	Chain	Res	Type
1	A	15	GLU
1	A	19	HIS
1	A	20	ASN
1	A	21	LYS
1	A	23	ASP
1	A	27	VAL
1	A	28	VAL
1	A	32	TYR
1	A	38	ARG
1	A	64	PRO
1	A	65	LEU
1	A	72	ASP
1	A	78	GLU
1	A	81	LEU
1	A	90	PRO
1	A	101	GLU
1	A	113	LYS
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	137	THR
1	A	152	VAL
1	A	169	LYS
1	A	170	ILE
1	A	175	ARG
1	A	178	ASP
1	A	184	LEU
1	A	190	VAL
1	A	191	PRO
1	A	195	SER
1	A	197	THR
1	A	206	LEU
1	A	212	VAL
1	A	229	THR
1	A	230	LEU
1	A	232	SER
1	A	236	GLU
1	A	255	VAL
1	A	256	ASN
1	A	261	ILE
1	A	263	ASP
1	A	265	LEU

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Mol	Chain	Res	Type
1	A	271	LYS
1	A	292	ASP
1	A	294	LYS
1	A	325	PHE
1	A	329	SER
1	A	330	LEU
1	A	338	LEU
1	A	341	LYS
1	A	343	LYS
1	A	359	LYS
1	A	365	VAL
1	A	366	SER
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU
1	A	397	GLN
1	A	399	ASN
1	A	408	VAL
1	A	452	GLU
1	A	460	MET
1	A	464	LEU
1	A	483	LEU
1	A	490	VAL
1	A	492	ASN
1	A	494	VAL
1	A	506	THR
1	A	509	GLU
1	B	102	THR
1	B	103	LYS
1	B	108	ARG
1	B	112	LEU
1	B	125	LEU
1	B	131	LEU
1	B	136	LEU
1	B	139	GLN
1	B	152	VAL
1	B	163	ARG
1	B	167	LYS
1	B	170	ILE
1	B	184	LEU
1	B	197	THR

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Mol	Chain	Res	Type
1	B	199	LEU
1	B	202	LEU
1	B	206	LEU
1	B	209	GLU
1	B	222	LYS
1	B	227	ILE
1	B	236	GLU
1	B	243	PRO
1	B	244	SER
1	B	248	ILE
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	257	SER
1	B	262	THR
1	B	267	LYS
1	B	275	LYS
1	B	285	SER
1	B	286	LEU
1	B	294	LYS
1	B	295	LEU
1	B	319	SER
1	B	331	THR
1	B	338	LEU
1	B	342	THR
1	B	343	LYS
1	B	368	VAL
1	B	370	LEU
1	B	372	ASN
1	B	373	HIS
1	B	378	LEU
1	B	388	LEU
1	B	391	THR
1	B	408	VAL
1	B	413	ARG
1	B	416	THR
1	B	429	VAL
1	B	436	LEU
1	B	477	LEU
1	B	483	LEU
1	B	490	VAL
1	B	491	PRO

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Mol	Chain	Res	Type
1	B	492	ASN
1	B	504	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	85	GLN
1	A	124	ASN
1	A	157	ASN
1	A	159	ASN
1	A	162	HIS
1	A	218	GLN
1	A	252	GLN
1	A	256	ASN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	A	492	ASN
1	A	497	ASN
1	B	121	ASN
1	B	124	ASN
1	B	149	ASN
1	B	218	GLN
1	B	225	GLN
1	B	247	GLN
1	B	256	ASN
1	B	268	ASN
1	B	372	ASN
1	B	397	GLN
1	B	492	ASN
1	B	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

5 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
4	PPY	B	580	-	12,12,12	2.61	3 (25%)	14,15,15	1.48	4 (28%)
4	PPY	A	580	-	12,12,12	2.28	2 (16%)	14,15,15	1.73	2 (14%)
2	HEM	A	560	1	50,50,50	1.24	5 (10%)	67,82,82	1.03	2 (2%)
3	FMN	A	570	-	33,33,33	2.13	9 (27%)	48,50,50	2.45	20 (41%)
3	FMN	B	570	-	33,33,33	2.01	11 (33%)	48,50,50	2.26	18 (37%)

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
4	PPY	B	580	-	-	0/8/8/8	0/1/1/1
4	PPY	A	580	-	-	1/8/8/8	0/1/1/1
2	HEM	A	560	1	-	11/14/54/54	-
3	FMN	A	570	-	2/2/4/4	12/18/18/18	0/3/3/3
3	FMN	B	570	-	2/2/4/4	8/18/18/18	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	580	PPY	C2-C1	-7.62	1.42	1.53
4	A	580	PPY	C2-C1	-6.68	1.43	1.53
3	A	570	FMN	C1'-N10	-6.05	1.33	1.47
3	B	570	FMN	C1'-N10	-5.40	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	570	FMN	C2'-C3'	-5.12	1.44	1.53
3	B	570	FMN	C9-C8	-4.61	1.33	1.39
4	B	580	PPY	C3-C2	3.93	1.55	1.51
3	B	570	FMN	C2'-C3'	-3.81	1.46	1.53
3	A	570	FMN	C6-C7	-3.55	1.34	1.39
2	A	560	HEM	CBB-CAB	3.54	1.47	1.30
2	A	560	HEM	CAC-C3C	-3.22	1.38	1.47
4	A	580	PPY	C3-C2	3.17	1.55	1.51
3	A	570	FMN	C6-C5A	-3.17	1.35	1.40
2	A	560	HEM	CBC-CAC	3.15	1.45	1.30
3	A	570	FMN	C10-N1	3.13	1.39	1.33
3	B	570	FMN	C4A-N5	2.97	1.37	1.30
3	B	570	FMN	C10-N1	2.84	1.39	1.33
3	A	570	FMN	C9-C8	-2.82	1.35	1.39
3	B	570	FMN	C9-C9A	-2.64	1.35	1.39
3	A	570	FMN	C5A-N5	-2.63	1.34	1.39
3	B	570	FMN	C9A-N10	-2.63	1.36	1.41
3	B	570	FMN	C6-C7	-2.57	1.36	1.39
2	A	560	HEM	CAB-C3B	-2.57	1.40	1.47
3	A	570	FMN	C4A-N5	2.45	1.36	1.30
3	B	570	FMN	C6-C5A	-2.37	1.36	1.40
4	B	580	PPY	O2-C1	-2.21	1.24	1.30
2	A	560	HEM	O2A-CGA	-2.19	1.23	1.30
3	B	570	FMN	C5A-N5	-2.13	1.35	1.39
3	A	570	FMN	C9A-N10	-2.07	1.37	1.41
3	B	570	FMN	C9A-C5A	-2.07	1.37	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	FMN	O4'-C4'-C5'	5.62	122.38	109.99
3	A	570	FMN	C4A-C10-N1	-5.56	110.96	124.59
3	B	570	FMN	C4'-C3'-C2'	5.20	122.22	113.57
3	B	570	FMN	C10-N1-C2	4.86	127.38	116.85
3	B	570	FMN	C4A-C10-N1	-4.76	112.92	124.59
3	A	570	FMN	C4-C4A-C10	4.74	125.06	116.93
3	A	570	FMN	C7M-C7-C6	-4.63	111.41	119.57
4	A	580	PPY	C1'-C3-C2	-4.58	105.99	113.56
3	A	570	FMN	C10-N1-C2	4.50	126.59	116.85
3	B	570	FMN	C5A-C9A-N10	4.46	122.00	117.97
3	A	570	FMN	O4'-C4'-C3'	4.12	118.89	109.25
3	B	570	FMN	C4-C4A-C10	4.05	123.87	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	FMN	C4-C4A-N5	-3.77	112.99	118.21
2	A	560	HEM	C3B-C4B-NB	3.60	112.06	109.47
3	B	570	FMN	C8M-C8-C9	-3.54	113.34	119.57
3	A	570	FMN	N10-C10-N1	3.31	128.26	118.51
3	A	570	FMN	C7M-C7-C8	3.29	127.48	120.76
3	B	570	FMN	C4A-C10-N10	3.19	121.05	116.48
3	B	570	FMN	C9A-N10-C10	-3.04	116.12	120.75
3	B	570	FMN	C8M-C8-C7	2.99	126.87	120.76
3	B	570	FMN	C4-C4A-N5	-2.98	114.09	118.21
3	A	570	FMN	C4A-C10-N10	2.96	120.71	116.48
3	B	570	FMN	C9-C9A-N10	-2.94	117.89	121.85
4	B	580	PPY	C1'-C3-C2	2.89	118.33	113.56
3	A	570	FMN	O2'-C2'-C1'	2.87	121.99	110.20
4	B	580	PPY	O2-C1-O1	-2.87	117.08	123.90
3	B	570	FMN	O4'-C4'-C3'	2.86	115.95	109.25
3	A	570	FMN	C9A-N10-C10	-2.72	116.61	120.75
3	B	570	FMN	O5'-C5'-C4'	2.71	116.59	109.36
3	A	570	FMN	C4'-C3'-C2'	2.70	118.06	113.57
3	A	570	FMN	O3'-C3'-C4'	2.65	114.95	108.93
3	A	570	FMN	C8M-C8-C7	2.64	126.15	120.76
3	B	570	FMN	O2-C2-N3	2.63	123.64	118.58
3	A	570	FMN	C8M-C8-C9	-2.56	115.05	119.57
3	A	570	FMN	O3P-P-O5'	-2.50	100.16	106.67
4	B	580	PPY	O3-C2-C1	-2.48	116.12	119.67
4	A	580	PPY	O2-C1-O1	-2.42	118.13	123.90
3	B	570	FMN	O2'-C2'-C1'	2.41	120.12	110.20
4	B	580	PPY	O2-C1-C2	2.38	120.19	113.59
3	B	570	FMN	O3P-P-O5'	-2.38	100.48	106.67
3	B	570	FMN	O3P-P-O2P	2.37	116.70	107.80
3	B	570	FMN	N10-C10-N1	2.37	125.48	118.51
3	A	570	FMN	O3P-P-O2P	2.32	116.51	107.80
3	A	570	FMN	C5A-C9A-N10	2.30	120.05	117.97
3	A	570	FMN	C6-C5A-N5	-2.11	114.95	118.44
2	A	560	HEM	C2B-C1B-NB	2.03	112.17	109.84

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	570	FMN	C2'
3	A	570	FMN	C4'
3	B	570	FMN	C2'
3	B	570	FMN	C4'

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	560	HEM	C3A-C2A-CAA-CBA
2	A	560	HEM	C2C-C3C-CAC-CBC
2	A	560	HEM	C4C-C3C-CAC-CBC
3	A	570	FMN	N10-C1'-C2'-O2'
3	A	570	FMN	C1'-C2'-C3'-O3'
3	A	570	FMN	O2'-C2'-C3'-O3'
3	A	570	FMN	C2'-C3'-C4'-O4'
3	A	570	FMN	O3'-C3'-C4'-O4'
3	A	570	FMN	O3'-C3'-C4'-C5'
3	A	570	FMN	O4'-C4'-C5'-O5'
3	A	570	FMN	C5'-O5'-P-O2P
3	A	570	FMN	C5'-O5'-P-O3P
3	B	570	FMN	N10-C1'-C2'-O2'
3	B	570	FMN	C3'-C4'-C5'-O5'
3	B	570	FMN	O4'-C4'-C5'-O5'
4	A	580	PPY	O2-C1-C2-C3
2	A	560	HEM	C2A-CAA-CBA-CGA
3	B	570	FMN	O3'-C3'-C4'-O4'
2	A	560	HEM	C3D-CAD-CBD-CGD
3	B	570	FMN	C2'-C3'-C4'-O4'
2	A	560	HEM	C2B-C3B-CAB-CBB
3	A	570	FMN	C5'-O5'-P-O1P
3	B	570	FMN	C4'-C5'-O5'-P
3	A	570	FMN	C4'-C5'-O5'-P
2	A	560	HEM	C4B-C3B-CAB-CBB
3	B	570	FMN	C2'-C1'-N10-C10
3	A	570	FMN	O2'-C2'-C3'-C4'
2	A	560	HEM	CAD-CBD-CGD-O1D
2	A	560	HEM	CAD-CBD-CGD-O2D
2	A	560	HEM	CAA-CBA-CGA-O1A
3	B	570	FMN	O3'-C3'-C4'-C5'
2	A	560	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

5 monomers are involved in 16 short contacts:

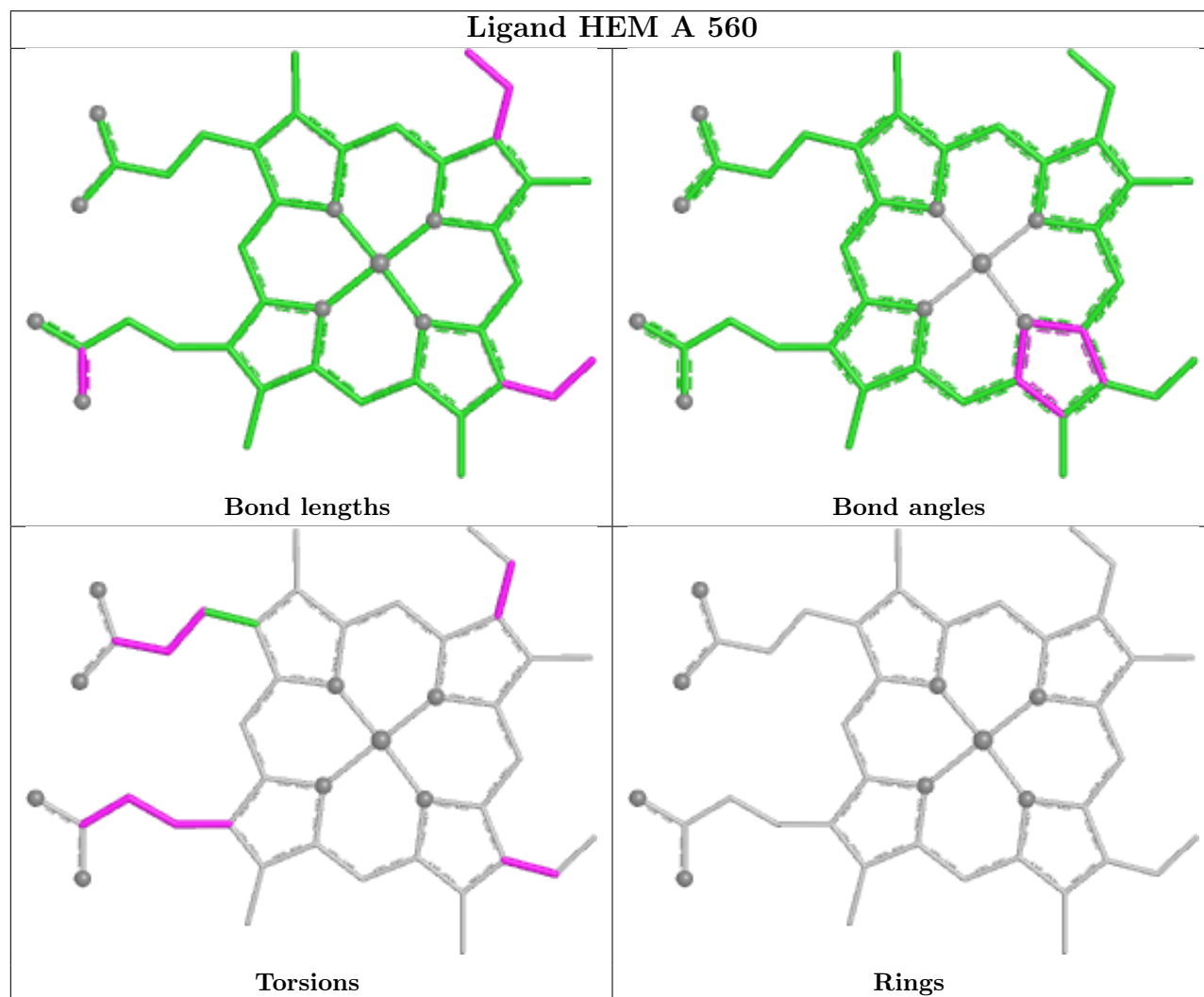
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	580	PPY	2	0
4	A	580	PPY	1	0
2	A	560	HEM	3	0
3	A	570	FMN	4	0

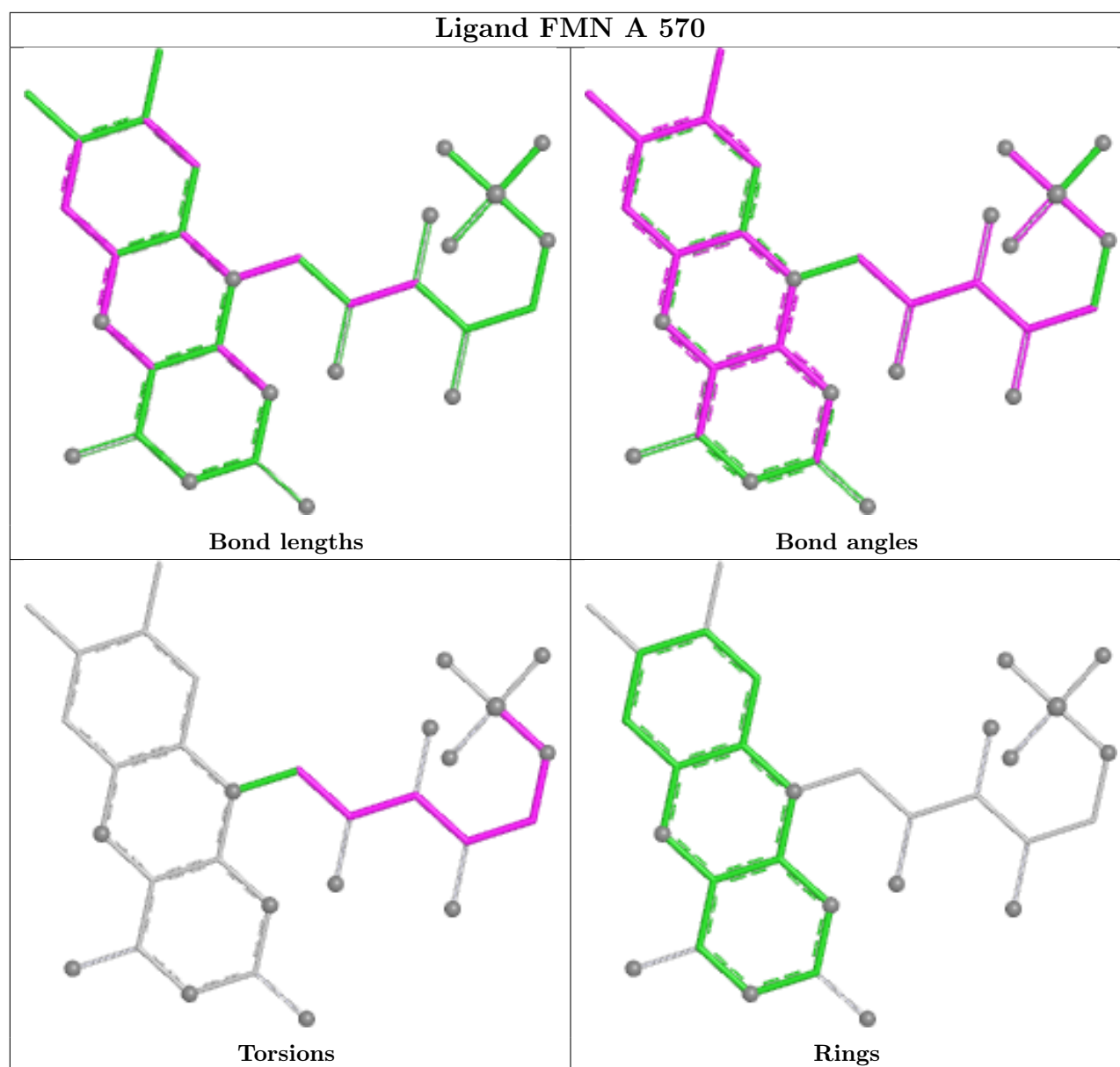
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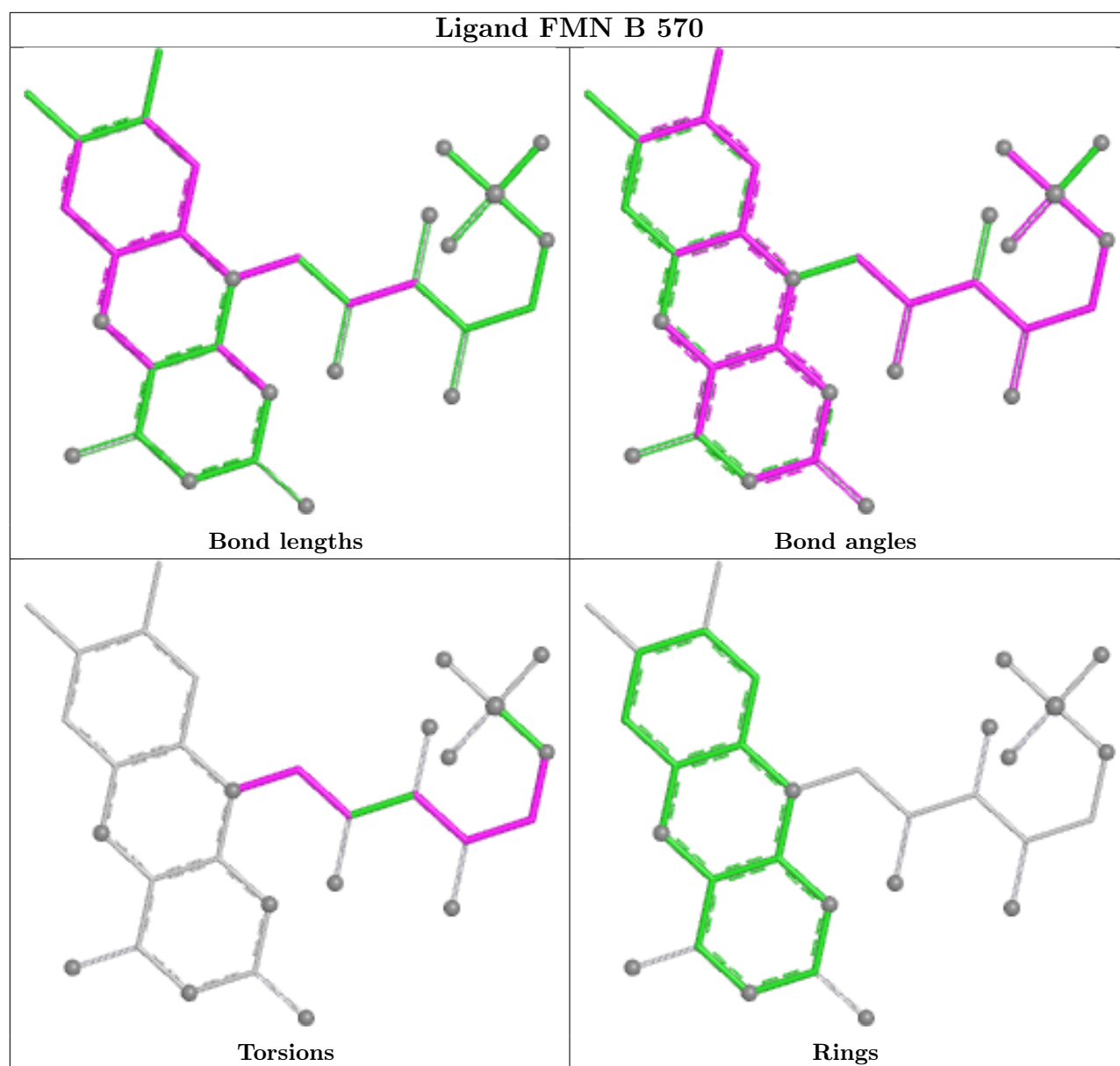
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	570	FMN	7	0

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.