



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 8XSV / pdb_00008xsv
Title : crystal structure of PPAT mutant P8A
Authors : Yin, H.S.
Deposited on : 2024-01-10
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

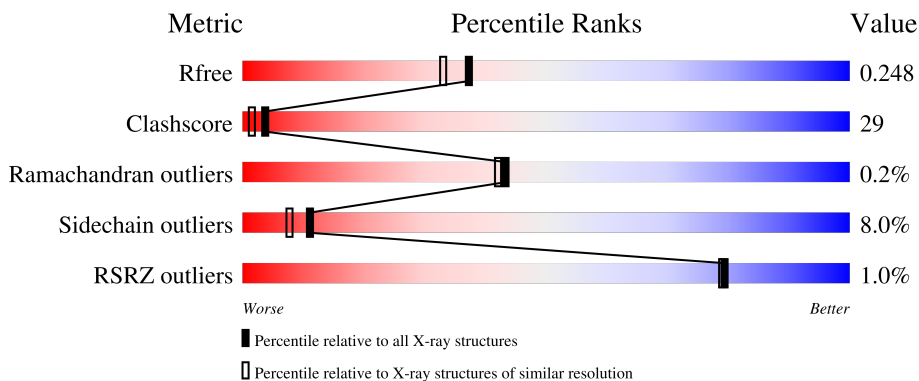
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



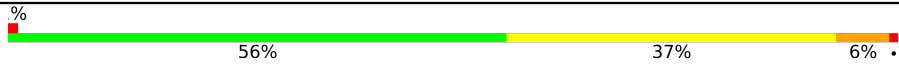
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	155	 53% 37% 8% ..
1	B	155	 62% 34% 5%
1	C	155	 55% 37% 7% .
1	D	155	 52% 41% 6% .
1	E	155	 50% 40% 9% .

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Mol	Chain	Length	Quality of chain
1	F	155	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '56%', a yellow segment in the middle labeled '37%', and a red segment on the right labeled '6%'. A small red square is positioned at the very beginning of the bar, and a small black dot is at the very end. A '%' symbol is located above the start of the bar.</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8233 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.

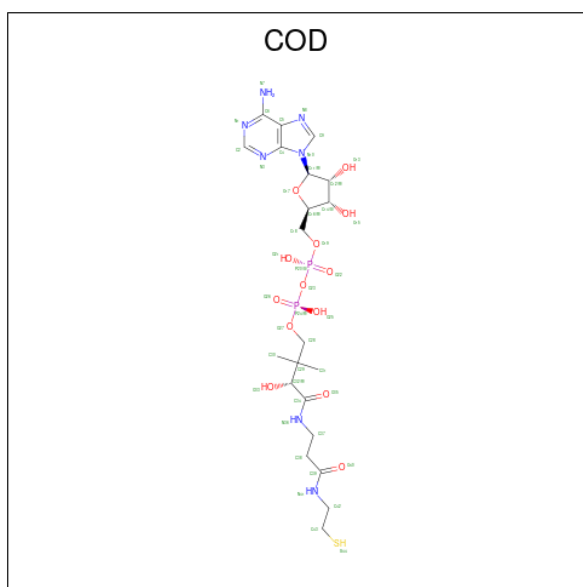
- Molecule 1 is a protein called Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1220	787	205	221	7	0	0	0
1	B	155	1226	790	206	223	7	0	0	0
1	C	155	1226	790	206	223	7	0	0	0
1	D	155	1226	790	206	223	7	0	0	0
1	E	155	1226	790	206	223	7	0	0	0
1	F	155	1226	790	206	223	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	PRO	engineered mutation	UNP O26010
B	8	ALA	PRO	engineered mutation	UNP O26010
C	8	ALA	PRO	engineered mutation	UNP O26010
D	8	ALA	PRO	engineered mutation	UNP O26010
E	8	ALA	PRO	engineered mutation	UNP O26010
F	8	ALA	PRO	engineered mutation	UNP O26010

- Molecule 2 is DEPHOSPHO COENZYME A (CCD ID: COD) (formula: $C_{21}H_{35}N_7O_{13}P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	44	21	7	13	2	1	0	0
2	B	1	44	21	7	13	2	1	0	0
2	C	1	44	21	7	13	2	1	0	0
2	D	1	44	21	7	13	2	1	0	0
2	E	1	44	21	7	13	2	1	0	0
2	F	1	44	21	7	13	2	1	0	0

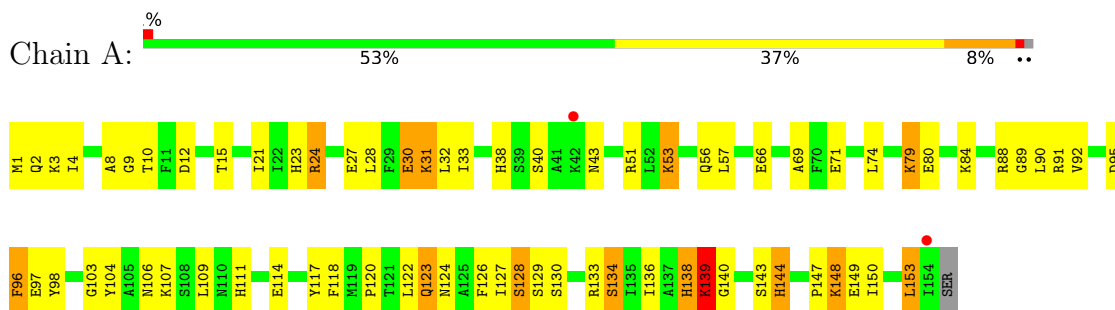
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total 109	O 109	0	0
3	B	112	Total 112	O 112	0	0
3	C	108	Total 108	O 108	0	0
3	D	104	Total 104	O 104	0	0
3	E	96	Total 96	O 96	0	0
3	F	90	Total 90	O 90	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

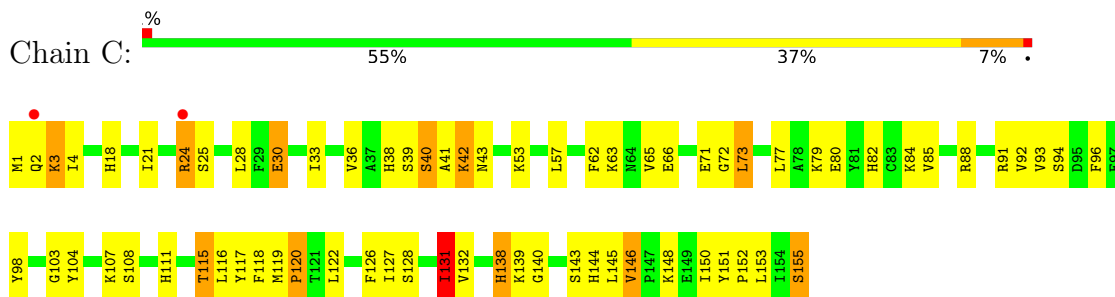
- Molecule 1: Phosphopantetheine adenylyltransferase



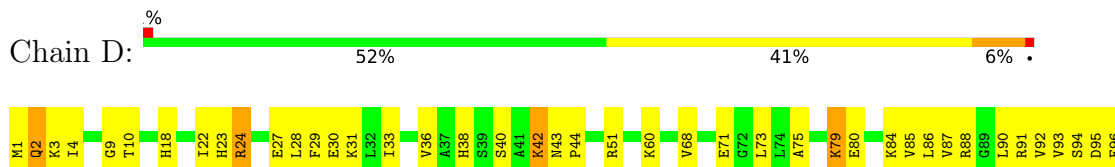
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

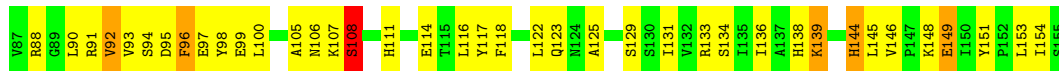
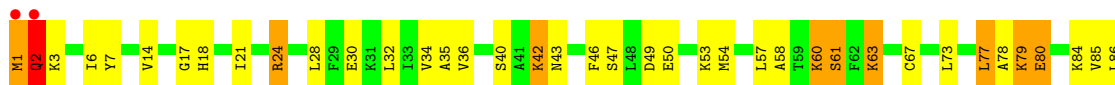


- Molecule 1: Phosphopantetheine adenylyltransferase

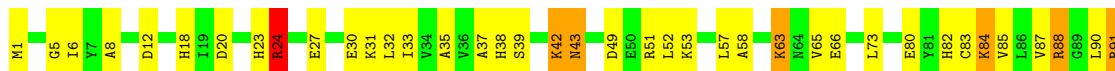




• Molecule 1: Phosphopantetheine adenylyltransferase



• Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.89Å 126.90Å 89.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.98 – 2.00 89.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (89.98-2.00) 96.3 (89.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.250 0.193 , 0.248	Depositor DCC
R_{free} test set	3661 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8233	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0605e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	1.88	24/1245 (1.9%)	1.47	8/1680 (0.5%)
1	B	1.78	15/1251 (1.2%)	1.32	3/1688 (0.2%)
1	C	1.84	25/1251 (2.0%)	1.62	10/1688 (0.6%)
1	D	1.75	20/1251 (1.6%)	1.54	11/1688 (0.7%)
1	E	1.75	18/1251 (1.4%)	1.57	17/1688 (1.0%)
1	F	1.87	24/1251 (1.9%)	1.59	14/1688 (0.8%)
All	All	1.81	126/7500 (1.7%)	1.52	63/10120 (0.6%)

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	146	VAL	C-O	-10.57	1.16	1.24
1	B	51	ARG	N-CA	10.31	1.59	1.46
1	F	51	ARG	N-CA	9.72	1.58	1.46
1	C	116	LEU	C-O	8.22	1.34	1.24
1	A	144	HIS	CG-CD2	8.21	1.44	1.35
1	A	33	ILE	CA-CB	-7.76	1.44	1.54
1	C	103	GLY	N-CA	7.72	1.55	1.45
1	A	31	LYS	CA-C	7.53	1.61	1.52
1	A	69	ALA	C-O	-7.53	1.15	1.23
1	C	144	HIS	CG-CD2	7.49	1.44	1.35
1	F	35	ALA	CA-C	7.46	1.62	1.52
1	D	114	GLU	N-CA	7.43	1.54	1.45
1	D	103	GLY	CA-C	7.35	1.60	1.51
1	B	49	ASP	C-O	-7.31	1.15	1.24
1	E	144	HIS	CG-CD2	7.19	1.43	1.35
1	A	2	GLN	CD-OE1	7.15	1.37	1.23
1	F	111	HIS	CG-CD2	6.99	1.43	1.35
1	B	132	VAL	CA-CB	6.98	1.62	1.54
1	F	52	LEU	C-O	6.98	1.32	1.24
1	A	15	THR	N-CA	6.96	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	ARG	CZ-NH2	-6.96	1.24	1.33
1	A	127	ILE	CA-C	-6.90	1.44	1.52
1	A	144	HIS	ND1-CE1	6.87	1.39	1.32
1	B	23	HIS	CG-CD2	6.84	1.43	1.35
1	A	95	ASP	N-CA	6.79	1.55	1.46
1	F	99	GLU	CA-C	-6.78	1.44	1.52
1	A	111	HIS	CG-CD2	6.77	1.43	1.35
1	E	99	GLU	N-CA	6.72	1.54	1.46
1	F	18	HIS	C-O	-6.66	1.16	1.24
1	B	18	HIS	CG-ND1	-6.64	1.30	1.38
1	E	117	TYR	N-CA	6.54	1.53	1.46
1	D	138	HIS	ND1-CE1	6.52	1.39	1.32
1	B	68	VAL	C-O	6.52	1.30	1.23
1	C	18	HIS	CE1-NE2	6.51	1.39	1.32
1	D	138	HIS	CE1-NE2	6.51	1.39	1.32
1	C	30	GLU	N-CA	6.51	1.54	1.46
1	D	144	HIS	CB-CG	6.29	1.58	1.50
1	E	125	ALA	N-CA	6.29	1.54	1.46
1	F	39	SER	C-O	6.25	1.31	1.23
1	C	103	GLY	C-O	6.25	1.31	1.23
1	C	18	HIS	CG-CD2	6.23	1.42	1.35
1	B	128	SER	C-O	6.23	1.31	1.23
1	F	99	GLU	N-CA	6.17	1.53	1.46
1	D	147	PRO	CA-C	6.14	1.60	1.52
1	C	115	THR	N-CA	6.11	1.53	1.46
1	F	43	ASN	C-O	-6.05	1.17	1.24
1	D	99	GLU	N-CA	6.05	1.53	1.46
1	C	111	HIS	CG-CD2	6.03	1.42	1.35
1	D	144	HIS	ND1-CE1	6.03	1.38	1.32
1	A	144	HIS	CE1-NE2	6.00	1.38	1.32
1	A	43	ASN	C-O	5.98	1.26	1.23
1	C	38	HIS	CG-CD2	5.96	1.42	1.35
1	F	87	VAL	C-O	5.94	1.31	1.24
1	E	43	ASN	CA-C	-5.91	1.45	1.52
1	D	68	VAL	C-O	5.88	1.29	1.23
1	E	49	ASP	CA-C	-5.88	1.45	1.52
1	F	111	HIS	ND1-CE1	5.87	1.38	1.32
1	C	144	HIS	ND1-CE1	5.87	1.38	1.32
1	C	24	ARG	C-O	-5.84	1.17	1.24
1	E	114	GLU	N-CA	5.81	1.52	1.45
1	F	143	SER	C-O	-5.80	1.16	1.24
1	A	8	ALA	C-O	5.77	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	32	LEU	C-O	5.75	1.30	1.24
1	C	144	HIS	CE1-NE2	5.74	1.38	1.32
1	D	18	HIS	CG-ND1	-5.73	1.31	1.38
1	E	17	GLY	C-O	-5.73	1.16	1.23
1	A	134	SER	C-O	5.70	1.30	1.24
1	D	138	HIS	CG-CD2	5.69	1.42	1.35
1	F	58	ALA	C-O	-5.69	1.16	1.24
1	C	146	VAL	C-O	-5.64	1.18	1.24
1	E	36	VAL	C-O	5.63	1.30	1.24
1	A	128	SER	N-CA	5.62	1.52	1.45
1	F	38	HIS	N-CA	5.62	1.52	1.46
1	C	39	SER	C-O	5.61	1.31	1.23
1	F	52	LEU	N-CA	5.58	1.53	1.46
1	E	17	GLY	N-CA	5.57	1.52	1.45
1	B	144	HIS	CB-CG	5.55	1.57	1.50
1	B	46	PHE	C-O	5.53	1.30	1.23
1	D	123	GLN	N-CA	5.50	1.53	1.46
1	A	74	LEU	C-O	5.49	1.30	1.24
1	C	73	LEU	C-O	5.49	1.30	1.23
1	E	77	LEU	C-O	5.47	1.30	1.24
1	A	51	ARG	N-CA	5.44	1.52	1.46
1	C	43	ASN	CA-C	-5.44	1.46	1.52
1	C	120	PRO	N-CA	-5.41	1.40	1.47
1	D	125	ALA	CA-C	5.38	1.60	1.52
1	B	38	HIS	CG-CD2	5.38	1.41	1.35
1	F	83	CYS	C-O	5.36	1.30	1.24
1	A	103	GLY	C-O	5.35	1.30	1.23
1	B	38	HIS	ND1-CE1	5.34	1.37	1.32
1	B	136	ILE	N-CA	-5.34	1.39	1.46
1	F	43	ASN	CA-C	-5.33	1.47	1.52
1	F	12	ASP	N-CA	5.32	1.52	1.46
1	E	148	LYS	N-CA	5.32	1.53	1.46
1	D	23	HIS	CG-CD2	5.29	1.41	1.35
1	F	8	ALA	CA-CB	-5.28	1.45	1.53
1	A	23	HIS	CG-CD2	5.27	1.41	1.35
1	D	97	GLU	CD-OE2	5.27	1.35	1.25
1	C	72	GLY	C-O	5.26	1.28	1.24
1	C	104	TYR	N-CA	5.26	1.52	1.46
1	F	65	VAL	CA-C	5.26	1.58	1.52
1	A	1	MET	N-CA	5.24	1.56	1.46
1	A	30	GLU	C-O	-5.23	1.17	1.24
1	C	38	HIS	ND1-CE1	5.23	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	HIS	CG-ND1	-5.23	1.32	1.38
1	D	97	GLU	N-CA	-5.22	1.40	1.46
1	D	38	HIS	N-CA	5.21	1.52	1.46
1	E	111	HIS	CG-CD2	5.16	1.41	1.35
1	B	135	ILE	N-CA	-5.15	1.40	1.46
1	E	146	VAL	CA-C	5.14	1.56	1.52
1	A	38	HIS	CG-CD2	5.14	1.41	1.35
1	B	111	HIS	CE1-NE2	5.13	1.37	1.32
1	F	30	GLU	C-O	-5.12	1.18	1.24
1	D	23	HIS	CA-C	-5.11	1.46	1.52
1	E	53	LYS	C-O	5.11	1.30	1.24
1	A	103	GLY	N-CA	5.11	1.52	1.45
1	E	35	ALA	CA-C	5.10	1.59	1.52
1	D	30	GLU	CA-C	-5.08	1.46	1.52
1	F	27	GLU	N-CA	5.07	1.52	1.46
1	C	36	VAL	C-O	5.07	1.29	1.24
1	C	138	HIS	ND1-CE1	5.07	1.37	1.32
1	A	53	LYS	N-CA	5.04	1.52	1.46
1	C	82	HIS	CG-CD2	5.03	1.41	1.35
1	D	22	ILE	N-CA	5.03	1.52	1.46
1	B	91	ARG	C-O	5.00	1.30	1.24
1	F	32	LEU	CA-C	5.00	1.58	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	42	LYS	CA-C-N	-18.65	98.28	123.46
1	F	42	LYS	C-N-CA	-18.65	98.28	123.46
1	C	42	LYS	CA-C-N	-15.55	104.04	123.16
1	C	42	LYS	C-N-CA	-15.55	104.04	123.16
1	E	42	LYS	CA-C-N	-14.43	105.41	123.16
1	E	42	LYS	C-N-CA	-14.43	105.41	123.16
1	D	42	LYS	CA-C-N	-13.45	105.30	123.46
1	D	42	LYS	C-N-CA	-13.45	105.30	123.46
1	C	42	LYS	N-CA-C	-10.63	97.01	110.19
1	F	42	LYS	N-CA-C	-8.79	99.19	110.53
1	E	42	LYS	N-CA-C	-8.26	96.91	109.79
1	C	24	ARG	N-CA-C	8.10	120.19	111.36
1	E	108	SER	CB-CA-C	-7.96	98.38	110.88
1	C	131	ILE	CB-CA-C	-7.81	101.79	112.02
1	F	88	ARG	CA-C-N	-7.40	114.39	122.38
1	F	88	ARG	C-N-CA	-7.40	114.39	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	LYS	N-CA-C	-7.02	100.66	110.35
1	F	24	ARG	N-CA-C	6.94	118.49	111.07
1	D	125	ALA	N-CA-C	-6.94	104.79	113.18
1	E	24	ARG	N-CA-C	6.80	118.77	111.36
1	D	3	LYS	N-CA-C	6.64	121.46	113.23
1	D	135	ILE	N-CA-C	6.63	117.33	110.36
1	E	61	SER	N-CA-C	6.32	120.67	113.15
1	F	24	ARG	CG-CD-NE	6.24	125.72	112.00
1	B	43	ASN	CB-CA-C	-6.20	105.61	111.00
1	F	84	LYS	CA-CB-CG	6.20	126.50	114.10
1	A	139	LYS	N-CA-C	6.15	120.11	112.24
1	D	30	GLU	N-CA-C	-6.07	104.67	111.28
1	C	43	ASN	CA-C-N	-6.06	113.54	119.78
1	C	43	ASN	C-N-CA	-6.06	113.54	119.78
1	F	42	LYS	O-C-N	-6.06	115.20	122.65
1	B	10	THR	N-CA-C	-6.04	104.98	112.90
1	A	136	ILE	N-CA-C	-6.03	104.63	110.42
1	E	107	LYS	CA-CB-CG	6.03	126.16	114.10
1	A	126	PHE	CA-C-N	-5.95	115.44	122.93
1	A	126	PHE	C-N-CA	-5.95	115.44	122.93
1	E	146	VAL	CA-C-N	-5.58	114.01	119.76
1	E	146	VAL	C-N-CA	-5.58	114.01	119.76
1	E	78	ALA	CA-C-N	5.57	128.06	120.54
1	E	78	ALA	C-N-CA	5.57	128.06	120.54
1	C	40	SER	N-CA-C	-5.57	105.30	111.71
1	A	138	HIS	N-CA-C	-5.31	106.67	112.72
1	A	143	SER	N-CA-C	-5.28	106.67	113.01
1	F	108	SER	CB-CA-C	-5.28	100.54	110.67
1	D	136	ILE	CB-CA-C	-5.28	105.02	112.14
1	E	106	ASN	N-CA-C	5.23	116.98	111.28
1	E	136	ILE	N-CA-C	-5.21	105.46	110.72
1	F	96	PHE	N-CA-C	5.20	116.95	111.28
1	C	85	VAL	N-CA-C	5.15	115.40	107.77
1	D	33	ILE	CB-CA-C	-5.14	104.73	110.96
1	F	84	LYS	CG-CD-CE	5.14	123.12	111.30
1	E	80	GLU	CB-CA-C	-5.12	101.98	110.68
1	B	96	PHE	N-CA-CB	-5.09	102.63	110.16
1	A	9	GLY	N-CA-C	-5.07	102.87	110.42
1	A	24	ARG	N-CA-C	5.07	116.88	111.36
1	C	93	VAL	N-CA-C	-5.06	107.41	111.91
1	D	131	ILE	CB-CA-C	5.06	119.20	112.22
1	D	36	VAL	CB-CA-C	-5.05	104.83	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	MET	N-CA-C	-5.05	96.84	111.00
1	E	107	LYS	CA-C-N	5.04	127.00	120.44
1	E	107	LYS	C-N-CA	5.04	127.00	120.44
1	F	24	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	F	149	GLU	N-CA-C	5.03	117.41	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1220	0	1245	80	2
1	B	1226	0	1250	69	0
1	C	1226	0	1250	91	0
1	D	1226	0	1250	96	0
1	E	1226	0	1250	80	0
1	F	1226	0	1250	60	1
2	A	44	0	33	2	0
2	B	44	0	33	2	0
2	C	44	0	33	7	0
2	D	44	0	33	3	0
2	E	44	0	33	2	0
2	F	44	0	33	4	0
3	A	109	0	0	51	0
3	B	112	0	0	35	0
3	C	108	0	0	51	0
3	D	104	0	0	59	2
3	E	96	0	0	41	2
3	F	90	0	0	44	1
All	All	8233	0	7693	442	4

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 29.

All (442) 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:119:MET:HE2	3:B:3184:HOH:O	1.20	1.36
1:C:146:VAL:HB	3:C:3101:HOH:O	1.25	1.32
1:A:32:LEU:HD13	3:A:3128:HOH:O	1.14	1.31
1:A:149:GLU:HB3	3:A:3172:HOH:O	1.19	1.29
1:A:150:ILE:HG23	3:A:3156:HOH:O	1.26	1.29
1:F:5:GLY:HA2	3:F:3104:HOH:O	1.20	1.29
1:D:119:MET:HB2	3:D:3174:HOH:O	1.17	1.29
1:E:84:LYS:HB2	3:E:3159:HOH:O	1.23	1.29
1:C:33:ILE:HD13	3:C:3179:HOH:O	1.24	1.28
3:D:3176:HOH:O	1:E:100:LEU:HD13	1.33	1.28
1:A:31:LYS:HB3	3:A:3140:HOH:O	1.27	1.27
1:C:143:SER:HB3	3:C:3115:HOH:O	1.13	1.26
1:D:1:MET:HE1	3:E:3146:HOH:O	1.19	1.26
1:A:106:ASN:HA	3:A:3105:HOH:O	1.12	1.26
1:F:123:GLN:HA	3:F:3155:HOH:O	1.10	1.25
1:B:73:LEU:HB3	3:B:3132:HOH:O	1.34	1.24
1:D:87:VAL:HG23	3:D:3133:HOH:O	1.30	1.23
1:E:118:PHE:HB2	3:E:3165:HOH:O	1.35	1.23
1:B:98:TYR:HB3	3:B:3106:HOH:O	1.39	1.23
1:C:77:LEU:HD12	3:C:3113:HOH:O	1.34	1.23
1:D:9:GLY:HA3	3:D:3119:HOH:O	1.06	1.22
3:A:3174:HOH:O	1:D:92:VAL:HG12	1.06	1.21
1:E:30:GLU:HG2	3:E:3185:HOH:O	1.37	1.21
1:C:62:PHE:HB2	3:C:3174:HOH:O	1.36	1.21
1:A:27:GLU:HB2	1:B:1:MET:CE	1.70	1.21
1:B:107:LYS:HA	3:B:3103:HOH:O	1.06	1.20
1:A:24:ARG:O	1:B:1:MET:HE1	1.42	1.20
1:E:61:SER:HB3	3:E:3158:HOH:O	1.42	1.20
1:D:75:ALA:HB2	3:D:3162:HOH:O	1.37	1.19
1:E:116:LEU:HB3	3:E:3184:HOH:O	1.42	1.18
1:F:116:LEU:HB2	3:F:3167:HOH:O	1.03	1.18
1:B:95:ASP:HB3	3:B:3106:HOH:O	1.37	1.18
1:B:124:ASN:HB3	3:B:3112:HOH:O	1.42	1.17
1:D:124:ASN:HB2	3:D:3105:HOH:O	1.44	1.16
1:C:88:ARG:HG2	3:C:3173:HOH:O	1.44	1.15
1:D:120:PRO:HB2	3:D:3105:HOH:O	1.44	1.14
1:C:66:GLU:HB3	3:C:3179:HOH:O	1.46	1.12
1:A:3:LYS:HE3	3:A:3104:HOH:O	1.49	1.12
1:F:85:VAL:HB	3:F:3104:HOH:O	1.48	1.11
1:A:130:SER:HB2	3:A:3106:HOH:O	0.94	1.11
1:A:27:GLU:HB2	1:B:1:MET:HE2	1.13	1.10
1:B:117:TYR:CE2	3:B:3101:HOH:O	2.04	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LEU:HB3	3:F:3182:HOH:O	1.53	1.09
1:D:116:LEU:CD1	3:D:3142:HOH:O	2.00	1.08
1:D:28:LEU:HG	3:D:3125:HOH:O	1.50	1.07
1:D:28:LEU:HD21	1:E:28:LEU:HD21	1.06	1.05
1:D:100:LEU:HD13	3:E:3128:HOH:O	1.55	1.04
1:E:100:LEU:HD23	3:E:3104:HOH:O	1.55	1.04
1:A:148:LYS:HE3	3:A:3172:HOH:O	1.58	1.04
1:C:24:ARG:NH1	1:C:118:PHE:HA	1.71	1.04
1:E:85:VAL:HG12	3:E:3113:HOH:O	1.55	1.04
1:C:3:LYS:HE3	3:C:3152:HOH:O	1.58	1.03
1:D:24:ARG:HG2	1:D:24:ARG:HH21	1.15	1.03
1:D:102:MET:HB3	3:D:3151:HOH:O	1.57	1.03
2:F:3000:COD:S44	3:F:3173:HOH:O	2.14	1.03
1:D:24:ARG:HH21	1:D:24:ARG:CG	1.70	1.02
1:C:65:VAL:HB	3:C:3174:HOH:O	1.58	1.02
1:A:3:LYS:CE	3:A:3104:HOH:O	2.02	1.02
1:C:24:ARG:NE	1:C:118:PHE:HD1	1.58	1.01
1:C:28:LEU:HB2	1:F:1:MET:CE	1.89	1.01
1:D:96:PHE:CD1	3:E:3174:HOH:O	2.12	1.01
1:A:148:LYS:HB3	3:A:3176:HOH:O	1.61	0.99
3:A:3196:HOH:O	1:B:1:MET:SD	2.20	0.99
1:D:28:LEU:CD2	1:E:28:LEU:HD21	1.92	0.99
1:D:60:LYS:HE2	3:D:3165:HOH:O	1.61	0.99
1:E:6:ILE:HB	3:E:3103:HOH:O	1.62	0.99
1:E:122:LEU:CD2	3:F:3155:HOH:O	2.10	0.99
1:E:21:ILE:HD12	3:E:3165:HOH:O	1.64	0.98
1:E:122:LEU:HD22	3:F:3155:HOH:O	1.64	0.97
1:A:90:LEU:HD23	3:A:3121:HOH:O	1.63	0.97
1:C:28:LEU:CB	1:F:1:MET:HE2	1.95	0.96
1:C:28:LEU:HB2	1:F:1:MET:HE2	0.98	0.96
1:E:47:SER:OG	1:E:50:GLU:HG3	1.66	0.96
2:F:3000:COD:C30	3:F:3107:HOH:O	2.14	0.95
2:C:3000:COD:H181	3:C:3116:HOH:O	1.65	0.95
1:A:31:LYS:HE3	3:A:3158:HOH:O	1.67	0.94
1:B:127:ILE:HD12	3:B:3112:HOH:O	1.67	0.94
1:C:25:SER:HB3	3:C:3107:HOH:O	1.67	0.94
1:A:96:PHE:CB	3:A:3175:HOH:O	2.16	0.93
1:B:42:LYS:HE3	3:B:3176:HOH:O	1.67	0.93
2:F:3000:COD:H302	3:F:3107:HOH:O	1.66	0.92
1:E:96:PHE:HB3	3:E:3174:HOH:O	1.68	0.92
1:A:96:PHE:HB2	3:A:3200:HOH:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LEU:HD23	3:E:3103:HOH:O	1.69	0.91
1:D:131:ILE:HG22	3:D:3157:HOH:O	1.70	0.91
1:D:28:LEU:HD21	1:E:28:LEU:CD2	2.00	0.91
1:A:57:LEU:HD23	3:A:3195:HOH:O	1.72	0.90
1:E:116:LEU:HD23	3:E:3184:HOH:O	1.68	0.90
1:A:97:GLU:HG3	3:B:3186:HOH:O	1.71	0.90
2:C:3000:COD:C18	3:C:3116:HOH:O	2.19	0.90
1:A:118:PHE:HB2	3:A:3103:HOH:O	1.72	0.89
1:F:23:HIS:HE1	3:F:3124:HOH:O	1.55	0.89
1:D:116:LEU:HD12	3:D:3142:HOH:O	1.66	0.89
1:B:113:LEU:HB3	3:B:3103:HOH:O	1.72	0.89
1:E:85:VAL:CG1	3:E:3113:HOH:O	2.16	0.88
1:E:42:LYS:HE3	3:E:3177:HOH:O	1.73	0.88
1:E:1:MET:O	1:E:3:LYS:N	2.06	0.88
1:A:27:GLU:CB	1:B:1:MET:HE2	2.02	0.88
1:D:119:MET:SD	3:D:3174:HOH:O	2.31	0.88
1:B:95:ASP:CB	3:B:3106:HOH:O	2.05	0.87
1:C:132:VAL:HG21	3:C:3181:HOH:O	1.73	0.87
2:C:3000:COD:HC14	3:C:3116:HOH:O	1.74	0.87
1:A:97:GLU:HB3	3:A:3174:HOH:O	1.73	0.87
1:B:42:LYS:NZ	2:B:3000:COD:O26	2.07	0.87
1:F:20:ASP:HB3	3:F:3143:HOH:O	1.72	0.86
1:A:96:PHE:HB3	3:A:3175:HOH:O	1.73	0.86
1:B:112:GLU:HB2	3:B:3113:HOH:O	1.75	0.86
1:C:1:MET:SD	1:C:84:LYS:HG2	2.15	0.86
1:C:96:PHE:CD1	3:F:3141:HOH:O	2.28	0.85
1:F:85:VAL:HA	3:F:3101:HOH:O	1.76	0.85
1:C:1:MET:CE	1:C:84:LYS:HG2	2.06	0.85
1:F:42:LYS:NZ	2:F:3000:COD:O26	2.09	0.85
1:D:96:PHE:CE1	3:E:3174:HOH:O	2.22	0.85
1:D:102:MET:HE2	3:D:3151:HOH:O	1.78	0.84
1:D:116:LEU:HD11	3:D:3142:HOH:O	1.67	0.84
1:A:21:ILE:HD12	3:A:3103:HOH:O	1.76	0.84
1:A:104:TYR:CE1	3:B:3184:HOH:O	2.31	0.84
1:E:145:LEU:HD13	3:E:3133:HOH:O	1.77	0.83
1:D:111:HIS:HB2	3:D:3189:HOH:O	1.78	0.83
1:C:4:ILE:CD1	3:C:3188:HOH:O	2.26	0.83
1:D:79:LYS:HG3	3:D:3172:HOH:O	1.79	0.83
1:E:98:TYR:HB2	3:E:3168:HOH:O	1.78	0.82
1:C:1:MET:HE1	1:C:84:LYS:HG2	1.61	0.82
1:D:148:LYS:HD3	3:D:3107:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ILE:HG23	3:E:3165:HOH:O	1.80	0.82
1:A:92:VAL:CG1	3:F:3165:HOH:O	2.27	0.81
1:F:138:HIS:CD2	3:F:3158:HOH:O	2.34	0.81
1:E:96:PHE:CB	3:E:3174:HOH:O	2.28	0.81
1:A:98:TYR:CD2	3:A:3194:HOH:O	2.33	0.81
1:A:28:LEU:N	1:B:1:MET:HE3	1.96	0.80
3:D:3125:HOH:O	1:E:28:LEU:HD11	1.81	0.80
1:A:89:GLY:HA2	3:A:3103:HOH:O	1.79	0.80
1:D:99:GLU:HA	3:D:3151:HOH:O	1.81	0.80
1:A:109:LEU:HB2	3:A:3105:HOH:O	1.79	0.80
1:C:150:ILE:HD11	3:C:3101:HOH:O	1.80	0.80
1:D:24:ARG:CG	1:D:24:ARG:NH2	2.38	0.80
1:C:65:VAL:CB	3:C:3174:HOH:O	2.19	0.80
1:C:139:LYS:HD2	3:C:3189:HOH:O	1.83	0.79
1:D:9:GLY:CA	3:D:3119:HOH:O	1.84	0.79
1:A:150:ILE:CG2	3:A:3156:HOH:O	2.00	0.78
1:D:109:LEU:HB2	3:D:3162:HOH:O	1.83	0.78
1:B:95:ASP:CG	3:B:3106:HOH:O	2.25	0.78
1:B:28:LEU:HD23	1:B:118:PHE:CE1	2.19	0.78
2:C:3000:COD:C14	3:C:3116:HOH:O	2.30	0.78
1:B:98:TYR:CE1	3:B:3194:HOH:O	2.36	0.78
1:D:73:LEU:HD23	3:F:3158:HOH:O	1.84	0.78
1:F:138:HIS:CG	3:F:3158:HOH:O	2.37	0.78
1:C:127:ILE:HD13	3:C:3155:HOH:O	1.84	0.77
1:D:119:MET:CB	3:D:3174:HOH:O	1.92	0.77
1:A:96:PHE:HB2	3:A:3175:HOH:O	1.81	0.76
1:D:119:MET:CG	3:D:3174:HOH:O	2.27	0.76
1:C:53:LYS:HE3	1:C:153:LEU:HD13	1.66	0.76
1:E:50:GLU:HG2	3:E:3162:HOH:O	1.86	0.76
1:A:53:LYS:NZ	1:A:56:GLN:HE22	1.85	0.75
2:C:3000:COD:C16	3:C:3116:HOH:O	2.36	0.74
1:A:153:LEU:HD13	3:A:3195:HOH:O	1.88	0.74
1:C:96:PHE:HB3	3:C:3169:HOH:O	1.88	0.73
1:D:96:PHE:HB3	3:D:3156:HOH:O	1.86	0.73
1:C:4:ILE:HD12	3:C:3188:HOH:O	1.84	0.73
1:C:115:THR:HG23	3:C:3173:HOH:O	1.86	0.73
1:C:132:VAL:CG2	3:C:3181:HOH:O	2.30	0.73
1:C:2:GLN:OE1	1:C:30:GLU:HG2	1.89	0.73
1:D:152:PRO:HD3	3:D:3181:HOH:O	1.88	0.72
1:B:117:TYR:HE2	3:B:3101:HOH:O	1.55	0.72
1:D:24:ARG:HG2	1:D:24:ARG:NH2	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HZ2	1:A:56:GLN:HE22	1.38	0.72
1:D:96:PHE:CB	3:D:3156:HOH:O	2.37	0.71
1:E:100:LEU:HD22	3:E:3145:HOH:O	1.90	0.71
1:C:122:LEU:HD23	1:C:122:LEU:C	2.17	0.70
1:B:144:HIS:CD2	1:B:144:HIS:H	2.09	0.70
1:A:98:TYR:HD2	3:A:3194:HOH:O	1.70	0.69
1:C:127:ILE:CG2	3:C:3155:HOH:O	2.40	0.69
1:C:96:PHE:CB	3:C:3169:HOH:O	2.40	0.69
1:C:24:ARG:NE	1:C:118:PHE:CD1	2.44	0.69
1:E:85:VAL:HG13	1:E:116:LEU:HD13	1.75	0.68
1:A:98:TYR:HE2	3:A:3180:HOH:O	1.76	0.68
1:D:42:LYS:NZ	2:D:3000:COD:O26	2.26	0.68
1:C:77:LEU:HA	3:C:3113:HOH:O	1.92	0.68
1:A:147:PRO:HG2	3:A:3156:HOH:O	1.94	0.68
1:D:9:GLY:C	3:D:3119:HOH:O	2.25	0.68
1:F:66:GLU:HB2	3:F:3144:HOH:O	1.94	0.67
1:A:24:ARG:O	1:B:1:MET:CE	2.32	0.67
1:E:105:ALA:O	1:E:108:SER:HB2	1.94	0.67
1:C:118:PHE:HE1	1:F:1:MET:HE1	1.59	0.67
1:A:79:LYS:HG3	3:A:3149:HOH:O	1.93	0.67
1:C:128:SER:H	1:C:131:ILE:HD12	1.59	0.66
1:D:42:LYS:HE3	3:D:3184:HOH:O	1.96	0.66
1:B:117:TYR:HD1	3:B:3105:HOH:O	1.78	0.65
1:D:60:LYS:HE3	3:D:3163:HOH:O	1.95	0.65
1:E:42:LYS:NZ	2:E:3000:COD:O26	2.30	0.65
1:B:28:LEU:HD23	1:B:118:PHE:HE1	1.59	0.65
3:C:3169:HOH:O	1:F:96:PHE:CD1	2.49	0.65
1:F:53:LYS:HE2	1:F:57:LEU:HD11	1.78	0.65
1:E:50:GLU:O	1:E:54:MET:HG3	1.97	0.65
1:D:153:LEU:HD13	3:D:3164:HOH:O	1.96	0.65
1:B:98:TYR:CD1	3:B:3106:HOH:O	2.50	0.64
1:C:96:PHE:HZ	1:F:91:ARG:O	1.80	0.64
1:A:120:PRO:HD3	2:A:3000:COD:HC2	1.80	0.64
1:F:24:ARG:HD2	3:F:3143:HOH:O	1.98	0.64
1:D:43:ASN:HB2	3:D:3185:HOH:O	1.96	0.64
1:C:96:PHE:CE1	3:F:3141:HOH:O	2.45	0.64
1:D:151:TYR:N	1:D:152:PRO:HD2	2.12	0.64
1:C:143:SER:CB	3:C:3115:HOH:O	1.95	0.64
1:C:127:ILE:CD1	3:C:3155:HOH:O	2.44	0.63
1:C:128:SER:H	1:C:131:ILE:CD1	2.11	0.63
1:A:144:HIS:HE2	1:F:108:SER:HB3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:HH11	1:C:118:PHE:HA	1.62	0.62
1:B:80:GLU:HG3	3:B:3188:HOH:O	1.99	0.62
1:E:40:SER:O	1:E:42:LYS:O	2.17	0.62
1:B:124:ASN:CB	3:B:3112:HOH:O	2.19	0.61
3:D:3156:HOH:O	1:E:96:PHE:CE1	2.51	0.61
1:D:108:SER:OG	1:F:144:HIS:HE1	1.83	0.61
1:D:85:VAL:HG12	3:D:3133:HOH:O	2.00	0.61
1:B:144:HIS:HE1	1:E:108:SER:OG	1.84	0.61
1:A:148:LYS:HG3	3:A:3153:HOH:O	2.00	0.61
1:D:24:ARG:NE	3:D:3101:HOH:O	2.32	0.61
1:A:106:ASN:CA	3:A:3105:HOH:O	1.96	0.61
1:C:40:SER:O	1:C:42:LYS:O	2.18	0.61
1:C:127:ILE:CG1	3:C:3155:HOH:O	2.47	0.61
1:F:104:TYR:HE2	3:F:3182:HOH:O	1.84	0.61
1:A:31:LYS:CE	3:A:3158:HOH:O	2.38	0.60
1:D:1:MET:SD	1:E:28:LEU:HB2	2.40	0.60
3:D:3113:HOH:O	1:E:116:LEU:HG	2.02	0.60
1:E:46:PHE:CZ	1:E:154:ILE:HG22	2.37	0.60
1:D:102:MET:CB	3:D:3151:HOH:O	2.28	0.60
1:F:144:HIS:CD2	1:F:144:HIS:H	2.20	0.60
1:A:98:TYR:CE2	3:A:3194:HOH:O	2.53	0.60
3:A:3175:HOH:O	1:B:96:PHE:CD1	2.51	0.60
1:C:24:ARG:NH1	1:F:116:LEU:HD12	2.17	0.60
1:D:118:PHE:HA	3:D:3113:HOH:O	2.00	0.60
1:C:4:ILE:HD13	3:C:3188:HOH:O	1.95	0.60
1:D:100:LEU:HD22	3:D:3109:HOH:O	2.00	0.59
2:D:3000:COD:C38	3:F:3158:HOH:O	2.50	0.59
1:C:24:ARG:CZ	1:C:119:MET:H	2.15	0.59
1:E:122:LEU:HD21	3:F:3155:HOH:O	1.84	0.59
1:B:73:LEU:HD11	1:C:140:GLY:HA3	1.84	0.59
3:D:3156:HOH:O	1:E:96:PHE:CD1	2.55	0.59
1:C:53:LYS:HA	3:C:3124:HOH:O	2.03	0.59
1:C:150:ILE:CD1	3:C:3101:HOH:O	2.45	0.59
1:D:24:ARG:NH2	1:D:24:ARG:HG3	2.16	0.59
1:D:93:VAL:HG22	3:D:3143:HOH:O	2.03	0.59
1:A:92:VAL:HG12	3:F:3165:HOH:O	1.99	0.59
1:F:104:TYR:CE2	3:F:3182:HOH:O	2.52	0.59
1:D:151:TYR:CD1	1:D:154:ILE:HD11	2.38	0.58
1:A:153:LEU:CD1	3:A:3195:HOH:O	2.50	0.58
1:E:24:ARG:HD2	3:E:3102:HOH:O	2.03	0.58
1:B:144:HIS:CE1	1:E:108:SER:OG	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:NH1	1:F:115:THR:O	2.35	0.58
1:A:123:GLN:HG2	1:A:124:ASN:N	2.18	0.58
1:F:116:LEU:HD13	3:F:3101:HOH:O	2.01	0.58
1:E:93:VAL:HG22	3:E:3142:HOH:O	2.03	0.58
1:D:79:LYS:CG	3:D:3172:HOH:O	2.43	0.58
1:E:24:ARG:NH1	3:E:3102:HOH:O	2.37	0.57
1:E:79:LYS:HE3	3:E:3147:HOH:O	2.03	0.57
1:B:89:GLY:C	3:B:3105:HOH:O	2.46	0.57
1:D:123:GLN:CG	3:D:3180:HOH:O	2.52	0.57
1:B:84:LYS:CE	3:B:3113:HOH:O	2.53	0.57
1:C:25:SER:CB	3:C:3107:HOH:O	2.38	0.56
1:D:75:ALA:CB	3:D:3162:HOH:O	2.18	0.56
1:F:88:ARG:HD2	3:F:3127:HOH:O	2.04	0.56
1:F:37:ALA:HB3	3:F:3107:HOH:O	2.04	0.56
1:B:84:LYS:HE3	3:B:3113:HOH:O	2.04	0.56
1:A:144:HIS:NE2	1:F:108:SER:HB3	2.21	0.56
1:C:30:GLU:HA	3:C:3103:HOH:O	2.04	0.56
1:D:71:GLU:HG3	3:D:3177:HOH:O	2.04	0.56
2:D:3000:COD:H381	3:F:3158:HOH:O	2.03	0.56
1:C:1:MET:HE1	1:C:84:LYS:CG	2.35	0.56
1:D:73:LEU:HD11	1:F:140:GLY:HA3	1.88	0.56
1:A:134:SER:O	1:A:138:HIS:HD2	1.89	0.56
1:D:92:VAL:HG23	3:D:3176:HOH:O	2.06	0.56
1:B:53:LYS:HE3	1:B:57:LEU:HD11	1.87	0.55
1:D:90:LEU:CD2	3:D:3191:HOH:O	2.54	0.55
1:C:127:ILE:HG12	3:C:3155:HOH:O	2.07	0.55
1:F:131:ILE:HB	3:F:3102:HOH:O	2.07	0.55
1:A:96:PHE:HZ	1:B:91:ARG:O	1.88	0.55
1:C:24:ARG:NH1	1:C:118:PHE:CA	2.60	0.54
1:C:24:ARG:NH2	1:C:119:MET:H	2.05	0.54
1:A:4:ILE:HG21	3:A:3186:HOH:O	2.07	0.54
1:C:1:MET:SD	1:C:84:LYS:CG	2.94	0.54
1:E:63:LYS:HA	3:E:3161:HOH:O	2.07	0.54
1:C:4:ILE:HD11	1:C:33:ILE:HG13	1.88	0.54
1:C:65:VAL:CG2	3:C:3174:HOH:O	2.49	0.54
1:C:108:SER:OG	1:E:144:HIS:HE1	1.90	0.54
1:C:117:TYR:HB2	1:F:117:TYR:HB2	1.88	0.54
1:D:123:GLN:HG3	3:D:3180:HOH:O	2.08	0.54
1:A:27:GLU:CB	1:B:1:MET:CE	2.65	0.53
1:A:109:LEU:HD12	3:A:3105:HOH:O	2.08	0.53
1:C:24:ARG:HG3	1:C:118:PHE:CD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:LEU:CB	3:F:3167:HOH:O	1.88	0.53
1:E:88:ARG:HD2	3:E:3114:HOH:O	2.07	0.53
1:A:4:ILE:HB	3:A:3140:HOH:O	2.08	0.53
1:B:63:LYS:NZ	3:B:3102:HOH:O	2.28	0.53
1:F:122:LEU:C	1:F:122:LEU:HD23	2.34	0.53
1:F:66:GLU:HG3	3:F:3183:HOH:O	2.09	0.52
1:A:150:ILE:HG12	3:A:3156:HOH:O	2.10	0.52
1:D:96:PHE:HB2	3:D:3156:HOH:O	2.07	0.52
1:C:4:ILE:HD11	1:C:33:ILE:CG1	2.40	0.51
1:D:40:SER:O	1:D:42:LYS:O	2.28	0.51
1:D:90:LEU:HD21	3:D:3191:HOH:O	2.10	0.51
1:B:57:LEU:HD12	1:B:153:LEU:HD11	1.93	0.51
1:B:93:VAL:HG22	3:B:3174:HOH:O	2.10	0.51
1:C:80:GLU:HB2	3:C:3113:HOH:O	2.10	0.51
1:E:151:TYR:CD1	1:E:154:ILE:HD11	2.45	0.51
1:B:57:LEU:CD1	1:B:153:LEU:HD11	2.41	0.51
1:A:21:ILE:HG23	3:A:3103:HOH:O	2.10	0.51
1:D:27:GLU:OE2	1:E:1:MET:HE3	2.10	0.51
1:E:105:ALA:O	1:E:108:SER:CB	2.59	0.51
1:E:1:MET:C	1:E:3:LYS:H	2.12	0.50
1:D:153:LEU:HD22	3:D:3190:HOH:O	2.11	0.50
1:A:92:VAL:HG12	1:F:97:GLU:HB3	1.93	0.50
1:B:91:ARG:HD2	3:B:3174:HOH:O	2.11	0.50
1:C:53:LYS:HE3	1:C:153:LEU:CD1	2.39	0.50
1:B:140:GLY:HA3	1:E:73:LEU:HD11	1.93	0.50
1:A:21:ILE:HD11	2:A:3000:COD:HC2	1.92	0.50
1:C:151:TYR:CE2	1:C:155:SER:OG	2.65	0.50
1:C:24:ARG:NE	1:C:118:PHE:HB3	2.27	0.50
1:D:29:PHE:CZ	1:D:85:VAL:HG11	2.47	0.50
1:E:134:SER:O	1:E:138:HIS:HD2	1.94	0.49
1:E:129:SER:HB3	1:E:133:ARG:NH1	2.27	0.49
1:A:4:ILE:CG2	3:A:3186:HOH:O	2.60	0.49
1:C:57:LEU:CD2	3:C:3172:HOH:O	2.61	0.49
1:A:122:LEU:C	1:A:122:LEU:HD23	2.37	0.49
1:C:41:ALA:C	1:C:42:LYS:O	2.49	0.49
1:D:123:GLN:HG2	3:D:3180:HOH:O	2.12	0.49
1:C:118:PHE:CE1	1:F:1:MET:HE1	2.44	0.48
1:B:144:HIS:H	1:B:144:HIS:HD2	1.54	0.48
1:D:71:GLU:CG	3:D:3177:HOH:O	2.58	0.48
1:C:127:ILE:HG23	3:C:3155:HOH:O	2.07	0.48
1:D:155:SER:HB2	3:D:3196:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:SER:OG	1:F:144:HIS:CE1	2.66	0.48
3:D:3150:HOH:O	1:E:24:ARG:HG3	2.13	0.48
1:F:109:LEU:CD1	3:F:3173:HOH:O	2.60	0.48
1:C:92:VAL:HG11	1:C:126:PHE:CE2	2.49	0.48
1:B:63:LYS:CE	3:B:3102:HOH:O	2.62	0.48
1:F:20:ASP:CB	3:F:3143:HOH:O	2.46	0.48
1:C:21:ILE:HD11	2:C:3000:COD:HC2	1.96	0.48
1:D:84:LYS:NZ	3:D:3103:HOH:O	2.46	0.48
1:F:90:LEU:HD23	3:F:3126:HOH:O	2.13	0.47
1:D:2:GLN:OE1	1:E:2:GLN:HB3	2.14	0.47
1:D:27:GLU:OE2	1:E:1:MET:CE	2.63	0.47
1:E:144:HIS:H	1:E:144:HIS:CD2	2.30	0.47
1:A:147:PRO:HB2	3:A:3156:HOH:O	2.14	0.47
1:C:57:LEU:HD23	3:C:3172:HOH:O	2.13	0.47
1:A:4:ILE:CB	3:A:3140:HOH:O	2.61	0.47
1:B:134:SER:O	1:B:138:HIS:HD2	1.96	0.47
1:C:53:LYS:HD3	3:C:3159:HOH:O	2.14	0.47
1:C:145:LEU:HD22	3:C:3155:HOH:O	2.14	0.47
1:D:94:SER:HB2	1:E:96:PHE:CZ	2.50	0.47
1:A:88:ARG:HB2	1:A:117:TYR:CD1	2.50	0.47
1:F:6:ILE:HG12	1:F:33:ILE:HB	1.96	0.47
1:C:96:PHE:HB2	3:C:3169:HOH:O	2.10	0.46
1:D:116:LEU:CD1	3:E:3184:HOH:O	2.63	0.46
1:F:92:VAL:HG11	1:F:126:PHE:CE2	2.49	0.46
1:E:122:LEU:HD23	1:E:122:LEU:C	2.40	0.46
3:A:3175:HOH:O	1:B:96:PHE:CE1	2.68	0.46
1:D:118:PHE:CG	3:D:3113:HOH:O	2.68	0.46
1:E:7:TYR:CE1	2:E:3000:COD:HC16	2.51	0.46
1:E:58:ALA:HA	1:E:149:GLU:HG2	1.97	0.46
1:B:124:ASN:CG	3:B:3112:HOH:O	2.56	0.46
1:A:31:LYS:NZ	1:A:66:GLU:OE2	2.48	0.46
1:A:139:LYS:HB2	1:A:139:LYS:HE3	1.51	0.46
1:B:90:LEU:HG	1:B:117:TYR:HB3	1.98	0.46
1:D:24:ARG:CD	3:D:3101:HOH:O	2.62	0.46
1:F:82:HIS:CD2	3:F:3184:HOH:O	2.69	0.46
3:B:3152:HOH:O	1:C:138:HIS:HE1	1.99	0.46
1:E:92:VAL:HG23	3:E:3128:HOH:O	2.16	0.46
1:F:134:SER:O	1:F:138:HIS:HD2	1.99	0.46
3:A:3174:HOH:O	1:D:92:VAL:CG1	1.94	0.45
1:C:152:PRO:HA	3:C:3176:HOH:O	2.16	0.45
1:D:151:TYR:CE1	1:D:154:ILE:HD11	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:PHE:HB2	3:E:3174:HOH:O	2.08	0.45
1:E:95:ASP:CG	1:E:98:TYR:HB3	2.40	0.45
1:E:144:HIS:CD2	3:E:3178:HOH:O	2.70	0.45
1:E:100:LEU:CD2	3:E:3104:HOH:O	2.36	0.45
1:B:7:TYR:CE1	2:B:3000:COD:HC16	2.52	0.45
1:B:92:VAL:HG11	1:B:126:PHE:CE2	2.52	0.45
1:B:98:TYR:CG	3:B:3106:HOH:O	2.64	0.45
1:D:90:LEU:HD11	1:E:90:LEU:HD11	1.99	0.45
1:B:54:MET:HG2	1:B:150:ILE:HB	1.98	0.45
1:A:92:VAL:HB	3:F:3165:HOH:O	2.16	0.45
3:C:3184:HOH:O	1:F:91:ARG:HA	2.17	0.45
1:E:85:VAL:HG11	1:E:116:LEU:HD22	1.98	0.45
1:A:92:VAL:CB	3:F:3165:HOH:O	2.62	0.45
1:A:96:PHE:CZ	1:B:94:SER:HB2	2.52	0.45
1:D:4:ILE:HA	1:D:31:LYS:O	2.17	0.45
1:D:119:MET:CG	3:E:3104:HOH:O	2.65	0.44
1:F:90:LEU:HG	1:F:117:TYR:HB3	2.00	0.44
1:B:97:GLU:CD	1:B:97:GLU:H	2.25	0.44
1:B:107:LYS:CA	3:B:3103:HOH:O	1.94	0.44
1:D:96:PHE:CZ	1:E:94:SER:HB2	2.53	0.44
1:D:42:LYS:O	1:D:44:PRO:HD3	2.17	0.44
1:D:84:LYS:HE3	1:D:112:GLU:OE2	2.17	0.44
1:C:1:MET:SD	1:C:84:LYS:HD3	2.58	0.44
1:C:145:LEU:HB3	3:C:3155:HOH:O	2.17	0.44
1:D:95:ASP:CG	1:D:98:TYR:HB3	2.43	0.44
3:C:3169:HOH:O	1:F:96:PHE:CE1	2.69	0.44
1:F:85:VAL:HG13	3:F:3101:HOH:O	2.17	0.44
1:C:107:LYS:O	1:C:107:LYS:HG2	2.17	0.44
1:B:144:HIS:CD2	1:B:144:HIS:N	2.84	0.43
1:D:88:ARG:HB2	1:D:117:TYR:CD1	2.53	0.43
1:D:119:MET:HG2	3:E:3104:HOH:O	2.18	0.43
1:A:106:ASN:C	3:A:3105:HOH:O	2.46	0.43
1:E:97:GLU:CD	1:E:97:GLU:H	2.27	0.43
1:D:86:LEU:HD11	1:D:113:LEU:HD21	2.00	0.43
1:E:1:MET:HB3	1:E:2:GLN:H	1.62	0.43
1:E:34:VAL:O	1:E:67:CYS:HA	2.19	0.43
1:C:122:LEU:C	1:C:122:LEU:CD2	2.90	0.43
1:B:155:SER:HB3	3:B:3133:HOH:O	2.19	0.43
1:C:88:ARG:HB2	1:C:117:TYR:CD1	2.54	0.42
1:E:139:LYS:HZ2	1:E:139:LYS:HG2	1.47	0.42
1:A:107:LYS:NZ	1:A:114:GLU:OE1	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:HIS:H	1:F:144:HIS:HD2	1.66	0.42
1:A:140:GLY:HA3	1:F:73:LEU:HD11	2.02	0.42
1:F:109:LEU:HD12	3:F:3173:HOH:O	2.19	0.42
1:A:92:VAL:HG11	3:F:3165:HOH:O	2.10	0.42
3:A:3169:HOH:O	1:B:24:ARG:HD2	2.19	0.42
1:C:120:PRO:HD3	2:C:3000:COD:HC2	2.01	0.42
1:B:63:LYS:HE3	3:B:3102:HOH:O	2.18	0.42
1:A:10:THR:HG22	1:A:12:ASP:HB2	2.01	0.42
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.82	0.42
1:A:129:SER:HB3	1:A:133:ARG:NH1	2.35	0.42
1:E:30:GLU:CG	3:E:3185:HOH:O	2.22	0.42
1:E:77:LEU:O	1:E:80:GLU:HB2	2.20	0.42
1:F:31:LYS:HG3	3:F:3166:HOH:O	2.18	0.42
1:C:65:VAL:HG21	3:C:3174:HOH:O	2.15	0.42
1:B:24:ARG:HA	1:B:24:ARG:HD3	1.80	0.41
1:D:10:THR:O	1:D:51:ARG:HD2	2.20	0.41
1:A:117:TYR:HB2	1:B:117:TYR:HB2	2.01	0.41
1:C:24:ARG:HE	1:C:118:PHE:HD1	0.74	0.41
1:B:107:LYS:O	1:B:107:LYS:HG2	2.20	0.41
1:A:98:TYR:CE2	3:A:3180:HOH:O	2.57	0.41
1:E:60:LYS:HG3	3:E:3179:HOH:O	2.19	0.41
1:F:100:LEU:HD13	3:F:3182:HOH:O	2.19	0.41
1:A:128:SER:HB3	1:F:101:GLN:OE1	2.20	0.41
1:E:85:VAL:CB	3:E:3113:HOH:O	2.59	0.41
1:F:151:TYR:N	1:F:152:PRO:HD2	2.36	0.41
1:B:28:LEU:CD2	1:B:118:PHE:HE1	2.31	0.41
1:D:116:LEU:HD11	3:E:3184:HOH:O	2.20	0.41
1:C:94:SER:HB2	1:F:96:PHE:CZ	2.55	0.40
1:A:147:PRO:CG	3:A:3156:HOH:O	2.62	0.40
1:B:3:LYS:CD	3:B:3207:HOH:O	2.68	0.40
1:D:97:GLU:HB3	1:F:92:VAL:HG12	2.03	0.40

All (4) 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:149:GLU:OE1	3:D:3163:HOH:O[3_446]	2.07	0.13
1:F:63:LYS:NZ	3:E:3180:HOH:O[4_455]	2.10	0.10
3:E:3112:HOH:O	3:F:3180:HOH:O[4_555]	2.14	0.06
1:A:149:GLU:OE2	3:D:3163:HOH:O[3_446]	2.18	0.02

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	152/155 (98%)	151 (99%)	1 (1%)	0	100	100
1	B	153/155 (99%)	151 (99%)	1 (1%)	1 (1%)	18	14
1	C	153/155 (99%)	151 (99%)	2 (1%)	0	100	100
1	D	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
1	E	153/155 (99%)	149 (97%)	3 (2%)	1 (1%)	18	14
1	F	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
All	All	917/930 (99%)	902 (98%)	13 (1%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	GLN
1	B	139	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/136 (99%)	123 (91%)	12 (9%)	9	6
1	B	136/136 (100%)	127 (93%)	9 (7%)	15	12
1	C	136/136 (100%)	126 (93%)	10 (7%)	13	9
1	D	136/136 (100%)	128 (94%)	8 (6%)	18	14
1	E	136/136 (100%)	121 (89%)	15 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	136/136 (100%)	125 (92%)	11 (8%)	11	7
All	All	815/816 (100%)	750 (92%)	65 (8%)	11	8

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	40	SER
1	A	71	GLU
1	A	79	LYS
1	A	80	GLU
1	A	84	LYS
1	A	91	ARG
1	A	96	PHE
1	A	123	GLN
1	A	139	LYS
1	A	148	LYS
1	A	153	LEU
1	B	28	LEU
1	B	31	LYS
1	B	60	LYS
1	B	66	GLU
1	B	123	GLN
1	B	131	ILE
1	B	136	ILE
1	B	139	LYS
1	B	150	ILE
1	C	3	LYS
1	C	63	LYS
1	C	71	GLU
1	C	73	LEU
1	C	79	LYS
1	C	91	ARG
1	C	98	TYR
1	C	131	ILE
1	C	148	LYS
1	C	155	SER
1	D	2	GLN
1	D	24	ARG
1	D	79	LYS
1	D	80	GLU
1	D	91	ARG

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Mol	Chain	Res	Type
1	D	116	LEU
1	D	123	GLN
1	D	148	LYS
1	E	2	GLN
1	E	14	VAL
1	E	57	LEU
1	E	60	LYS
1	E	63	LYS
1	E	79	LYS
1	E	91	ARG
1	E	92	VAL
1	E	96	PHE
1	E	108	SER
1	E	123	GLN
1	E	131	ILE
1	E	139	LYS
1	E	149	GLU
1	E	153	LEU
1	F	24	ARG
1	F	43	ASN
1	F	49	ASP
1	F	63	LYS
1	F	80	GLU
1	F	84	LYS
1	F	91	ARG
1	F	111	HIS
1	F	148	LYS
1	F	153	LEU
1	F	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	23	HIS
1	A	56	GLN
1	A	106	ASN
1	A	138	HIS
1	B	56	GLN
1	B	138	HIS
1	B	144	HIS
1	C	56	GLN

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Mol	Chain	Res	Type
1	C	106	ASN
1	C	123	GLN
1	C	124	ASN
1	C	138	HIS
1	D	56	GLN
1	D	138	HIS
1	E	23	HIS
1	E	38	HIS
1	E	56	GLN
1	E	106	ASN
1	E	123	GLN
1	E	138	HIS
1	E	144	HIS
1	F	23	HIS
1	F	56	GLN
1	F	123	GLN
1	F	124	ASN
1	F	138	HIS
1	F	144	HIS

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](#)

6 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	COD	B	3000	-	43,46,46	1.34	5 (11%)	62,68,68	1.89	19 (30%)
2	COD	C	3000	-	43,46,46	1.66	9 (20%)	62,68,68	2.20	23 (37%)
2	COD	E	3000	-	43,46,46	1.72	12 (27%)	62,68,68	1.81	19 (30%)
2	COD	A	3000	-	43,46,46	1.51	9 (20%)	62,68,68	2.06	16 (25%)
2	COD	F	3000	-	43,46,46	1.42	4 (9%)	62,68,68	2.06	24 (38%)
2	COD	D	3000	-	43,46,46	1.62	9 (20%)	62,68,68	2.13	18 (29%)

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	COD	B	3000	-	-	0/43/59/59	0/3/3/3
2	COD	C	3000	-	-	2/43/59/59	0/3/3/3
2	COD	E	3000	-	-	0/43/59/59	0/3/3/3
2	COD	A	3000	-	-	3/43/59/59	0/3/3/3
2	COD	F	3000	-	-	3/43/59/59	0/3/3/3
2	COD	D	3000	-	-	1/43/59/59	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	COD	C5-C4	5.16	1.48	1.39
2	B	3000	COD	C5-C4	4.87	1.47	1.39
2	D	3000	COD	C5-C4	4.66	1.47	1.39
2	C	3000	COD	P20-O23	4.51	1.64	1.59
2	F	3000	COD	C5-C4	4.34	1.46	1.39
2	E	3000	COD	C5-C4	4.11	1.46	1.39
2	F	3000	COD	P20-O23	4.00	1.63	1.59
2	E	3000	COD	C9-N8	3.86	1.39	1.31
2	D	3000	COD	P20-O23	3.79	1.63	1.59
2	A	3000	COD	O33-C32	3.77	1.49	1.42
2	E	3000	COD	C4-N10	-3.70	1.30	1.37
2	F	3000	COD	C4-N10	-3.56	1.30	1.37
2	D	3000	COD	P24-O23	-3.55	1.55	1.59
2	C	3000	COD	C9-N8	3.41	1.38	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	COD	C5-C4	3.25	1.44	1.39
2	E	3000	COD	O33-C32	3.08	1.47	1.42
2	D	3000	COD	O40-C39	2.96	1.29	1.23
2	A	3000	COD	C5-C6	2.90	1.49	1.41
2	D	3000	COD	C5-C6	2.88	1.49	1.41
2	B	3000	COD	C4-N3	2.79	1.39	1.34
2	E	3000	COD	P20-O23	2.73	1.62	1.59
2	B	3000	COD	C5-C6	2.72	1.48	1.41
2	E	3000	COD	C28-C29	2.66	1.57	1.52
2	C	3000	COD	C34-N36	2.58	1.39	1.33
2	C	3000	COD	C4-N10	-2.55	1.32	1.37
2	A	3000	COD	C9-N10	2.47	1.41	1.37
2	B	3000	COD	O33-C32	2.46	1.46	1.42
2	B	3000	COD	P20-O23	2.46	1.62	1.59
2	D	3000	COD	C4-N10	-2.44	1.32	1.37
2	E	3000	COD	C6-N1	-2.39	1.29	1.35
2	E	3000	COD	C34-N36	2.39	1.39	1.33
2	F	3000	COD	C5-C6	2.36	1.47	1.41
2	E	3000	COD	P24-O23	-2.34	1.57	1.59
2	C	3000	COD	C5-C6	2.32	1.47	1.41
2	A	3000	COD	O35-C34	2.30	1.27	1.23
2	D	3000	COD	P20-O22	2.28	1.58	1.50
2	D	3000	COD	C37-C38	2.27	1.58	1.51
2	E	3000	COD	P24-O25	-2.26	1.44	1.55
2	E	3000	COD	C5-C6	2.25	1.47	1.41
2	A	3000	COD	C42-N41	2.22	1.51	1.46
2	E	3000	COD	C39-N41	-2.22	1.28	1.33
2	C	3000	COD	P24-O23	2.21	1.61	1.59
2	C	3000	COD	O40-C39	2.20	1.27	1.23
2	D	3000	COD	C9-N8	2.20	1.35	1.31
2	A	3000	COD	P20-O23	2.18	1.61	1.59
2	C	3000	COD	C42-N41	2.13	1.51	1.46
2	A	3000	COD	C28-C29	2.05	1.56	1.52
2	A	3000	COD	C4-N10	-2.05	1.33	1.37

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3000	COD	C4-N10-C9	5.91	111.94	105.74
2	C	3000	COD	C2-N1-C6	5.77	128.21	118.73
2	A	3000	COD	N3-C2-N1	-5.74	119.89	128.58
2	C	3000	COD	N3-C2-N1	-5.65	120.03	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3000	COD	N3-C2-N1	-5.34	120.50	128.58
2	C	3000	COD	C42-N41-C39	-5.15	113.23	122.82
2	D	3000	COD	C4-N10-C9	5.15	111.14	105.74
2	B	3000	COD	C2-N1-C6	5.08	127.07	118.73
2	C	3000	COD	C4-N10-C9	5.04	111.03	105.74
2	B	3000	COD	N3-C2-N1	-4.77	121.35	128.58
2	A	3000	COD	C4-N10-C9	4.76	110.74	105.74
2	F	3000	COD	C30-C29-C28	4.60	115.82	108.22
2	D	3000	COD	C43-C42-N41	-4.56	101.96	112.31
2	C	3000	COD	C43-C42-N41	-4.56	101.97	112.31
2	A	3000	COD	O23-P20-O22	-4.51	97.15	110.70
2	D	3000	COD	C5-C4-N3	-4.46	120.58	126.72
2	A	3000	COD	C43-C42-N41	-4.46	102.19	112.31
2	D	3000	COD	C42-N41-C39	-4.39	114.65	122.82
2	D	3000	COD	C2-N1-C6	4.30	125.80	118.73
2	A	3000	COD	C2-N1-C6	4.22	125.67	118.73
2	D	3000	COD	N3-C4-N10	4.14	134.21	127.17
2	B	3000	COD	O27-C28-C29	-4.12	103.92	110.55
2	E	3000	COD	O25-P24-O23	4.11	118.37	107.27
2	A	3000	COD	C2-N3-C4	4.08	121.80	111.83
2	A	3000	COD	N10-C9-N8	-3.96	108.32	113.94
2	C	3000	COD	O33-C32-C29	-3.94	101.06	110.18
2	E	3000	COD	C2-N1-C6	3.84	125.04	118.73
2	A	3000	COD	N3-C4-N10	3.83	133.68	127.17
2	D	3000	COD	C37-C38-C39	-3.80	106.06	112.39
2	A	3000	COD	C5-C4-N3	-3.79	121.50	126.72
2	E	3000	COD	C4-N10-C9	3.64	109.56	105.74
2	D	3000	COD	C2-N3-C4	3.62	120.66	111.83
2	F	3000	COD	C43-C42-N41	-3.57	104.21	112.31
2	F	3000	COD	N10-C9-N8	-3.51	108.95	113.94
2	E	3000	COD	O40-C39-N41	-3.48	116.19	123.03
2	F	3000	COD	C38-C39-N41	-3.43	110.09	116.34
2	B	3000	COD	C4-N10-C9	3.38	109.28	105.74
2	F	3000	COD	C4-N10-C11	-3.31	118.89	126.63
2	C	3000	COD	C30-C29-C32	3.27	114.34	108.77
2	A	3000	COD	O33-C32-C29	-3.26	102.64	110.18
2	E	3000	COD	C5-C4-N3	-3.25	122.24	126.72
2	B	3000	COD	C42-N41-C39	3.25	128.87	122.82
2	B	3000	COD	C31-C29-C28	3.20	113.50	108.22
2	C	3000	COD	C31-C29-C28	3.20	113.50	108.22
2	F	3000	COD	O15-C14-C16	-3.19	101.93	111.08
2	F	3000	COD	N3-C4-N10	3.14	132.51	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3000	COD	C2-N1-C6	3.13	123.86	118.73
2	C	3000	COD	C4-N10-C11	-3.11	119.35	126.63
2	F	3000	COD	O27-C28-C29	-3.11	105.55	110.55
2	C	3000	COD	C14-C12-C11	-3.09	95.63	101.46
2	B	3000	COD	C6-C5-N8	3.08	138.04	132.09
2	A	3000	COD	C14-C12-C11	-3.08	95.63	101.46
2	E	3000	COD	C42-N41-C39	-3.07	117.11	122.82
2	B	3000	COD	C4-N10-C11	-3.05	119.49	126.63
2	E	3000	COD	C30-C29-C32	2.92	113.75	108.77
2	F	3000	COD	O21-P20-O22	2.92	126.01	112.44
2	D	3000	COD	N7-C6-N1	2.91	124.86	118.38
2	D	3000	COD	C37-N36-C34	-2.90	117.33	122.55
2	D	3000	COD	O23-P24-O26	-2.86	102.09	110.70
2	F	3000	COD	O33-C32-C29	-2.85	103.58	110.18
2	D	3000	COD	C30-C29-C28	2.81	112.86	108.22
2	C	3000	COD	C37-C38-C39	-2.80	107.72	112.39
2	E	3000	COD	O27-C28-C29	-2.80	106.04	110.55
2	B	3000	COD	C30-C29-C32	2.80	113.55	108.77
2	B	3000	COD	O33-C32-C29	-2.79	103.72	110.18
2	E	3000	COD	C4-C5-N8	-2.78	107.40	110.58
2	B	3000	COD	N3-C4-N10	2.78	131.89	127.17
2	B	3000	COD	C5-C4-N3	-2.70	123.00	126.72
2	B	3000	COD	O25-P24-O23	2.68	114.53	107.27
2	F	3000	COD	O40-C39-C38	2.68	126.88	122.02
2	C	3000	COD	C30-C29-C28	-2.68	103.80	108.22
2	C	3000	COD	C2-N3-C4	2.67	118.36	111.83
2	E	3000	COD	N3-C2-N1	-2.63	124.60	128.58
2	A	3000	COD	C5-N8-C9	2.62	107.57	103.45
2	B	3000	COD	C2-N3-C4	2.60	118.17	111.83
2	F	3000	COD	N3-C2-N1	-2.59	124.66	128.58
2	E	3000	COD	C43-C42-N41	-2.58	106.45	112.31
2	F	3000	COD	C5-C4-N3	-2.56	123.19	126.72
2	A	3000	COD	C4-N10-C11	-2.53	120.72	126.63
2	F	3000	COD	C37-N36-C34	-2.53	118.01	122.55
2	E	3000	COD	O25-P24-O26	2.50	124.09	112.44
2	F	3000	COD	C4-C5-N8	-2.48	107.74	110.58
2	E	3000	COD	C6-C5-N8	2.48	136.87	132.09
2	C	3000	COD	N10-C9-N8	-2.48	110.42	113.94
2	F	3000	COD	C6-C5-N8	2.47	136.84	132.09
2	E	3000	COD	O17-C11-N10	-2.43	103.42	108.09
2	B	3000	COD	C6-C5-C4	-2.41	113.89	117.18
2	F	3000	COD	C31-C29-C32	2.38	112.83	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	COD	N7-C6-N1	2.38	123.68	118.38
2	C	3000	COD	O23-P24-O26	-2.37	103.58	110.70
2	E	3000	COD	N10-C9-N8	-2.35	110.60	113.94
2	A	3000	COD	C30-C29-C32	2.34	112.75	108.77
2	D	3000	COD	O25-P24-O23	2.33	113.56	107.27
2	E	3000	COD	C14-C12-C11	-2.32	97.08	101.46
2	A	3000	COD	C31-C29-C32	2.30	112.69	108.77
2	C	3000	COD	O25-P24-O26	2.30	123.15	112.44
2	D	3000	COD	C4-N10-C11	-2.30	121.25	126.63
2	C	3000	COD	C6-C5-N8	2.28	136.49	132.09
2	F	3000	COD	C5-N8-C9	2.26	107.01	103.45
2	E	3000	COD	C5-C6-N7	2.26	128.88	123.29
2	D	3000	COD	N10-C9-N8	-2.25	110.74	113.94
2	B	3000	COD	O15-C14-C16	-2.23	104.67	111.08
2	C	3000	COD	C31-C29-C32	2.23	112.57	108.77
2	F	3000	COD	O23-P20-O22	-2.23	104.01	110.70
2	B	3000	COD	C4-C5-N8	-2.20	108.07	110.58
2	E	3000	COD	C31-C29-C30	2.19	113.57	109.20
2	D	3000	COD	O21-P20-O22	2.19	122.64	112.44
2	A	3000	COD	C6-C5-N8	2.17	136.26	132.09
2	C	3000	COD	C6-C5-C4	-2.15	114.24	117.18
2	E	3000	COD	C38-C39-N41	2.14	120.23	116.34
2	C	3000	COD	O25-P24-O23	2.10	112.94	107.27
2	D	3000	COD	O25-P24-O26	2.10	122.19	112.44
2	C	3000	COD	N3-C4-N10	2.08	130.71	127.17
2	B	3000	COD	C31-C29-C30	-2.06	105.09	109.20
2	F	3000	COD	C30-C29-C32	-2.06	105.26	108.77
2	F	3000	COD	O21-P20-O23	2.05	112.80	107.27
2	C	3000	COD	O15-C14-C16	-2.04	105.23	111.08
2	F	3000	COD	C42-N41-C39	2.04	126.61	122.82
2	B	3000	COD	O21-P20-O22	2.01	121.78	112.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3000	COD	C28-O27-P24-O23
2	D	3000	COD	O40-C39-N41-C42
2	A	3000	COD	O27-C28-C29-C30
2	A	3000	COD	C28-O27-P24-O26
2	F	3000	COD	O40-C39-N41-C42
2	F	3000	COD	P24-O23-P20-O21

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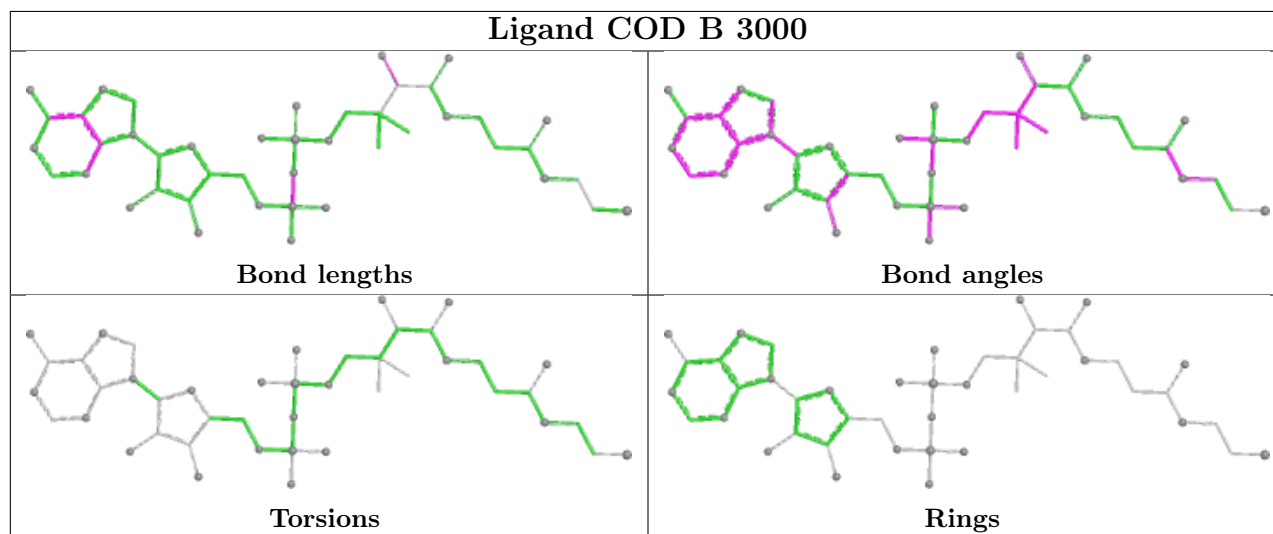
Mol	Chain	Res	Type	Atoms
2	F	3000	COD	C38-C39-N41-C42
2	A	3000	COD	O27-C28-C29-C32
2	C	3000	COD	O40-C39-N41-C42

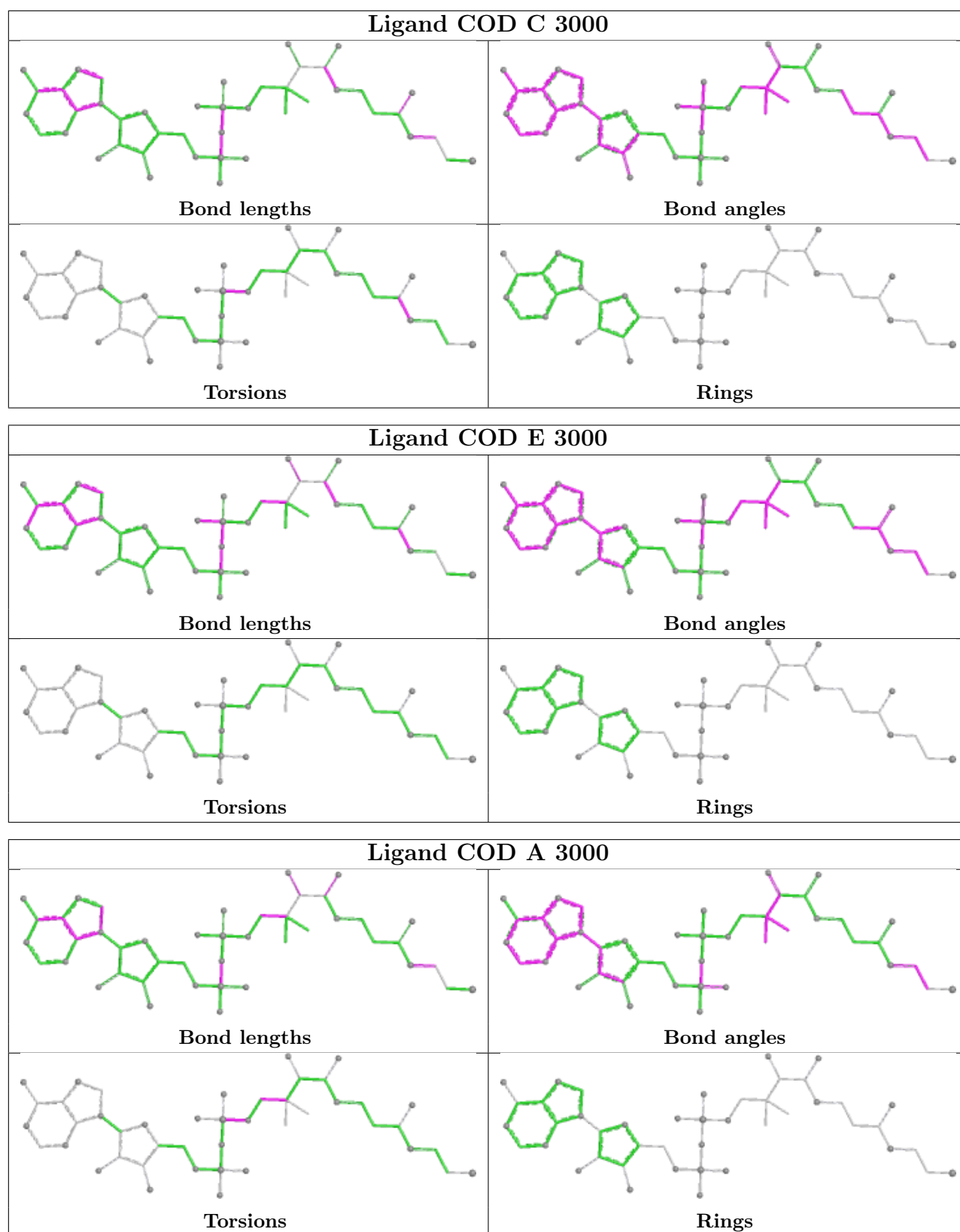
There are no ring outliers.

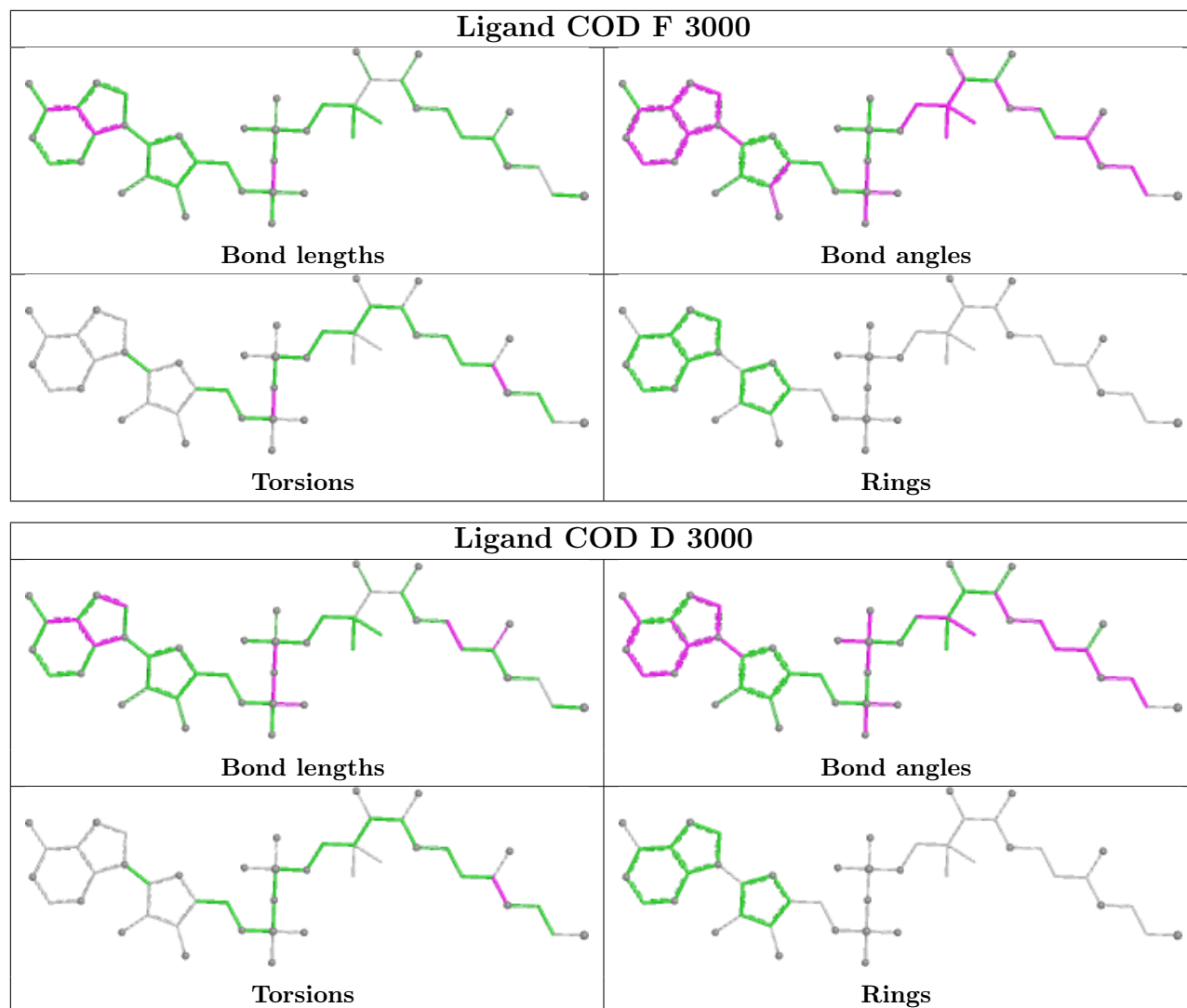
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3000	COD	2	0
2	C	3000	COD	7	0
2	E	3000	COD	2	0
2	A	3000	COD	2	0
2	F	3000	COD	4	0
2	D	3000	COD	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	154/155 (99%)	-0.41	2 (1%) 75 74	15, 23, 41, 55	0
1	B	155/155 (100%)	-0.41	0 100 100	16, 25, 48, 67	0
1	C	155/155 (100%)	-0.36	2 (1%) 75 74	14, 24, 45, 72	0
1	D	155/155 (100%)	-0.33	1 (0%) 85 85	16, 26, 44, 74	0
1	E	155/155 (100%)	-0.31	2 (1%) 75 74	16, 26, 49, 71	0
1	F	155/155 (100%)	-0.32	2 (1%) 75 74	15, 25, 50, 68	0
All	All	929/930 (99%)	-0.36	9 (0%) 79 79	14, 25, 48, 74	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	LYS	2.9
1	F	155	SER	2.8
1	F	111	HIS	2.7
1	D	155	SER	2.7
1	E	1	MET	2.5
1	C	24	ARG	2.5
1	C	2	GLN	2.2
1	E	2	GLN	2.2
1	A	154	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

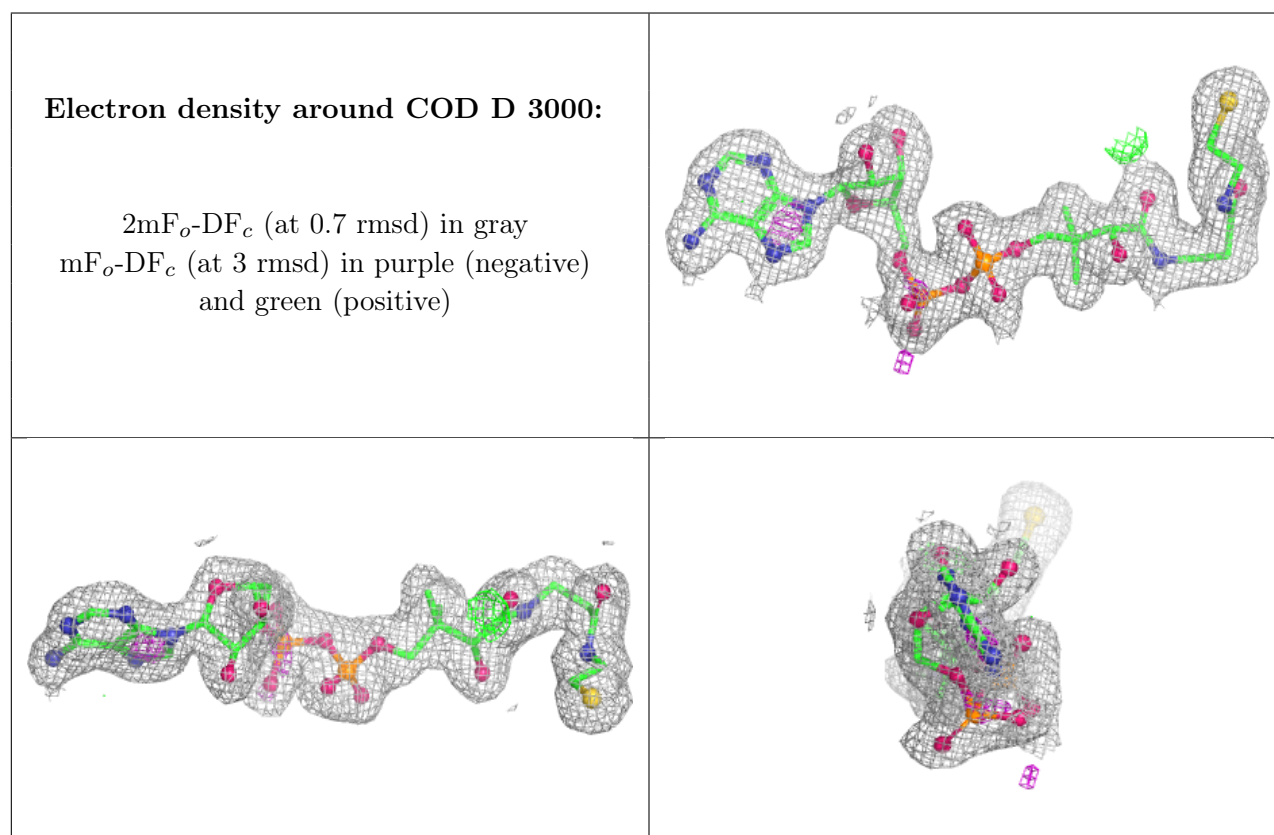
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

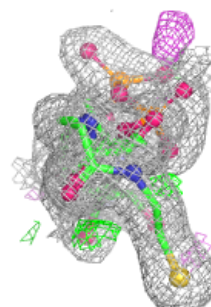
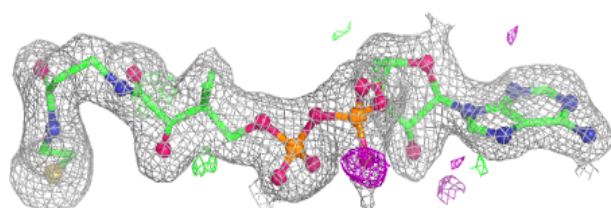
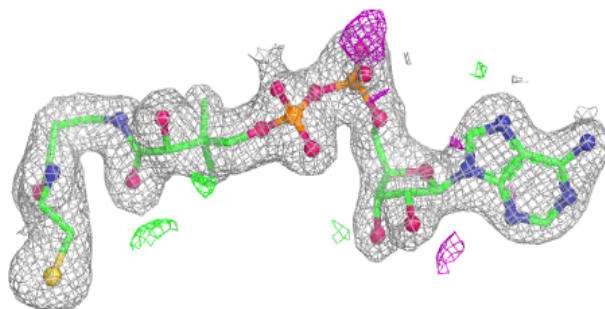
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	COD	D	3000	44/44	0.94	0.08	15,24,33,41	0
2	COD	B	3000	44/44	0.95	0.07	16,27,34,46	0
2	COD	E	3000	44/44	0.95	0.07	15,26,35,38	0
2	COD	A	3000	44/44	0.96	0.07	14,25,32,40	0
2	COD	C	3000	44/44	0.96	0.07	15,28,34,36	0
2	COD	F	3000	44/44	0.96	0.07	19,28,34,45	0

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

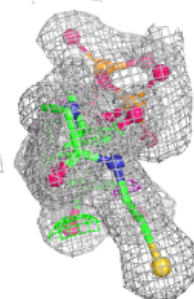
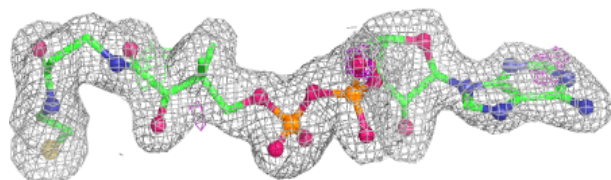
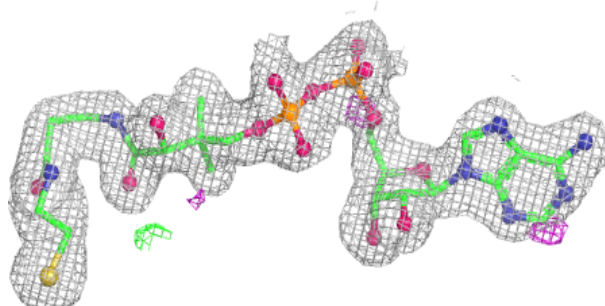


Electron density around COD B 3000:

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

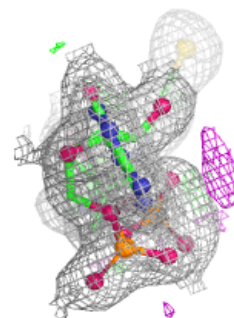
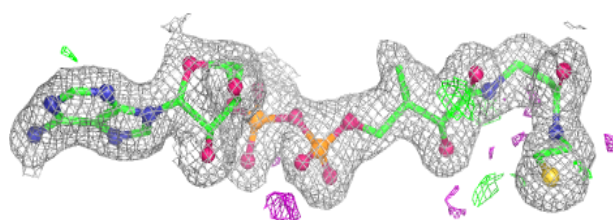
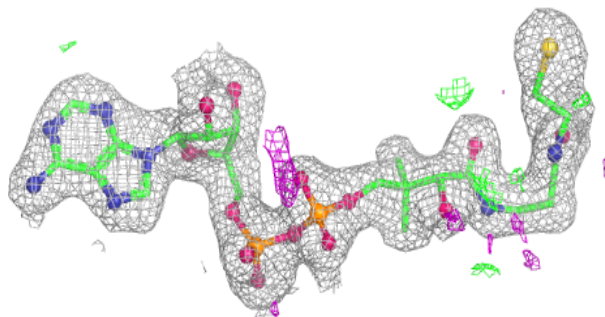
**Electron density around COD E 3000:**

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

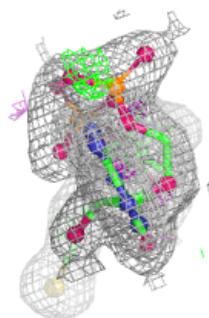
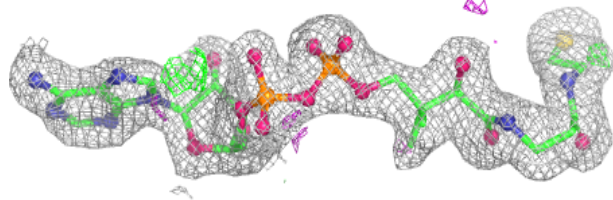
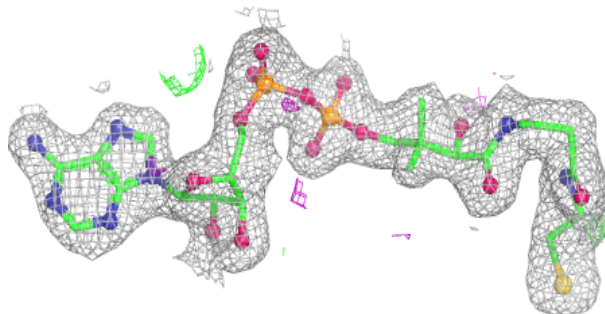


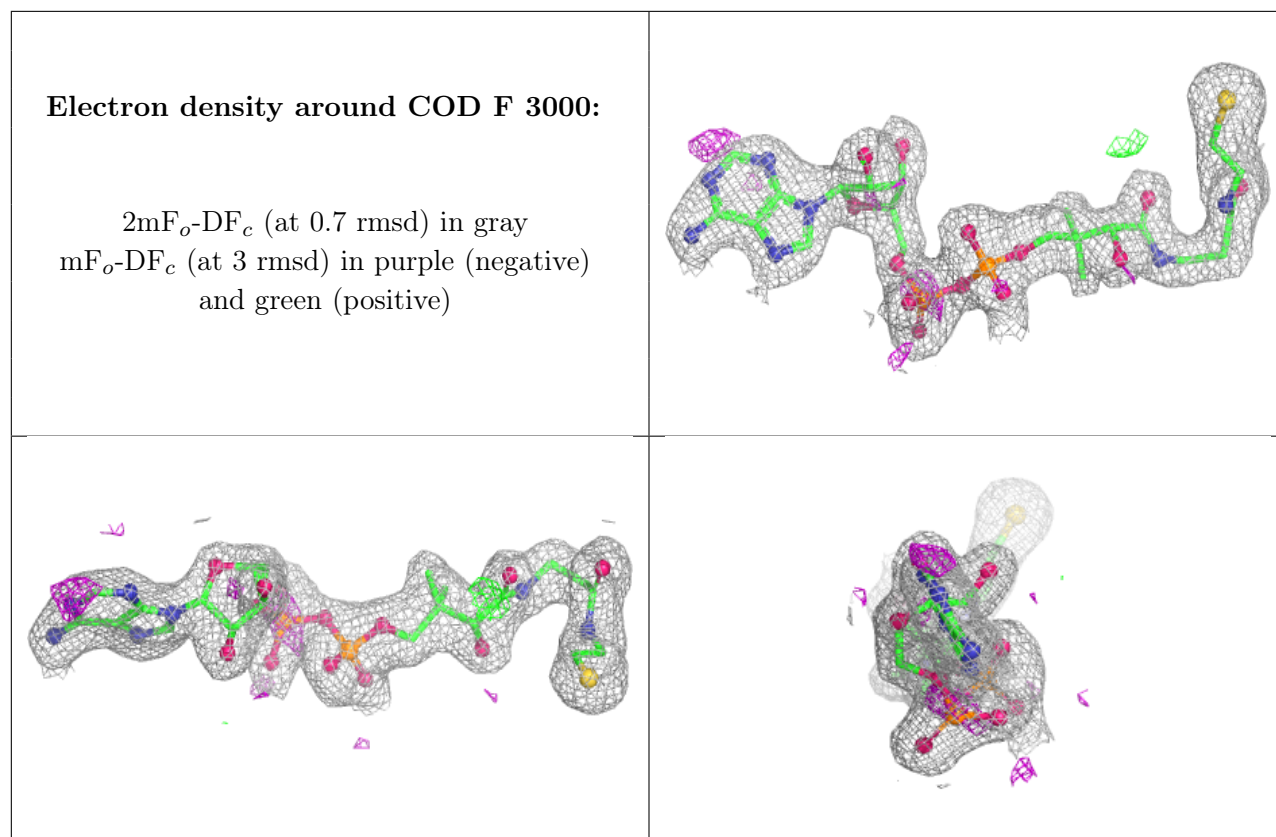
Electron density around COD A 3000:

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

**Electron density around COD C 3000:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.