



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 7VVX / pdb_00007vvx
Title : MmtN-SAH-Met complex
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Deposited on : 2021-11-09
Resolution : 2.51 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

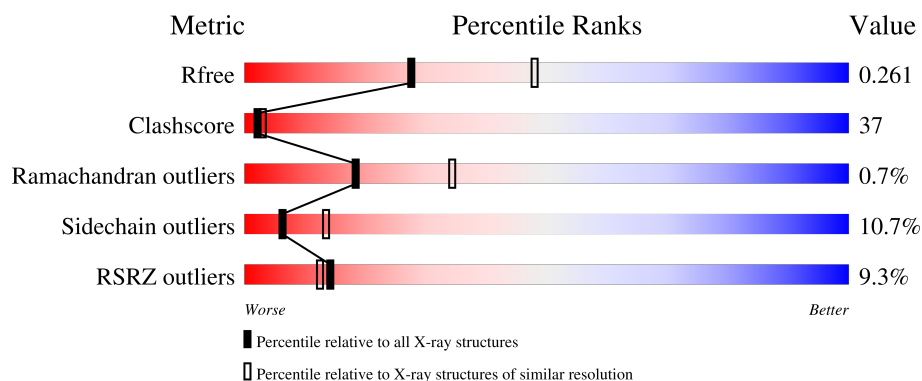
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	305	8% 50% 27% 7% • 15%
1	B	305	8% 45% 31% 14% • 8%
1	C	305	9% 46% 38% 7% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6316 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 SAM-dependent methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1966	1238	345	378	5			
1	B	281	Total	C	N	O	S	0	0	0
			2140	1344	379	412	5			
1	C	280	Total	C	N	O	S	0	0	0
			2129	1343	375	406	5			

There are 9 discrepancies between the modelled and reference sequences:

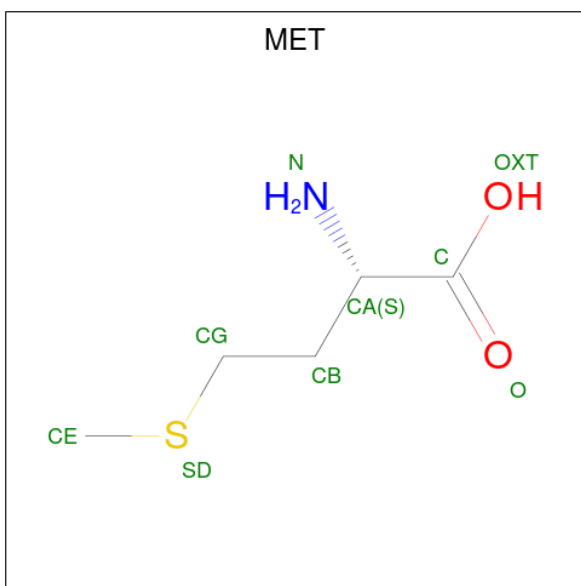
Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
A	143	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
A	146	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
B	141	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
B	143	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
B	146	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
C	141	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
C	143	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
C	146	ALA	LYS	engineered mutation	UNP A0A0T5PCK9

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

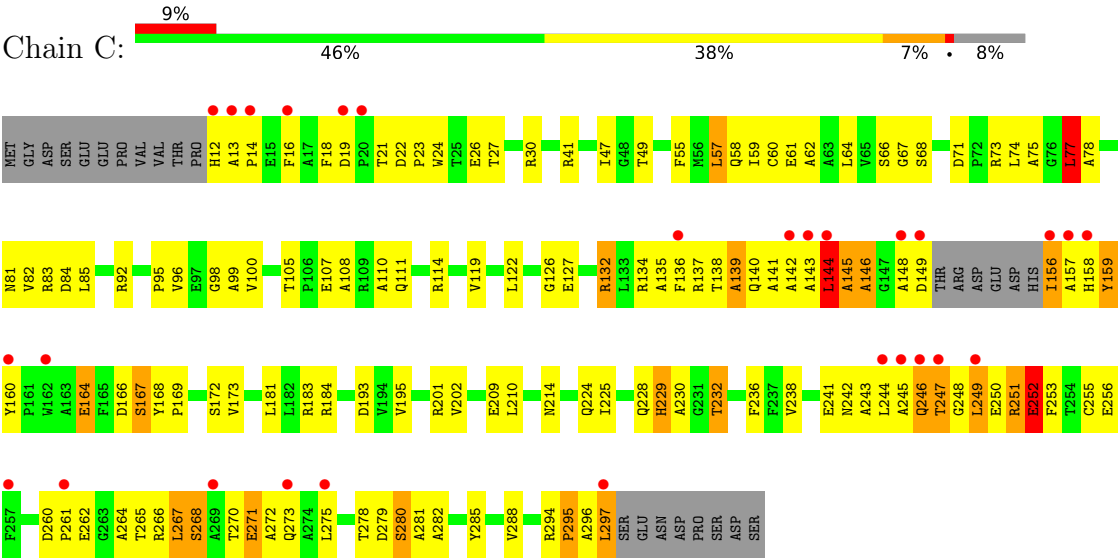
- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	3	Total	O	0	0
			3	3		
5	C	6	Total	O	0	0
			6	6		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.91Å 131.10Å 134.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.57 – 2.51 41.57 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.57-2.51) 99.8 (41.57-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.232 , 0.255 0.237 , 0.261	Depositor DCC
R_{free} test set	2071 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6316	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SAH

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	1.49	38/2006 (1.9%)	0.94	10/2728 (0.4%)
1	B	1.59	42/2184 (1.9%)	1.17	24/2974 (0.8%)
1	C	1.57	41/2174 (1.9%)	1.00	16/2960 (0.5%)
All	All	1.55	121/6364 (1.9%)	1.05	50/8662 (0.6%)

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	22	ASP	C-O	-9.92	1.16	1.25
1	A	227	LEU	CA-C	-8.69	1.42	1.52
1	C	59	ILE	C-O	-8.15	1.16	1.24
1	B	251	ARG	CA-C	-7.88	1.43	1.52
1	C	110	ALA	C-O	-7.69	1.14	1.24
1	A	41	ARG	C-O	-7.55	1.14	1.24
1	B	188	THR	C-O	-7.33	1.15	1.24
1	A	175	LEU	C-O	-7.27	1.14	1.23
1	A	173	VAL	C-O	-7.04	1.15	1.24
1	A	62	ALA	C-O	-6.95	1.15	1.23
1	B	294	ARG	C-O	-6.94	1.16	1.24
1	C	164	GLU	C-O	-6.90	1.15	1.24
1	B	229	HIS	CA-C	-6.84	1.44	1.52
1	A	219	GLU	C-O	-6.81	1.16	1.23
1	C	166	ASP	C-O	-6.71	1.15	1.24
1	B	218	PRO	C-O	-6.67	1.16	1.23
1	A	281	ALA	CA-C	-6.66	1.44	1.52
1	A	225	ILE	C-O	-6.65	1.16	1.24
1	C	13	ALA	CA-C	-6.65	1.45	1.53
1	B	294	ARG	CA-C	-6.63	1.45	1.52
1	C	229	HIS	CA-C	-6.58	1.44	1.52
1	C	167	SER	C-O	-6.55	1.16	1.24
1	C	135	ALA	CA-C	-6.54	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	ALA	CA-C	-6.54	1.44	1.52
1	A	295	PRO	C-O	-6.53	1.15	1.23
1	B	94	HIS	C-O	-6.25	1.18	1.24
1	A	40	LYS	C-O	-6.23	1.15	1.23
1	C	24	TRP	C-O	-6.20	1.16	1.24
1	B	65	VAL	C-O	-6.19	1.18	1.24
1	B	154	ASP	CA-C	-6.19	1.46	1.53
1	B	274	ALA	N-CA	-6.18	1.40	1.46
1	C	98	GLY	C-O	-6.18	1.17	1.23
1	C	57	LEU	C-O	-6.14	1.16	1.24
1	B	227	LEU	C-O	-6.13	1.16	1.23
1	A	223	SER	C-O	-6.09	1.16	1.23
1	A	220	LYS	C-O	-6.09	1.16	1.24
1	A	225	ILE	CA-C	-6.08	1.45	1.52
1	C	253	PHE	CA-C	-6.07	1.45	1.52
1	B	41	ARG	C-O	-6.05	1.16	1.24
1	A	254	THR	C-O	-6.04	1.16	1.23
1	B	260	ASP	C-N	-6.00	1.28	1.34
1	A	41	ARG	CA-C	-5.96	1.45	1.52
1	C	62	ALA	C-O	-5.96	1.16	1.23
1	A	95	PRO	CA-C	-5.95	1.45	1.52
1	C	83	ARG	C-O	-5.94	1.16	1.24
1	B	96	VAL	C-O	-5.94	1.17	1.24
1	B	30	ARG	N-CA	-5.91	1.39	1.46
1	C	271	GLU	C-O	-5.86	1.16	1.24
1	A	106	PRO	C-O	-5.86	1.17	1.24
1	A	172	SER	C-O	-5.85	1.16	1.24
1	A	108	ALA	C-O	-5.85	1.17	1.24
1	C	107	GLU	C-O	-5.82	1.17	1.24
1	B	116	ASP	C-O	-5.79	1.16	1.24
1	B	136	PHE	C-O	-5.79	1.17	1.24
1	B	219	GLU	C-O	-5.73	1.17	1.23
1	B	220	LYS	CA-C	-5.73	1.45	1.52
1	B	284	ILE	CA-C	-5.70	1.45	1.52
1	C	267	LEU	CA-C	-5.69	1.45	1.52
1	A	164	GLU	C-O	-5.69	1.16	1.24
1	B	63	ALA	C-O	-5.69	1.17	1.24
1	B	164	GLU	C-O	-5.66	1.16	1.24
1	B	95	PRO	CA-C	-5.66	1.46	1.52
1	B	187	ALA	C-O	-5.65	1.16	1.24
1	B	30	ARG	CA-C	-5.64	1.45	1.52
1	A	260	ASP	C-O	-5.63	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	ILE	CA-CB	-5.58	1.46	1.54
1	A	229	HIS	CA-C	-5.57	1.45	1.52
1	C	267	LEU	C-O	-5.57	1.17	1.23
1	A	128	PRO	C-O	-5.57	1.17	1.23
1	A	254	THR	CA-C	-5.54	1.45	1.52
1	C	295	PRO	C-O	-5.53	1.17	1.23
1	A	96	VAL	C-O	-5.52	1.18	1.24
1	B	42	VAL	C-O	-5.48	1.18	1.24
1	C	95	PRO	CA-C	-5.46	1.47	1.52
1	A	95	PRO	C-O	-5.46	1.16	1.23
1	B	186	ARG	C-O	-5.45	1.17	1.24
1	A	228	GLN	C-O	-5.41	1.17	1.23
1	C	99	ALA	C-O	-5.40	1.17	1.24
1	C	252	GLU	CA-C	-5.40	1.46	1.52
1	A	224	GLN	C-O	-5.40	1.16	1.23
1	A	227	LEU	C-O	-5.40	1.17	1.24
1	B	284	ILE	C-O	-5.40	1.17	1.24
1	C	255	CYS	C-O	-5.35	1.16	1.23
1	B	276	VAL	N-CA	-5.34	1.40	1.46
1	C	272	ALA	CA-C	-5.33	1.45	1.52
1	A	271	GLU	C-O	-5.32	1.17	1.24
1	C	256	GLU	C-O	-5.30	1.17	1.23
1	A	295	PRO	CA-C	-5.30	1.46	1.52
1	C	134	ARG	C-O	-5.29	1.17	1.24
1	C	268	SER	C-O	-5.29	1.16	1.23
1	C	295	PRO	CA-C	-5.26	1.45	1.52
1	A	84	ASP	C-O	-5.24	1.17	1.24
1	A	253	PHE	C-O	-5.22	1.17	1.24
1	C	98	GLY	CA-C	-5.22	1.45	1.52
1	A	89	ARG	C-O	-5.18	1.16	1.24
1	B	232	THR	C-O	-5.18	1.18	1.24
1	B	129	ASP	C-O	-5.16	1.17	1.24
1	C	99	ALA	CA-C	-5.16	1.46	1.52
1	C	272	ALA	C-O	-5.14	1.17	1.24
1	A	97	GLU	C-O	-5.12	1.17	1.23
1	B	98	GLY	C-O	-5.11	1.18	1.23
1	B	89	ARG	CA-C	-5.11	1.46	1.52
1	B	266	ARG	CA-C	-5.10	1.46	1.53
1	B	220	LYS	C-O	-5.10	1.17	1.24
1	C	84	ASP	C-O	-5.09	1.17	1.24
1	C	62	ALA	CA-C	-5.08	1.46	1.52
1	C	159	TYR	CA-C	-5.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	GLN	C-O	-5.08	1.17	1.24
1	B	262	GLU	CA-C	-5.08	1.46	1.52
1	B	275	LEU	C-N	-5.08	1.27	1.34
1	C	134	ARG	CA-C	-5.08	1.45	1.52
1	C	280	SER	C-O	-5.07	1.17	1.23
1	A	40	LYS	CA-C	-5.06	1.46	1.52
1	C	253	PHE	C-O	-5.05	1.18	1.23
1	A	35	ALA	N-CA	-5.05	1.40	1.46
1	B	114	ARG	CA-C	-5.05	1.46	1.53
1	B	31	GLY	C-O	-5.03	1.17	1.23
1	C	127	GLU	C-N	5.03	1.39	1.33
1	C	268	SER	CA-C	-5.01	1.46	1.52
1	C	77	LEU	C-O	-5.01	1.17	1.24
1	A	219	GLU	CA-C	-5.00	1.46	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ASP	N-CA-C	-13.41	90.80	109.71
1	B	91	ASP	N-CA-C	-12.46	98.08	113.28
1	B	155	HIS	N-CA-C	11.55	126.83	107.20
1	B	150	THR	N-CA-C	10.05	125.47	109.79
1	B	163	ALA	N-CA-C	9.19	122.48	111.82
1	B	160	TYR	C-N-CD	-8.68	101.51	120.60
1	C	252	GLU	N-CA-C	-7.70	96.69	109.24
1	C	144	LEU	N-CA-C	-7.45	102.76	111.03
1	A	96	VAL	N-CA-C	-7.27	98.00	108.17
1	B	89	ARG	CA-C-N	-7.26	115.46	126.86
1	B	89	ARG	C-N-CA	-7.26	115.46	126.86
1	C	148	ALA	N-CA-C	7.25	121.47	111.90
1	A	131	VAL	N-CA-C	6.68	117.66	108.84
1	C	280	SER	CA-C-N	-6.55	116.58	126.86
1	C	280	SER	C-N-CA	-6.55	116.58	126.86
1	A	249	LEU	N-CA-C	6.53	120.69	110.32
1	B	277	ASP	N-CA-C	-6.50	103.82	111.03
1	C	242	ASN	N-CA-C	-6.41	100.76	110.70
1	C	58	GLN	N-CA-C	6.04	119.84	112.23
1	B	279	ASP	N-CA-C	6.00	120.33	112.89
1	A	278	THR	N-CA-C	-5.99	105.98	113.28
1	B	274	ALA	N-CA-C	-5.92	101.86	111.04
1	C	296	ALA	N-CA-C	-5.91	98.21	110.80
1	A	277	ASP	N-CA-C	-5.88	105.36	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ALA	N-CA-C	-5.83	99.63	108.67
1	A	251	ARG	N-CA-C	5.70	117.78	108.55
1	B	283	GLU	N-CA-C	-5.70	103.01	110.53
1	C	146	ALA	N-CA-C	-5.67	107.36	114.56
1	B	142	ALA	N-CA-C	5.66	118.38	111.82
1	C	139	ALA	N-CA-C	-5.61	105.08	111.14
1	A	218	PRO	N-CA-C	5.53	121.00	111.77
1	B	18	PHE	N-CA-C	5.47	117.59	110.53
1	C	127	GLU	CA-C-N	-5.47	114.08	119.93
1	C	127	GLU	C-N-CA	-5.47	114.08	119.93
1	A	174	GLY	N-CA-C	5.46	122.90	115.30
1	B	294	ARG	CA-C-N	-5.46	114.70	120.66
1	B	294	ARG	C-N-CA	-5.46	114.70	120.66
1	A	61	GLU	N-CA-C	5.34	118.95	111.74
1	B	155	HIS	N-CA-CB	-5.34	102.64	110.86
1	C	23	PRO	N-CA-C	5.32	120.57	114.03
1	C	250	GLU	N-CA-C	-5.32	102.33	110.14
1	B	58	GLN	N-CA-C	5.25	119.78	112.90
1	A	244	LEU	N-CA-C	5.24	117.97	109.79
1	B	230	ALA	N-CA-C	-5.16	102.85	110.48
1	C	24	TRP	N-CA-C	-5.10	105.18	111.40
1	B	94	HIS	CA-C-N	-5.09	115.48	120.52
1	B	94	HIS	C-N-CA	-5.09	115.48	120.52
1	C	280	SER	N-CA-C	-5.08	103.44	110.35
1	B	250	GLU	CA-C-N	-5.05	113.96	122.29
1	B	250	GLU	C-N-CA	-5.05	113.96	122.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1966	0	1913	133	0
1	B	2140	0	2073	200	0
1	C	2129	0	2065	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	26	0	19	2	0
2	B	26	0	19	2	0
3	B	9	0	8	1	0
4	C	5	0	0	1	0
5	A	6	0	0	0	0
5	B	3	0	0	0	0
5	C	6	0	0	0	0
All	All	6316	0	6097	460	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 37.

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:HB3	1:A:74:LEU:CD1	1.45	1.44
1:C:132:ARG:HG2	1:C:159:TYR:CE2	1.57	1.38
1:A:71:ASP:CB	1:A:74:LEU:HD11	1.57	1.33
1:B:41:ARG:HG2	1:B:64:LEU:CD2	1.63	1.27
1:A:252:GLU:N	1:B:162:TRP:HH2	1.37	1.22
1:A:257:PHE:HB2	1:A:267:LEU:HD12	1.23	1.20
1:C:243:ALA:HB1	1:C:251:ARG:HE	1.06	1.16
1:B:247:THR:HG21	1:B:249:LEU:HD22	1.28	1.15
1:C:245:ALA:HA	1:C:249:LEU:O	1.47	1.14
1:A:273:GLN:HE21	1:A:276:VAL:CG2	1.61	1.13
1:B:148:ALA:HB3	1:B:149:ASP:HA	1.16	1.13
1:B:41:ARG:HG2	1:B:64:LEU:HD21	1.20	1.12
1:B:41:ARG:CG	1:B:64:LEU:HD21	1.80	1.09
1:B:144:LEU:HA	1:B:148:ALA:HB2	1.34	1.08
1:C:132:ARG:CG	1:C:159:TYR:HE2	1.65	1.08
1:A:228:GLN:CG	1:A:232:THR:HG21	1.84	1.07
1:A:74:LEU:HD12	1:A:74:LEU:H	1.19	1.07
1:A:279:ASP:OD1	1:A:280:SER:N	1.89	1.06
1:A:228:GLN:HG3	1:A:232:THR:HG21	1.07	1.05
1:B:41:ARG:CG	1:B:64:LEU:CD2	2.36	1.04
1:B:159:TYR:H	1:B:160:TYR:HB3	1.23	1.04
1:C:246:GLN:HG3	1:C:249:LEU:HD12	1.38	1.01
1:C:243:ALA:HB1	1:C:251:ARG:NE	1.75	1.01
1:B:158:HIS:HB3	1:B:160:TYR:O	1.62	1.00
1:C:246:GLN:HG3	1:C:249:LEU:CD1	1.91	1.00
1:A:273:GLN:NE2	1:A:276:VAL:CG2	2.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NE	1:C:159:TYR:CD2	2.30	0.98
1:C:246:GLN:HA	1:C:248:GLY:HA2	1.47	0.96
1:B:18:PHE:HE2	1:B:30:ARG:HH11	1.10	0.96
1:C:248:GLY:CA	1:C:249:LEU:HD13	1.95	0.96
1:A:267:LEU:HD13	1:A:272:ALA:HB2	1.46	0.96
1:C:266:ARG:C	1:C:267:LEU:HD22	1.91	0.96
1:A:252:GLU:N	1:B:162:TRP:CH2	2.21	0.95
1:C:132:ARG:CG	1:C:159:TYR:CE2	2.44	0.95
1:C:248:GLY:C	1:C:249:LEU:HD22	1.92	0.95
1:A:257:PHE:HB3	1:A:267:LEU:HD11	1.44	0.94
1:A:257:PHE:CB	1:A:267:LEU:HD12	1.97	0.94
1:A:273:GLN:NE2	1:A:276:VAL:HG21	1.83	0.94
1:C:132:ARG:HG2	1:C:159:TYR:HE2	0.89	0.94
1:B:247:THR:CG2	1:B:249:LEU:HD22	1.98	0.94
1:B:93:PHE:CZ	1:B:95:PRO:HG3	2.02	0.93
1:B:56:MET:HE1	1:B:119:VAL:HG21	1.48	0.93
1:A:272:ALA:HA	1:A:275:LEU:HD21	1.51	0.93
1:A:89:ARG:HH11	1:A:89:ARG:HG2	1.31	0.92
1:A:273:GLN:HE21	1:A:276:VAL:HG23	1.33	0.92
1:C:132:ARG:HE	1:C:159:TYR:HD2	1.10	0.92
1:B:148:ALA:HB3	1:B:149:ASP:CA	1.98	0.92
1:C:280:SER:O	1:C:281:ALA:HB3	1.66	0.92
1:A:257:PHE:CB	1:A:267:LEU:CD1	2.47	0.92
1:B:58:GLN:HE22	1:B:86:ALA:HA	1.35	0.91
1:A:202:VAL:HG12	1:A:206:VAL:HG11	1.53	0.91
1:C:243:ALA:CB	1:C:251:ARG:HE	1.84	0.90
1:B:18:PHE:CE2	1:B:30:ARG:HD2	2.07	0.89
1:C:132:ARG:HH11	1:C:159:TYR:HB3	1.37	0.88
1:B:89:ARG:O	1:B:90:ALA:HB3	1.72	0.87
1:A:257:PHE:HB2	1:A:267:LEU:CD1	2.03	0.87
1:C:246:GLN:H	1:C:249:LEU:HA	1.40	0.86
1:B:57:LEU:HD22	1:B:92:ARG:HG3	1.55	0.86
1:C:261:PRO:HG3	1:C:285:TYR:CE2	2.11	0.86
1:B:18:PHE:HE2	1:B:30:ARG:NH1	1.74	0.86
1:B:159:TYR:H	1:B:160:TYR:CB	1.89	0.85
1:B:267:LEU:HD21	1:B:271:GLU:HB2	1.59	0.84
1:C:248:GLY:HA2	1:C:249:LEU:HD13	1.56	0.84
1:A:27:THR:HG22	1:A:224:GLN:CD	2.03	0.84
1:B:41:ARG:CD	1:B:64:LEU:HD21	2.08	0.84
1:A:132:ARG:HA	1:A:133:LEU:O	1.78	0.83
1:B:158:HIS:CB	1:B:160:TYR:O	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:HB3	1:A:267:LEU:CD1	2.07	0.82
1:B:260:ASP:OD1	1:B:265:THR:HG22	1.78	0.82
1:A:275:LEU:O	1:A:279:ASP:HB3	1.80	0.82
1:A:88:ARG:HG2	1:A:88:ARG:HH21	1.44	0.81
1:B:131:VAL:HG21	2:B:401:SAH:HB1	1.63	0.81
1:A:132:ARG:H	1:A:133:LEU:HB3	1.45	0.81
1:A:228:GLN:HG3	1:A:232:THR:CG2	2.01	0.81
1:B:159:TYR:N	1:B:160:TYR:O	2.14	0.81
1:A:273:GLN:NE2	1:A:276:VAL:HG23	1.92	0.81
1:A:275:LEU:HD22	1:A:275:LEU:H	1.45	0.81
1:B:32:LEU:HD13	1:B:56:MET:HE3	1.62	0.80
1:C:280:SER:O	1:C:281:ALA:CB	2.28	0.80
1:B:18:PHE:CZ	1:B:30:ARG:HD2	2.16	0.80
1:A:88:ARG:HG2	1:A:88:ARG:NH2	1.97	0.79
1:A:273:GLN:HE21	1:A:273:GLN:HA	1.46	0.79
1:B:89:ARG:O	1:B:90:ALA:CB	2.30	0.79
1:C:144:LEU:O	1:C:146:ALA:N	2.16	0.79
1:B:58:GLN:NE2	1:B:86:ALA:HA	1.98	0.78
1:B:159:TYR:OH	1:B:162:TRP:CZ2	2.35	0.78
1:C:132:ARG:HH11	1:C:159:TYR:CB	1.95	0.78
1:C:77:LEU:HD22	1:C:77:LEU:O	1.83	0.78
1:B:41:ARG:HG2	1:B:64:LEU:HD23	1.61	0.78
1:C:141:ALA:O	1:C:143:ALA:N	2.18	0.77
1:B:250:GLU:CD	1:B:250:GLU:H	1.93	0.76
1:B:86:ALA:O	1:B:90:ALA:HB2	1.84	0.76
1:A:273:GLN:HA	1:A:276:VAL:CG2	2.14	0.76
1:B:143:ALA:O	1:B:148:ALA:HB1	1.84	0.76
1:B:247:THR:HG21	1:B:249:LEU:CD2	2.14	0.76
1:C:19:ASP:CG	1:C:21:THR:HG22	2.11	0.75
1:B:45:VAL:HG23	1:B:122:LEU:HD21	1.69	0.75
1:B:41:ARG:NE	1:B:64:LEU:HD21	2.02	0.74
1:B:27:THR:HG22	1:B:224:GLN:CD	2.12	0.74
1:A:225:ILE:N	1:A:225:ILE:HD12	2.03	0.74
1:B:93:PHE:CE1	1:B:95:PRO:HG3	2.22	0.74
1:C:267:LEU:HD22	1:C:267:LEU:N	2.01	0.74
1:A:129:ASP:OD1	1:A:129:ASP:N	2.22	0.73
1:C:144:LEU:HG	1:C:145:ALA:H	1.52	0.73
1:C:156:ILE:O	1:C:158:HIS:N	2.22	0.73
1:B:159:TYR:CZ	1:B:162:TRP:CZ2	2.77	0.73
1:C:297:LEU:C	1:C:297:LEU:HD22	2.14	0.72
1:A:228:GLN:CG	1:A:232:THR:CG2	2.65	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:O	1:C:267:LEU:HD13	1.89	0.72
1:C:260:ASP:OD2	1:C:262:GLU:HB2	1.90	0.72
1:A:132:ARG:HA	1:A:133:LEU:C	2.15	0.72
1:B:143:ALA:O	1:B:148:ALA:CB	2.38	0.72
1:B:150:THR:OG1	1:B:151:ARG:N	2.22	0.71
1:C:261:PRO:HG3	1:C:285:TYR:CZ	2.25	0.71
1:C:248:GLY:HA3	1:C:249:LEU:HD13	1.72	0.71
1:A:27:THR:HG22	1:A:224:GLN:OE1	1.91	0.71
1:C:19:ASP:OD1	1:C:21:THR:HG22	1.89	0.71
1:A:251:ARG:HA	1:B:162:TRP:CZ3	2.26	0.71
1:B:245:ALA:O	1:B:248:GLY:HA2	1.92	0.70
1:B:83:ARG:O	1:B:87:PRO:HG3	1.92	0.70
1:A:74:LEU:HD12	1:A:74:LEU:N	2.02	0.70
1:B:57:LEU:CD2	1:B:92:ARG:HG3	2.22	0.70
1:B:148:ALA:H	1:B:149:ASP:CG	2.00	0.70
1:C:229:HIS:O	1:C:232:THR:HG22	1.92	0.70
1:C:249:LEU:HD22	1:C:249:LEU:N	2.06	0.69
1:A:71:ASP:CG	1:A:74:LEU:HD11	2.17	0.69
1:A:89:ARG:HG2	1:A:89:ARG:NH1	2.02	0.69
1:B:267:LEU:HD23	1:B:268:SER:N	2.07	0.69
1:A:200:ALA:HB3	1:A:287:GLU:HB3	1.73	0.68
1:A:252:GLU:HB2	1:B:162:TRP:CZ2	2.29	0.68
1:B:151:ARG:CG	1:B:152:ASP:H	2.05	0.68
1:B:91:ASP:N	1:B:91:ASP:OD1	2.23	0.68
1:C:139:ALA:O	1:C:143:ALA:HB3	1.93	0.68
1:B:41:ARG:CG	1:B:64:LEU:HD23	2.15	0.68
1:A:71:ASP:HB3	1:A:74:LEU:HD11	0.73	0.67
1:A:71:ASP:HB3	1:A:74:LEU:HD13	1.68	0.67
1:C:19:ASP:OD2	1:C:21:THR:HG22	1.95	0.67
1:C:122:LEU:HD11	1:C:181:LEU:HD22	1.77	0.67
1:C:68:SER:HB3	1:C:96:VAL:CG2	2.25	0.67
1:B:18:PHE:CE2	1:B:30:ARG:NH1	2.60	0.66
1:A:161:PRO:O	1:A:162:TRP:HE3	1.78	0.66
1:B:86:ALA:N	1:B:87:PRO:HD3	2.11	0.66
1:A:133:LEU:C	1:A:133:LEU:HD23	2.19	0.66
1:B:158:HIS:O	1:B:159:TYR:HB2	1.95	0.66
1:A:164:GLU:OE2	1:A:164:GLU:N	2.27	0.65
1:A:275:LEU:HD22	1:A:275:LEU:N	2.09	0.65
1:B:273:GLN:HA	1:B:276:VAL:CG2	2.26	0.65
1:B:212:GLU:HG2	1:C:184:ARG:CZ	2.26	0.65
1:A:251:ARG:HA	1:B:162:TRP:HZ3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:O	1:A:74:LEU:HD12	1.97	0.65
1:A:121:CYS:SG	2:A:401:SAH:HA	2.37	0.65
1:B:271:GLU:O	1:B:274:ALA:HB3	1.96	0.65
1:C:238:VAL:HG13	1:C:270:THR:HG22	1.79	0.65
1:A:273:GLN:NE2	1:A:273:GLN:HA	2.11	0.64
1:A:236:PHE:CE2	1:C:247:THR:HG22	2.33	0.64
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.10	0.64
1:C:19:ASP:O	1:C:26:GLU:HB2	1.97	0.64
1:B:136:PHE:HD1	1:B:154:ASP:O	1.79	0.64
1:A:267:LEU:CD1	1:A:272:ALA:HB2	2.24	0.64
1:C:158:HIS:CD2	1:C:159:TYR:CE1	2.86	0.64
1:B:86:ALA:N	1:B:87:PRO:CD	2.61	0.64
1:B:151:ARG:HG3	1:B:152:ASP:H	1.63	0.63
1:A:272:ALA:HA	1:A:275:LEU:CD2	2.27	0.63
1:C:158:HIS:HD2	1:C:159:TYR:CE1	2.15	0.63
1:A:273:GLN:HE21	1:A:273:GLN:CA	2.12	0.63
1:A:132:ARG:N	1:A:133:LEU:HB3	2.13	0.63
1:B:148:ALA:CB	1:B:149:ASP:HA	2.07	0.62
1:A:247:THR:C	1:A:249:LEU:H	2.07	0.62
1:B:295:PRO:O	1:B:297:LEU:HD22	1.98	0.62
1:C:30:ARG:HD2	1:C:224:GLN:NE2	2.14	0.62
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.63	0.62
1:B:18:PHE:CE2	1:B:30:ARG:CD	2.82	0.62
1:A:228:GLN:OE1	1:A:284:ILE:HB	2.00	0.62
1:A:71:ASP:O	1:A:74:LEU:CD1	2.48	0.62
1:C:142:ALA:C	1:C:144:LEU:H	2.06	0.61
1:B:283:GLU:O	1:B:284:ILE:HD13	2.00	0.61
1:C:159:TYR:O	1:C:160:TYR:C	2.43	0.61
1:A:78:ALA:O	1:A:82:VAL:HG23	2.00	0.61
1:C:252:GLU:HG3	1:C:252:GLU:O	2.00	0.61
1:B:158:HIS:C	1:B:160:TYR:O	2.42	0.61
1:C:144:LEU:CG	1:C:145:ALA:H	2.13	0.61
1:B:126:GLY:O	1:B:201:ARG:NH2	2.33	0.61
1:A:252:GLU:HB2	1:B:162:TRP:CH2	2.36	0.60
1:A:71:ASP:CB	1:A:74:LEU:CD1	2.40	0.60
1:A:275:LEU:N	1:A:275:LEU:HD13	2.16	0.60
1:A:246:GLN:HG3	1:B:166:ASP:O	2.00	0.60
1:A:73:ARG:HG2	1:A:73:ARG:HH11	1.66	0.60
1:C:132:ARG:NH1	1:C:159:TYR:HB3	2.13	0.60
1:B:61:GLU:OE1	1:B:89:ARG:NH2	2.34	0.59
1:C:14:PRO:CG	1:C:16:PHE:CE2	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:THR:O	1:C:265:THR:HG23	2.01	0.59
1:A:273:GLN:HA	1:A:276:VAL:HG22	1.84	0.59
1:C:243:ALA:HB1	1:C:251:ARG:CD	2.32	0.59
1:B:121:CYS:SG	2:B:401:SAH:HA	2.43	0.59
1:A:119:VAL:HG12	1:A:195:VAL:HB	1.83	0.59
1:B:204:SER:OG	1:B:220:LYS:NZ	2.35	0.59
1:B:279:ASP:O	1:B:280:SER:HB3	2.03	0.58
1:B:279:ASP:C	1:B:281:ALA:H	2.10	0.58
1:C:241:GLU:C	1:C:243:ALA:H	2.11	0.58
1:A:275:LEU:H	1:A:275:LEU:HD13	1.66	0.58
1:B:160:TYR:HD1	1:B:161:PRO:HB3	1.69	0.58
1:C:246:GLN:H	1:C:249:LEU:CA	2.16	0.58
1:A:89:ARG:HH12	1:A:92:ARG:NH1	2.01	0.58
1:B:273:GLN:HA	1:B:276:VAL:HG22	1.84	0.58
1:B:93:PHE:CZ	1:B:95:PRO:CG	2.82	0.58
1:B:48:GLY:HA2	1:B:74:LEU:HD13	1.86	0.58
1:B:56:MET:O	1:B:60:CYS:HB2	2.05	0.57
1:B:247:THR:CB	1:B:249:LEU:H	2.16	0.57
1:B:77:LEU:HD11	1:B:143:ALA:HB2	1.84	0.57
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.17	0.57
1:C:14:PRO:HG2	1:C:16:PHE:CE2	2.40	0.57
1:C:141:ALA:O	1:C:142:ALA:HB3	2.04	0.57
1:B:159:TYR:N	1:B:160:TYR:HB3	2.06	0.57
1:B:88:ARG:HA	1:B:88:ARG:CZ	2.35	0.57
1:B:285:TYR:CD1	1:B:285:TYR:N	2.73	0.57
1:C:156:ILE:O	1:C:157:ALA:HB3	2.05	0.57
1:C:126:GLY:O	1:C:201:ARG:NH2	2.38	0.56
1:C:245:ALA:O	1:C:246:GLN:O	2.22	0.56
1:B:283:GLU:C	1:B:284:ILE:HG12	2.29	0.56
1:C:246:GLN:N	1:C:249:LEU:HA	2.16	0.56
1:A:23:PRO:O	1:A:27:THR:HG23	2.06	0.56
1:B:71:ASP:HB3	1:B:74:LEU:HG	1.86	0.56
1:C:201:ARG:NH1	1:C:228:GLN:OE1	2.38	0.56
1:B:247:THR:CB	1:B:249:LEU:N	2.69	0.56
1:B:247:THR:HB	1:B:249:LEU:N	2.21	0.56
1:B:132:ARG:HD3	3:B:402:MET:HE2	1.88	0.56
1:B:244:LEU:HD12	1:B:250:GLU:HA	1.88	0.56
1:C:158:HIS:CD2	1:C:159:TYR:HE1	2.22	0.56
1:B:86:ALA:O	1:B:90:ALA:CB	2.53	0.56
1:B:266:ARG:HH11	1:B:266:ARG:HG2	1.70	0.56
1:C:225:ILE:HG21	1:C:261:PRO:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:O	1:B:284:ILE:CD1	2.54	0.56
1:A:275:LEU:O	1:A:279:ASP:CB	2.53	0.55
1:B:247:THR:HG22	1:C:236:PHE:CD2	2.41	0.55
1:B:23:PRO:O	1:B:27:THR:HG23	2.06	0.55
1:A:222:HIS:NE2	1:A:224:GLN:NE2	2.48	0.55
1:B:283:GLU:O	1:B:284:ILE:HG12	2.07	0.55
1:A:44:GLU:HG3	1:A:119:VAL:HG23	1.86	0.55
1:C:169:PRO:HG2	4:C:401:PO4:O3	2.06	0.55
1:B:136:PHE:CD1	1:B:154:ASP:O	2.59	0.55
1:A:246:GLN:OE1	1:B:168:TYR:O	2.25	0.54
1:A:273:GLN:HG3	1:A:273:GLN:O	2.07	0.54
1:A:238:VAL:HG12	1:A:269:ALA:C	2.32	0.54
1:C:16:PHE:CD1	1:C:16:PHE:C	2.85	0.54
1:B:245:ALA:O	1:B:248:GLY:CA	2.54	0.54
1:A:238:VAL:HG12	1:A:269:ALA:O	2.08	0.54
1:B:193:ASP:OD1	1:B:294:ARG:HG3	2.07	0.54
1:A:61:GLU:OE2	1:A:89:ARG:NH2	2.41	0.54
1:A:252:GLU:HB2	1:B:159:TYR:OH	2.08	0.54
1:B:221:LEU:HD11	1:B:292:ARG:HB2	1.90	0.54
1:B:144:LEU:C	1:B:146:ALA:H	2.15	0.53
1:A:77:LEU:O	1:A:80:ARG:HG3	2.08	0.53
1:B:144:LEU:CA	1:B:148:ALA:HB2	2.24	0.53
1:C:132:ARG:NE	1:C:159:TYR:HD2	1.83	0.53
1:A:241:GLU:CD	1:A:269:ALA:HB3	2.34	0.53
1:B:80:ARG:O	1:B:81:ASN:C	2.50	0.53
1:C:156:ILE:CG2	1:C:157:ALA:N	2.72	0.53
1:B:227:LEU:HD13	1:B:285:TYR:CE2	2.44	0.52
1:B:32:LEU:CD1	1:B:56:MET:HE3	2.35	0.52
1:B:266:ARG:HG2	1:B:266:ARG:NH1	2.23	0.52
1:C:295:PRO:O	1:C:297:LEU:N	2.43	0.52
1:B:247:THR:N	1:B:248:GLY:HA2	2.24	0.52
1:B:158:HIS:O	1:B:159:TYR:CB	2.58	0.52
1:C:77:LEU:CD2	1:C:81:ASN:OD1	2.58	0.52
1:C:144:LEU:CG	1:C:145:ALA:N	2.73	0.52
1:C:241:GLU:C	1:C:243:ALA:N	2.64	0.51
1:A:202:VAL:HG12	1:A:206:VAL:CG1	2.32	0.51
1:A:225:ILE:N	1:A:225:ILE:CD1	2.73	0.51
1:B:40:LYS:O	1:B:63:ALA:HB3	2.10	0.51
1:A:275:LEU:H	1:A:275:LEU:CD2	2.10	0.51
1:B:19:ASP:OD1	1:B:20:PRO:HD2	2.10	0.51
1:C:246:GLN:HA	1:C:249:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:OD1	1:A:72:PRO:HD2	2.11	0.51
1:A:273:GLN:O	1:A:276:VAL:HG23	2.11	0.51
1:C:78:ALA:O	1:C:82:VAL:HG23	2.11	0.51
1:C:249:LEU:N	1:C:249:LEU:CD2	2.73	0.51
1:A:132:ARG:CA	1:A:133:LEU:C	2.84	0.51
1:B:88:ARG:HA	1:B:88:ARG:NE	2.26	0.51
1:B:94:HIS:ND1	1:B:94:HIS:N	2.60	0.50
1:B:159:TYR:CZ	1:B:162:TRP:HZ2	2.26	0.50
1:B:283:GLU:O	1:B:284:ILE:CG1	2.59	0.50
1:C:67:GLY:O	1:C:96:VAL:HG22	2.11	0.50
1:B:27:THR:HG21	1:B:224:GLN:HB2	1.92	0.50
1:C:243:ALA:CB	1:C:251:ARG:NE	2.59	0.50
1:B:18:PHE:CZ	1:B:30:ARG:CD	2.92	0.50
1:C:27:THR:HG21	1:C:288:VAL:HG12	1.94	0.50
1:B:148:ALA:CB	1:B:149:ASP:CA	2.76	0.50
1:B:159:TYR:N	1:B:160:TYR:C	2.70	0.50
1:A:169:PRO:HB3	1:B:167:SER:O	2.12	0.50
1:C:268:SER:H	1:C:271:GLU:HB2	1.75	0.50
1:A:47:ILE:HD11	1:A:75:ALA:HA	1.93	0.50
1:C:158:HIS:C	1:C:159:TYR:CD1	2.90	0.50
1:C:68:SER:HB2	1:C:100:VAL:HB	1.94	0.50
1:B:41:ARG:HG2	1:B:64:LEU:CG	2.35	0.50
1:B:38:GLY:HA2	1:B:61:GLU:O	2.12	0.49
1:C:111:GLN:OE1	1:C:114:ARG:NH2	2.44	0.49
1:B:247:THR:CB	1:B:248:GLY:CA	2.91	0.49
1:B:159:TYR:H	1:B:160:TYR:CA	2.26	0.49
1:C:267:LEU:N	1:C:267:LEU:CD2	2.73	0.49
1:A:132:ARG:H	1:A:133:LEU:CB	2.20	0.49
1:B:151:ARG:CG	1:B:152:ASP:N	2.72	0.49
1:B:278:THR:HG22	1:B:279:ASP:N	2.27	0.49
1:C:74:LEU:O	1:C:77:LEU:N	2.45	0.49
1:C:157:ALA:C	1:C:159:TYR:H	2.19	0.49
1:A:132:ARG:N	1:A:133:LEU:CB	2.75	0.49
1:A:131:VAL:HG23	1:A:131:VAL:O	2.12	0.49
1:B:156:ILE:HG22	1:B:158:HIS:CE1	2.47	0.49
1:C:144:LEU:HD12	1:C:145:ALA:N	2.28	0.49
1:B:158:HIS:CD2	1:B:158:HIS:H	2.30	0.48
1:C:14:PRO:HG3	1:C:16:PHE:CE2	2.48	0.48
1:C:142:ALA:C	1:C:144:LEU:N	2.71	0.48
1:C:229:HIS:ND1	1:C:230:ALA:N	2.60	0.48
1:B:159:TYR:CG	1:B:159:TYR:O	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ARG:HD2	1:C:114:ARG:O	2.13	0.48
1:C:49:THR:O	1:C:78:ALA:HA	2.13	0.48
1:A:247:THR:O	1:A:249:LEU:N	2.45	0.48
1:A:272:ALA:O	1:A:275:LEU:CD2	2.61	0.48
1:B:247:THR:OG1	1:B:249:LEU:N	2.29	0.48
1:B:267:LEU:HD23	1:B:267:LEU:C	2.37	0.48
1:C:229:HIS:HD1	1:C:230:ALA:N	2.11	0.48
1:B:70:LEU:HD21	1:B:161:PRO:HD3	1.95	0.48
1:C:260:ASP:OD1	1:C:265:THR:HG22	2.12	0.48
1:B:159:TYR:OH	1:B:162:TRP:HZ2	1.95	0.48
1:C:30:ARG:HD2	1:C:224:GLN:HE21	1.78	0.48
1:A:133:LEU:C	1:A:133:LEU:CD2	2.85	0.48
1:A:246:GLN:CG	1:B:166:ASP:O	2.62	0.48
1:B:253:PHE:HD1	1:B:254:THR:N	2.11	0.48
1:C:241:GLU:OE1	1:C:270:THR:HG23	2.14	0.48
1:B:144:LEU:C	1:B:146:ALA:N	2.72	0.48
1:B:159:TYR:CE1	1:B:162:TRP:NE1	2.82	0.48
1:B:41:ARG:HG3	1:B:64:LEU:HD23	1.92	0.48
1:C:66:SER:OG	1:C:111:GLN:HG2	2.14	0.48
1:A:73:ARG:HG2	1:A:73:ARG:NH1	2.26	0.47
1:B:159:TYR:CE1	1:B:162:TRP:CE2	3.01	0.47
1:B:160:TYR:CD1	1:B:161:PRO:HB3	2.49	0.47
1:B:27:THR:HG22	1:B:224:GLN:NE2	2.29	0.47
1:B:143:ALA:O	1:B:148:ALA:HB2	2.13	0.47
1:C:248:GLY:HA3	1:C:249:LEU:CD1	2.44	0.47
1:A:229:HIS:ND1	1:A:229:HIS:N	2.60	0.47
1:B:247:THR:HG22	1:C:236:PHE:CE2	2.48	0.47
1:B:200:ALA:HB3	1:B:287:GLU:HB3	1.96	0.47
1:A:88:ARG:HH21	1:A:88:ARG:CG	2.16	0.47
1:B:23:PRO:O	1:B:24:TRP:C	2.55	0.47
1:B:279:ASP:C	1:B:281:ALA:N	2.72	0.47
1:A:261:PRO:HB3	1:A:285:TYR:CE2	2.50	0.47
1:C:141:ALA:C	1:C:143:ALA:N	2.72	0.47
1:C:144:LEU:C	1:C:146:ALA:N	2.73	0.47
1:C:156:ILE:C	1:C:158:HIS:N	2.72	0.47
1:C:260:ASP:OD1	1:C:264:ALA:N	2.42	0.47
1:B:159:TYR:N	1:B:160:TYR:CA	2.78	0.47
1:A:252:GLU:HB2	1:B:162:TRP:HZ2	1.76	0.47
1:B:267:LEU:CD2	1:B:271:GLU:HB2	2.40	0.46
1:C:136:PHE:O	1:C:139:ALA:N	2.43	0.46
1:C:273:GLN:HA	1:C:273:GLN:OE1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:CYS:O	1:B:61:GLU:HB2	2.16	0.46
1:A:227:LEU:HD12	1:A:285:TYR:CE2	2.51	0.46
1:C:92:ARG:HG2	1:C:92:ARG:HH11	1.81	0.46
1:C:105:THR:HG23	1:C:108:ALA:H	1.81	0.46
1:B:235:SER:O	1:B:238:VAL:HG22	2.15	0.46
1:C:77:LEU:HD22	1:C:81:ASN:OD1	2.14	0.46
1:B:244:LEU:N	1:B:244:LEU:HD22	2.30	0.46
1:A:258:TYR:HB2	1:A:285:TYR:HB2	1.97	0.46
1:B:272:ALA:O	1:B:276:VAL:HG22	2.16	0.45
1:A:80:ARG:O	1:A:83:ARG:N	2.50	0.45
1:B:244:LEU:HB3	1:B:249:LEU:O	2.16	0.45
1:B:247:THR:CB	1:B:248:GLY:HA2	2.47	0.45
1:B:159:TYR:O	1:B:159:TYR:CD2	2.70	0.45
1:B:246:GLN:HG2	1:C:172:SER:HA	1.98	0.45
1:C:278:THR:OG1	1:C:279:ASP:N	2.50	0.45
1:C:173:VAL:HB	1:C:202:VAL:HG11	1.98	0.45
1:B:58:GLN:CD	1:B:86:ALA:HA	2.41	0.45
1:C:105:THR:CG2	1:C:108:ALA:H	2.30	0.45
1:B:73:ARG:H	1:B:73:ARG:HG2	1.57	0.44
1:C:105:THR:HG22	1:C:108:ALA:HB3	1.98	0.44
1:C:132:ARG:NE	1:C:159:TYR:CE2	2.73	0.44
1:A:168:TYR:OH	1:C:209:GLU:OE2	2.24	0.44
1:A:275:LEU:H	1:A:275:LEU:CD1	2.26	0.44
1:A:89:ARG:NH1	1:A:92:ARG:NH1	2.64	0.44
1:B:260:ASP:OD1	1:B:265:THR:CG2	2.59	0.44
1:A:30:ARG:HD2	1:A:224:GLN:NE2	2.31	0.44
1:B:267:LEU:C	1:B:267:LEU:CD2	2.90	0.44
1:B:155:HIS:ND1	1:B:155:HIS:C	2.73	0.44
1:A:273:GLN:CA	1:A:276:VAL:HG22	2.45	0.44
1:C:193:ASP:OD1	1:C:294:ARG:HD3	2.18	0.44
1:C:243:ALA:CB	1:C:251:ARG:HG3	2.48	0.43
1:A:273:GLN:CA	1:A:276:VAL:CG2	2.90	0.43
1:B:279:ASP:O	1:B:281:ALA:N	2.50	0.43
1:C:138:THR:O	1:C:138:THR:HG22	2.17	0.43
1:C:281:ALA:O	1:C:282:ALA:C	2.53	0.43
1:A:272:ALA:HB1	1:A:284:ILE:HD12	2.00	0.43
1:C:281:ALA:C	1:C:282:ALA:O	2.57	0.43
1:C:14:PRO:HG3	1:C:16:PHE:HE2	1.83	0.43
1:B:44:GLU:HA	1:B:119:VAL:O	2.18	0.43
1:B:92:ARG:HE	1:B:92:ARG:HB3	1.69	0.43
1:A:121:CYS:O	2:A:401:SAH:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HB	1:B:202:VAL:HG11	2.01	0.43
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.83	0.43
1:C:156:ILE:HG22	1:C:157:ALA:H	1.84	0.43
1:B:156:ILE:CG2	1:B:158:HIS:CE1	3.02	0.43
1:B:203:GLY:HA2	1:B:256:GLU:OE1	2.18	0.43
1:B:283:GLU:C	1:B:284:ILE:CG1	2.92	0.43
1:C:142:ALA:O	1:C:144:LEU:N	2.46	0.43
1:A:34:ILE:O	1:A:34:ILE:HG22	2.19	0.42
1:C:251:ARG:HH11	1:C:251:ARG:HD2	1.70	0.42
1:B:19:ASP:OD1	1:B:21:THR:OG1	2.26	0.42
1:B:156:ILE:O	1:B:156:ILE:HG13	2.18	0.42
1:C:14:PRO:HG2	1:C:16:PHE:CD2	2.54	0.42
1:C:68:SER:HB3	1:C:96:VAL:HG22	1.99	0.42
1:C:243:ALA:HB1	1:C:251:ARG:CG	2.48	0.42
1:A:60:CYS:O	1:A:61:GLU:HB2	2.19	0.42
1:B:223:SER:HB2	1:B:289:CYS:HB3	2.01	0.42
1:B:275:LEU:O	1:B:276:VAL:C	2.59	0.42
1:C:136:PHE:O	1:C:139:ALA:HB3	2.19	0.42
1:B:276:VAL:O	1:B:280:SER:HA	2.19	0.42
1:A:272:ALA:C	1:A:275:LEU:CD2	2.92	0.42
1:B:274:ALA:O	1:B:277:ASP:HB2	2.20	0.42
1:C:60:CYS:O	1:C:61:GLU:HB2	2.18	0.42
1:A:30:ARG:O	1:A:34:ILE:HG13	2.20	0.42
1:B:156:ILE:O	1:B:156:ILE:CG1	2.67	0.42
1:B:144:LEU:CD2	1:B:149:ASP:OD1	2.68	0.42
1:B:209:GLU:HG2	1:C:164:GLU:O	2.18	0.42
1:C:41:ARG:HG3	1:C:64:LEU:HB3	2.01	0.42
1:C:246:GLN:CA	1:C:248:GLY:HA2	2.34	0.42
1:A:252:GLU:CA	1:B:162:TRP:HH2	2.24	0.42
1:C:57:LEU:HA	1:C:57:LEU:HD23	1.83	0.42
1:B:85:LEU:C	1:B:87:PRO:CD	2.92	0.42
1:B:267:LEU:HD23	1:B:268:SER:H	1.81	0.42
1:A:129:ASP:O	1:A:130:ASP:C	2.61	0.42
1:B:235:SER:HA	1:B:238:VAL:HG22	2.01	0.42
1:A:236:PHE:CD2	1:C:247:THR:HG22	2.55	0.41
1:B:158:HIS:CD2	1:B:158:HIS:N	2.87	0.41
1:B:162:TRP:CD1	1:B:162:TRP:N	2.88	0.41
1:C:246:GLN:HA	1:C:248:GLY:CA	2.35	0.41
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.89	0.41
1:C:18:PHE:HE1	1:C:55:PHE:HZ	1.67	0.41
1:C:71:ASP:OD1	1:C:73:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:HIS:O	1:C:159:TYR:CD1	2.73	0.41
1:C:168:TYR:HE1	1:C:183:ARG:HG3	1.86	0.41
1:A:201:ARG:HD2	1:A:237:PHE:CZ	2.56	0.41
1:B:92:ARG:H	1:B:92:ARG:HG2	1.59	0.41
1:B:245:ALA:C	1:B:247:THR:N	2.77	0.41
1:B:274:ALA:O	1:B:275:LEU:C	2.62	0.41
1:B:276:VAL:O	1:B:280:SER:N	2.53	0.41
1:C:119:VAL:HG12	1:C:195:VAL:HB	2.03	0.41
1:C:210:LEU:O	1:C:214:ASN:ND2	2.47	0.41
1:A:273:GLN:C	1:A:276:VAL:HG22	2.45	0.40
1:B:209:GLU:OE2	1:C:168:TYR:OH	2.25	0.40
1:A:275:LEU:HD23	1:A:284:ILE:HD11	2.02	0.40
1:B:251:ARG:CG	1:B:252:GLU:N	2.84	0.40
1:B:297:LEU:HD13	1:B:297:LEU:HA	1.93	0.40
1:B:253:PHE:C	1:B:253:PHE:CD1	2.99	0.40
1:B:283:GLU:H	1:B:283:GLU:HG2	1.67	0.40
1:C:47:ILE:HD11	1:C:75:ALA:HB2	2.03	0.40
1:C:77:LEU:HD21	1:C:81:ASN:OD1	2.20	0.40
1:A:14:PRO:C	1:A:16:PHE:H	2.30	0.40
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.90	0.40
1:A:209:GLU:OE2	1:B:168:TYR:OH	2.34	0.40
1:A:229:HIS:O	1:A:232:THR:HG22	2.21	0.40
1:A:279:ASP:OD1	1:A:281:ALA:N	2.40	0.40
1:B:122:LEU:HD11	1:B:181:LEU:HD22	2.03	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	254/305 (83%)	230 (91%)	24 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	279/305 (92%)	245 (88%)	31 (11%)	3 (1%)	11	22
1	C	276/305 (90%)	247 (90%)	26 (9%)	3 (1%)	11	22
All	All	809/915 (88%)	722 (89%)	81 (10%)	6 (1%)	18	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	TYR
1	C	145	ALA
1	C	246	GLN
1	B	161	PRO
1	B	162	TRP
1	C	140	GLN

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	202/238 (85%)	178 (88%)	24 (12%)	5	11
1	B	216/238 (91%)	188 (87%)	28 (13%)	4	8
1	C	214/238 (90%)	199 (93%)	15 (7%)	14	29
All	All	632/714 (88%)	565 (89%)	67 (11%)	6	14

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	18	PHE
1	A	74	LEU
1	A	80	ARG
1	A	83	ARG
1	A	89	ARG
1	A	97	GLU
1	A	129	ASP

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Mol	Chain	Res	Type
1	A	130	ASP
1	A	131	VAL
1	A	132	ARG
1	A	134	ARG
1	A	226	VAL
1	A	228	GLN
1	A	229	HIS
1	A	246	GLN
1	A	247	THR
1	A	249	LEU
1	A	250	GLU
1	A	252	GLU
1	A	266	ARG
1	A	267	LEU
1	A	270	THR
1	A	275	LEU
1	B	20	PRO
1	B	21	THR
1	B	30	ARG
1	B	40	LYS
1	B	58	GLN
1	B	64	LEU
1	B	73	ARG
1	B	80	ARG
1	B	87	PRO
1	B	91	ASP
1	B	92	ARG
1	B	94	HIS
1	B	97	GLU
1	B	144	LEU
1	B	151	ARG
1	B	153	GLU
1	B	156	ILE
1	B	158	HIS
1	B	160	TYR
1	B	220	LYS
1	B	247	THR
1	B	249	LEU
1	B	252	GLU
1	B	262	GLU
1	B	267	LEU
1	B	278	THR

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Mol	Chain	Res	Type
1	B	283	GLU
1	B	297	LEU
1	C	12	HIS
1	C	77	LEU
1	C	132	ARG
1	C	137	ARG
1	C	144	LEU
1	C	149	ASP
1	C	156	ILE
1	C	167	SER
1	C	232	THR
1	C	244	LEU
1	C	247	THR
1	C	249	LEU
1	C	251	ARG
1	C	252	GLU
1	C	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	273	GLN
1	B	81	ASN
1	B	158	HIS
1	B	224	GLN
1	C	58	GLN
1	C	158	HIS
1	C	171	ASN
1	C	242	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	C	401	-	4,4,4	0.95	0	6,6,6	0.46	0
3	MET	B	402	-	7,8,8	0.68	0	5,9,9	0.56	0
2	SAH	A	401	-	27,28,28	1.20	4 (14%)	36,40,40	1.93	10 (27%)
2	SAH	B	401	-	27,28,28	1.18	5 (18%)	36,40,40	2.20	14 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MET	B	402	-	-	3/8/8/8	-
2	SAH	A	401	-	-	1/15/31/31	0/3/3/3
2	SAH	B	401	-	-	7/15/31/31	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	C2-N1	2.85	1.39	1.33
2	A	401	SAH	C2-N3	2.72	1.38	1.33
2	B	401	SAH	C2-N3	2.66	1.38	1.33
2	B	401	SAH	C2-N1	2.63	1.38	1.33
2	B	401	SAH	C8-N7	2.35	1.36	1.31
2	A	401	SAH	C8-N7	2.35	1.36	1.31
2	B	401	SAH	C5-N7	-2.10	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	OXT-C	-2.09	1.24	1.30
2	B	401	SAH	OXT-C	-2.06	1.24	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAH	N3-C2-N1	-5.48	120.29	128.58
2	B	401	SAH	C5-C4-N3	-5.37	119.33	126.72
2	A	401	SAH	N3-C2-N1	-5.14	120.80	128.58
2	A	401	SAH	C5-C4-N3	-4.05	121.13	126.72
2	A	401	SAH	N9-C8-N7	-3.96	108.31	113.94
2	B	401	SAH	N3-C4-N9	3.60	133.29	127.17
2	A	401	SAH	C5-N7-C8	3.52	108.99	103.45
2	B	401	SAH	C2-N3-C4	3.52	120.42	111.83
2	B	401	SAH	C5-N7-C8	3.51	108.97	103.45
2	B	401	SAH	C5'-SD-CG	-3.26	92.60	102.26
2	B	401	SAH	N9-C8-N7	-3.23	109.36	113.94
2	A	401	SAH	N3-C4-N9	3.02	132.30	127.17
2	A	401	SAH	C5'-SD-CG	-2.79	93.99	102.26
2	A	401	SAH	C2-N3-C4	2.77	118.60	111.83
2	B	401	SAH	OXT-C-O	-2.74	117.87	124.08
2	B	401	SAH	O4'-C1'-N9	2.73	113.33	108.09
2	B	401	SAH	C5'-C4'-C3'	-2.66	108.42	115.06
2	A	401	SAH	OXT-C-O	-2.56	118.27	124.08
2	B	401	SAH	C6-C5-C4	2.52	120.62	117.18
2	B	401	SAH	C4-C5-N7	-2.47	107.76	110.58
2	B	401	SAH	O4'-C4'-C5'	2.11	114.27	108.83
2	B	401	SAH	O2'-C2'-C1'	2.09	117.31	110.10
2	A	401	SAH	C4-C5-N7	-2.02	108.27	110.58
2	A	401	SAH	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	SAH	N-CA-CB-CG
2	B	401	SAH	C-CA-CB-CG
2	B	401	SAH	O4'-C4'-C5'-SD
2	B	401	SAH	C3'-C4'-C5'-SD
2	B	401	SAH	CA-CB-CG-SD
3	B	402	MET	CA-CB-CG-SD
3	B	402	MET	C-CA-CB-CG

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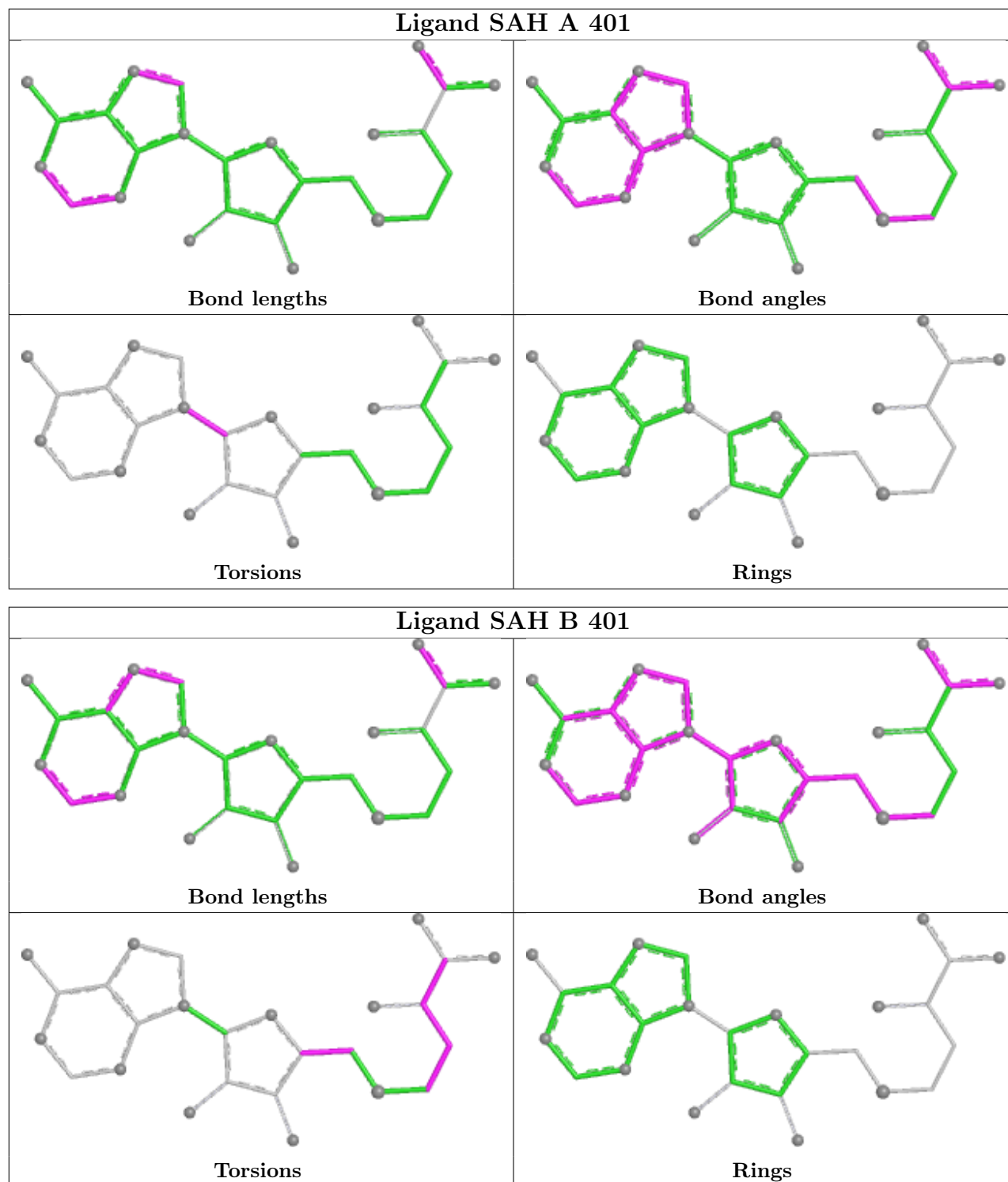
Mol	Chain	Res	Type	Atoms
2	B	401	SAH	O-C-CA-N
3	B	402	MET	OXT-C-CA-N
2	B	401	SAH	OXT-C-CA-N
2	A	401	SAH	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	PO4	1	0
3	B	402	MET	1	0
2	A	401	SAH	2	0
2	B	401	SAH	2	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	258/305 (84%)	0.77	25 (9%)	13 11	55, 72, 107, 124	0
1	B	281/305 (92%)	0.75	23 (8%)	17 15	24, 76, 108, 125	0
1	C	280/305 (91%)	0.71	28 (10%)	12 10	24, 67, 111, 141	0
All	All	819/915 (89%)	0.74	76 (9%)	14 12	24, 73, 108, 141	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	8.2
1	B	21	THR	7.1
1	A	244	LEU	5.6
1	A	161	PRO	5.6
1	A	14	PRO	5.5
1	C	12	HIS	5.0
1	C	14	PRO	4.6
1	B	19	ASP	4.6
1	B	20	PRO	4.6
1	A	247	THR	4.5
1	B	18	PHE	4.4
1	C	13	ALA	4.3
1	B	297	LEU	4.3
1	A	135	ALA	4.2
1	C	245	ALA	4.2
1	B	159	TYR	4.1
1	A	249	LEU	4.0
1	C	244	LEU	3.9
1	B	160	TYR	3.9
1	C	20	PRO	3.9
1	C	144	LEU	3.7
1	B	17	ALA	3.6
1	A	246	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	297	LEU	3.4
1	C	156	ILE	3.4
1	A	269	ALA	3.4
1	B	148	ALA	3.3
1	A	276	VAL	3.2
1	B	245	ALA	3.1
1	C	269	ALA	3.1
1	B	161	PRO	3.0
1	C	162	TRP	3.0
1	B	162	TRP	3.0
1	A	296	ALA	3.0
1	B	156	ILE	2.9
1	A	162	TRP	2.9
1	C	148	ALA	2.9
1	B	247	THR	2.9
1	A	230	ALA	2.9
1	C	143	ALA	2.8
1	C	157	ALA	2.8
1	A	133	LEU	2.8
1	B	249	LEU	2.8
1	A	243	ALA	2.8
1	B	244	LEU	2.8
1	A	15	GLU	2.8
1	B	79	GLU	2.8
1	C	158	HIS	2.8
1	C	160	TYR	2.8
1	C	149	ASP	2.7
1	C	249	LEU	2.6
1	C	19	ASP	2.5
1	A	278	THR	2.5
1	B	150	THR	2.5
1	B	93	PHE	2.4
1	B	64	LEU	2.4
1	C	275	LEU	2.4
1	C	16	PHE	2.4
1	A	192	ALA	2.4
1	A	259	GLY	2.3
1	A	236	PHE	2.3
1	A	17	ALA	2.3
1	C	246	GLN	2.3
1	A	267	LEU	2.3
1	C	247	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	273	GLN	2.2
1	B	57	LEU	2.2
1	A	16	PHE	2.2
1	C	257	PHE	2.2
1	A	281	ALA	2.1
1	C	261	PRO	2.1
1	A	229	HIS	2.1
1	B	155	HIS	2.1
1	B	147	GLY	2.1
1	C	136	PHE	2.0
1	C	142	ALA	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](#)

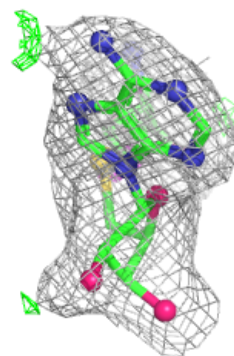
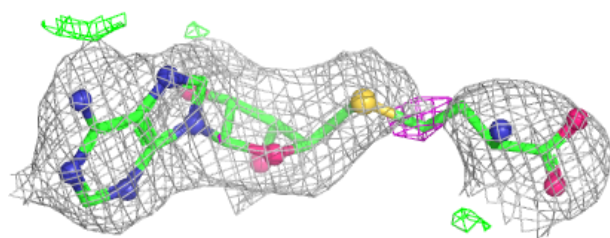
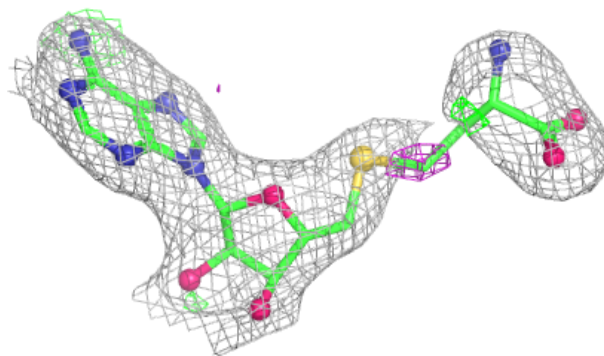
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MET	B	402	9/9	0.52	0.20	76,81,93,107	0
2	SAH	B	401	26/26	0.84	0.14	69,82,95,104	0
4	PO4	C	401	5/5	0.84	0.28	66,73,79,86	5
2	SAH	A	401	26/26	0.86	0.13	69,87,91,92	0

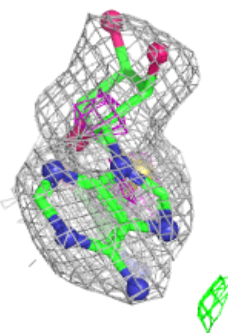
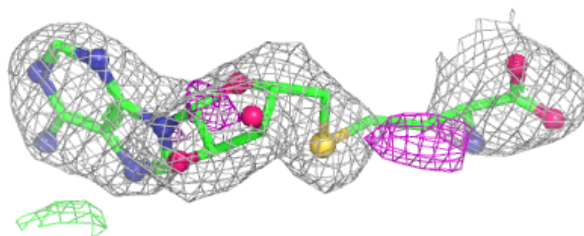
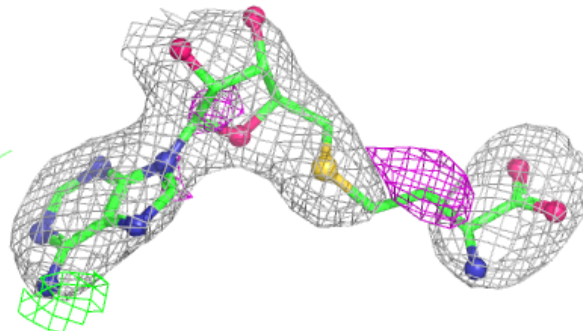
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH B 401:

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

**Electron density around SAH A 401:**

$2mF_o-DF_c$ (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.