



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:40 pm GMT

PDB ID : 4C68
Title : Plasmodium vivax N-myristoyltransferase in complex with a peptidomimetic inhibitor
Authors : Olaleye, T.O.; Brannigan, J.A.; Goncalves, V.; Roberts, S.M.; Leatherbarrow, R.J.; Wilkinson, A.J.; Tate, E.W.
Deposited on : 2013-09-17
Resolution : 1.38 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

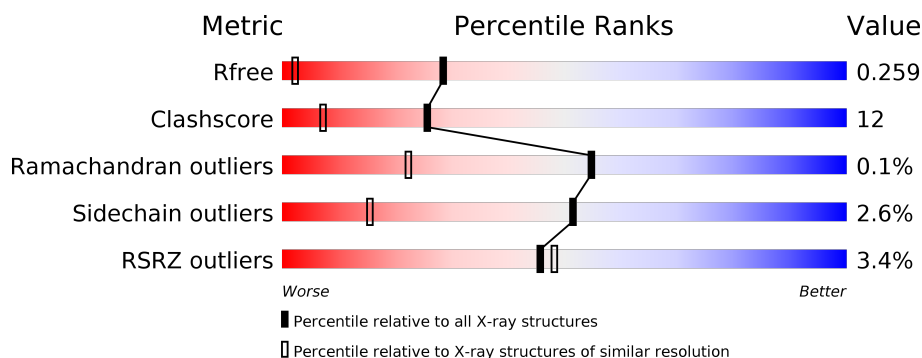
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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}	100719	2133 (1.40-1.36)
Clashscore	112137	2266 (1.40-1.36)
Ramachandran outliers	110173	2215 (1.40-1.36)
Sidechain outliers	110143	2214 (1.40-1.36)
RSRZ outliers	101464	2141 (1.40-1.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	384	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	384	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	384	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>...</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMT	A	997	-	-	X	-
3	DMS	A	1415	-	-	X	X
3	DMS	A	999	-	X	-	X
3	DMS	B	1414	-	-	X	X
3	DMS	B	999	-	-	-	X
3	DMS	C	999	-	-	-	X
4	EN5	A	1000[A]	-	-	-	X
4	EN5	A	1000[B]	-	-	-	X

2 Entry composition [i](#)

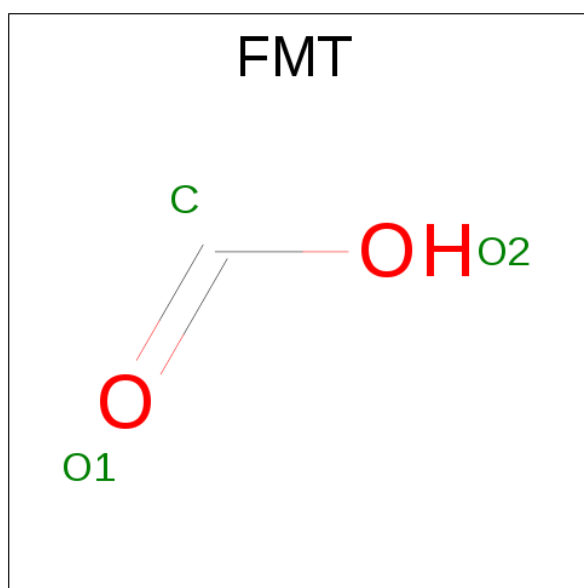
There are 9 unique types of molecules in this entry. The entry contains 11510 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

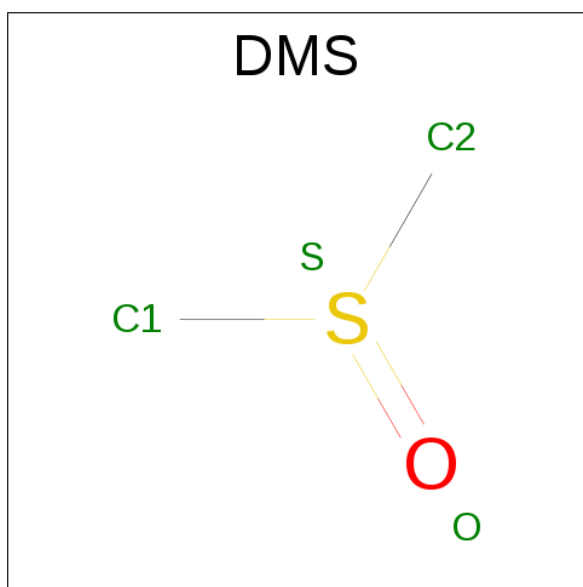
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	32	0
			3375	2199	543	619	14			
1	B	384	Total	C	N	O	S	0	20	0
			3319	2162	534	611	12			
1	C	370	Total	C	N	O	S	0	18	0
			3191	2082	511	587	11			

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



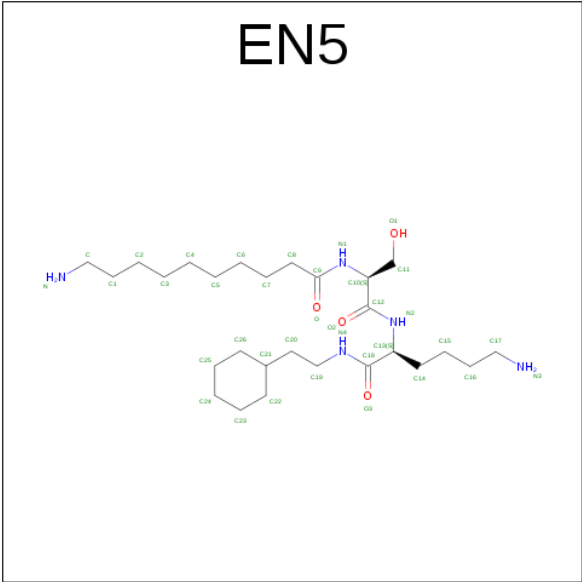
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



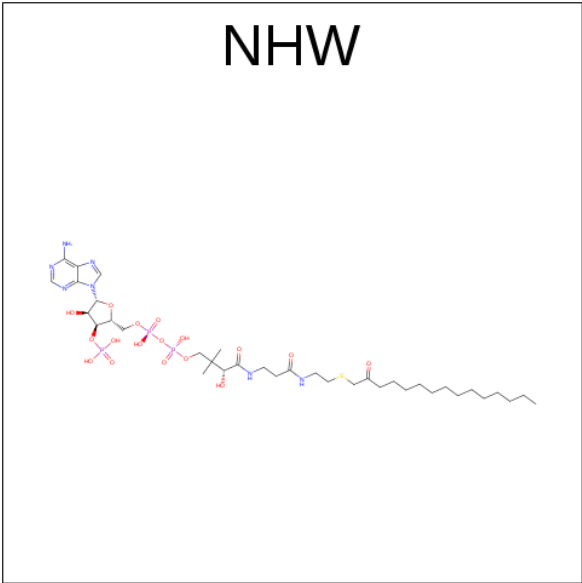
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is N-(10-AMINODECANOYL)-L-SERYL-N-(2-CYCLOHEXYLETHYL)-L-LY SINAMIDE (three-letter code: EN5) (formula: C₂₇H₅₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			72	54	10	8		
4	B	1	Total	C	N	O	0	0
			36	27	5	4		

- Molecule 5 is 2-OXOPENTADECYL-COA (three-letter code: NHW) (formula: C₃₆H₆₄N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

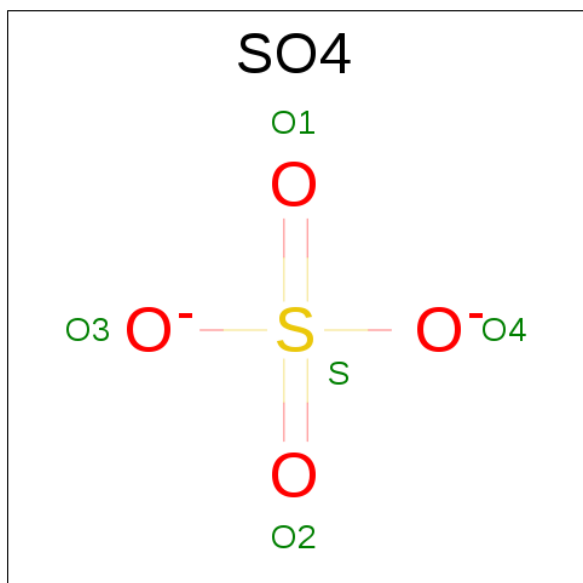
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		
6	C	3	Total	Cl	0	0
			3	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

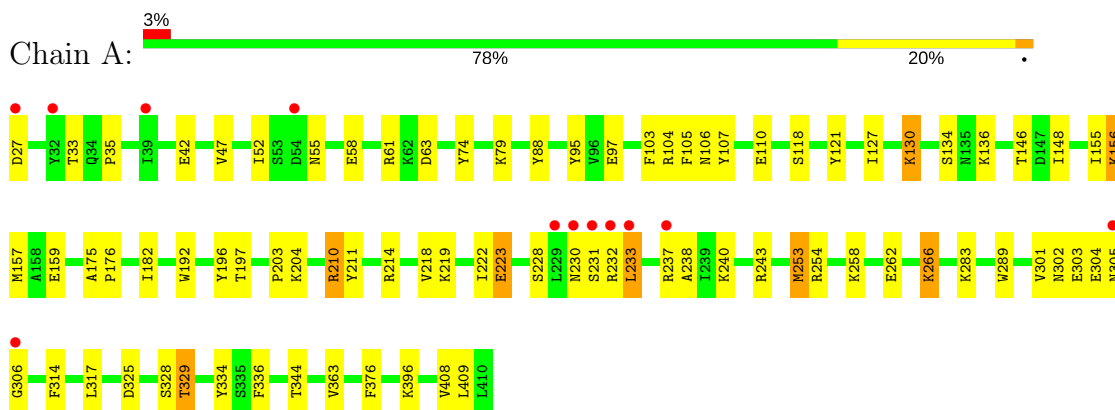
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	479	Total	O	0	0
			479	479		
9	B	453	Total	O	0	0
			453	453		
9	C	357	Total	O	0	0
			357	357		

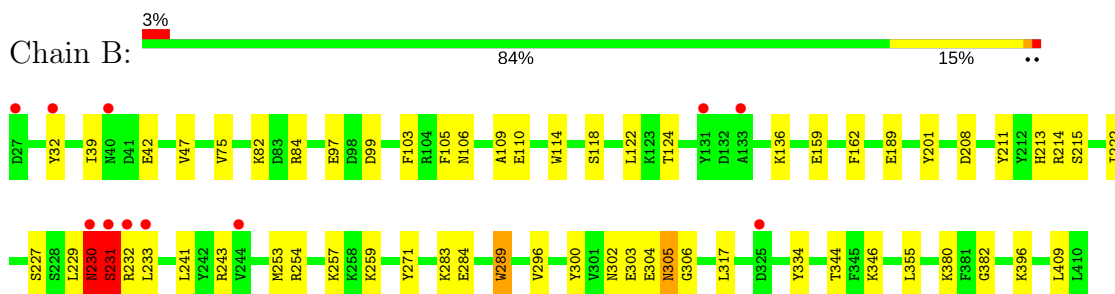
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

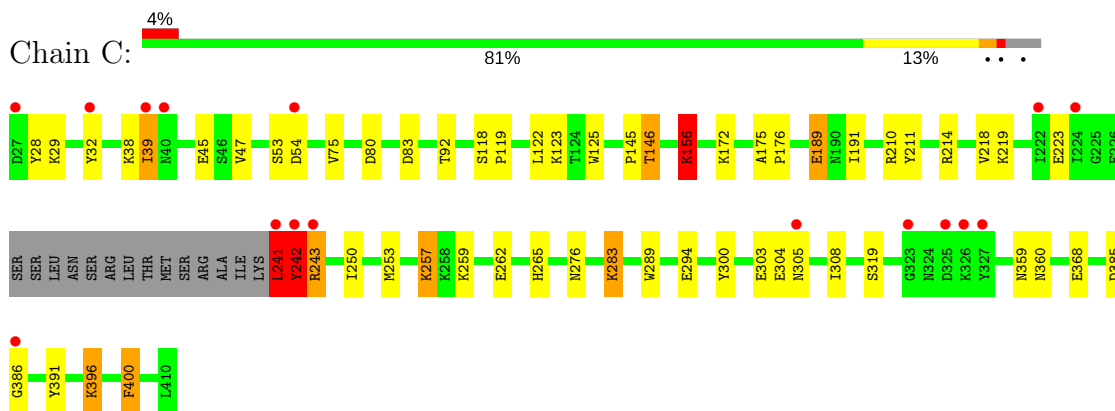
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.33Å 121.43Å 178.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.97 – 1.38 41.94 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.97-1.38) 99.8 (41.94-1.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.38Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.220 , 0.260 0.219 , 0.259	Depositor DCC
R_{free} test set	12819 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11510	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, FMT, NHW, DMS, SO4, EN5

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	1.26	4/3531 (0.1%)	1.29	19/4770 (0.4%)
1	B	1.27	7/3433 (0.2%)	1.27	6/4642 (0.1%)
1	C	1.25	6/3307 (0.2%)	1.29	21/4477 (0.5%)
All	All	1.26	17/10271 (0.2%)	1.28	46/13889 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	4
All	All	0	7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243[A]	ARG	CA-C	7.61	1.72	1.52
1	C	243[B]	ARG	CA-C	7.61	1.72	1.52
1	B	215	SER	CB-OG	-6.75	1.33	1.42
1	C	300	TYR	CE1-CZ	-6.57	1.30	1.38
1	B	162	PHE	CG-CD2	5.82	1.47	1.38
1	C	319	SER	CB-OG	-5.70	1.34	1.42
1	A	336	PHE	CG-CD1	5.53	1.47	1.38
1	A	254	ARG	C-O	-5.47	1.12	1.23
1	A	88	TYR	CG-CD2	5.44	1.46	1.39
1	C	368	GLU	CD-OE2	-5.37	1.19	1.25
1	B	284[A]	GLU	CA-C	5.29	1.66	1.52
1	B	284[B]	GLU	CA-C	5.29	1.66	1.52
1	B	114	TRP	CZ3-CH2	5.28	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	PHE	CG-CD1	5.26	1.46	1.38
1	B	271	TYR	CE2-CZ	-5.21	1.31	1.38
1	B	289	TRP	CG-CD1	-5.16	1.29	1.36
1	C	189	GLU	CG-CD	5.00	1.59	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243[A]	ARG	N-CA-CB	-10.18	92.27	110.60
1	C	243[B]	ARG	N-CA-CB	-10.18	92.27	110.60
1	B	283[A]	LYS	CA-C-N	-8.20	99.16	117.20
1	B	283[B]	LYS	CA-C-N	-8.20	99.16	117.20
1	C	241	LEU	CA-CB-CG	7.91	133.50	115.30
1	A	63	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	104	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	172	LYS	CD-CE-NZ	-6.25	97.31	111.70
1	C	80	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	130	LYS	CD-CE-NZ	-5.96	97.98	111.70
1	C	283[A]	LYS	CD-CE-NZ	5.95	125.38	111.70
1	C	283[B]	LYS	CD-CE-NZ	5.95	125.38	111.70
1	C	83	ASP	CB-CG-OD2	-5.82	113.07	118.30
1	A	210	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	95	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	233	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	61	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	104	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	242	TYR	C-N-CA	-5.64	107.59	121.70
1	C	243[A]	ARG	CA-C-N	-5.59	104.90	117.20
1	C	243[B]	ARG	CA-C-N	-5.59	104.90	117.20
1	C	80	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	C	400	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	A	363	VAL	CG1-CB-CG2	5.42	119.58	110.90
1	C	391	TYR	CG-CD1-CE1	-5.42	116.96	121.30
1	A	223	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	A	253[A]	MET	CB-CA-C	-5.37	99.67	110.40
1	A	253[B]	MET	CB-CA-C	-5.37	99.67	110.40
1	C	385[A]	ASP	CB-CA-C	-5.36	99.68	110.40
1	C	385[B]	ASP	CB-CA-C	-5.36	99.68	110.40
1	A	376	PHE	CB-CG-CD1	5.34	124.54	120.80
1	C	156[A]	LYS	CB-CG-CD	5.33	125.45	111.60
1	C	156[B]	LYS	CB-CG-CD	5.33	125.45	111.60
1	A	95	TYR	CG-CD2-CE2	-5.22	117.13	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	B	231	SER	CB-CA-C	5.15	119.89	110.10
1	B	284[A]	GLU	CA-C-N	-5.15	105.88	117.20
1	B	284[B]	GLU	CA-C-N	-5.15	105.88	117.20
1	A	196	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	A	325	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	211	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	C	242	TYR	CA-CB-CG	5.10	123.09	113.40
1	A	334	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
1	C	304	GLU	CB-CA-C	-5.05	100.29	110.40
1	B	208	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	33	THR	CA-CB-CG2	-5.00	105.40	112.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	ASN	Peptide
1	B	231	SER	Mainchain,Peptide
1	C	242	TYR	Peptide
1	C	243[A]	ARG	Mainchain
1	C	243[B]	ARG	Mainchain

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	3375	0	3417	65	0
1	B	3319	0	3326	85	0
1	C	3191	0	3182	56	0
2	A	3	0	2	2	0
3	A	8	0	12	30	0
3	B	8	0	12	19	0
3	C	4	0	6	0	0
4	A	72	0	106	30	0
4	B	36	0	53	7	0
5	A	64	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	64	0	60	0	0
5	C	64	0	60	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	5	0	0	0	0
9	A	479	0	0	11	0
9	B	453	0	0	12	0
9	C	357	0	0	3	0
All	All	11510	0	10296	245	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 12.

All (245) 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:257[B]:LYS:HD2	1:B:259[B]:LYS:NZ	1.27	1.42
1:B:75[A]:VAL:HG22	9:B:2107:HOH:O	1.32	1.29
1:B:257[B]:LYS:CD	1:B:259[B]:LYS:HZ2	1.49	1.25
1:B:257[B]:LYS:CD	1:B:259[B]:LYS:NZ	2.01	1.23
1:B:231:SER:N	1:B:233:LEU:H	1.39	1.19
1:B:231:SER:H	1:B:233:LEU:N	1.45	1.13
1:B:75[B]:VAL:HG22	9:B:2196:HOH:O	1.51	1.08
1:A:408:VAL:HG13	2:A:997:FMT:H	1.39	1.04
1:B:257[B]:LYS:CE	1:B:259[B]:LYS:HZ1	1.70	1.04
4:A:1000[A]:EN5:HN	4:A:1000[A]:EN5:H3	1.21	1.02
4:A:1000[A]:EN5:N1	3:A:1415:DMS:H22	1.75	1.01
4:A:1000[B]:EN5:N1	3:A:1415:DMS:H22	1.75	1.00
4:A:1000[B]:EN5:HN1	3:A:1415:DMS:H22	1.30	0.95
1:A:136[B]:LYS:HD3	9:A:2211:HOH:O	1.67	0.95
1:C:145:PRO:HB2	1:C:156[A]:LYS:HE3	1.46	0.94
1:C:122[B]:LEU:HD11	1:C:189:GLU:HG3	1.47	0.94
1:B:231:SER:N	1:B:233:LEU:N	2.05	0.93
4:A:1000[A]:EN5:H8A	3:A:1415:DMS:C2	1.99	0.93
4:A:1000[B]:EN5:H8A	3:A:1415:DMS:C2	1.99	0.93
1:B:230:ASN:HD22	1:B:231:SER:HA	1.32	0.92
1:B:257[B]:LYS:HE3	1:B:259[B]:LYS:HZ1	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:HB2	1:A:136[A]:LYS:HE3	1.50	0.92
4:A:1000[A]:EN5:HN1	3:A:1415:DMS:H22	1.30	0.91
4:B:1000:EN5:H8A	3:B:1414:DMS:H22	1.53	0.91
1:B:75[B]:VAL:HG21	9:B:2239:HOH:O	1.72	0.90
1:A:283[B]:LYS:HB2	1:A:283[B]:LYS:NZ	1.83	0.89
1:C:122[B]:LEU:HD12	1:C:125:TRP:NE1	1.88	0.88
1:A:253[A]:MET:HE2	1:A:302:ASN:N	1.89	0.87
1:B:230:ASN:ND2	1:B:231:SER:HA	1.89	0.86
3:A:1415:DMS:H21	9:A:2397:HOH:O	1.77	0.84
1:A:283[B]:LYS:HB2	1:A:283[B]:LYS:HZ1	1.41	0.83
1:C:122[B]:LEU:HD12	1:C:125:TRP:CE2	2.14	0.83
1:B:213:HIS:HE1	3:B:1414:DMS:H12	1.46	0.81
4:A:1000[A]:EN5:H8A	3:A:1415:DMS:H23	1.62	0.80
1:C:211[B]:TYR:CD2	1:C:386:GLY:O	2.34	0.80
4:A:1000[B]:EN5:H8A	3:A:1415:DMS:H23	1.63	0.80
1:C:32[A]:TYR:CE1	1:C:38:LYS:HE3	2.16	0.80
1:A:253[A]:MET:CE	1:A:302:ASN:N	2.46	0.79
1:B:32[B]:TYR:CD1	9:B:2013:HOH:O	2.36	0.78
1:A:240[B]:LYS:HD3	1:A:243[B]:ARG:NH1	1.98	0.78
1:B:230:ASN:HB2	1:B:231:SER:HA	1.65	0.78
4:A:1000[A]:EN5:C3	4:A:1000[A]:EN5:HN	1.97	0.77
1:A:253[A]:MET:HE2	1:A:301:VAL:C	2.05	0.77
1:B:257[B]:LYS:CE	1:B:259[B]:LYS:NZ	2.40	0.77
1:C:265:HIS:ND1	1:C:283[A]:LYS:HG2	2.00	0.77
4:A:1000[A]:EN5:C8	3:A:1415:DMS:H22	2.15	0.76
4:A:1000[B]:EN5:C8	3:A:1415:DMS:H22	2.15	0.76
1:A:262:GLU:HG3	9:A:2356:HOH:O	1.86	0.75
1:C:257:LYS:HE2	1:C:259:LYS:CE	2.17	0.74
1:C:32[A]:TYR:CD1	1:C:38:LYS:HE3	2.23	0.74
1:C:241:LEU:HD22	1:C:242:TYR:CE1	2.23	0.74
4:A:1000[B]:EN5:C9	3:A:1415:DMS:H22	2.17	0.73
1:A:156[B]:LYS:HE3	9:A:2235:HOH:O	1.87	0.73
1:C:257:LYS:HE2	1:C:259:LYS:HE2	1.67	0.73
4:A:1000[A]:EN5:H3	4:A:1000[A]:EN5:N	2.01	0.73
4:A:1000[A]:EN5:HN1	3:A:1415:DMS:C2	2.01	0.72
4:A:1000[B]:EN5:HN1	3:A:1415:DMS:C2	2.01	0.72
1:A:303:GLU:OE2	1:A:306:GLY:HA2	1.91	0.71
1:C:219:LYS:O	1:C:223:GLU:HG3	1.91	0.71
1:B:257[B]:LYS:CD	1:B:259[B]:LYS:HZ1	1.86	0.70
1:B:230:ASN:CB	1:B:231:SER:HA	2.21	0.70
1:A:58[A]:GLU:CD	1:A:58[A]:GLU:H	1.95	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1000[A]:EN5:C8	3:A:1415:DMS:C2	2.69	0.70
4:B:1000:EN5:H8A	3:B:1414:DMS:C2	2.20	0.70
3:A:1415:DMS:C2	9:A:2397:HOH:O	2.39	0.69
1:A:283[B]:LYS:CB	1:A:283[B]:LYS:NZ	2.54	0.69
4:A:1000[A]:EN5:C9	3:A:1415:DMS:H22	2.17	0.69
1:B:159:GLU:CD	1:B:409[A]:LEU:CD2	2.62	0.68
1:B:230:ASN:HB2	1:B:231:SER:CA	2.23	0.68
4:B:1000:EN5:H11A	3:B:1414:DMS:H12	1.75	0.68
1:B:159:GLU:CD	1:B:409[A]:LEU:HD22	2.12	0.68
1:B:257[B]:LYS:HE3	1:B:259[B]:LYS:NZ	2.05	0.68
1:B:230:ASN:ND2	1:B:231:SER:OG	2.27	0.68
4:A:1000[B]:EN5:N	9:A:2240:HOH:O	2.28	0.67
1:C:211[B]:TYR:HD2	1:C:386:GLY:O	1.77	0.67
1:A:253[A]:MET:CE	1:A:301:VAL:C	2.63	0.67
1:B:231:SER:H	1:B:233:LEU:CA	2.07	0.67
4:A:1000[A]:EN5:H8A	3:A:1415:DMS:H22	1.70	0.67
3:B:999:DMS:H22	9:B:2396:HOH:O	1.94	0.66
1:B:75[B]:VAL:CG2	9:B:2239:HOH:O	2.36	0.66
4:A:1000[B]:EN5:H8A	3:A:1415:DMS:H22	1.71	0.66
1:B:304[B]:GLU:O	1:B:305:ASN:ND2	2.28	0.66
1:A:253[A]:MET:CE	1:A:302:ASN:HB2	2.26	0.65
1:A:134:SER:HB2	1:A:136[A]:LYS:CE	2.26	0.64
1:C:145:PRO:O	1:C:146[A]:THR:HG22	1.98	0.64
1:C:122[B]:LEU:HD11	1:C:189:GLU:CG	2.24	0.64
1:C:211[B]:TYR:CD2	1:C:386:GLY:C	2.71	0.64
1:B:222:ILE:HD12	1:B:229:LEU:HG	1.78	0.64
4:B:1000:EN5:H11A	3:B:1414:DMS:C1	2.28	0.63
1:A:42[A]:GLU:HG2	1:B:344:THR:HG21	1.79	0.62
1:C:145:PRO:CB	1:C:156[A]:LYS:HE3	2.25	0.62
3:B:1414:DMS:H21	9:B:2267:HOH:O	2.00	0.60
1:C:257:LYS:HE2	1:C:259:LYS:NZ	2.16	0.60
1:B:110[A]:GLU:HG3	1:B:296:VAL:HG21	1.83	0.60
1:B:211[B]:TYR:CD1	3:B:1414:DMS:H11	2.37	0.60
1:A:197:THR:HG23	1:A:409:LEU:HD12	1.83	0.60
1:B:211[B]:TYR:CG	3:B:1414:DMS:H11	2.37	0.59
1:C:257:LYS:CE	1:C:259:LYS:HE2	2.32	0.59
1:C:241:LEU:CD2	1:C:242:TYR:CE1	2.85	0.59
1:B:230:ASN:CB	1:B:231:SER:CA	2.81	0.59
1:A:253[A]:MET:HE2	1:A:302:ASN:CA	2.34	0.58
1:C:218:VAL:HG22	1:C:242:TYR:CE2	2.39	0.58
1:C:211[B]:TYR:CE2	1:C:386:GLY:HA3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:CG1	1:B:396:LYS:HG2	2.34	0.58
1:A:156[B]:LYS:HD2	9:A:2237:HOH:O	2.02	0.58
1:C:241:LEU:HD22	1:C:242:TYR:CD1	2.38	0.58
1:B:213:HIS:CE1	3:B:1414:DMS:H12	2.35	0.57
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.39	0.57
1:B:32[B]:TYR:CE1	9:B:2013:HOH:O	2.55	0.57
4:A:1000[B]:EN5:C8	3:A:1415:DMS:C2	2.69	0.57
1:A:240[B]:LYS:HD3	1:A:243[B]:ARG:CZ	2.34	0.57
1:B:211[A]:TYR:CD2	3:B:1414:DMS:H11	2.39	0.57
1:B:243:ARG:HG3	9:B:2301:HOH:O	2.03	0.57
4:A:1000[A]:EN5:O2	3:A:1415:DMS:O	2.23	0.56
4:A:1000[B]:EN5:O2	3:A:1415:DMS:O	2.23	0.56
1:C:122[B]:LEU:HD12	1:C:125:TRP:CD1	2.40	0.56
1:A:148:ILE:HG13	1:A:157[B]:MET:HE2	1.88	0.56
1:B:124:THR:HG23	9:B:2195:HOH:O	2.05	0.55
1:C:156[B]:LYS:HE2	1:C:191:ILE:HD11	1.87	0.55
1:B:47:VAL:HG11	1:B:396:LYS:HG2	1.88	0.55
1:A:266:LYS:NZ	1:A:266:LYS:HB2	2.23	0.54
1:A:266:LYS:HZ2	1:A:266:LYS:HB2	1.72	0.54
1:B:230:ASN:C	1:B:233:LEU:H	2.05	0.54
1:C:276:ASN:ND2	1:C:400:PHE:CE2	2.76	0.54
1:C:303[B]:GLU:HB3	1:C:308:ILE:HD13	1.90	0.54
1:A:253[A]:MET:HE3	1:A:302:ASN:HB2	1.88	0.54
4:B:1000:EN5:H1	9:B:2145:HOH:O	2.08	0.54
1:C:211[B]:TYR:HE2	1:C:386:GLY:HA3	1.71	0.54
1:A:253[A]:MET:HE2	1:A:302:ASN:HB2	1.88	0.53
1:B:229:LEU:C	1:B:230:ASN:OD1	2.47	0.53
1:C:265:HIS:HB3	1:C:283[A]:LYS:HD3	1.91	0.53
1:C:211[B]:TYR:CE2	1:C:386:GLY:C	2.82	0.53
1:A:344:THR:HG21	1:B:42[B]:GLU:HG3	1.91	0.53
1:B:231:SER:H	1:B:233:LEU:CB	2.22	0.53
1:B:230:ASN:CG	1:B:231:SER:HA	2.28	0.52
1:C:265:HIS:CB	1:C:283[A]:LYS:HD3	2.39	0.52
1:A:105:PHE:HE1	3:A:1415:DMS:H23	1.73	0.52
1:B:382:GLY:HA3	4:B:1000:EN5:H24	1.91	0.52
1:B:159:GLU:OE2	3:B:999:DMS:C1	2.57	0.52
1:A:127:ILE:HG13	1:A:182:ILE:HD13	1.92	0.52
1:C:156[B]:LYS:HG2	1:C:191:ILE:HG12	1.91	0.52
1:A:146:THR:HG23	1:A:148:ILE:HG12	1.92	0.52
1:B:303:GLU:OE2	1:B:306:GLY:HA2	2.10	0.51
1:A:35:PRO:HB3	1:A:52:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:ND2	1:A:232:ARG:HB2	2.25	0.51
1:C:276:ASN:ND2	1:C:400:PHE:CD2	2.78	0.51
1:C:75:VAL:HG12	1:C:123:LYS:HE2	1.93	0.51
1:A:155:ILE:HB	1:A:157[B]:MET:SD	2.51	0.51
1:B:211[A]:TYR:CG	3:B:1414:DMS:H11	2.45	0.51
1:C:45:GLU:OE1	1:C:45:GLU:HA	2.12	0.50
1:A:210:ARG:HB3	9:A:2283:HOH:O	2.11	0.50
1:B:253[B]:MET:SD	1:B:302:ASN:HB2	2.51	0.50
1:C:303[A]:GLU:OE2	9:C:2250:HOH:O	2.20	0.50
1:B:231:SER:HB2	1:B:232:ARG:C	2.32	0.50
1:A:127:ILE:HD11	1:A:182:ILE:HD12	1.93	0.50
1:A:134:SER:CB	1:A:136[A]:LYS:HE3	2.34	0.49
1:B:122:LEU:HD22	1:B:189:GLU:HG3	1.93	0.49
1:A:233:LEU:HG	1:A:238:ALA:HB2	1.94	0.49
1:B:105:PHE:HZ	3:B:1414:DMS:C2	2.26	0.49
1:B:105:PHE:CZ	3:B:1414:DMS:H22	2.47	0.49
4:A:1000[A]:EN5:HN1	3:A:1415:DMS:C1	2.25	0.48
4:A:1000[B]:EN5:HN1	3:A:1415:DMS:C1	2.25	0.48
1:A:328:SER:OG	1:A:329[A]:THR:HG22	2.13	0.48
1:C:250:ILE:HB	1:C:253[B]:MET:HG3	1.96	0.48
1:A:408:VAL:CG1	2:A:997:FMT:H	2.27	0.48
1:A:304:GLU:O	1:A:305:ASN:HB2	2.12	0.48
1:C:265:HIS:CE1	1:C:283[A]:LYS:HG2	2.49	0.48
1:C:92:THR:HG21	9:C:2095:HOH:O	2.14	0.48
1:A:74:TYR:CD2	1:A:130:LYS:HE3	2.49	0.48
1:B:257[B]:LYS:HD2	1:B:259[B]:LYS:HZ2	0.54	0.48
1:B:32[B]:TYR:OH	1:B:39:ILE:HB	2.13	0.48
1:C:262:GLU:HG3	1:C:283[A]:LYS:HE3	1.96	0.48
1:C:303[B]:GLU:HB3	1:C:308:ILE:CD1	2.44	0.48
1:C:359:ASN:O	1:C:360:ASN:HB3	2.14	0.48
3:A:999:DMS:C1	9:A:2412:HOH:O	2.61	0.47
1:B:39:ILE:CD1	1:B:201:TYR:HE2	2.27	0.47
1:A:47:VAL:CG1	1:A:396:LYS:HG2	2.45	0.47
1:B:159:GLU:OE2	1:B:409[A]:LEU:HD22	2.13	0.47
1:A:253[A]:MET:HE1	1:A:302:ASN:N	2.27	0.47
4:A:1000[A]:EN5:C8	3:A:1415:DMS:H23	2.40	0.47
1:A:253[A]:MET:HE2	1:A:302:ASN:CB	2.45	0.47
1:B:105:PHE:CZ	3:B:1414:DMS:C2	2.98	0.47
1:B:211[B]:TYR:CD1	3:B:1414:DMS:C1	2.98	0.46
4:A:1000[A]:EN5:C3	4:A:1000[A]:EN5:N	2.71	0.46
1:A:134:SER:OG	1:A:136[B]:LYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:VAL:HG22	1:C:242:TYR:HE2	1.81	0.46
1:B:231:SER:HB2	1:B:232:ARG:CB	2.46	0.46
1:B:105:PHE:CE1	3:B:1414:DMS:H22	2.51	0.45
1:C:257:LYS:HE3	1:C:257:LYS:HB2	1.50	0.45
1:B:254:ARG:NH1	1:B:257[B]:LYS:HE2	2.32	0.45
1:B:159:GLU:OE2	1:B:409[A]:LEU:CD2	2.65	0.45
1:B:84:ARG:HD2	1:B:109:ALA:O	2.17	0.45
1:A:55:ASN:HB3	1:A:192:TRP:CZ3	2.51	0.45
1:B:229:LEU:O	1:B:230:ASN:OD1	2.35	0.45
1:A:97:GLU:HA	1:A:103:PHE:O	2.16	0.45
1:A:107:TYR:CD1	1:A:317:LEU:HD13	2.52	0.45
4:A:1000[A]:EN5:HN1	3:A:1415:DMS:H11	1.81	0.45
1:A:47:VAL:HG12	1:A:396:LYS:HG2	1.99	0.45
1:B:230:ASN:HD22	1:B:231:SER:CA	2.18	0.45
1:B:122:LEU:CD2	1:B:189:GLU:HG3	2.47	0.44
1:B:241:LEU:HD12	1:B:380:LYS:HE2	1.99	0.44
1:C:241:LEU:O	1:C:242:TYR:CG	2.70	0.44
1:C:47:VAL:HG11	1:C:396:LYS:HD2	2.00	0.44
1:A:218:VAL:O	1:A:222:ILE:HG12	2.17	0.44
1:B:230:ASN:HD22	1:B:231:SER:CB	2.30	0.44
1:B:75[B]:VAL:HG12	1:B:75[B]:VAL:O	2.17	0.44
1:B:227:SER:HB3	4:B:1000:EN5:H26	1.99	0.44
1:B:230:ASN:O	1:B:233:LEU:O	2.35	0.43
1:B:317:LEU:HB3	1:B:334:TYR:CE1	2.53	0.43
1:A:253[A]:MET:CE	1:A:302:ASN:CB	2.95	0.43
1:C:211[B]:TYR:CE2	1:C:386:GLY:CA	3.02	0.43
1:C:265:HIS:ND1	1:C:283[A]:LYS:CG	2.74	0.43
1:A:79:LYS:HE3	1:A:121:TYR:OH	2.19	0.43
4:A:1000[B]:EN5:HN1	3:A:1415:DMS:H11	1.81	0.43
1:A:283[B]:LYS:CB	1:A:283[B]:LYS:HZ2	2.30	0.43
1:B:97:GLU:HA	1:B:103:PHE:O	2.19	0.43
1:C:360:ASN:HB2	9:C:2329:HOH:O	2.18	0.43
1:A:233:LEU:HD12	1:A:237[A]:ARG:HG2	2.00	0.42
1:B:39:ILE:HD12	1:B:201:TYR:HE2	1.83	0.42
1:B:159:GLU:OE2	3:B:999:DMS:H11	2.19	0.42
1:B:231:SER:CB	1:B:232:ARG:CB	2.97	0.42
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.54	0.42
1:A:243[B]:ARG:HB3	1:A:243[B]:ARG:HE	1.65	0.42
1:C:28:TYR:CE2	1:C:39:ILE:HG13	2.54	0.42
3:A:999:DMS:H13	9:A:2412:HOH:O	2.18	0.42
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156[B]:LYS:C	1:A:157[B]:MET:HG3	2.39	0.41
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.02	0.41
1:C:175:ALA:HB3	1:C:176:PRO:HD3	2.02	0.41
1:B:230:ASN:ND2	1:B:231:SER:CA	2.71	0.41
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.56	0.41
1:A:228:SER:HB2	9:A:2309:HOH:O	2.20	0.41
1:B:304[B]:GLU:HG2	1:B:305:ASN:ND2	2.36	0.41
1:C:211[B]:TYR:CD2	1:C:386:GLY:CA	3.04	0.41
1:B:253[A]:MET:HG3	1:B:300:TYR:HB3	2.03	0.41
1:C:262:GLU:HA	1:C:283[A]:LYS:CD	2.51	0.41
1:A:219:LYS:O	1:A:223:GLU:HG3	2.22	0.40
1:C:250:ILE:HG22	1:C:253[B]:MET:HG2	2.03	0.40
1:A:203:PRO:HA	1:A:204:LYS:HA	1.94	0.40
1:B:300:TYR:CG	1:B:355:LEU:HD13	2.57	0.40
1:B:346[A]:LYS:HD3	9:B:2403:HOH:O	2.22	0.40
1:C:29:LYS:HA	1:C:29:LYS:HD3	1.87	0.40
1:A:110[B]:GLU:CD	1:A:110[B]:GLU:H	2.23	0.40
1:B:230:ASN:HB2	1:B:231:SER:O	2.22	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	413/384 (108%)	401 (97%)	12 (3%)	0	100	100
1	B	401/384 (104%)	390 (97%)	10 (2%)	1 (0%)	51	21
1	C	384/384 (100%)	372 (97%)	12 (3%)	0	100	100
All	All	1198/1152 (104%)	1163 (97%)	34 (3%)	1 (0%)	55	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ASN

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	382/350 (109%)	370 (97%)	12 (3%)	45	11
1	B	370/350 (106%)	362 (98%)	8 (2%)	57	21
1	C	355/350 (101%)	339 (96%)	16 (4%)	32	4
All	All	1107/1050 (105%)	1071 (97%)	36 (3%)	51	10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27[A]	ASP
1	A	27[B]	ASP
1	A	106	ASN
1	A	156[B]	LYS
1	A	156[C]	LYS
1	A	214	ARG
1	A	231	SER
1	A	258[A]	LYS
1	A	258[B]	LYS
1	A	266	LYS
1	A	329[A]	THR
1	A	329[B]	THR
1	B	82	LYS
1	B	99	ASP
1	B	106	ASN
1	B	136[A]	LYS
1	B	136[B]	LYS
1	B	214	ARG
1	B	230	ASN
1	B	305	ASN
1	C	39	ILE
1	C	53	SER

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Mol	Chain	Res	Type
1	C	54[A]	ASP
1	C	54[B]	ASP
1	C	119	PRO
1	C	146[A]	THR
1	C	146[B]	THR
1	C	156[A]	LYS
1	C	156[B]	LYS
1	C	214[A]	ARG
1	C	214[B]	ARG
1	C	241	LEU
1	C	257	LYS
1	C	294	GLU
1	C	305	ASN
1	C	396	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	44	ASN
1	A	106	ASN
1	A	249	ASN
1	A	295	ASN
1	A	350	GLN
1	B	34	GLN
1	B	151	HIS
1	B	230	ASN
1	B	249	ASN
1	B	350	GLN
1	C	34	GLN
1	C	106	ASN
1	C	249	ASN
1	C	350	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

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	EN5	A	1000[A]	-	36,36,36	1.16	3 (8%)	42,42,42	1.14	3 (7%)
4	EN5	A	1000[B]	-	36,36,36	1.16	3 (8%)	42,42,42	1.16	3 (7%)
5	NHW	A	1411	7	59,66,66	1.40	9 (15%)	66,92,92	1.97	19 (28%)
8	SO4	A	1414	-	4,4,4	0.51	0	6,6,6	1.51	1 (16%)
3	DMS	A	1415	-	3,3,3	0.59	0	3,3,3	1.59	1 (33%)
2	FMT	A	997	-	0,2,2	0.00	-	0,1,1	0.00	-
3	DMS	A	999	-	3,3,3	0.40	0	3,3,3	2.88	3 (100%)
4	EN5	B	1000	-	36,36,36	0.95	1 (2%)	42,42,42	1.50	7 (16%)
5	NHW	B	1411	-	59,66,66	1.59	8 (13%)	66,92,92	1.56	9 (13%)
3	DMS	B	1414	-	3,3,3	0.75	0	3,3,3	2.50	2 (66%)
3	DMS	B	999	-	3,3,3	0.89	0	3,3,3	2.02	1 (33%)
5	NHW	C	1411	7	59,66,66	1.76	8 (13%)	66,92,92	1.37	11 (16%)
3	DMS	C	999	-	3,3,3	0.46	0	3,3,3	1.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EN5	A	1000[A]	-	-	0/39/47/47	0/1/1/1
4	EN5	A	1000[B]	-	-	0/39/47/47	0/1/1/1
5	NHW	A	1411	7	-	0/61/81/81	0/3/3/3
8	SO4	A	1414	-	-	0/0/0/0	0/0/0/0
3	DMS	A	1415	-	-	0/0/0/0	0/0/0/0
2	FMT	A	997	-	-	0/0/0/0	0/0/0/0
3	DMS	A	999	-	-	0/0/0/0	0/0/0/0
4	EN5	B	1000	-	-	0/39/47/47	0/1/1/1
5	NHW	B	1411	-	-	0/61/81/81	0/3/3/3
3	DMS	B	1414	-	-	0/0/0/0	0/0/0/0
3	DMS	B	999	-	-	0/0/0/0	0/0/0/0
5	NHW	C	1411	7	-	0/61/81/81	0/3/3/3
3	DMS	C	999	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000[A]	EN5	O2-C12	-4.05	1.15	1.23
4	A	1000[B]	EN5	O2-C12	-4.05	1.15	1.23
4	A	1000[A]	EN5	O3-C18	-4.02	1.15	1.23
4	A	1000[B]	EN5	O3-C18	-4.02	1.15	1.23
5	A	1411	NHW	CP-C1M	-2.91	1.46	1.51
5	B	1411	NHW	P2A-O5A	-2.90	1.40	1.50
5	A	1411	NHW	P1A-O2A	-2.82	1.40	1.55
5	B	1411	NHW	P3X-O7A	-2.73	1.43	1.54
5	C	1411	NHW	P3X-O7A	-2.56	1.44	1.54
5	C	1411	NHW	C9-N8	-2.52	1.28	1.33
4	A	1000[A]	EN5	O-C9	-2.50	1.18	1.23
4	A	1000[B]	EN5	O-C9	-2.46	1.18	1.23
5	A	1411	NHW	C13-C11	-2.43	1.48	1.53
5	C	1411	NHW	C2M-C1M	-2.38	1.44	1.50
5	B	1411	NHW	P2A-O4A	-2.25	1.43	1.55
5	B	1411	NHW	CP-C1M	-2.15	1.47	1.51
5	C	1411	NHW	C5A-N7A	-2.00	1.32	1.39
5	A	1411	NHW	C4A-N3A	2.05	1.38	1.35
4	B	1000	EN5	O2-C12	2.38	1.28	1.23
5	A	1411	NHW	O4X-C4X	2.46	1.50	1.45
5	A	1411	NHW	P3X-O3X	2.58	1.64	1.59
5	A	1411	NHW	P3X-O8A	2.64	1.65	1.54
5	C	1411	NHW	C4A-N3A	2.66	1.39	1.35
5	A	1411	NHW	O1M-C1M	3.06	1.27	1.21
5	C	1411	NHW	CP-C1M	3.08	1.56	1.51
5	B	1411	NHW	O4X-C1X	3.08	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1411	NHW	O4X-C1X	4.00	1.46	1.41
5	B	1411	NHW	CP-S1	4.03	1.90	1.81
5	B	1411	NHW	O10-C10	4.15	1.50	1.42
5	C	1411	NHW	O4X-C4X	5.73	1.58	1.45
5	B	1411	NHW	P3X-O3X	6.88	1.71	1.59
5	C	1411	NHW	P3X-O3X	8.53	1.74	1.59

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1411	NHW	C13-C11-C12	-5.82	99.82	108.37
5	B	1411	NHW	N3A-C2A-N1A	-5.38	124.17	128.86
5	B	1411	NHW	C6-C5-N4	-5.37	107.23	116.49
5	A	1411	NHW	O6A-C12-C11	-4.94	102.61	110.55
5	A	1411	NHW	C4X-O4X-C1X	-4.13	105.37	109.77
5	A	1411	NHW	O1M-C1M-CP	-3.93	116.56	122.17
5	A	1411	NHW	C6-C7-N8	-3.59	104.45	111.87
4	B	1000	EN5	C8-C9-N1	-3.27	110.07	115.82
5	C	1411	NHW	C1X-N9A-C4A	-3.06	121.35	126.64
5	C	1411	NHW	O1M-C1M-CP	-2.88	118.06	122.17
5	B	1411	NHW	C4X-O4X-C1X	-2.86	106.73	109.77
5	A	1411	NHW	C7-C6-C5	-2.69	107.89	112.22
5	A	1411	NHW	N3A-C2A-N1A	-2.60	126.59	128.86
5	A	1411	NHW	C6-C5-N4	-2.55	112.09	116.49
8	A	1414	SO4	O4-S-O3	-2.50	97.70	108.96
5	A	1411	NHW	C2-S1-CP	-2.50	97.59	101.77
4	B	1000	EN5	C18-C13-N2	-2.46	104.43	111.20
5	C	1411	NHW	C2-S1-CP	-2.38	97.80	101.77
5	C	1411	NHW	C6-C7-N8	-2.25	107.21	111.87
4	B	1000	EN5	C14-C13-N2	-2.24	106.26	110.90
5	C	1411	NHW	C4A-C5A-N7A	-2.24	107.25	109.41
5	C	1411	NHW	O5-C5-C6	-2.19	117.89	122.01
5	A	1411	NHW	O5-C5-N4	-2.15	118.86	122.97
5	B	1411	NHW	C13-C11-C10	2.04	112.36	108.82
5	B	1411	NHW	C2-S1-CP	2.06	105.21	101.77
5	C	1411	NHW	O4A-P2A-O5A	2.07	123.01	112.28
3	A	999	DMS	O-S-C1	2.13	117.77	106.54
3	B	1414	DMS	O-S-C2	2.20	118.15	106.54
5	A	1411	NHW	C3-N4-C5	2.21	127.08	122.84
5	A	1411	NHW	C5A-C6A-N6A	2.24	125.04	120.47
4	A	1000[A]	EN5	C20-C21-C22	2.28	117.30	112.11
4	A	1000[B]	EN5	C20-C21-C22	2.28	117.30	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1411	NHW	CP-C1M-C2M	2.33	120.52	115.52
4	B	1000	EN5	C7-C8-C9	2.38	120.00	113.32
5	A	1411	NHW	O4A-P2A-O5A	2.41	124.76	112.28
5	A	1411	NHW	CP-C1M-C2M	2.48	120.83	115.52
5	A	1411	NHW	C13-C11-C10	2.48	113.12	108.82
5	A	1411	NHW	C7-N8-C9	2.51	127.27	122.59
4	A	1000[A]	EN5	C25-C26-C21	2.59	116.94	112.19
4	A	1000[B]	EN5	C25-C26-C21	2.59	116.94	112.19
5	B	1411	NHW	C2A-N1A-C6A	2.70	123.50	118.77
3	A	1415	DMS	C2-S-C1	2.71	112.49	98.44
4	B	1000	EN5	C3-C2-C1	2.73	128.53	114.45
5	B	1411	NHW	O7A-P3X-O9A	2.75	121.27	110.50
5	B	1411	NHW	C5A-C6A-N6A	2.84	126.26	120.47
5	C	1411	NHW	C7-N8-C9	2.91	128.01	122.59
5	C	1411	NHW	C13-C11-C10	2.91	113.87	108.82
5	B	1411	NHW	C14-C11-C10	2.99	114.00	108.82
5	A	1411	NHW	O9-C9-N8	3.12	129.07	123.07
4	B	1000	EN5	C22-C21-C26	3.16	117.08	109.27
3	A	999	DMS	O-S-C2	3.17	123.28	106.54
3	B	999	DMS	O-S-C1	3.19	123.39	106.54
3	A	999	DMS	C2-S-C1	3.21	115.10	98.44
5	C	1411	NHW	O6A-C12-C11	3.23	115.73	110.55
3	B	1414	DMS	C2-S-C1	3.26	115.35	98.44
5	A	1411	NHW	O5-C5-C6	3.61	128.79	122.01
4	A	1000[A]	EN5	C24-C23-C22	3.80	119.28	111.42
4	A	1000[B]	EN5	C24-C23-C22	3.80	119.28	111.42
4	B	1000	EN5	O-C9-C8	4.26	130.01	122.01
5	A	1411	NHW	C14-C11-C10	4.90	117.32	108.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000[A]	EN5	17	0
4	A	1000[B]	EN5	13	0
3	A	1415	DMS	28	0
2	A	997	FMT	2	0
3	A	999	DMS	2	0
4	B	1000	EN5	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1414	DMS	16	0
3	B	999	DMS	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	384/384 (100%)	0.14	12 (3%)	49	53	6, 11, 20, 57	12 (3%)
1	B	384/384 (100%)	0.02	11 (2%)	52	55	5, 10, 21, 60	11 (2%)
1	C	370/384 (96%)	0.23	16 (4%)	36	38	7, 12, 26, 66	14 (3%)
All	All	1138/1152 (98%)	0.13	39 (3%)	46	48	5, 11, 23, 66	37 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	TYR	13.6
1	C	241	LEU	9.9
1	B	232	ARG	6.7
1	A	231	SER	6.3
1	B	231	SER	5.1
1	A	39	ILE	4.8
1	C	323	GLY	4.1
1	A	230	ASN	3.7
1	A	233	LEU	3.6
1	C	326	LYS	3.6
1	C	243[A]	ARG	3.4
1	A	54	ASP	3.3
1	C	27	ASP	3.2
1	A	32[A]	TYR	2.9
1	A	27[A]	ASP	2.9
1	A	232	ARG	2.8
1	C	222	ILE	2.7
1	B	27[A]	ASP	2.7
1	A	306	GLY	2.6
1	B	32[A]	TYR	2.6
1	C	386	GLY	2.6
1	C	40	ASN	2.6
1	A	237[A]	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	131	TYR	2.4
1	B	40	ASN	2.3
1	B	244	VAL	2.3
1	C	39	ILE	2.3
1	C	32[A]	TYR	2.3
1	C	325	ASP	2.3
1	B	230	ASN	2.2
1	C	305	ASN	2.2
1	C	54[A]	ASP	2.2
1	A	305	ASN	2.2
1	C	327	TYR	2.2
1	A	229	LEU	2.2
1	C	224	ILE	2.2
1	B	133	ALA	2.2
1	B	233	LEU	2.1
1	B	325	ASP	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	DMS	C	999	4/4	0.53	0.43	29.94	27,28,31,34	4
3	DMS	A	999	4/4	0.64	0.30	13.74	15,17,21,24	4
3	DMS	B	1414	4/4	0.82	0.22	11.24	18,20,21,25	4
3	DMS	A	1415	4/4	0.73	0.26	11.18	23,24,25,27	4
3	DMS	B	999	4/4	0.62	0.21	9.44	20,20,24,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EN5	A	1000[B]	36/36	0.88	0.13	2.03	16,19,22,23	36
4	EN5	A	1000[A]	36/36	0.88	0.13	2.00	14,16,18,19	36
4	EN5	B	1000	36/36	0.90	0.11	1.64	12,15,22,22	0
8	SO4	A	1414	5/5	0.92	0.12	1.48	31,36,38,43	0
7	MG	C	1415	1/1	0.98	0.08	1.16	21,21,21,21	0
6	CL	C	1413	1/1	0.93	0.13	1.04	41,41,41,41	0
6	CL	C	1414	1/1	0.87	0.18	0.26	54,54,54,54	0
6	CL	B	1412	1/1	0.99	0.07	0.07	9,9,9,9	0
5	NHW	C	1411	64/64	0.97	0.07	-0.35	6,10,13,16	0
5	NHW	B	1411	64/64	0.98	0.07	-0.42	5,8,11,14	0
5	NHW	A	1411	64/64	0.97	0.07	-0.48	6,8,11,14	0
2	FMT	A	997	3/3	0.96	0.09	-0.85	16,16,17,18	0
7	MG	B	1413	1/1	0.99	0.04	-2.05	21,21,21,21	0
7	MG	A	1413	1/1	0.96	0.06	-2.14	21,21,21,21	0
6	CL	A	1412	1/1	1.00	0.04	-4.55	8,8,8,8	0
6	CL	C	1412	1/1	1.00	0.04	-5.91	10,10,10,10	0

6.5 Other polymers

There are no such residues in this entry.