



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:33 am BST

PDB ID : 3REQ
Title : METHYLMALONYL-COA MUTASE, SUBSTRATE-FREE STATE (POOR QUALITY STRUCTURE)
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1997-12-04
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

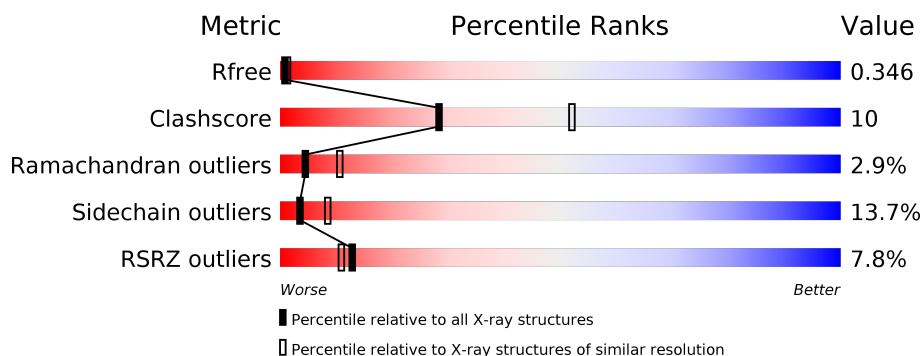
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	727	<div> <div>9%</div> <div>58%</div> <div>32%</div> <div>9%</div> <div>.</div> </div>
2	B	637	<div> <div>6%</div> <div>57%</div> <div>32%</div> <div>8%</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
3	B12	A	800	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10285 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 METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5552	3508	964	1056	24			

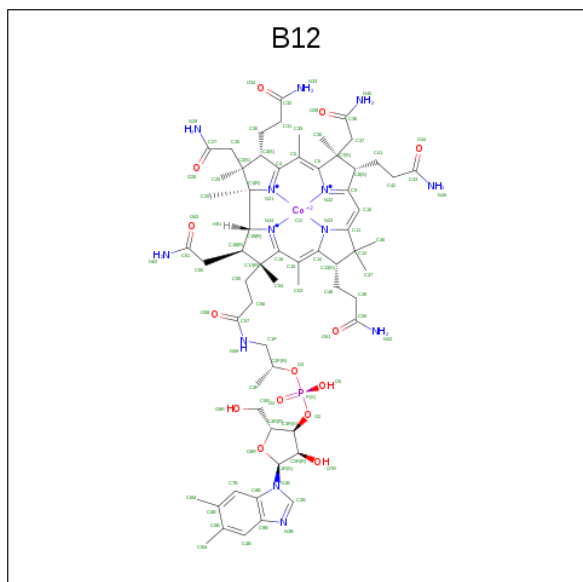
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	620	Total	C	N	O	S	0	0	0
			4624	2918	796	897	13			

There are 3 discrepancies between the modelled and reference sequences:

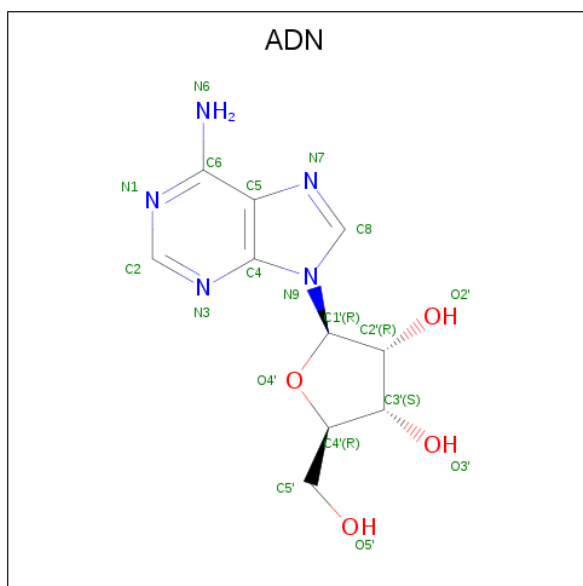
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	CONFLICT	UNP P11652
B	330	GLU	ASP	CONFLICT	UNP P11652
B	331	LEU	VAL	CONFLICT	UNP P11652

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	
			91	62	1	13	14	1	
								0	0

- Molecule 4 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).

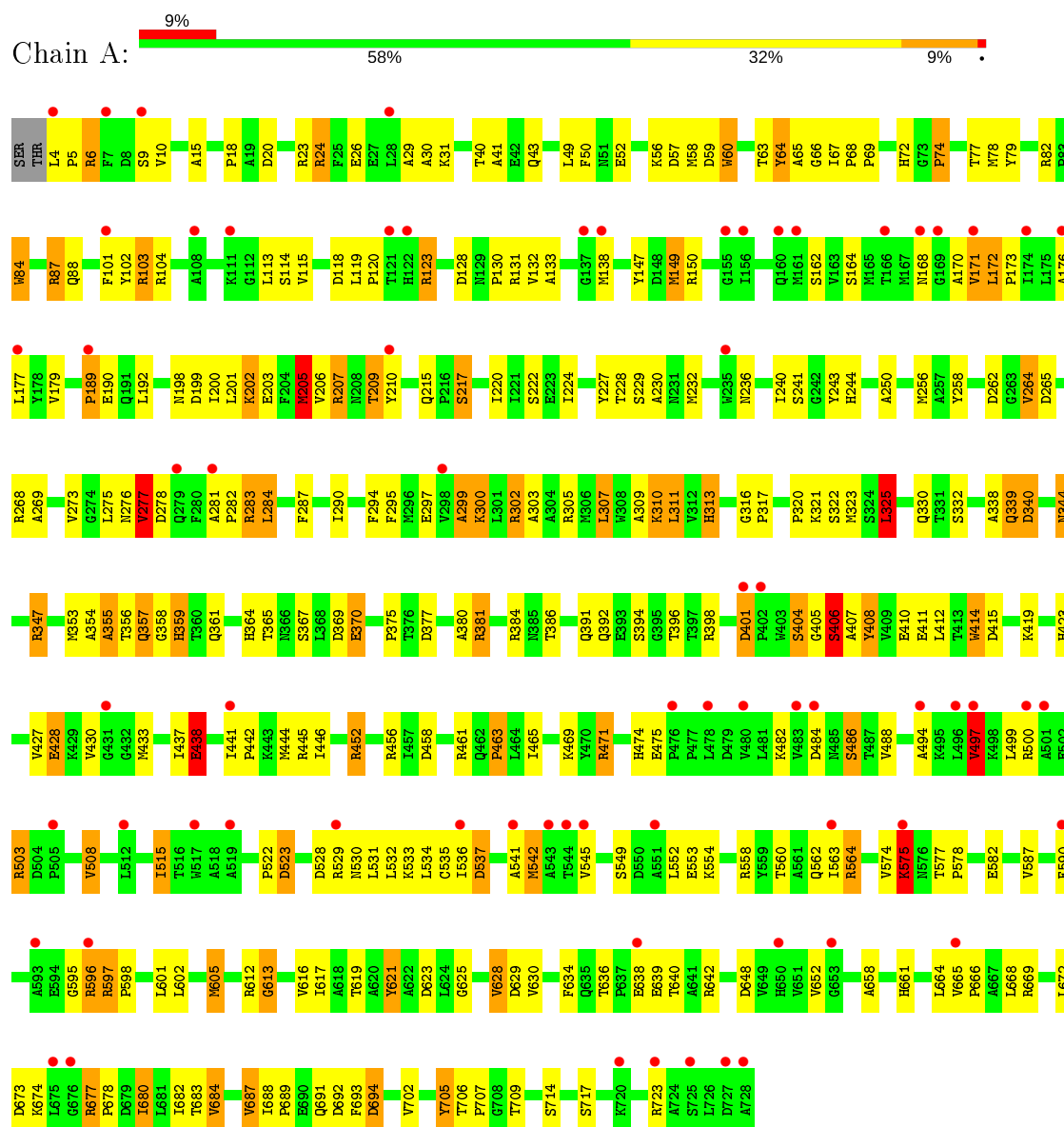


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O		
			18	10	5	3	0	0

3 Residue-property plots

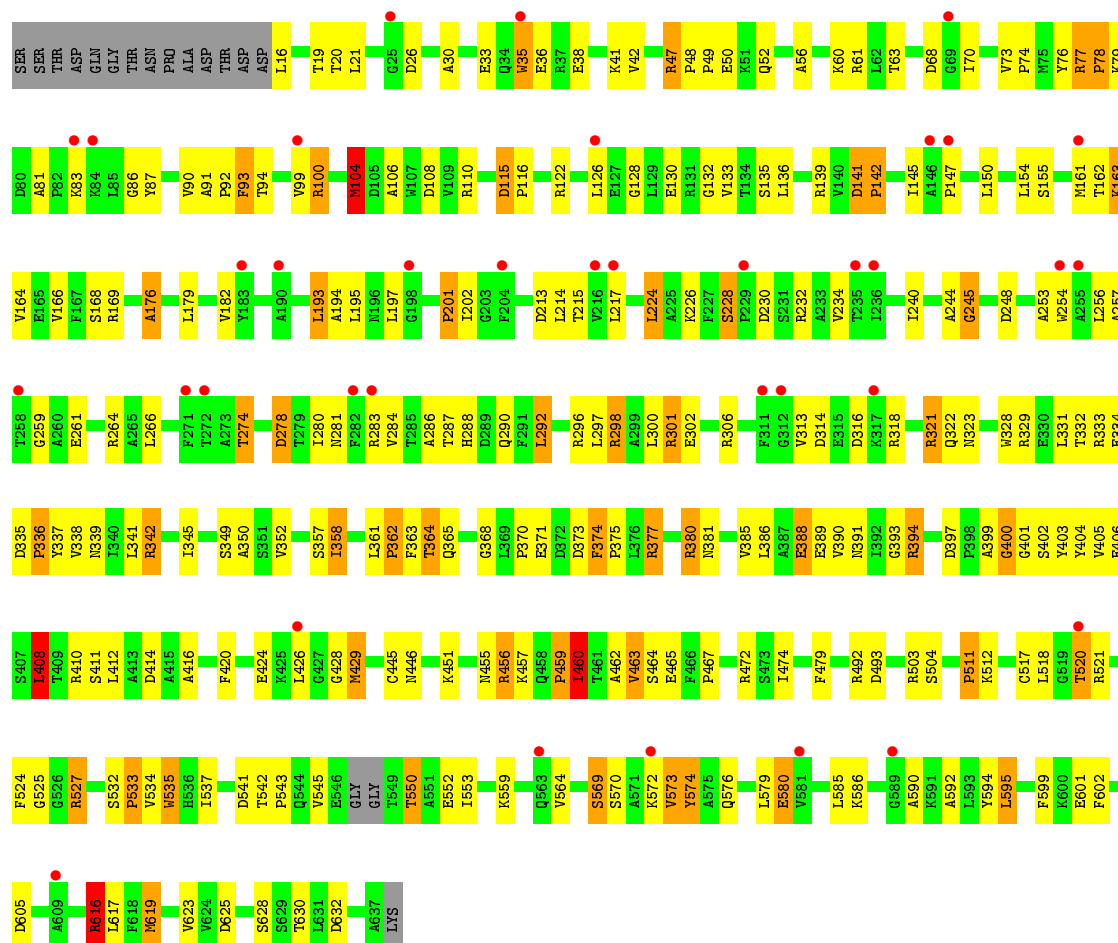
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 2: METHYLMALONYL-COA MUTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.91Å 110.91Å 257.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.70) 97.7 (29.92-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.313 , 0.393 0.277 , 0.346	Depositor DCC
R_{free} test set	2225 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10285	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: ADN, B12

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	0.66	0/5667	2.13	204/7699 (2.6%)
2	B	0.61	0/4714	2.04	140/6425 (2.2%)
All	All	0.64	0/10381	2.09	344/14124 (2.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
2	B	0	8
All	All	0	20

There are no bond length outliers.

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ARG	NE-CZ-NH2	21.17	130.89	120.30
2	B	77	ARG	CD-NE-CZ	19.48	150.87	123.60
1	A	597	ARG	NE-CZ-NH1	18.04	129.32	120.30
1	A	131	ARG	CD-NE-CZ	14.94	144.52	123.60
1	A	340	ASP	CB-CG-OD2	14.86	131.67	118.30
1	A	23	ARG	CD-NE-CZ	14.48	143.88	123.60
2	B	404	TYR	CB-CG-CD1	14.45	129.67	121.00
2	B	503	ARG	CD-NE-CZ	14.14	143.40	123.60
1	A	529	ARG	CD-NE-CZ	13.72	142.81	123.60
2	B	377	ARG	NE-CZ-NH1	13.57	127.09	120.30
2	B	388	GLU	OE1-CD-OE2	-13.54	107.05	123.30
1	A	597	ARG	NE-CZ-NH2	-13.22	113.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ARG	CD-NE-CZ	12.93	141.70	123.60
1	A	347	ARG	NE-CZ-NH2	-12.77	113.91	120.30
2	B	403	TYR	CB-CG-CD1	12.36	128.42	121.00
1	A	384	ARG	NE-CZ-NH1	-11.83	114.39	120.30
2	B	493	ASP	CB-CG-OD1	11.70	128.83	118.30
2	B	456	ARG	NE-CZ-NH2	11.61	126.10	120.30
2	B	394	ARG	CD-NE-CZ	11.37	139.52	123.60
1	A	452	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	A	597	ARG	CD-NE-CZ	11.19	139.26	123.60
2	B	342	ARG	CD-NE-CZ	11.13	139.18	123.60
2	B	321	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	452	ARG	CD-NE-CZ	10.91	138.87	123.60
1	A	458	ASP	CB-CG-OD1	10.88	128.09	118.30
1	A	669	ARG	CD-NE-CZ	10.87	138.82	123.60
1	A	79	TYR	CB-CG-CD1	10.77	127.46	121.00
2	B	77	ARG	NE-CZ-NH1	-10.66	114.97	120.30
2	B	380	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	A	612	ARG	NH1-CZ-NH2	-10.49	107.86	119.40
2	B	404	TYR	CB-CG-CD2	-10.49	114.71	121.00
1	A	612	ARG	CD-NE-CZ	10.46	138.24	123.60
2	B	403	TYR	CB-CG-CD2	-10.42	114.75	121.00
1	A	118	ASP	CB-CG-OD1	10.07	127.36	118.30
2	B	377	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	406	SER	CA-C-O	10.02	141.14	120.10
2	B	100	ARG	CD-NE-CZ	9.88	137.43	123.60
2	B	169	ARG	NE-CZ-NH2	9.86	125.23	120.30
1	A	131	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	299	ALA	O-C-N	-9.81	107.00	122.70
2	B	306	ARG	NE-CZ-NH2	-9.78	115.41	120.30
2	B	493	ASP	CB-CG-OD2	-9.69	109.58	118.30
2	B	264	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	87	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	401	ASP	CB-CG-OD1	9.66	126.99	118.30
1	A	461	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	A	79	TYR	CB-CG-CD2	-9.60	115.24	121.00
2	B	472	ARG	NE-CZ-NH2	9.35	124.97	120.30
2	B	394	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	596	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	407	ALA	N-CA-CB	-9.21	97.20	110.10
2	B	321	ARG	NE-CZ-NH2	-9.10	115.75	120.30
2	B	100	ARG	NE-CZ-NH2	-9.02	115.79	120.30
2	B	394	ARG	NE-CZ-NH1	9.01	124.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	410	GLU	OE1-CD-OE2	-8.95	112.56	123.30
2	B	26	ASP	CB-CG-OD2	-8.75	110.43	118.30
2	B	457	LYS	C-N-CA	8.75	143.57	121.70
1	A	692	ASP	CB-CG-OD2	-8.74	110.44	118.30
2	B	616	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	380	ALA	C-N-CA	8.63	143.29	121.70
1	A	103	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	325	LEU	CA-CB-CG	8.48	134.80	115.30
2	B	380	ARG	CD-NE-CZ	8.46	135.44	123.60
1	A	391	GLN	CB-CG-CD	8.41	133.47	111.60
2	B	625	ASP	CB-CG-OD1	-8.39	110.75	118.30
2	B	306	ARG	CD-NE-CZ	8.34	135.28	123.60
1	A	150	ARG	NE-CZ-NH1	-8.30	116.15	120.30
2	B	410	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	B	264	ARG	CD-NE-CZ	8.21	135.10	123.60
2	B	616	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	283	ARG	NE-CZ-NH1	8.11	124.36	120.30
2	B	232	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	415	ASP	CB-CG-OD2	8.05	125.54	118.30
1	A	59	ASP	CB-CG-OD2	8.05	125.54	118.30
2	B	492	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	A	147	TYR	CB-CG-CD1	7.94	125.76	121.00
2	B	296	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	A	634	PHE	CB-CG-CD2	-7.87	115.29	120.80
1	A	287	PHE	CB-CG-CD1	7.83	126.28	120.80
1	A	340	ASP	OD1-CG-OD2	-7.82	108.44	123.30
1	A	677	ARG	NE-CZ-NH2	-7.81	116.39	120.30
2	B	318	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	B	335	ASP	CB-CG-OD2	7.74	125.26	118.30
2	B	139	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	268	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	82	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	596	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	24	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	B	147	PRO	C-N-CA	7.62	140.75	121.70
1	A	207	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	B	52	GLN	N-CA-CB	7.59	124.27	110.60
2	B	334	GLU	OE1-CD-OE2	-7.54	114.25	123.30
2	B	52	GLN	CA-CB-CG	7.51	129.91	113.40
2	B	619	MET	CA-CB-CG	7.48	126.01	113.30
2	B	388	GLU	CG-CD-OE1	7.42	133.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	693	PHE	CB-CG-CD1	7.41	125.98	120.80
1	A	24	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	497	VAL	CA-CB-CG1	7.27	121.80	110.90
2	B	318	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	673	ASP	CB-CG-OD2	7.24	124.82	118.30
1	A	694	ASP	CB-CG-OD1	-7.23	111.79	118.30
2	B	329	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	258	TYR	CB-CG-CD1	7.21	125.32	121.00
1	A	484	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	23	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	303	ALA	O-C-N	-7.11	111.32	122.70
1	A	384	ARG	NH1-CZ-NH2	7.07	127.18	119.40
1	A	381	ARG	CB-CG-CD	7.02	129.86	111.60
1	A	558	ARG	CD-NE-CZ	6.96	133.35	123.60
1	A	408	TYR	CB-CG-CD1	6.93	125.16	121.00
1	A	377	ASP	CB-CG-OD1	6.92	124.53	118.30
2	B	38	GLU	C-N-CA	6.92	138.99	121.70
1	A	398	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	619	THR	O-C-N	-6.89	111.68	122.70
2	B	318	ARG	CD-NE-CZ	6.88	133.24	123.60
1	A	410	GLU	CA-CB-CG	6.88	128.53	113.40
1	A	401	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	406	SER	CA-C-N	-6.84	102.16	117.20
1	A	262	ASP	CA-C-N	6.83	129.85	116.20
1	A	503	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	241	SER	CA-C-O	6.82	134.41	120.10
1	A	723	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	B	363	PHE	CA-CB-CG	6.76	130.12	113.90
1	A	623	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	578	PRO	N-CA-CB	6.70	111.34	103.30
1	A	347	ARG	NH1-CZ-NH2	6.70	126.77	119.40
2	B	47	ARG	CD-NE-CZ	6.67	132.94	123.60
1	A	621	TYR	CB-CG-CD1	6.64	124.98	121.00
2	B	78	PRO	O-C-N	-6.64	112.08	122.70
1	A	241	SER	O-C-N	-6.63	111.93	123.20
1	A	60	TRP	C-N-CA	6.57	138.13	121.70
2	B	100	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	31	LYS	O-C-N	-6.55	112.22	122.70
2	B	169	ARG	CD-NE-CZ	6.53	132.75	123.60
1	A	303	ALA	CA-C-N	6.51	131.51	117.20
1	A	310	LYS	O-C-N	-6.47	112.35	122.70
1	A	438	GLU	OE1-CD-OE2	-6.47	115.54	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	B	316	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	284	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	118	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	658	ALA	C-N-CA	6.43	135.80	122.30
1	A	564	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	406	SER	N-CA-CB	6.40	120.10	110.50
1	A	356	THR	CA-C-N	6.37	131.22	117.20
2	B	193	LEU	CA-CB-CG	6.37	129.95	115.30
2	B	493	ASP	CA-CB-CG	6.37	127.41	113.40
1	A	658	ALA	O-C-N	-6.36	112.38	123.20
1	A	52	GLU	CA-CB-CG	6.30	127.26	113.40
1	A	367	SER	O-C-N	-6.30	112.62	122.70
2	B	176	ALA	O-C-N	-6.28	112.65	122.70
1	A	320	PRO	O-C-N	-6.27	112.67	122.70
2	B	381	ASN	O-C-N	-6.26	112.68	122.70
1	A	613	GLY	O-C-N	-6.25	112.69	122.70
1	A	673	ASP	OD1-CG-OD2	-6.22	111.48	123.30
2	B	283	ARG	NE-CZ-NH1	-6.22	117.19	120.30
2	B	100	ARG	CG-CD-NE	6.22	124.85	111.80
1	A	463	PRO	N-CA-CB	6.21	110.76	103.30
1	A	147	TYR	CB-CG-CD2	-6.18	117.29	121.00
2	B	26	ASP	CB-CG-OD1	6.17	123.86	118.30
2	B	133	VAL	CA-CB-CG1	6.16	120.14	110.90
1	A	20	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	66	GLY	CA-C-O	6.15	131.66	120.60
2	B	408	LEU	O-C-N	-6.15	112.87	122.70
1	A	358	GLY	C-N-CA	6.13	137.02	121.70
1	A	590	PHE	CB-CG-CD1	6.10	125.07	120.80
2	B	248	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	A	723	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	B	594	TYR	CB-CG-CD2	6.06	124.64	121.00
1	A	210	TYR	CB-CG-CD1	6.03	124.62	121.00
1	A	84	TRP	C-N-CA	6.02	136.76	121.70
1	A	309	ALA	N-CA-CB	-6.01	101.68	110.10
1	A	673	ASP	CB-CG-OD1	6.01	123.70	118.30
1	A	68	PRO	N-CA-CB	6.00	110.49	103.30
2	B	465	GLU	CG-CD-OE1	5.99	130.28	118.30
1	A	82	ARG	CD-NE-CZ	5.98	131.98	123.60
2	B	115	ASP	N-CA-CB	-5.98	99.84	110.60
2	B	380	ARG	NE-CZ-NH1	5.97	123.28	120.30
2	B	106	ALA	C-N-CA	5.97	136.62	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ASP	C-N-CA	5.96	136.61	121.70
1	A	553	GLU	CA-CB-CG	5.96	126.51	113.40
1	A	295	PHE	CG-CD2-CE2	5.95	127.35	120.80
1	A	658	ALA	CA-C-N	5.95	128.11	116.20
1	A	40	THR	O-C-N	-5.95	113.18	122.70
2	B	298	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	B	132	GLY	CA-C-O	-5.93	109.93	120.60
1	A	617	ILE	O-C-N	-5.92	113.22	122.70
2	B	79	LYS	O-C-N	-5.92	113.22	122.70
2	B	492	ARG	CD-NE-CZ	5.92	131.89	123.60
2	B	460	ILE	CB-CA-C	5.92	123.44	111.60
1	A	642	ARG	NE-CZ-NH1	-5.89	117.35	120.30
2	B	63	THR	CA-CB-CG2	5.89	120.65	112.40
1	A	278	ASP	O-C-N	-5.89	113.28	122.70
2	B	512	LYS	O-C-N	-5.89	113.28	122.70
2	B	533	PRO	CA-C-N	5.89	130.15	117.20
1	A	294	PHE	CA-C-O	5.88	132.45	120.10
1	A	452	ARG	NH1-CZ-NH2	5.87	125.86	119.40
2	B	336	PRO	O-C-N	-5.86	113.32	122.70
1	A	465	ILE	CA-C-O	5.85	132.38	120.10
1	A	693	PHE	CB-CG-CD2	-5.85	116.71	120.80
2	B	56	ALA	O-C-N	-5.83	113.37	122.70
1	A	190	GLU	OE1-CD-OE2	5.82	130.28	123.30
2	B	349	SER	CA-C-N	5.82	130.00	117.20
2	B	377	ARG	CG-CD-NE	5.82	124.01	111.80
2	B	169	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	A	228	THR	N-CA-CB	5.79	121.30	110.30
1	A	52	GLU	O-C-N	-5.79	113.44	122.70
2	B	524	PHE	CB-CG-CD1	5.78	124.84	120.80
2	B	56	ALA	CB-CA-C	5.77	118.76	110.10
1	A	684	VAL	CA-CB-CG1	5.76	119.54	110.90
1	A	537	ASP	CB-CG-OD1	5.75	123.47	118.30
2	B	337	TYR	O-C-N	-5.74	113.52	122.70
2	B	333	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	118	ASP	CA-CB-CG	5.72	125.99	113.40
1	A	295	PHE	CB-CG-CD1	5.71	124.80	120.80
1	A	445	ARG	CD-NE-CZ	5.69	131.56	123.60
2	B	286	ALA	N-CA-CB	5.69	118.06	110.10
2	B	60	LYS	C-N-CA	5.67	135.88	121.70
2	B	108	ASP	CB-CG-OD1	5.67	123.40	118.30
2	B	357	SER	N-CA-CB	5.66	118.99	110.50
2	B	456	ARG	NE-CZ-NH1	-5.66	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	TYR	CB-CG-CD1	5.66	124.39	121.00
2	B	298	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	149	MET	CA-CB-CG	-5.65	103.69	113.30
2	B	463	VAL	CG1-CB-CG2	-5.65	101.87	110.90
2	B	278	ASP	CA-CB-CG	5.64	125.80	113.40
1	A	115	VAL	CB-CA-C	-5.63	100.70	111.40
2	B	574	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	445	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	340	ASP	O-C-N	-5.62	113.71	122.70
1	A	428	GLU	C-N-CA	5.60	135.70	121.70
2	B	543	PRO	N-CA-CB	5.59	110.00	103.30
1	A	575	LYS	CA-CB-CG	5.58	125.68	113.40
1	A	300	LYS	C-N-CA	5.57	135.63	121.70
1	A	705	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	189	PRO	CA-C-N	5.56	129.43	117.20
1	A	6	ARG	CA-CB-CG	5.55	125.60	113.40
1	A	465	ILE	C-N-CA	5.54	133.94	122.30
1	A	41	ALA	C-N-CA	5.54	135.56	121.70
2	B	617	LEU	N-CA-CB	5.54	121.48	110.40
1	A	605	MET	CA-CB-CG	5.54	122.71	113.30
1	A	170	ALA	C-N-CA	5.54	135.54	121.70
1	A	313	HIS	O-C-N	-5.52	113.86	122.70
1	A	57	ASP	CB-CG-OD2	5.52	123.27	118.30
2	B	115	ASP	CA-C-O	5.51	131.67	120.10
1	A	347	ARG	CG-CD-NE	-5.50	100.24	111.80
2	B	467	PRO	N-CA-CB	5.50	109.90	103.30
1	A	49	LEU	N-CA-CB	5.50	121.39	110.40
2	B	301	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	590	PHE	CB-CG-CD2	-5.49	116.96	120.80
2	B	321	ARG	CD-NE-CZ	5.49	131.28	123.60
2	B	580	GLU	CA-CB-CG	5.48	125.45	113.40
2	B	462	ALA	C-N-CA	5.47	135.38	121.70
1	A	358	GLY	CA-C-O	5.47	130.45	120.60
1	A	486	SER	C-N-CA	5.47	135.37	121.70
1	A	241	SER	C-N-CA	5.45	133.75	122.30
1	A	541	ALA	C-N-CA	5.44	135.31	121.70
2	B	104	MET	CA-CB-CG	5.43	122.53	113.30
2	B	456	ARG	CG-CD-NE	5.43	123.20	111.80
2	B	20	THR	N-CA-CB	5.42	120.60	110.30
1	A	18	PRO	N-CA-CB	5.41	109.80	103.30
1	A	133	ALA	CA-C-N	5.41	127.03	116.20
2	B	512	LYS	CB-CA-C	5.41	121.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	380	ARG	N-CA-CB	5.39	120.31	110.60
1	A	332	SER	O-C-N	-5.39	114.03	123.20
1	A	320	PRO	C-N-CA	5.39	135.17	121.70
2	B	142	PRO	C-N-CA	5.38	135.14	121.70
2	B	87	TYR	CB-CG-CD2	5.37	124.22	121.00
1	A	132	VAL	CB-CA-C	-5.35	101.23	111.40
2	B	352	VAL	C-N-CA	5.34	133.51	122.30
2	B	459	PRO	N-CA-CB	5.33	109.70	103.30
1	A	357	GLN	C-N-CA	5.33	133.50	122.30
1	A	398	ARG	CB-CA-C	5.33	121.06	110.40
1	A	582	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	A	256	MET	CB-CG-SD	-5.32	96.43	112.40
2	B	632	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	673	ASP	O-C-N	-5.31	114.20	122.70
1	A	621	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	66	GLY	O-C-N	-5.29	114.23	122.70
2	B	213	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	648	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	201	PRO	O-C-N	-5.28	114.25	122.70
1	A	361	GLN	CG-CD-OE1	5.26	132.13	121.60
2	B	292	LEU	CB-CA-C	5.26	120.19	110.20
1	A	278	ASP	C-N-CA	5.25	134.83	121.70
2	B	76	TYR	CB-CA-C	5.25	120.89	110.40
1	A	84	TRP	O-C-N	-5.25	114.31	122.70
1	A	344	ASN	O-C-N	-5.24	114.32	122.70
2	B	128	GLY	O-C-N	-5.22	114.34	122.70
1	A	277	VAL	O-C-N	-5.22	114.34	122.70
2	B	385	VAL	O-C-N	-5.22	114.35	122.70
1	A	375	PRO	N-CA-CB	5.21	109.56	103.30
2	B	318	ARG	CA-CB-CG	5.21	124.87	113.40
1	A	369	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	595	GLY	C-N-CA	5.19	134.67	121.70
2	B	122	ARG	CA-C-N	5.18	128.60	117.20
1	A	677	ARG	N-CA-C	5.18	124.99	111.00
2	B	570	SER	N-CA-CB	-5.18	102.73	110.50
2	B	147	PRO	O-C-N	-5.18	114.41	122.70
2	B	176	ALA	C-N-CA	5.18	134.65	121.70
1	A	322	SER	C-N-CA	5.17	134.62	121.70
1	A	683	THR	O-C-N	5.17	130.97	122.70
1	A	355	ALA	O-C-N	-5.16	114.44	122.70
2	B	463	VAL	CA-CB-CG1	5.16	118.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLU	N-CA-CB	-5.16	101.31	110.60
1	A	201	LEU	O-C-N	-5.16	114.45	122.70
1	A	307	LEU	N-CA-CB	5.15	120.70	110.40
1	A	687	VAL	CA-C-N	5.15	128.52	117.20
2	B	373	ASP	CB-CG-OD1	5.14	122.93	118.30
2	B	377	ARG	CD-NE-CZ	-5.14	116.40	123.60
1	A	358	GLY	O-C-N	-5.13	114.50	122.70
1	A	684	VAL	CA-CB-CG2	-5.13	103.21	110.90
1	A	74	PRO	C-N-CA	5.12	134.51	121.70
1	A	428	GLU	O-C-N	-5.12	114.51	122.70
1	A	203	GLU	OE1-CD-OE2	5.12	129.44	123.30
2	B	619	MET	CB-CA-C	5.11	120.62	110.40
1	A	6	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	598	PRO	N-CA-CB	5.11	109.43	103.30
2	B	74	PRO	N-CA-CB	5.11	109.43	103.30
1	A	102	TYR	CB-CG-CD1	5.10	124.06	121.00
1	A	564	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	B	535	TRP	O-C-N	-5.10	114.55	122.70
2	B	329	ARG	CA-CB-CG	5.08	124.58	113.40
1	A	82	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	269	ALA	C-N-CA	5.08	132.97	122.30
2	B	389	GLU	CA-CB-CG	5.08	124.57	113.40
1	A	628	VAL	CA-CB-CG1	5.08	118.51	110.90
2	B	337	TYR	C-N-CA	5.07	134.39	121.70
1	A	354	ALA	N-CA-CB	5.07	117.20	110.10
2	B	527	ARG	CD-NE-CZ	5.07	130.69	123.60
1	A	177	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	177	LEU	C-N-CA	5.06	134.34	121.70
2	B	632	ASP	C-N-CA	5.06	134.34	121.70
1	A	206	VAL	N-CA-C	5.05	124.63	111.00
1	A	88	GLN	CA-C-O	-5.04	109.51	120.10
1	A	297	GLU	OE1-CD-OE2	-5.04	117.25	123.30
2	B	364	THR	O-C-N	-5.04	114.63	122.70
1	A	638	GLU	CA-CB-CG	5.04	124.49	113.40
1	A	537	ASP	CA-CB-CG	5.04	124.48	113.40
1	A	243	TYR	CB-CG-CD1	5.02	124.01	121.00
2	B	414	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	678	PRO	N-CA-CB	5.00	109.31	103.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	LEU	Mainchain
1	A	215	GLN	Mainchain
1	A	264	VAL	Mainchain
1	A	277	VAL	Mainchain
1	A	30	ALA	Mainchain
1	A	339	GLN	Mainchain
1	A	340	ASP	Mainchain
1	A	438	GLU	Mainchain
1	A	621	TYR	Mainchain
1	A	640	THR	Mainchain
1	A	687	VAL	Mainchain
1	A	74	PRO	Mainchain
2	B	336	PRO	Mainchain
2	B	338	VAL	Mainchain
2	B	35	TRP	Mainchain
2	B	362	PRO	Mainchain
2	B	451	LYS	Mainchain
2	B	535	TRP	Mainchain
2	B	599	PHE	Mainchain
2	B	86	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5552	0	5447	102	0
2	B	4624	0	4438	101	0
3	A	91	0	88	22	0
4	A	18	0	10	0	0
All	All	10285	0	9983	198	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 10.

All (198) 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:406:SER:HB2	2:B:400:GLY:O	1.34	1.22
3:A:800:B12:H362	3:A:800:B12:H351	1.35	1.06
3:A:800:B12:H302	3:A:800:B12:H353	1.37	1.06
1:A:406:SER:CB	2:B:400:GLY:O	2.02	1.05
3:A:800:B12:H312	3:A:800:B12:C25	1.90	1.01
1:A:406:SER:N	2:B:401:GLY:O	2.04	0.91
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.55	0.87
1:A:406:SER:HA	2:B:400:GLY:O	1.76	0.85
3:A:800:B12:H251	3:A:800:B12:H312	1.58	0.85
1:A:706:THR:HB	1:A:707:PRO:HD2	1.61	0.83
1:A:405:GLY:C	2:B:401:GLY:O	2.18	0.81
1:A:316:GLY:H	1:A:317:PRO:HD3	1.43	0.81
3:A:800:B12:O28	3:A:800:B12:H3	1.80	0.79
3:A:800:B12:H253	3:A:800:B12:H312	1.65	0.78
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.69	0.75
1:A:305:ARG:HG2	1:A:325:LEU:HB3	1.69	0.75
3:A:800:B12:H302	3:A:800:B12:C35	2.15	0.74
1:A:224:ILE:HG12	1:A:532:LEU:HD22	1.70	0.74
1:A:665:VAL:HG13	1:A:682:ILE:HG21	1.70	0.73
3:A:800:B12:H482	3:A:800:B12:H533	1.72	0.72
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.71	0.72
2:B:361:LEU:HD22	2:B:365:GLN:HG2	1.71	0.71
1:A:173:PRO:HB2	1:A:545:VAL:HG22	1.71	0.71
1:A:406:SER:CA	2:B:400:GLY:O	2.37	0.71
3:A:800:B12:H531	3:A:800:B12:H552	1.73	0.71
1:A:205:MET:HG2	1:A:437:ILE:HD11	1.73	0.70
2:B:331:LEU:HD13	2:B:365:GLN:HB3	1.75	0.68
3:A:800:B12:C30	3:A:800:B12:H353	2.21	0.68
1:A:601:LEU:HA	1:A:629:ASP:HB2	1.75	0.68
2:B:202:ILE:HD13	2:B:429:MET:HB3	1.76	0.67
1:A:406:SER:CB	2:B:399:ALA:O	2.42	0.67
1:A:101:PHE:HA	1:A:104:ARG:HD2	1.76	0.67
2:B:284:VAL:HG11	2:B:322:GLN:HE21	1.60	0.67
1:A:353:MET:HE3	2:B:345:ILE:HG13	1.76	0.67
2:B:332:THR:HG21	2:B:460:ILE:HD11	1.76	0.66
2:B:391:ASN:ND2	2:B:394:ARG:HE	1.93	0.66
2:B:386:LEU:HD23	2:B:390:VAL:HG21	1.78	0.65
1:A:172:LEU:HB2	1:A:173:PRO:HD3	1.78	0.65
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.45	0.65
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.78	0.65
1:A:15:ALA:HB1	2:B:92:PRO:HB3	1.78	0.64
3:A:800:B12:H362	3:A:800:B12:C35	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:HB2	2:B:400:GLY:C	2.18	0.63
2:B:550:THR:HG21	2:B:580:GLU:HG2	1.80	0.63
1:A:405:GLY:CA	2:B:401:GLY:O	2.46	0.63
2:B:104:MET:HG3	2:B:388:GLU:HG2	1.81	0.63
1:A:171:VAL:HG11	1:A:198:ASN:HD22	1.65	0.62
1:A:406:SER:HB3	2:B:399:ALA:O	2.00	0.61
1:A:406:SER:N	2:B:401:GLY:C	2.53	0.61
1:A:63:THR:HG21	1:A:69:PRO:HD2	1.82	0.61
2:B:92:PRO:O	2:B:93:PHE:HB2	2.01	0.61
1:A:316:GLY:N	1:A:317:PRO:HD3	2.15	0.60
3:A:800:B12:C2B	3:A:800:B12:O7R	2.49	0.60
2:B:254:TRP:HA	2:B:257:ALA:HB3	1.82	0.60
1:A:172:LEU:HD11	1:A:220:ILE:HG12	1.83	0.60
3:A:800:B12:H2B	3:A:800:B12:O7R	2.01	0.60
2:B:202:ILE:HG21	2:B:429:MET:HG3	1.85	0.58
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.84	0.58
2:B:91:ALA:HA	2:B:92:PRO:C	2.22	0.58
1:A:437:ILE:HG13	1:A:442:PRO:HG2	1.85	0.58
1:A:405:GLY:HA3	2:B:401:GLY:O	2.04	0.58
2:B:460:ILE:HG23	2:B:464:SER:H	1.69	0.58
3:A:800:B12:H351	3:A:800:B12:C36	2.17	0.58
2:B:150:LEU:HD21	2:B:166:VAL:HG11	1.85	0.58
1:A:665:VAL:HB	1:A:666:PRO:HD3	1.86	0.57
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.86	0.57
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.86	0.57
1:A:494:ALA:HA	1:A:497:VAL:HB	1.87	0.57
1:A:240:ILE:HD11	1:A:284:LEU:HD22	1.86	0.56
2:B:234:VAL:HB	2:B:280:ILE:HG12	1.86	0.56
1:A:406:SER:HB3	2:B:402:SER:N	2.21	0.56
3:A:800:B12:C31	3:A:800:B12:C25	2.72	0.56
3:A:800:B12:H2B	3:A:800:B12:O2	2.06	0.56
1:A:64:TYR:HB3	2:B:35:TRP:HB2	1.88	0.55
2:B:534:VAL:HA	2:B:537:ILE:HD12	1.88	0.54
2:B:424:GLU:HA	2:B:428:GLY:HA2	1.89	0.54
2:B:390:VAL:O	2:B:391:ASN:HB2	2.08	0.54
1:A:587:VAL:HG11	1:A:625:GLY:HA3	1.89	0.53
1:A:665:VAL:HB	1:A:666:PRO:CD	2.38	0.53
1:A:123:ARG:HD2	1:A:209:THR:HA	1.89	0.53
1:A:705:TYR:HB3	1:A:709:THR:HG21	1.90	0.53
1:A:406:SER:HB3	2:B:401:GLY:C	2.29	0.53
2:B:602:PHE:HB3	2:B:605:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:LEU:HD22	1:A:680:ILE:HD12	1.91	0.52
1:A:406:SER:HA	2:B:401:GLY:HA3	1.91	0.52
2:B:460:ILE:HD12	2:B:463:VAL:HB	1.91	0.52
1:A:281:ALA:N	1:A:282:PRO:HD2	2.25	0.52
2:B:595:LEU:HD23	2:B:616:ARG:HG2	1.90	0.52
1:A:264:VAL:HG21	1:A:311:LEU:HD22	1.92	0.51
2:B:154:LEU:HD21	2:B:164:VAL:HG11	1.91	0.51
1:A:522:PRO:O	1:A:523:ASP:HB2	2.09	0.51
3:A:800:B12:H621	3:A:800:B12:H541	1.75	0.51
1:A:503:ARG:NH1	1:A:508:VAL:HG11	2.26	0.51
1:A:344:ASN:HA	1:A:347:ARG:HB2	1.93	0.51
3:A:800:B12:N62	3:A:800:B12:H541	2.25	0.51
2:B:374:PHE:HB3	2:B:375:PRO:CD	2.34	0.51
2:B:166:VAL:HG13	2:B:179:LEU:HD22	1.92	0.50
2:B:81:ALA:HA	2:B:406:GLU:HB3	1.93	0.50
2:B:364:THR:HG22	2:B:474:ILE:HG21	1.93	0.50
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.59	0.49
1:A:515:ILE:HG23	1:A:552:LEU:HG	1.94	0.49
2:B:534:VAL:HG13	2:B:623:VAL:HG12	1.93	0.49
2:B:253:ALA:HB2	2:B:416:ALA:HA	1.94	0.49
1:A:202:LYS:HA	1:A:205:MET:HG3	1.93	0.49
2:B:399:ALA:HB1	2:B:405:VAL:HG11	1.93	0.49
1:A:330:GLN:HG3	1:A:364:HIS:HB3	1.95	0.49
1:A:67:ILE:HG21	2:B:30:ALA:HB2	1.95	0.49
2:B:201:PRO:HB2	2:B:214:LEU:HD12	1.95	0.49
1:A:563:ILE:HG21	1:A:630:VAL:HB	1.94	0.48
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.95	0.48
1:A:574:VAL:O	1:A:575:LYS:HB2	2.13	0.48
1:A:406:SER:CB	2:B:400:GLY:C	2.81	0.48
1:A:338:ALA:HB3	1:A:339:GLN:NE2	2.30	0.47
1:A:503:ARG:HD2	1:A:508:VAL:HG21	1.97	0.47
2:B:328:TRP:HA	2:B:331:LEU:HG	1.96	0.46
2:B:274:THR:HA	2:B:313:VAL:HG13	1.98	0.46
2:B:292:LEU:HD23	2:B:408:LEU:HD21	1.97	0.46
2:B:518:LEU:HB2	2:B:569:SER:HB2	1.96	0.46
2:B:100:ARG:HD3	2:B:393:GLY:O	2.15	0.46
2:B:532:SER:HB2	2:B:533:PRO:CD	2.46	0.46
2:B:48:PRO:CB	2:B:49:PRO:HD2	2.46	0.45
2:B:572:LYS:HE2	2:B:573:VAL:HG22	1.99	0.45
1:A:299:ALA:O	1:A:300:LYS:C	2.54	0.45
2:B:564:VAL:HG11	2:B:630:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD23	1:A:224:ILE:HD11	1.99	0.45
1:A:441:ILE:HB	1:A:442:PRO:CD	2.47	0.45
2:B:361:LEU:HD23	2:B:362:PRO:HD2	1.99	0.44
1:A:531:LEU:HD22	1:A:552:LEU:HD21	1.99	0.44
1:A:499:LEU:HD11	1:A:542:MET:HG2	1.98	0.44
1:A:65:ALA:HA	1:A:72:HIS:HB2	1.98	0.44
3:A:800:B12:O2	3:A:800:B12:C2B	2.65	0.44
2:B:163:LYS:HE2	2:B:194:ALA:HB1	1.98	0.44
1:A:338:ALA:HB3	1:A:339:GLN:HE21	1.81	0.44
1:A:359:HIS:CE1	1:A:401:ASP:H	2.35	0.44
1:A:503:ARG:HH11	1:A:508:VAL:HG11	1.81	0.44
2:B:281:ASN:ND2	2:B:323:ASN:HD21	2.15	0.44
2:B:115:ASP:HA	2:B:116:PRO:HD2	1.83	0.44
2:B:77:ARG:HB3	2:B:78:PRO:HD2	1.99	0.44
1:A:119:LEU:N	1:A:120:PRO:HD2	2.32	0.44
1:A:500:ARG:HG3	1:A:503:ARG:HH21	1.83	0.44
2:B:553:ILE:HG22	2:B:585:LEU:HD21	1.99	0.44
2:B:517:CYS:HB2	2:B:545:VAL:O	2.18	0.44
2:B:94:THR:OG1	2:B:302:GLU:HG3	2.18	0.44
1:A:605:MET:HB2	1:A:664:LEU:HD13	2.00	0.43
2:B:278:ASP:HA	2:B:321:ARG:HH22	1.83	0.43
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.48	0.43
2:B:110:ARG:HA	2:B:135:SER:O	2.17	0.43
1:A:392:GLN:HB3	2:B:459:PRO:HG2	2.00	0.43
1:A:77:THR:OG1	2:B:42:VAL:HG11	2.19	0.43
1:A:29:ALA:HA	2:B:99:VAL:HG11	2.00	0.43
1:A:302:ARG:O	1:A:305:ARG:HB2	2.18	0.43
2:B:298:ARG:HH11	2:B:405:VAL:HG12	1.84	0.43
1:A:227:TYR:HB2	1:A:530:ASN:HD21	1.84	0.42
1:A:652:VAL:HG11	1:A:668:LEU:HD21	2.01	0.42
2:B:245:GLY:HA3	2:B:446:ASN:HD21	1.85	0.42
2:B:504:SER:HB3	2:B:511:PRO:HG2	2.01	0.42
1:A:4:LEU:HB3	1:A:5:PRO:HD2	2.00	0.42
1:A:404:SER:O	2:B:402:SER:HA	2.20	0.42
3:A:800:B12:H91	3:A:800:B12:H262	1.70	0.42
1:A:394:SER:HB2	1:A:396:THR:HG23	2.02	0.42
2:B:532:SER:HB2	2:B:533:PRO:HD3	2.01	0.42
1:A:613:GLY:HA2	1:A:616:VAL:HG22	2.00	0.42
2:B:455:ASN:O	2:B:456:ARG:HB2	2.19	0.42
1:A:172:LEU:HB2	1:A:173:PRO:CD	2.47	0.41
3:A:800:B12:H10	3:A:800:B12:H472	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ARG:HA	2:B:48:PRO:HD3	1.88	0.41
1:A:50:PHE:HE2	1:A:411:GLU:HG2	1.85	0.41
1:A:176:ALA:HB1	1:A:536:ILE:HG13	2.02	0.41
2:B:48:PRO:HB3	2:B:49:PRO:HD2	2.02	0.41
2:B:176:ALA:HB1	2:B:197:LEU:HD13	2.02	0.41
1:A:307:LEU:O	1:A:311:LEU:HD12	2.21	0.41
2:B:339:ASN:HA	2:B:342:ARG:HB2	2.02	0.41
1:A:386:THR:HA	2:B:341:LEU:HD13	2.01	0.41
3:A:800:B12:C36	3:A:800:B12:C35	2.90	0.41
2:B:126:LEU:HG	2:B:130:GLU:OE2	2.20	0.41
2:B:332:THR:CG2	2:B:460:ILE:HD11	2.49	0.41
1:A:179:VAL:HG11	1:A:536:ILE:HD13	2.02	0.41
1:A:305:ARG:HG2	1:A:325:LEU:HG	2.02	0.41
1:A:414:TRP:HE3	1:A:414:TRP:HA	1.84	0.41
2:B:377:ARG:HG3	2:B:380:ARG:NH2	2.36	0.41
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.69	0.41
1:A:199:ASP:HB3	1:A:202:LYS:HZ2	1.85	0.41
1:A:414:TRP:CE3	1:A:414:TRP:HA	2.55	0.41
1:A:58:MET:HG2	1:A:60:TRP:CH2	2.56	0.41
2:B:33:GLU:HA	2:B:36:GLU:HB2	2.02	0.41
1:A:406:SER:HB2	2:B:399:ALA:O	2.21	0.41
1:A:463:PRO:HB3	1:A:469:LYS:HD2	2.02	0.41
1:A:661:HIS:NE2	1:A:689:PRO:HD2	2.36	0.41
1:A:172:LEU:HD21	1:A:220:ILE:HG23	2.01	0.40
1:A:176:ALA:HB2	1:A:532:LEU:HD12	2.03	0.40
2:B:350:ALA:HB3	2:B:358:ILE:HD13	2.02	0.40
1:A:408:TYR:CE1	1:A:412:LEU:HD11	2.56	0.40
2:B:195:LEU:HD11	2:B:224:LEU:HD11	2.02	0.40
1:A:452:ARG:O	1:A:456:ARG:HG3	2.21	0.40
1:A:277:VAL:HG22	1:A:281:ALA:HB2	2.03	0.40
1:A:471:ARG:HB2	1:A:471:ARG:HE	1.77	0.40
2:B:297:LEU:HD23	2:B:322:GLN:NE2	2.37	0.40
2:B:368:GLY:HA2	2:B:479:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	723/727 (99%)	615 (85%)	87 (12%)	21 (3%)	4	10
2	B	616/637 (97%)	521 (85%)	77 (12%)	18 (3%)	4	10
All	All	1339/1364 (98%)	1136 (85%)	164 (12%)	39 (3%)	4	10

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	HIS
1	A	523	ASP
1	A	596	ARG
2	B	93	PHE
1	A	56	LYS
1	A	205	MET
1	A	486	SER
2	B	400	GLY
2	B	525	GLY
2	B	586	LYS
1	A	43	GLN
1	A	230	ALA
1	A	359	HIS
1	A	475	GLU
1	A	542	MET
2	B	50	GLU
2	B	240	ILE
2	B	245	GLY
2	B	371	GLU
2	B	576	GLN
1	A	192	LEU
1	A	229	SER
1	A	404	SER
1	A	575	LYS
2	B	244	ALA

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Mol	Chain	Res	Type
1	A	10	VAL
1	A	84	TRP
1	A	406	SER
2	B	259	GLY
2	B	520	THR
1	A	130	PRO
2	B	145	ILE
2	B	228	SER
2	B	590	ALA
2	B	374	PHE
1	A	189	PRO
1	A	680	ILE
2	B	397	ASP
2	B	511	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	568/590 (96%)	488 (86%)	80 (14%)	3	8
2	B	458/509 (90%)	397 (87%)	61 (13%)	4	9
All	All	1026/1099 (93%)	885 (86%)	141 (14%)	3	8

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	9	SER
1	A	24	ARG
1	A	26	GLU
1	A	78	MET
1	A	87	ARG
1	A	103	ARG
1	A	113	LEU
1	A	114	SER

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Mol	Chain	Res	Type
1	A	123	ARG
1	A	128	ASP
1	A	138	MET
1	A	149	MET
1	A	162	SER
1	A	164	SER
1	A	168	ASN
1	A	171	VAL
1	A	202	LYS
1	A	205	MET
1	A	207	ARG
1	A	209	THR
1	A	217	SER
1	A	222	SER
1	A	232	MET
1	A	236	ASN
1	A	244	HIS
1	A	265	ASP
1	A	273	VAL
1	A	275	LEU
1	A	276	ASN
1	A	283	ARG
1	A	310	LYS
1	A	311	LEU
1	A	313	HIS
1	A	321	LYS
1	A	323	MET
1	A	325	LEU
1	A	365	THR
1	A	370	GLU
1	A	381	ARG
1	A	414	TRP
1	A	419	LYS
1	A	423	HIS
1	A	427	VAL
1	A	428	GLU
1	A	430	VAL
1	A	433	MET
1	A	438	GLU
1	A	444	MET
1	A	471	ARG
1	A	482	LYS

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Mol	Chain	Res	Type
1	A	488	VAL
1	A	497	VAL
1	A	508	VAL
1	A	515	ILE
1	A	528	ASP
1	A	533	LYS
1	A	534	LEU
1	A	535	CYS
1	A	537	ASP
1	A	549	SER
1	A	554	LYS
1	A	560	THR
1	A	562	GLN
1	A	564	ARG
1	A	577	THR
1	A	597	ARG
1	A	602	LEU
1	A	628	VAL
1	A	636	THR
1	A	639	GLU
1	A	674	LYS
1	A	677	ARG
1	A	684	VAL
1	A	688	ILE
1	A	691	GLN
1	A	694	ASP
1	A	702	VAL
1	A	714	SER
1	A	717	SER
2	B	16	LEU
2	B	19	THR
2	B	21	LEU
2	B	41	LYS
2	B	61	ARG
2	B	68	ASP
2	B	70	ILE
2	B	73	VAL
2	B	83	LYS
2	B	90	VAL
2	B	104	MET
2	B	136	LEU
2	B	141	ASP

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Mol	Chain	Res	Type
2	B	155	SER
2	B	161	MET
2	B	162	THR
2	B	163	LYS
2	B	168	SER
2	B	182	VAL
2	B	193	LEU
2	B	215	THR
2	B	217	LEU
2	B	224	LEU
2	B	226	LYS
2	B	228	SER
2	B	230	ASP
2	B	256	LEU
2	B	261	GLU
2	B	266	LEU
2	B	274	THR
2	B	287	THR
2	B	288	HIS
2	B	300	LEU
2	B	301	ARG
2	B	314	ASP
2	B	358	ILE
2	B	408	LEU
2	B	411	SER
2	B	412	LEU
2	B	420	PHE
2	B	426	LEU
2	B	429	MET
2	B	445	CYS
2	B	460	ILE
2	B	520	THR
2	B	521	ARG
2	B	527	ARG
2	B	541	ASP
2	B	542	THR
2	B	550	THR
2	B	552	GLU
2	B	559	LYS
2	B	569	SER
2	B	573	VAL
2	B	574	TYR

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Mol	Chain	Res	Type
2	B	579	LEU
2	B	595	LEU
2	B	601	GLU
2	B	616	ARG
2	B	619	MET
2	B	628	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	198	ASN
1	A	215	GLN
1	A	339	GLN
1	A	359	HIS
1	A	385	ASN
1	A	425	GLN
1	A	635	GLN
1	A	643	GLN
2	B	113	HIS
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	391	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	B12	A	800	1,4	80,101,101	1.21	7 (8%)	101,166,166	2.07	27 (26%)
4	ADN	A	801	3	17,20,21	1.01	2 (11%)	15,30,31	2.15	5 (33%)

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	B12	A	800	1,4	-	13/51/223/223	0/3/11/11
4	ADN	A	801	3	-	0/0/20/22	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	CO-N23	-5.58	1.67	1.94
3	A	800	B12	CO-N24	2.73	1.95	1.89
3	A	800	B12	C11-C10	-2.67	1.36	1.40
3	A	800	B12	C2-C3	-2.58	1.54	1.58
3	A	800	B12	C55-C56	2.50	1.58	1.53
3	A	800	B12	C17-C18	2.49	1.57	1.54
4	A	801	ADN	C8-N7	-2.27	1.30	1.34
3	A	800	B12	C56-C57	2.25	1.55	1.51
4	A	801	ADN	O4'-C1'	2.01	1.43	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C56-C57-N59	-5.77	106.70	116.42
3	A	800	B12	C54-C17-C18	-5.31	105.14	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	ADN	O2'-C2'-C3'	-5.20	94.99	111.82
3	A	800	B12	C25-C2-C1	5.15	121.45	113.80
3	A	800	B12	C7B-C8B-C9B	4.89	125.38	120.54
3	A	800	B12	C55-C56-C57	-4.60	101.18	111.23
3	A	800	B12	O34-C32-C31	-3.76	110.03	121.07
3	A	800	B12	O58-C57-N59	3.75	130.08	123.01
3	A	800	B12	C13-C14-C15	-3.65	118.45	131.68
4	A	801	ADN	O4'-C1'-C2'	-3.58	101.70	106.93
3	A	800	B12	O34-C32-N33	3.56	132.23	122.50
3	A	800	B12	C55-C17-C16	3.49	121.55	109.92
3	A	800	B12	C4B-C9B-C8B	-3.41	117.61	121.10
3	A	800	B12	C36-C7-C8	3.35	118.14	112.11
4	A	801	ADN	O3'-C3'-C2'	-3.27	101.24	111.82
3	A	800	B12	C2P-C1P-N59	3.15	117.57	112.93
3	A	800	B12	C3-C4-C5	-3.09	120.46	131.68
3	A	800	B12	O6R-C1R-C2R	-3.05	102.47	106.93
3	A	800	B12	C30-C31-C32	-2.94	102.62	112.59
3	A	800	B12	C15-C14-N23	2.89	129.51	124.64
3	A	800	B12	C26-C2-C3	-2.80	102.33	107.47
3	A	800	B12	C26-C2-C1	-2.78	105.71	110.02
3	A	800	B12	O8R-C5R-C4R	-2.71	102.00	111.29
3	A	800	B12	C37-C7-C6	-2.52	101.54	109.92
3	A	800	B12	C19-C1-N21	2.42	104.64	102.16
3	A	800	B12	C17-C18-C19	-2.38	98.74	102.37
3	A	800	B12	C7B-C6B-C5B	-2.37	115.92	119.91
3	A	800	B12	C36-C7-C37	2.32	114.78	110.83
3	A	800	B12	C4B-C5B-C6B	2.26	123.72	119.91
4	A	801	ADN	C5'-C4'-C3'	2.24	118.05	115.70
3	A	800	B12	C2-C1-C19	-2.20	115.12	118.60
4	A	801	ADN	O3'-C3'-C4'	-2.11	105.30	110.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2P-C1P-N59-C57
3	A	800	B12	C18-C17-C55-C56
3	A	800	B12	C16-C17-C55-C56
3	A	800	B12	C17-C18-C60-C61
3	A	800	B12	C18-C60-C61-O63
3	A	800	B12	C18-C60-C61-N62
3	A	800	B12	C2P-O3-P-O2

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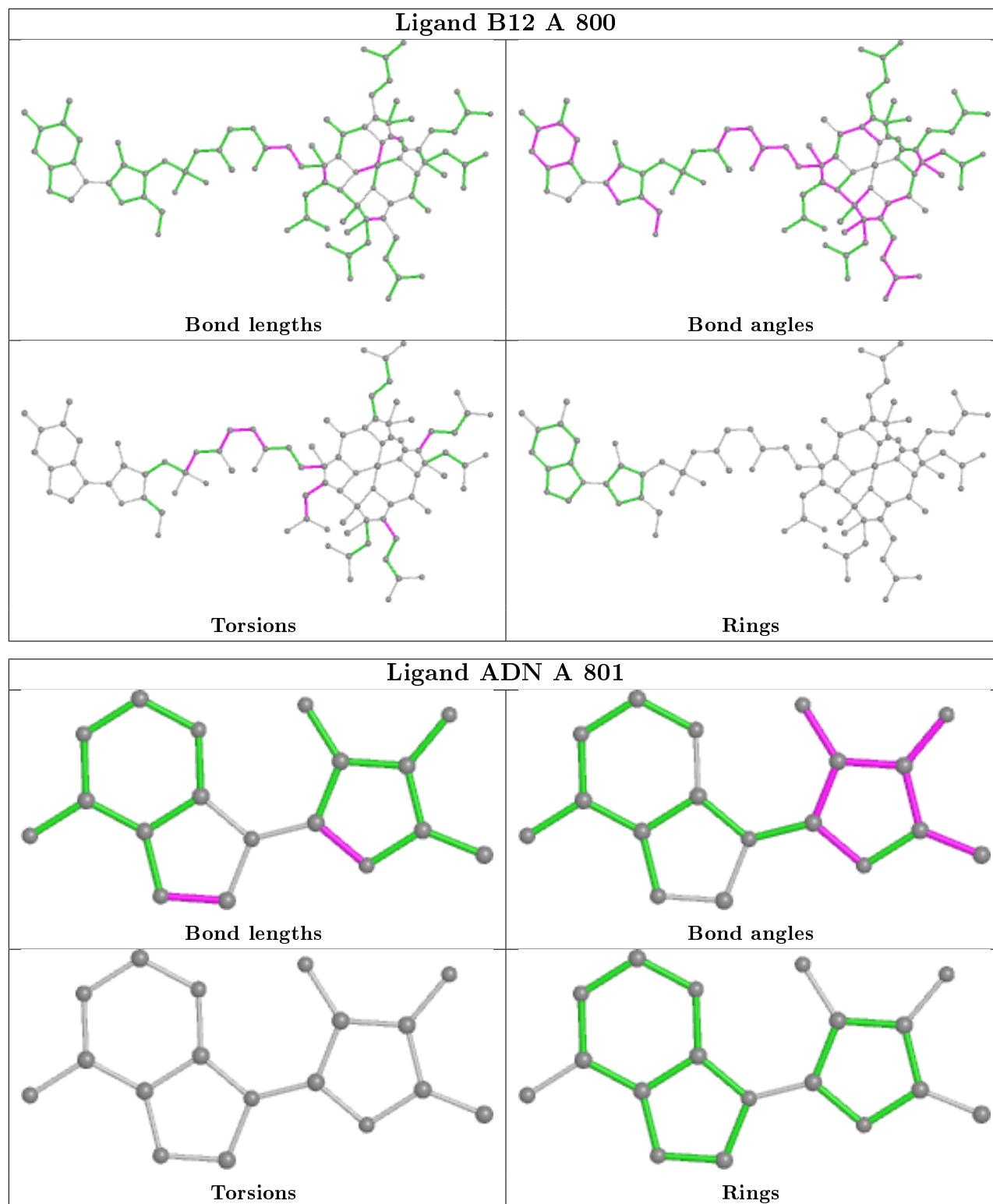
Mol	Chain	Res	Type	Atoms
3	A	800	B12	O58-C57-N59-C1P
3	A	800	B12	C42-C41-C8-C7
3	A	800	B12	N59-C1P-C2P-O3
3	A	800	B12	C42-C41-C8-C9
3	A	800	B12	C2-C3-C30-C31
3	A	800	B12	C56-C57-N59-C1P

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	22	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	725/727 (99%)	0.62	69 (9%)	8 6	27, 71, 94, 102	0
2	B	620/637 (97%)	0.47	36 (5%)	23 22	29, 72, 94, 109	0
All	All	1345/1364 (98%)	0.55	105 (7%)	13 11	27, 71, 94, 109	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ALA	7.1
1	A	161	MET	6.3
1	A	517	TRP	5.4
2	B	311	PHE	5.4
1	A	156	ILE	4.8
1	A	723	ARG	4.4
2	B	581	VAL	4.4
1	A	529	ARG	4.4
2	B	229	PRO	4.3
2	B	183	TYR	4.3
1	A	155	GLY	4.2
1	A	676	GLY	3.9
1	A	727	ASP	3.9
2	B	190	ALA	3.9
1	A	478	LEU	3.9
1	A	483	VAL	3.7
1	A	497	VAL	3.7
1	A	519	ALA	3.6
1	A	111	LYS	3.6
2	B	589	GLY	3.5
1	A	441	ILE	3.4
2	B	258	THR	3.3
2	B	83	LYS	3.3
1	A	505	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	3.3
1	A	101	PHE	3.3
1	A	9	SER	3.2
2	B	235	THR	3.2
1	A	500	ARG	3.2
2	B	271	PHE	3.2
1	A	541	ALA	3.2
2	B	282	PHE	3.1
2	B	161	MET	3.0
2	B	283	ARG	2.9
1	A	484	ASP	2.9
2	B	312	GLY	2.9
1	A	596	ARG	2.8
2	B	217	LEU	2.8
1	A	675	LEU	2.7
1	A	169	GLY	2.7
1	A	544	THR	2.7
1	A	177	LEU	2.7
2	B	426	LEU	2.7
1	A	650	HIS	2.7
1	A	174	ILE	2.6
1	A	279	GLN	2.6
1	A	501	ALA	2.6
2	B	126	LEU	2.6
1	A	210	TYR	2.6
1	A	725	SER	2.6
1	A	728	ALA	2.6
1	A	235	TRP	2.6
1	A	402	PRO	2.6
1	A	108	ALA	2.6
2	B	254	TRP	2.5
1	A	496	LEU	2.5
1	A	281	ALA	2.5
2	B	272	THR	2.5
1	A	4	LEU	2.5
1	A	168	ASN	2.5
1	A	189	PRO	2.5
2	B	146	ALA	2.5
1	A	480	VAL	2.5
1	A	176	ALA	2.4
1	A	575	LYS	2.4
1	A	121	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	122	HIS	2.4
1	A	545	VAL	2.4
1	A	476	PRO	2.4
1	A	590	PHE	2.4
2	B	147	PRO	2.4
2	B	609	ALA	2.4
1	A	720	LYS	2.4
1	A	138	MET	2.3
1	A	638	GLU	2.3
2	B	563	GLN	2.3
2	B	84	LYS	2.3
2	B	216	VAL	2.3
1	A	171	VAL	2.3
2	B	69	GLY	2.3
1	A	551	ALA	2.3
1	A	401	ASP	2.3
2	B	35	TRP	2.2
1	A	563	ILE	2.2
1	A	166	THR	2.2
1	A	137	GLY	2.2
1	A	298	VAL	2.2
2	B	198	GLY	2.2
2	B	255	ALA	2.2
1	A	536	ILE	2.1
2	B	99	VAL	2.1
1	A	7	PHE	2.1
1	A	431	GLY	2.1
1	A	28	LEU	2.1
2	B	317	LYS	2.1
1	A	653	GLY	2.1
1	A	665	VAL	2.0
2	B	236	ILE	2.0
2	B	25	GLY	2.0
1	A	543	ALA	2.0
1	A	593	ALA	2.0
2	B	520	THR	2.0
2	B	572	LYS	2.0
2	B	204	PHE	2.0
1	A	160	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

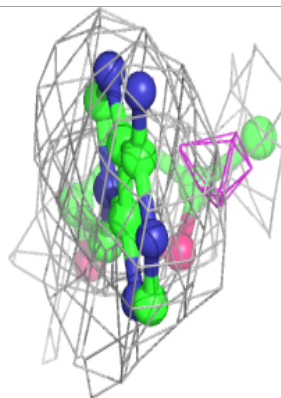
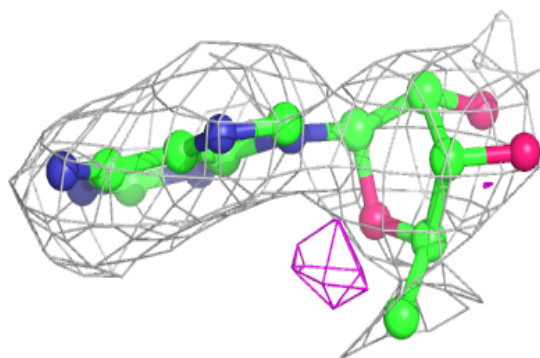
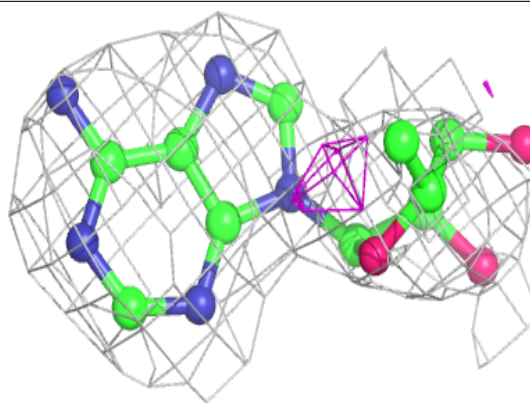
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ADN	A	801	18/19	0.90	0.28	56,79,82,83	0
3	B12	A	800	91/91	0.94	0.19	26,48,67,75	0

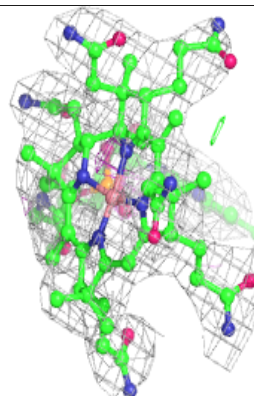
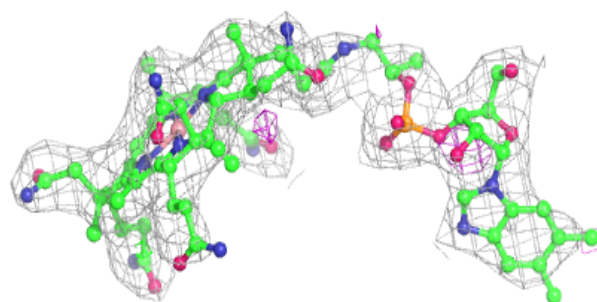
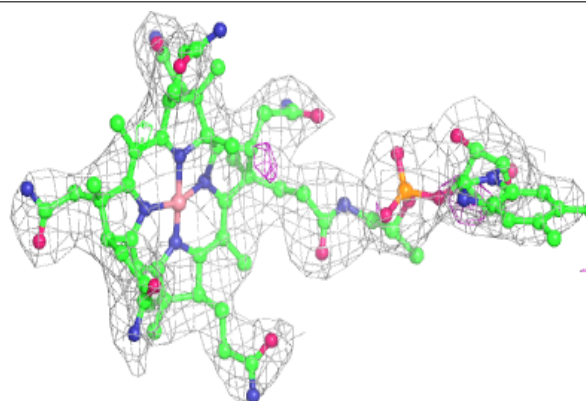
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN A 801:

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

**Electron density around B12 A 800:**

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



6.5 Other polymers

There are no such residues in this entry.