



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:18 pm BST

PDB ID : 1DIO  
Title : DIOL DEHYDRATASE-CYANOCOBALAMIN COMPLEX FROM KLEBSIELLA OXYTOCA  
Authors : Shibata, N.; Masuda, J.; Tobimatsu, T.; Toraya, T.; Suto, K.; Morimoto, Y.; Yasuoka, N.  
Deposited on : 1999-01-27  
Resolution : 2.20 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](mailto: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.

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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

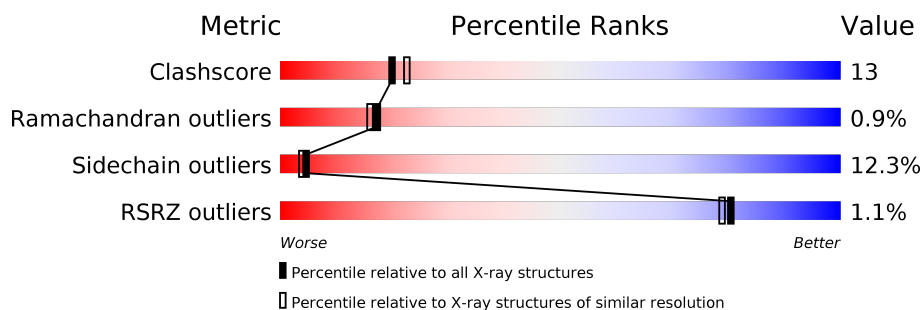
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	554	<div> <div>66%</div> <div>27%</div> <div>6%</div> <div>..</div> </div>
1	L	554	<div> <div>66%</div> <div>27%</div> <div>6%</div> <div>..</div> </div>
2	B	224	<div> <div>52%</div> <div>21%</div> <div>7%</div> <div>20%</div> </div>
2	E	224	<div> <div>5%</div> <div>43%</div> <div>28%</div> <div>6%</div> <div>•</div> <div>20%</div> </div>
3	G	173	<div> <div>45%</div> <div>28%</div> <div>6%</div> <div>•</div> <div>21%</div> </div>
3	M	173	<div> <div>2%</div> <div>51%</div> <div>21%</div> <div>6%</div> <div>•</div> <div>21%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13912 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 PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4201	2620	727	825	29			
1	L	551	Total	C	N	O	S	0	0	0
			4201	2620	727	825	29			

- Molecule 2 is a protein called PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	0	0
			1367	865	245	255	2			
2	E	179	Total	C	N	O	S	0	0	0
			1367	865	245	255	2			

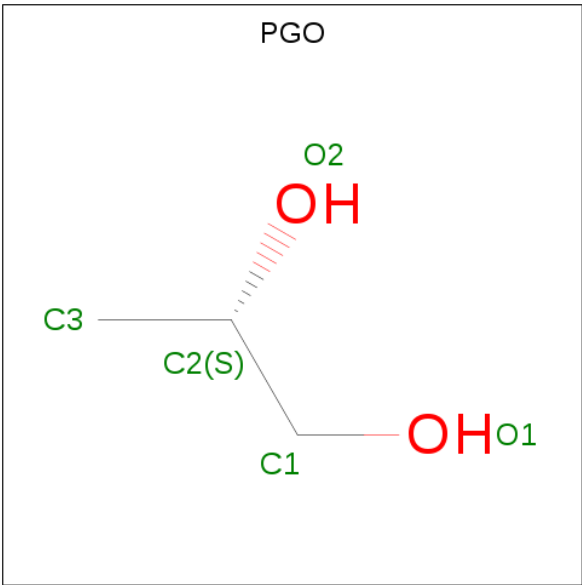
- Molecule 3 is a protein called PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	137	Total	C	N	O	S	0	0	0
			1093	681	195	214	3			
3	M	137	Total	C	N	O	S	0	0	0
			1093	681	195	214	3			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

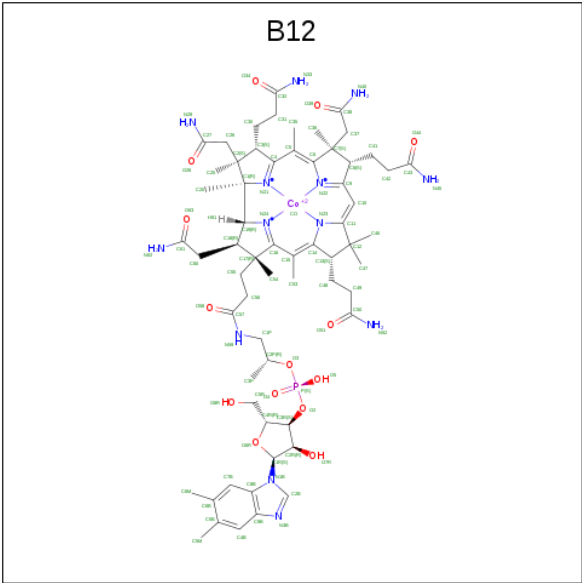
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	L	1	Total	K	0	0
			1	1		

- Molecule 5 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	3	2		
5	L	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

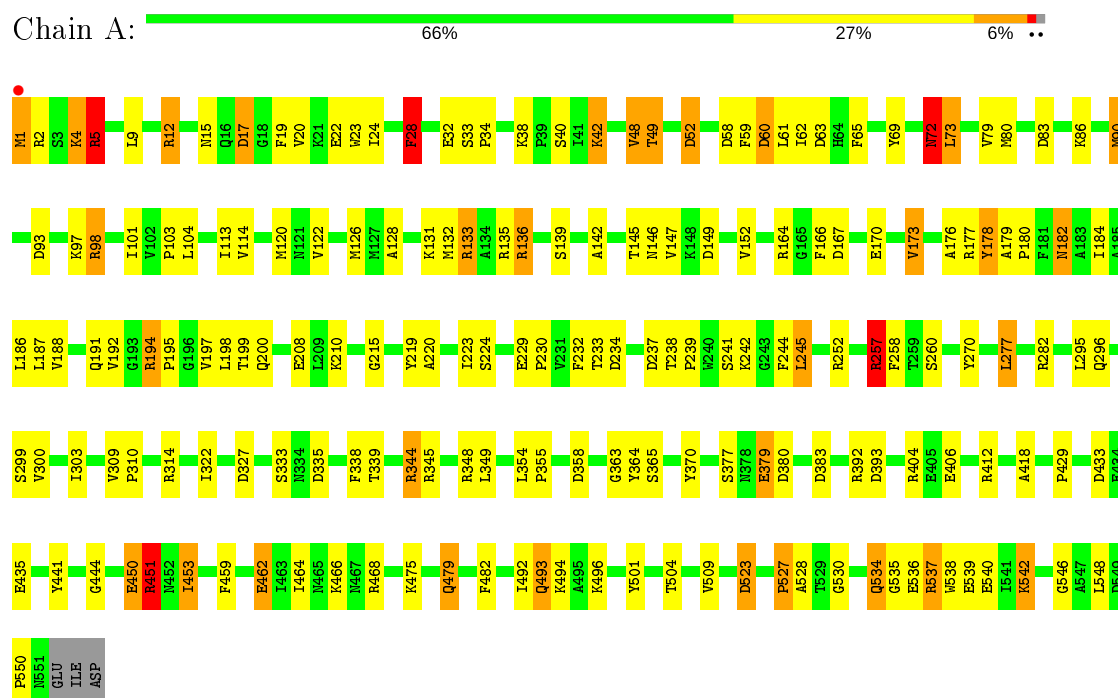
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	144	Total 144	O 144	0	0
7	B	41	Total 41	O 41	0	0
7	G	24	Total 24	O 24	0	0
7	L	150	Total 150	O 150	0	0
7	E	22	Total 22	O 22	0	0
7	M	15	Total 15	O 15	0	0

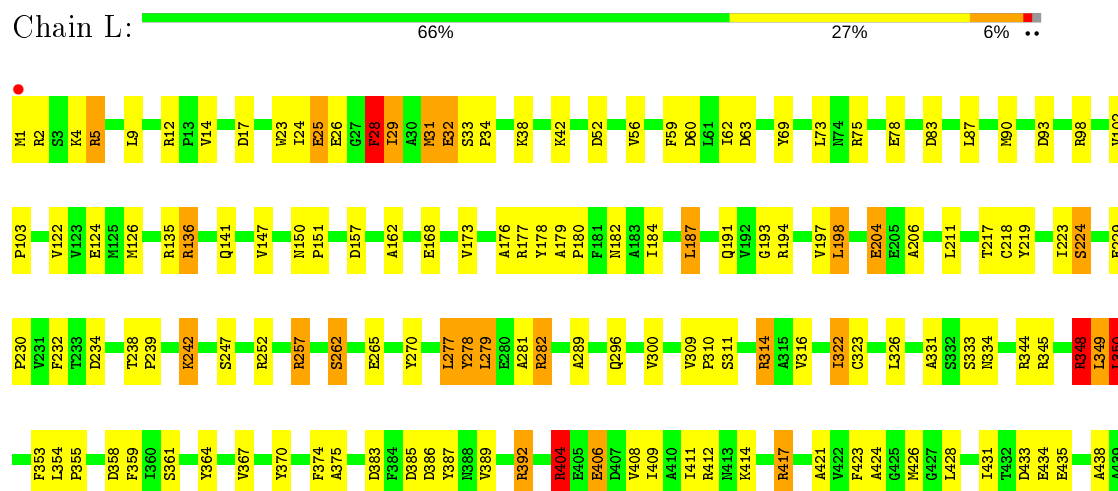
### 3 Residue-property plots

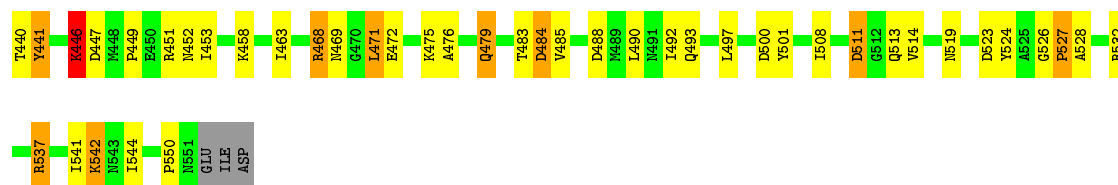
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



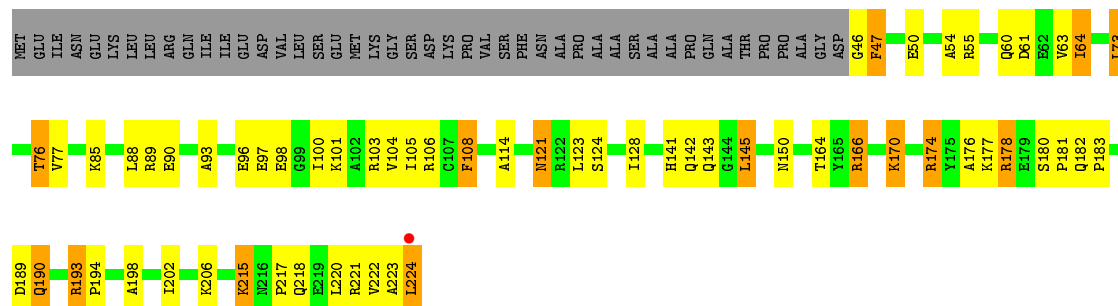
#### • Molecule 1: PROTEIN (DIOL DEHYDRATASE)





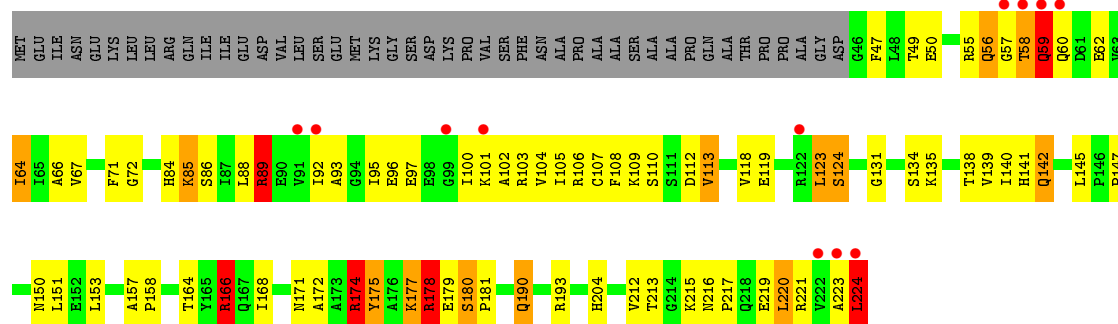
• Molecule 2: PROTEIN (DIOL DEHYDRATASE)

Chain B: 52% 21% 7% 20%



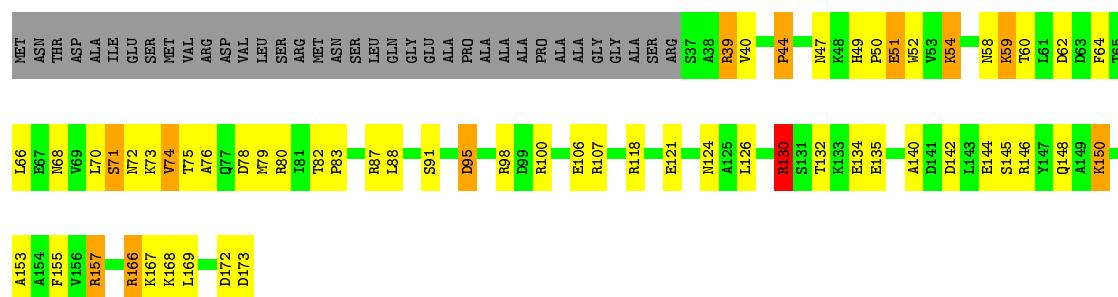
• Molecule 2: PROTEIN (DIOL DEHYDRATASE)

Chain E: 5% 43% 28% 6% 20%

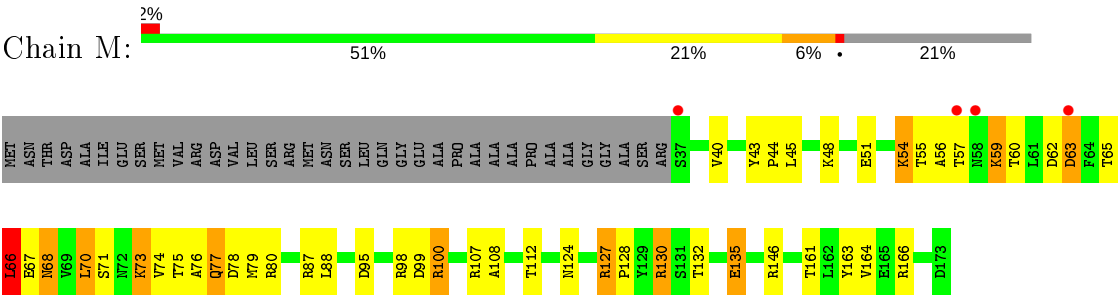


• Molecule 3: PROTEIN (DIOL DEHYDRATASE)

Chain G: 45% 28% 6% 21%



• Molecule 3: PROTEIN (DIOL DEHYDRATASE)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.20Å 122.30Å 209.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 47.46 – 2.17	Depositor EDS
% Data completeness (in resolution range)	83.5 (10.00-2.20) 83.5 (47.46-2.17)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.187 , 0.236 0.170 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGO, K, 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	0.74	0/4273	1.82	87/5787 (1.5%)
1	L	0.69	0/4273	1.67	73/5787 (1.3%)
2	B	0.58	0/1389	1.51	15/1879 (0.8%)
2	E	0.52	0/1389	1.48	13/1879 (0.7%)
3	G	0.62	0/1108	1.77	18/1497 (1.2%)
3	M	0.57	0/1108	1.71	19/1497 (1.3%)
All	All	0.67	0/13540	1.70	225/18326 (1.2%)

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	1	1
1	L	0	1
All	All	1	2

There are no bond length outliers.

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	NE-CZ-NH1	28.38	134.49	120.30
1	A	12	ARG	NE-CZ-NH2	-19.58	110.51	120.30
1	A	537	ARG	NE-CZ-NH2	-18.16	111.22	120.30
3	M	130	ARG	NE-CZ-NH2	-17.85	111.38	120.30
1	A	83	ASP	CB-CG-OD1	16.12	132.81	118.30
1	L	257	ARG	NE-CZ-NH2	-13.65	113.47	120.30
1	A	345	ARG	NE-CZ-NH2	13.62	127.11	120.30
1	L	532	ARG	NE-CZ-NH2	12.81	126.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	28	PHE	CB-CG-CD2	-12.63	111.96	120.80
3	M	98	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	A	257	ARG	NE-CZ-NH2	12.23	126.42	120.30
1	A	344	ARG	NE-CZ-NH2	-12.01	114.29	120.30
3	M	166	ARG	NE-CZ-NH1	12.01	126.31	120.30
1	A	52	ASP	CB-CG-OD1	11.85	128.96	118.30
1	A	28	PHE	CB-CG-CD2	-11.81	112.53	120.80
1	A	344	ARG	NE-CZ-NH1	-11.67	114.47	120.30
1	L	177	ARG	NE-CZ-NH1	11.62	126.11	120.30
3	G	39	ARG	NE-CZ-NH1	11.46	126.03	120.30
3	G	157	ARG	NE-CZ-NH2	-11.45	114.57	120.30
3	G	39	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	A	335	ASP	CB-CG-OD1	11.30	128.47	118.30
3	G	157	ARG	NE-CZ-NH1	11.10	125.85	120.30
3	G	155	PHE	CB-CG-CD1	-10.93	113.15	120.80
3	M	87	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	A	98	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	136	ARG	CD-NE-CZ	10.86	138.80	123.60
1	A	60	ASP	CB-CG-OD1	10.79	128.01	118.30
1	A	344	ARG	NH1-CZ-NH2	10.69	131.16	119.40
1	L	537	ARG	NE-CZ-NH1	-10.45	115.07	120.30
1	L	383	ASP	CB-CG-OD2	10.30	127.57	118.30
1	A	177	ARG	NE-CZ-NH2	-10.25	115.17	120.30
2	B	193	ARG	NE-CZ-NH1	-10.21	115.19	120.30
2	E	193	ARG	CD-NE-CZ	10.20	137.87	123.60
1	L	194	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	136	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	L	392	ARG	NE-CZ-NH2	-9.93	115.33	120.30
2	E	178	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	379	GLU	CA-CB-CG	9.84	135.04	113.40
1	L	12	ARG	NE-CZ-NH1	-9.61	115.49	120.30
1	L	12	ARG	CD-NE-CZ	9.50	136.90	123.60
1	A	135	ARG	NE-CZ-NH1	9.45	125.03	120.30
2	B	47	PHE	N-CA-CB	-9.41	93.67	110.60
2	E	224	LEU	CA-CB-CG	9.34	136.77	115.30
1	A	1	MET	N-CA-CB	9.31	127.36	110.60
2	B	166	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	A	17	ASP	CB-CG-OD1	9.22	126.60	118.30
1	A	60	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	L	278	TYR	CB-CG-CD2	-8.96	115.62	121.00
2	B	174	ARG	NE-CZ-NH1	-8.96	115.82	120.30
3	G	155	PHE	CB-CG-CD2	8.84	126.99	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ASP	CB-CG-OD1	8.84	126.25	118.30
1	L	93	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	A	537	ARG	NH1-CZ-NH2	8.77	129.05	119.40
2	B	178	ARG	CD-NE-CZ	8.65	135.71	123.60
3	G	98	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	A	133	ARG	CG-CD-NE	8.58	129.82	111.80
3	G	173	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	120	MET	CG-SD-CE	8.50	113.80	100.20
2	B	108	PHE	CB-CG-CD1	-8.44	114.89	120.80
1	A	237	ASP	CB-CG-OD1	8.43	125.88	118.30
1	A	412	ARG	CD-NE-CZ	8.42	135.39	123.60
2	E	166	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	L	257	ARG	CD-NE-CZ	8.32	135.25	123.60
1	A	149	ASP	CB-CG-OD2	8.27	125.75	118.30
3	M	66	LEU	CA-CB-CG	8.27	134.31	115.30
1	L	98	ARG	NE-CZ-NH2	-8.25	116.17	120.30
3	M	80	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	A	1	MET	O-C-N	-8.21	109.57	122.70
1	L	532	ARG	CD-NE-CZ	8.20	135.08	123.60
3	M	127	ARG	NE-CZ-NH2	-8.20	116.20	120.30
2	B	47	PHE	N-CA-C	8.17	133.05	111.00
1	A	380	ASP	CB-CG-OD1	8.10	125.59	118.30
1	L	278	TYR	CB-CG-CD1	8.10	125.86	121.00
1	L	345	ARG	NE-CZ-NH2	8.08	124.34	120.30
2	B	189	ASP	CB-CG-OD1	8.07	125.56	118.30
1	A	345	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	L	257	ARG	CA-CB-CG	7.96	130.90	113.40
1	A	28	PHE	CB-CG-CD1	7.83	126.28	120.80
1	L	441	TYR	CB-CG-CD1	7.83	125.70	121.00
3	G	39	ARG	CD-NE-CZ	7.81	134.53	123.60
1	L	441	TYR	CB-CG-CD2	-7.66	116.40	121.00
1	A	164	ARG	CD-NE-CZ	7.64	134.30	123.60
1	L	314	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	L	468	ARG	NE-CZ-NH1	-7.49	116.55	120.30
1	L	386	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	282	ARG	NE-CZ-NH2	-7.37	116.61	120.30
3	G	44	PRO	N-CA-CB	7.36	112.13	103.30
1	L	392	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	G	142	ASP	CB-CG-OD2	7.34	124.91	118.30
1	L	28	PHE	CB-CG-CD1	7.32	125.92	120.80
1	L	523	ASP	CB-CG-OD1	7.27	124.85	118.30
3	M	130	ARG	NH1-CZ-NH2	7.24	127.36	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	135	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	A	393	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	98	ARG	NH1-CZ-NH2	7.18	127.30	119.40
1	A	282	ARG	NE-CZ-NH1	7.17	123.88	120.30
2	E	174	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	A	135	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	32	GLU	OE1-CD-OE2	-7.08	114.81	123.30
1	L	333	SER	CA-C-N	7.05	132.71	117.20
1	L	177	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	L	83	ASP	CB-CG-OD2	-7.02	111.99	118.30
1	L	17	ASP	CB-CG-OD2	7.00	124.60	118.30
3	M	98	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	B	189	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	L	484	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	392	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	L	52	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	468	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	L	5	ARG	CG-CD-NE	-6.88	97.34	111.80
1	A	69	TYR	CB-CG-CD2	6.87	125.12	121.00
1	A	451	ARG	CG-CD-NE	6.80	126.09	111.80
2	B	61	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	L	344	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	L	194	ARG	NH1-CZ-NH2	-6.59	112.15	119.40
1	A	208	GLU	CG-CD-OE2	-6.58	105.14	118.30
3	G	44	PRO	CA-N-CD	-6.58	102.29	111.50
1	L	488	ASP	CB-CG-OD1	6.54	124.19	118.30
3	M	80	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	58	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	L	316	VAL	CA-CB-CG1	6.48	120.62	110.90
1	A	237	ASP	CA-CB-CG	6.44	127.57	113.40
1	A	451	ARG	CD-NE-CZ	-6.43	114.59	123.60
1	A	22	GLU	OE1-CD-OE2	-6.38	115.65	123.30
1	L	361	SER	CB-CA-C	-6.34	98.05	110.10
1	L	282	ARG	CD-NE-CZ	6.33	132.46	123.60
1	L	224	SER	N-CA-CB	-6.29	101.06	110.50
3	M	107	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	164	ARG	NE-CZ-NH1	-6.25	117.17	120.30
2	E	175	TYR	CB-CG-CD2	6.25	124.75	121.00
1	L	5	ARG	CB-CG-CD	6.23	127.81	111.60
1	L	417	ARG	CD-NE-CZ	6.23	132.33	123.60
1	A	19	PHE	CB-CG-CD1	6.22	125.15	120.80
1	A	252	ARG	NE-CZ-NH1	6.17	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	178	ARG	NH1-CZ-NH2	6.15	126.16	119.40
3	G	166	ARG	NE-CZ-NH1	6.14	123.37	120.30
3	M	135	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	A	65	PHE	CB-CG-CD2	6.13	125.09	120.80
1	L	31	MET	CA-CB-CG	6.10	123.67	113.30
2	B	46	GLY	N-CA-C	6.10	128.34	113.10
3	M	95	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	193	ARG	NH1-CZ-NH2	6.09	126.11	119.40
2	E	112	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	451	ARG	CB-CG-CD	6.07	127.37	111.60
1	A	133	ARG	CD-NE-CZ	6.06	132.08	123.60
3	M	127	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	237	ASP	N-CA-CB	5.97	121.35	110.60
1	L	387	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	L	242	LYS	CD-CE-NZ	5.96	125.39	111.70
1	L	262	SER	O-C-N	-5.92	113.13	123.20
1	A	178	TYR	N-CA-CB	-5.90	99.97	110.60
1	L	26	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	412	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	L	194	ARG	CG-CD-NE	5.83	124.05	111.80
1	A	83	ASP	OD1-CG-OD2	-5.82	112.24	123.30
3	M	43	TYR	CB-CG-CD2	-5.79	117.53	121.00
3	M	127	ARG	CD-NE-CZ	5.76	131.67	123.60
1	L	350	LEU	CB-CG-CD1	5.76	120.79	111.00
1	L	83	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	327	ASP	CB-CG-OD1	5.73	123.46	118.30
1	L	52	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	5	ARG	CD-NE-CZ	-5.71	115.60	123.60
1	L	358	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	338	PHE	CB-CG-CD2	-5.69	116.81	120.80
1	L	252	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	L	265	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	L	124	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	L	311	SER	N-CA-CB	5.67	119.01	110.50
3	G	39	ARG	CG-CD-NE	5.67	123.71	111.80
3	G	130	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	L	234	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	48	VAL	O-C-N	-5.62	113.70	122.70
2	B	106	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	M	78	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	L	511	ASP	CA-C-O	5.57	131.79	120.10
2	E	89	ARG	NE-CZ-NH2	-5.57	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	468	ARG	NH1-CZ-NH2	5.55	125.51	119.40
1	A	270	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	244	PHE	CB-CG-CD1	-5.52	116.94	120.80
3	M	163	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	358	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	E	224	LEU	CB-CG-CD1	5.47	120.31	111.00
1	L	277	LEU	CB-CG-CD2	5.47	120.30	111.00
2	B	61	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	383	ASP	CB-CG-OD2	5.44	123.20	118.30
3	M	99	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	345	ARG	CD-NE-CZ	5.38	131.13	123.60
2	B	221	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	G	146	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	208	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	A	468	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	252	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	93	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	136	ARG	CG-CD-NE	-5.31	100.65	111.80
1	A	380	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	L	135	ARG	CD-NE-CZ	5.30	131.03	123.60
1	A	234	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	90	MET	CA-CB-CG	5.25	122.22	113.30
1	L	519	ASN	CB-CG-ND2	5.22	129.22	116.70
2	E	166	ARG	CD-NE-CZ	-5.22	116.30	123.60
1	L	282	ARG	NE-CZ-NH2	-5.21	117.69	120.30
3	G	107	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	72	ASN	CB-CG-ND2	-5.19	104.25	116.70
1	A	296	GLN	O-C-N	5.19	131.00	122.70
3	G	95	ASP	CB-CG-OD2	5.18	122.96	118.30
1	L	252	ARG	CD-NE-CZ	-5.18	116.35	123.60
2	E	113	VAL	CA-CB-CG2	5.17	118.66	110.90
2	E	178	ARG	CG-CD-NE	-5.16	100.97	111.80
1	L	270	TYR	CA-CB-CG	5.15	123.18	113.40
1	L	404	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	65	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	A	244	PHE	CB-CG-CD2	5.13	124.39	120.80
1	L	219	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	L	136	ARG	CD-NE-CZ	-5.11	116.45	123.60
1	L	348	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	393	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	224	SER	N-CA-CB	-5.08	102.88	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	333	SER	CA-C-N	5.06	128.34	117.20
1	L	447	ASP	CB-CG-OD2	5.06	122.85	118.30
1	L	500	ASP	CB-CG-OD1	5.05	122.85	118.30
1	L	383	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	L	451	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	314	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ALA	Mainchain
1	L	322	ILE	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	4201	0	4140	92	0
1	L	4201	0	4140	83	0
2	B	1367	0	1419	43	0
2	E	1367	0	1419	51	0
3	G	1093	0	1101	38	0
3	M	1093	0	1101	33	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	A	5	0	6	1	0
5	L	5	0	5	1	0
6	B	91	0	88	6	0
6	E	91	0	88	9	0
7	A	144	0	0	2	0
7	B	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	22	0	0	3	0
7	G	24	0	0	1	0
7	L	150	0	0	2	0
7	M	15	0	0	0	0
All	All	13912	0	13507	340	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 13.

All (340) 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)
3:M:59:LYS:HE3	3:M:60:THR:H	1.20	1.01
2:B:76:THR:HG22	2:B:77:VAL:HG13	1.39	1.00
2:E:64:ILE:HG13	2:E:124:SER:HB2	1.41	1.00
3:M:59:LYS:HE2	3:M:63:ASP:HB2	1.46	0.93
2:E:179:GLU:O	2:E:180:SER:HB2	1.67	0.91
2:B:190:GLN:HE21	2:B:190:GLN:H	1.23	0.83
6:B:601:B12:H1R	7:B:630:HOH:O	1.78	0.81
2:B:128:ILE:HD13	2:B:176:ALA:HA	1.61	0.81
2:E:72:GLY:H	2:E:84:HIS:HD2	1.34	0.75
1:L:475:LYS:HG2	3:M:70:LEU:HD12	1.70	0.73
1:A:462:GLU:HG3	1:A:466:LYS:HD3	1.70	0.72
1:A:441:TYR:HE1	1:L:1:MET:HG3	1.53	0.72
3:G:54:LYS:HD2	3:G:58:ASN:HD21	1.55	0.72
1:A:98:ARG:HG3	1:A:132:MET:HE2	1.74	0.69
1:A:180:PRO:HG3	1:A:464:ILE:HD11	1.73	0.69
1:A:475:LYS:HD3	3:G:70:LEU:HD23	1.74	0.69
1:A:182:ASN:HD22	1:A:182:ASN:N	1.91	0.69
3:G:132:THR:OG1	3:G:135:GLU:HG3	1.93	0.69
2:E:72:GLY:H	2:E:84:HIS:CD2	2.10	0.69
1:L:484:ASP:OD1	1:L:485:VAL:HG23	1.93	0.69
2:B:47:PHE:HB2	2:B:223:ALA:HB3	1.76	0.68
1:A:23:TRP:HB2	1:L:550:PRO:HG3	1.75	0.68
1:A:131:LYS:HG2	1:A:132:MET:HE3	1.75	0.68
1:A:475:LYS:O	1:A:479:GLN:HG2	1.94	0.67
2:B:121:ASN:C	2:B:121:ASN:HD22	1.98	0.67
2:E:190:GLN:H	2:E:190:GLN:HE21	1.42	0.67
3:M:55:THR:HG22	3:M:57:THR:H	1.60	0.67
1:L:426:MET:HB2	1:L:428:LEU:HG	1.77	0.66
1:A:182:ASN:HD22	1:A:182:ASN:H	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:95:ILE:HG21	2:E:102:ALA:HB2	1.77	0.66
1:L:309:VAL:HB	1:L:310:PRO:HD2	1.78	0.66
1:A:534:GLN:HG2	1:A:535:GLY:N	2.11	0.66
3:G:134:GLU:H	3:G:134:GLU:CD	1.99	0.66
1:L:198:LEU:HD11	1:L:508:ILE:HD12	1.77	0.66
2:E:177:LYS:O	2:E:178:ARG:HB2	1.96	0.65
2:E:142:GLN:HG3	2:E:145:LEU:HD22	1.78	0.65
3:G:60:THR:HG22	3:G:62:ASP:H	1.60	0.65
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.77	0.65
2:E:58:THR:O	2:E:59:GLN:HB3	1.96	0.65
1:A:98:ARG:HA	1:A:132:MET:HE1	1.79	0.64
1:L:404:ARG:HG3	7:L:688:HOH:O	1.95	0.64
2:E:47:PHE:HA	2:E:223:ALA:HB2	1.79	0.64
1:L:173:VAL:HG12	1:L:182:ASN:ND2	2.11	0.64
1:A:441:TYR:CE1	1:L:1:MET:HG3	2.33	0.64
2:E:100:ILE:HD11	2:E:177:LYS:CD	2.28	0.64
2:B:104:VAL:HG12	2:B:220:LEU:HD12	1.79	0.64
3:G:153:ALA:O	3:G:157:ARG:HB2	1.98	0.64
2:E:223:ALA:O	2:E:224:LEU:HD13	1.98	0.63
1:A:114:VAL:HG13	1:A:277:LEU:HD13	1.79	0.63
1:L:23:TRP:HB3	1:L:28:PHE:HB2	1.80	0.63
1:A:494:LYS:HD3	3:G:64:PHE:HB2	1.80	0.63
2:B:141:HIS:HE1	2:B:145:LEU:HB3	1.64	0.62
1:A:23:TRP:HB3	1:A:28:PHE:HB2	1.80	0.62
2:E:103:ARG:HD2	2:E:219:GLU:OE2	1.99	0.62
2:E:47:PHE:HB2	2:E:223:ALA:HB3	1.82	0.62
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.80	0.62
3:G:54:LYS:HD2	3:G:58:ASN:ND2	2.14	0.62
2:E:174:ARG:HG2	2:E:181:PRO:HB3	1.81	0.62
3:M:59:LYS:HE2	3:M:63:ASP:CB	2.25	0.62
6:B:601:B12:H351	6:B:601:B12:H362	1.82	0.61
1:L:180:PRO:O	1:L:184:ILE:HD12	1.99	0.61
3:M:59:LYS:CE	3:M:63:ASP:HB2	2.25	0.61
6:E:601:B12:H492	6:E:601:B12:C2B	2.30	0.61
2:E:113:VAL:HG12	7:E:613:HOH:O	1.99	0.60
1:L:87:LEU:HA	1:L:90:MET:HE3	1.82	0.60
2:B:121:ASN:O	2:B:143:GLN:HG3	2.01	0.60
2:B:174:ARG:HB2	2:B:181:PRO:HG3	1.83	0.60
1:A:48:VAL:CG2	1:A:73:LEU:HD11	2.32	0.60
3:M:100:ARG:H	3:M:100:ARG:HE	1.49	0.60
1:L:409:ILE:HG23	1:L:440:THR:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:179:GLU:O	2:E:180:SER:CB	2.47	0.59
1:A:238:THR:HB	1:A:239:PRO:HD2	1.83	0.59
1:L:204:GLU:OE2	1:L:206:ALA:N	2.35	0.59
3:M:75:THR:HG22	3:M:76:ALA:N	2.18	0.59
2:B:50:GLU:HG2	2:B:218:GLN:HB3	1.83	0.59
2:B:142:GLN:O	2:B:145:LEU:HB2	2.02	0.59
1:A:538:TRP:CE2	1:A:542:LYS:HD2	2.37	0.59
3:M:60:THR:OG1	3:M:62:ASP:HB2	2.03	0.59
6:E:601:B12:H1R	7:E:618:HOH:O	2.03	0.59
3:G:118:ARG:NH1	3:G:121:GLU:OE1	2.35	0.58
1:L:475:LYS:HG2	3:M:70:LEU:CD1	2.33	0.58
2:E:67:VAL:HG13	2:E:71:PHE:HB3	1.85	0.58
3:G:60:THR:HG22	3:G:62:ASP:N	2.18	0.58
3:G:71:SER:OG	3:G:73:LYS:HE2	2.04	0.58
2:E:100:ILE:HD11	2:E:177:LYS:HD2	1.85	0.57
1:L:513:GLN:NE2	1:L:514:VAL:O	2.37	0.57
3:M:68:ASN:HB3	3:M:73:LYS:HD2	1.85	0.57
3:G:144:GLU:O	3:G:148:GLN:HA	2.04	0.57
1:A:435:GLU:OE2	1:A:451:ARG:HD2	2.05	0.57
1:A:131:LYS:HG2	1:A:132:MET:CE	2.34	0.56
1:A:220:ALA:HB1	1:A:223:ILE:HD11	1.88	0.56
1:A:527:PRO:O	1:A:528:ALA:HB3	2.05	0.56
3:G:87:ARG:NH1	7:G:185:HOH:O	2.39	0.55
2:E:66:ALA:O	2:E:131:GLY:HA2	2.07	0.55
1:A:86:LYS:O	1:A:90:MET:HG3	2.06	0.55
2:B:93:ALA:O	2:B:97:GLU:HG3	2.06	0.55
6:E:601:B12:H362	6:E:601:B12:H351	1.87	0.55
1:A:132:MET:HE2	1:A:132:MET:HA	1.88	0.55
1:A:229:GLU:N	1:A:230:PRO:HD2	2.22	0.55
1:A:132:MET:O	1:A:133:ARG:C	2.46	0.54
2:E:177:LYS:O	2:E:178:ARG:CB	2.53	0.54
1:L:31:MET:HG3	1:L:32:GLU:HG2	1.88	0.54
2:B:64:ILE:HG13	2:B:124:SER:HB2	1.88	0.54
3:G:74:VAL:HA	3:G:78:ASP:OD2	2.08	0.54
2:B:190:GLN:NE2	2:B:190:GLN:H	2.01	0.54
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.89	0.54
1:A:9:LEU:O	1:A:12:ARG:HB2	2.08	0.54
2:E:157:ALA:N	2:E:158:PRO:HD2	2.23	0.54
2:E:97:GLU:OE2	2:E:166:ARG:NH2	2.41	0.54
2:E:85:LYS:O	2:E:89:ARG:HB2	2.07	0.54
1:A:122:VAL:O	1:A:126:MET:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:VAL:HG23	2:B:100:ILE:HG21	1.89	0.53
2:B:198:ALA:O	2:B:202:ILE:HD12	2.08	0.53
1:L:370:TYR:CE1	1:L:446:LYS:HD3	2.43	0.53
3:G:68:ASN:HA	3:G:73:LYS:HE3	1.90	0.53
2:E:100:ILE:HD11	2:E:177:LYS:HD3	1.90	0.53
1:L:421:ALA:O	1:L:424:ALA:HB3	2.09	0.53
1:L:334:ASN:ND2	1:L:348:ARG:HD3	2.22	0.53
6:B:601:B12:C2B	6:B:601:B12:H492	2.39	0.53
3:M:68:ASN:HB3	3:M:73:LYS:CD	2.39	0.53
3:G:145:SER:HA	3:G:148:GLN:NE2	2.23	0.52
3:G:64:PHE:CE1	3:G:79:MET:HG2	2.45	0.52
2:B:47:PHE:H	2:B:47:PHE:HD1	1.58	0.52
3:G:49:HIS:N	3:G:50:PRO:HD3	2.25	0.52
3:M:75:THR:HG22	3:M:77:GLN:H	1.75	0.52
2:E:140:ILE:O	2:E:151:LEU:HB2	2.09	0.52
3:G:140:ALA:HB1	3:G:157:ARG:HD3	1.91	0.52
1:A:365:SER:HB2	1:A:377:SER:HB3	1.93	0.51
2:E:84:HIS:HE1	2:E:134:SER:O	1.94	0.51
1:L:468:ARG:NH2	1:L:472:GLU:OE1	2.35	0.51
1:L:238:THR:HB	1:L:239:PRO:HD2	1.92	0.51
1:L:331:ALA:HA	1:L:359:PHE:HB2	1.93	0.51
1:L:404:ARG:NH1	1:L:406:GLU:OE1	2.43	0.51
3:M:124:ASN:O	3:M:130:ARG:HG3	2.11	0.51
1:L:223:ILE:CG2	1:L:242:LYS:HE2	2.41	0.51
2:E:96:GLU:HA	2:E:100:ILE:O	2.11	0.50
3:G:75:THR:HG22	3:G:76:ALA:N	2.26	0.50
1:A:450:GLU:OE1	1:A:450:GLU:HA	2.11	0.50
1:A:61:LEU:HG	3:G:166:ARG:HG3	1.94	0.50
2:E:212:VAL:HG11	2:E:215:LYS:HG3	1.93	0.50
1:L:354:LEU:HB2	1:L:355:PRO:HD3	1.94	0.50
3:M:59:LYS:HE3	3:M:60:THR:N	2.05	0.50
2:B:193:ARG:HB3	2:B:194:PRO:HD3	1.94	0.50
1:L:322:ILE:O	1:L:323:CYS:C	2.50	0.50
2:B:222:VAL:HG12	2:B:223:ALA:H	1.78	0.49
2:B:89:ARG:HH11	2:B:90:GLU:HG2	1.77	0.49
1:A:260:SER:OG	1:A:295:LEU:HD11	2.12	0.49
3:G:124:ASN:O	3:G:130:ARG:HG2	2.11	0.49
1:A:233:THR:OG1	3:G:168:LYS:HE3	2.11	0.49
1:L:309:VAL:HB	1:L:310:PRO:CD	2.42	0.49
1:L:204:GLU:OE2	1:L:206:ALA:HB3	2.13	0.49
1:A:188:VAL:O	1:A:192:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ILE:HD11	2:B:183:PRO:HD2	1.95	0.49
2:B:114:ALA:HB2	6:B:601:B12:HM62	1.94	0.49
2:E:104:VAL:HG12	2:E:220:LEU:HD12	1.94	0.49
2:E:93:ALA:O	2:E:97:GLU:HG3	2.13	0.49
1:L:469:ASN:OD1	1:L:471:LEU:HB2	2.13	0.49
1:A:12:ARG:HD3	1:A:12:ARG:HA	1.68	0.48
1:A:418:ALA:HA	1:A:482:PHE:CE2	2.48	0.48
1:A:170:GLU:OE2	5:A:602:PGO:O1	2.30	0.48
2:E:153:LEU:HD13	6:E:601:B12:HM63	1.95	0.48
3:M:66:LEU:O	3:M:70:LEU:HB2	2.14	0.48
1:A:113:ILE:HD13	1:A:322:ILE:HG23	1.96	0.48
2:B:105:ILE:HD12	2:B:217:PRO:HB3	1.95	0.48
3:M:127:ARG:HB3	3:M:128:PRO:HD2	1.95	0.48
1:A:5:ARG:HD2	1:A:5:ARG:HH11	1.53	0.48
2:B:108:PHE:HB2	2:B:215:LYS:HB3	1.96	0.48
2:E:71:PHE:CE1	2:E:84:HIS:HB3	2.48	0.48
1:A:4:LYS:HG3	1:L:441:TYR:O	2.14	0.48
2:B:141:HIS:CE1	2:B:145:LEU:HB3	2.47	0.48
1:L:229:GLU:N	1:L:230:PRO:CD	2.77	0.48
1:L:484:ASP:OD1	1:L:485:VAL:N	2.47	0.48
3:M:55:THR:HG22	3:M:56:ALA:N	2.28	0.47
2:E:123:LEU:HD11	2:E:217:PRO:HG2	1.95	0.47
1:L:354:LEU:N	1:L:355:PRO:HD2	2.29	0.47
1:L:423:PHE:HA	1:L:428:LEU:HD12	1.97	0.47
2:B:108:PHE:CG	2:B:215:LYS:HD2	2.50	0.47
3:G:44:PRO:HG2	3:G:47:ASN:OD1	2.14	0.47
3:G:51:GLU:HG3	3:G:51:GLU:H	1.33	0.47
1:L:392:ARG:HG3	1:L:542:LYS:HA	1.95	0.47
1:L:24:ILE:HG22	1:L:25:GLU:OE1	2.15	0.47
1:L:122:VAL:O	1:L:126:MET:HG3	2.15	0.47
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.97	0.47
2:B:89:ARG:NH1	2:B:90:GLU:OE2	2.46	0.47
3:G:71:SER:O	3:G:72:ASN:HB2	2.14	0.47
1:A:180:PRO:O	1:A:184:ILE:HD12	2.15	0.46
1:A:242:LYS:HE3	1:A:245:LEU:HD12	1.97	0.46
3:M:132:THR:OG1	3:M:135:GLU:HG3	2.15	0.46
3:G:54:LYS:O	3:G:82:THR:HG23	2.15	0.46
1:A:537:ARG:NH1	1:A:540:GLU:OE1	2.49	0.46
2:B:98:GLU:HG3	2:B:177:LYS:HZ1	1.80	0.46
1:L:296:GLN:HE22	5:L:602:PGO:H12	1.79	0.46
1:A:229:GLU:N	1:A:230:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:HA	1:A:537:ARG:HD2	1.64	0.46
1:A:170:GLU:HA	1:A:200:GLN:HG3	1.98	0.46
2:E:47:PHE:HB2	2:E:223:ALA:CB	2.45	0.46
2:E:172:ALA:O	2:E:175:TYR:HB2	2.15	0.46
6:E:601:B12:C11	6:E:601:B12:H491	2.46	0.46
2:E:177:LYS:HA	2:E:177:LYS:HE3	1.98	0.46
6:E:601:B12:H601	6:E:601:B12:H261	1.97	0.46
1:L:136:ARG:HD3	1:L:136:ARG:HH11	1.50	0.46
1:L:408:VAL:O	1:L:411:ILE:HG22	2.16	0.46
3:M:44:PRO:O	3:M:48:LYS:HG2	2.16	0.46
2:E:138:THR:HG21	2:E:168:ILE:HD13	1.98	0.45
2:E:171:ASN:ND2	2:E:181:PRO:HB2	2.30	0.45
1:A:200:GLN:HG2	1:A:219:TYR:CZ	2.51	0.45
1:A:546:GLY:O	1:A:548:LEU:HG	2.16	0.45
1:L:23:TRP:HB3	1:L:28:PHE:CB	2.46	0.45
1:A:40:SER:H	1:A:52:ASP:HA	1.80	0.45
2:E:64:ILE:HD11	2:E:103:ARG:NH2	2.31	0.45
1:L:162:ALA:HB3	1:L:193:GLY:HA3	1.99	0.45
1:L:60:ASP:OD1	1:L:62:ILE:N	2.50	0.45
3:M:55:THR:HB	3:M:59:LYS:H	1.81	0.45
2:B:182:GLN:HG3	2:B:183:PRO:HD2	1.99	0.45
3:G:140:ALA:CB	3:G:157:ARG:HD3	2.47	0.45
3:M:68:ASN:HB3	3:M:73:LYS:HG2	1.98	0.45
1:L:56:VAL:HA	1:L:59:PHE:CD1	2.52	0.45
1:L:314:ARG:HH11	1:L:314:ARG:HD3	1.60	0.45
3:M:124:ASN:HA	3:M:127:ARG:HG3	1.98	0.45
1:A:17:ASP:OD2	1:A:339:THR:OG1	2.18	0.45
1:L:141:GLN:HB2	1:L:168:GLU:HB2	1.99	0.45
1:A:309:VAL:HB	1:A:310:PRO:HD2	1.98	0.44
1:A:42:LYS:HB3	1:A:49:THR:HG22	1.99	0.44
2:B:73:LEU:HD12	2:B:73:LEU:HA	1.86	0.44
1:A:23:TRP:CE3	1:L:550:PRO:HB2	2.52	0.44
1:A:194:ARG:HB3	1:A:197:VAL:HG23	1.99	0.44
1:L:476:ALA:O	1:L:479:GLN:HG3	2.18	0.44
2:E:135:LYS:HG2	7:E:615:HOH:O	2.18	0.44
1:L:4:LYS:HB2	1:L:4:LYS:HE3	1.57	0.44
3:M:108:ALA:O	3:M:112:THR:HG23	2.18	0.44
1:A:191:GLN:OE1	1:A:195:PRO:HA	2.18	0.44
6:E:601:B12:O7R	6:E:601:B12:C2B	2.66	0.44
3:M:55:THR:HG21	3:M:57:THR:HB	1.99	0.44
2:B:222:VAL:HG12	2:B:223:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PHE:CD1	2:B:47:PHE:N	2.85	0.44
3:M:100:ARG:NE	3:M:100:ARG:H	2.15	0.44
1:A:339:THR:HG21	1:A:344:ARG:HB3	1.99	0.44
1:L:431:ILE:HA	1:L:435:GLU:OE1	2.17	0.44
1:A:182:ASN:ND2	1:A:182:ASN:N	2.63	0.44
3:M:54:LYS:HB2	3:M:59:LYS:O	2.17	0.44
1:A:80:MET:HE2	7:A:729:HOH:O	2.16	0.43
1:L:157:ASP:OD1	1:L:412:ARG:NH1	2.39	0.43
1:A:145:THR:O	1:A:146:ASN:HB3	2.18	0.43
2:E:135:LYS:HE2	2:E:204:HIS:HB2	1.99	0.43
1:L:223:ILE:HG23	1:L:242:LYS:HE2	1.99	0.43
1:L:374:PHE:O	1:L:375:ALA:HB3	2.18	0.43
3:M:75:THR:CG2	3:M:76:ALA:N	2.80	0.43
1:L:198:LEU:CD1	1:L:508:ILE:HD12	2.47	0.43
3:M:55:THR:CG2	3:M:57:THR:HB	2.49	0.43
3:M:127:ARG:HB3	3:M:128:PRO:CD	2.48	0.43
1:A:257:ARG:HG3	1:A:258:PHE:O	2.18	0.43
1:A:435:GLU:HG2	7:A:619:HOH:O	2.17	0.43
2:B:128:ILE:HD13	2:B:176:ALA:CA	2.40	0.43
2:B:224:LEU:N	2:B:224:LEU:HD12	2.33	0.43
1:L:238:THR:HB	1:L:239:PRO:CD	2.49	0.43
2:E:118:VAL:HG21	2:E:147:PRO:HB3	1.99	0.43
1:A:98:ARG:CG	1:A:132:MET:HE2	2.47	0.43
1:A:142:ALA:HB2	1:A:166:PHE:CD1	2.54	0.43
6:B:601:B12:H533	6:B:601:B12:H481	2.01	0.43
2:B:97:GLU:OE1	2:B:170:LYS:NZ	2.47	0.43
1:A:139:SER:OG	1:A:167:ASP:OD2	2.30	0.43
1:L:102:VAL:HB	1:L:103:PRO:HD3	2.00	0.43
1:L:187:LEU:O	1:L:191:GLN:HG2	2.19	0.43
1:A:299:SER:OG	1:A:303:ILE:HA	2.18	0.42
1:L:279:LEU:HA	1:L:279:LEU:HD12	1.83	0.42
1:A:59:PHE:HB3	1:A:63:ASP:HB2	2.01	0.42
2:E:106:ARG:O	2:E:217:PRO:HA	2.19	0.42
3:G:169:LEU:O	3:G:172:ASP:HB2	2.19	0.42
1:L:537:ARG:O	1:L:541:ILE:HG13	2.18	0.42
1:A:60:ASP:OD1	1:A:62:ILE:HB	2.19	0.42
1:A:97:LYS:O	1:A:101:ILE:HD12	2.19	0.42
2:B:88:LEU:HA	2:B:88:LEU:HD12	1.86	0.42
1:L:278:TYR:O	1:L:281:ALA:HB3	2.19	0.42
1:A:536:GLU:H	1:A:536:GLU:CD	2.21	0.42
2:B:89:ARG:HH11	2:B:90:GLU:CG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLY:O	1:A:493:GLN:NE2	2.52	0.42
2:E:62:GLU:CD	2:E:103:ARG:HE	2.22	0.42
1:L:385:ASP:O	1:L:389:VAL:HG13	2.19	0.42
3:M:161:THR:O	3:M:164:VAL:HB	2.20	0.42
2:E:88:LEU:O	2:E:92:ILE:HD12	2.19	0.42
3:G:66:LEU:HD12	3:G:66:LEU:HA	1.84	0.42
1:L:282:ARG:HD2	7:L:620:HOH:O	2.19	0.42
2:B:224:LEU:H	2:B:224:LEU:HD12	1.83	0.42
2:E:107:CYS:HB3	2:E:119:GLU:OE1	2.20	0.42
1:L:463:ILE:HG12	1:L:463:ILE:H	1.70	0.42
1:A:418:ALA:HA	1:A:482:PHE:CD2	2.55	0.42
2:E:105:ILE:HD12	2:E:217:PRO:HB3	2.01	0.42
1:L:179:ALA:HB3	1:L:180:PRO:HD3	2.02	0.42
1:A:132:MET:CE	1:A:132:MET:HA	2.49	0.42
2:B:103:ARG:HD2	2:B:103:ARG:HH11	1.63	0.42
1:L:438:ALA:CB	1:L:449:PRO:HD3	2.50	0.42
1:A:539:GLU:OE2	1:A:542:LYS:NZ	2.52	0.41
3:G:83:PRO:O	3:G:87:ARG:HG3	2.20	0.41
1:L:162:ALA:HB1	1:L:197:VAL:HG21	2.01	0.41
1:A:33:SER:HA	1:A:34:PRO:HD2	1.78	0.41
1:A:370:TYR:OH	1:A:444:GLY:HA3	2.20	0.41
2:B:105:ILE:O	2:B:105:ILE:HG13	2.19	0.41
1:L:349:LEU:HD22	1:L:353:PHE:HB2	2.03	0.41
1:A:523:ASP:OD1	1:A:530:GLY:HA2	2.20	0.41
2:B:54:ALA:HB3	2:B:123:LEU:HD13	2.00	0.41
6:E:601:B12:H202	6:E:601:B12:N3B	2.36	0.41
1:L:414:LYS:HA	1:L:417:ARG:NH2	2.35	0.41
1:L:75:ARG:HH21	1:L:78:GLU:CD	2.24	0.41
2:E:106:ARG:HD2	2:E:108:PHE:CE2	2.54	0.41
1:L:350:LEU:HA	1:L:353:PHE:HB3	2.03	0.41
1:A:241:SER:O	1:A:245:LEU:HB2	2.21	0.41
1:A:550:PRO:HG2	1:L:23:TRP:HB2	2.02	0.41
2:B:100:ILE:HD11	2:B:177:LYS:CG	2.50	0.41
1:A:142:ALA:HB2	1:A:166:PHE:CG	2.55	0.41
1:A:186:LEU:CD2	1:A:199:THR:HB	2.50	0.41
6:B:601:B12:C35	6:B:601:B12:H362	2.48	0.41
3:G:49:HIS:HB3	3:G:52:TRP:CG	2.55	0.41
1:L:524:TYR:CZ	1:L:526:GLY:HA2	2.55	0.41
3:G:150:LYS:HB2	3:G:150:LYS:NZ	2.35	0.41
3:G:54:LYS:HB2	3:G:54:LYS:HE2	1.63	0.41
3:G:40:VAL:HG13	3:G:95:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:59:LYS:NZ	3:G:59:LYS:HB3	2.36	0.41
1:L:229:GLU:HB3	1:L:230:PRO:HD3	2.03	0.41
1:A:12:ARG:HB2	1:A:15:ASN:HD22	1.86	0.41
1:A:493:GLN:HE21	1:A:496:LYS:HZ2	1.69	0.41
2:B:98:GLU:HG3	2:B:177:LYS:NZ	2.36	0.41
2:E:108:PHE:CD1	2:E:215:LYS:HD2	2.56	0.41
6:E:601:B12:H362	6:E:601:B12:C35	2.50	0.41
1:L:354:LEU:N	1:L:355:PRO:CD	2.83	0.41
1:A:23:TRP:HB3	1:A:28:PHE:CB	2.47	0.41
1:A:429:PRO:HD3	1:A:459:PHE:CG	2.56	0.41
3:G:75:THR:O	3:G:78:ASP:HB2	2.21	0.41
1:L:392:ARG:HD2	1:L:544:ILE:HG12	2.03	0.41
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.88	0.40
2:E:113:VAL:HG22	2:E:139:VAL:HG12	2.02	0.40
1:L:150:ASN:HA	1:L:151:PRO:HD3	1.96	0.40
1:L:33:SER:HA	1:L:34:PRO:HD2	1.73	0.40
3:M:51:GLU:O	3:M:54:LYS:HE3	2.22	0.40
1:A:79:VAL:HG22	1:A:104:LEU:HD22	2.04	0.40
1:L:63:ASP:OD1	1:L:282:ARG:NH1	2.54	0.40
1:A:354:LEU:N	1:A:355:PRO:HD2	2.36	0.40
1:A:534:GLN:CG	1:A:535:GLY:N	2.83	0.40
3:G:70:LEU:HA	3:G:70:LEU:HD23	1.86	0.40
1:L:527:PRO:O	1:L:528:ALA:HB3	2.21	0.40
3:M:65:THR:HB	3:M:68:ASN:ND2	2.37	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	549/554 (99%)	512 (93%)	33 (6%)	4 (1%)	22 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	549/554 (99%)	508 (92%)	37 (7%)	4 (1%)	22	22
2	B	177/224 (79%)	171 (97%)	6 (3%)	0	100	100
2	E	177/224 (79%)	155 (88%)	16 (9%)	6 (3%)	3	1
3	G	135/173 (78%)	130 (96%)	5 (4%)	0	100	100
3	M	135/173 (78%)	128 (95%)	6 (4%)	1 (1%)	22	22
All	All	1722/1902 (90%)	1604 (93%)	103 (6%)	15 (1%)	17	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	180	SER
1	L	2	ARG
1	L	446	LYS
2	E	59	GLN
2	E	178	ARG
1	A	72	ASN
2	E	56	GLN
1	A	300	VAL
1	A	504	THR
1	L	300	VAL
2	E	123	LEU
3	M	67	GLU
2	E	57	GLY
1	A	363	GLY
1	L	29	ILE

### 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	450/453 (99%)	405 (90%)	45 (10%)	7	7
1	L	450/453 (99%)	400 (89%)	50 (11%)	6	5
2	B	147/183 (80%)	127 (86%)	20 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	147/183 (80%)	118 (80%)	29 (20%)	1	1
3	G	116/141 (82%)	101 (87%)	15 (13%)	4	3
3	M	116/141 (82%)	100 (86%)	16 (14%)	3	3
All	All	1426/1554 (92%)	1251 (88%)	175 (12%)	4	4

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	4	LYS
1	A	5	ARG
1	A	20	VAL
1	A	24	ILE
1	A	28	PHE
1	A	38	LYS
1	A	42	LYS
1	A	49	THR
1	A	72	ASN
1	A	73	LEU
1	A	103	PRO
1	A	136	ARG
1	A	147	VAL
1	A	152	VAL
1	A	173	VAL
1	A	178	TYR
1	A	182	ASN
1	A	187	LEU
1	A	198	LEU
1	A	210	LYS
1	A	232	PHE
1	A	245	LEU
1	A	257	ARG
1	A	277	LEU
1	A	348	ARG
1	A	349	LEU
1	A	364	TYR
1	A	379	GLU
1	A	404	ARG
1	A	406	GLU
1	A	433	ASP

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Mol	Chain	Res	Type
1	A	450	GLU
1	A	451	ARG
1	A	453	ILE
1	A	462	GLU
1	A	479	GLN
1	A	492	ILE
1	A	493	GLN
1	A	501	TYR
1	A	509	VAL
1	A	527	PRO
1	A	534	GLN
1	A	542	LYS
2	B	55	ARG
2	B	60	GLN
2	B	64	ILE
2	B	73	LEU
2	B	76	THR
2	B	85	LYS
2	B	96	GLU
2	B	101	LYS
2	B	121	ASN
2	B	145	LEU
2	B	150	ASN
2	B	164	THR
2	B	166	ARG
2	B	170	LYS
2	B	178	ARG
2	B	180	SER
2	B	190	GLN
2	B	206	LYS
2	B	215	LYS
2	B	224	LEU
3	G	39	ARG
3	G	51	GLU
3	G	54	LYS
3	G	59	LYS
3	G	71	SER
3	G	74	VAL
3	G	80	ARG
3	G	88	LEU
3	G	91	SER
3	G	100	ARG

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Mol	Chain	Res	Type
3	G	106	GLU
3	G	126	LEU
3	G	130	ARG
3	G	150	LYS
3	G	167	LYS
1	L	5	ARG
1	L	9	LEU
1	L	14	VAL
1	L	25	GLU
1	L	28	PHE
1	L	29	ILE
1	L	32	GLU
1	L	38	LYS
1	L	42	LYS
1	L	73	LEU
1	L	147	VAL
1	L	178	TYR
1	L	187	LEU
1	L	198	LEU
1	L	204	GLU
1	L	211	LEU
1	L	217	THR
1	L	218	CYS
1	L	224	SER
1	L	232	PHE
1	L	247	SER
1	L	257	ARG
1	L	262	SER
1	L	277	LEU
1	L	279	LEU
1	L	326	LEU
1	L	348	ARG
1	L	349	LEU
1	L	350	LEU
1	L	364	TYR
1	L	367	VAL
1	L	404	ARG
1	L	406	GLU
1	L	433	ASP
1	L	434	GLU
1	L	446	LYS
1	L	452	ASN

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Mol	Chain	Res	Type
1	L	453	ILE
1	L	458	LYS
1	L	471	LEU
1	L	479	GLN
1	L	483	THR
1	L	490	LEU
1	L	492	ILE
1	L	493	GLN
1	L	497	LEU
1	L	501	TYR
1	L	511	ASP
1	L	527	PRO
1	L	542	LYS
2	E	49	THR
2	E	50	GLU
2	E	55	ARG
2	E	56	GLN
2	E	58	THR
2	E	59	GLN
2	E	60	GLN
2	E	64	ILE
2	E	85	LYS
2	E	86	SER
2	E	89	ARG
2	E	101	LYS
2	E	109	LYS
2	E	110	SER
2	E	124	SER
2	E	141	HIS
2	E	142	GLN
2	E	150	ASN
2	E	164	THR
2	E	166	ARG
2	E	174	ARG
2	E	177	LYS
2	E	178	ARG
2	E	190	GLN
2	E	213	THR
2	E	216	ASN
2	E	220	LEU
2	E	221	ARG
2	E	224	LEU

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Mol	Chain	Res	Type
3	M	40	VAL
3	M	45	LEU
3	M	54	LYS
3	M	59	LYS
3	M	63	ASP
3	M	66	LEU
3	M	68	ASN
3	M	70	LEU
3	M	71	SER
3	M	73	LYS
3	M	74	VAL
3	M	77	GLN
3	M	79	MET
3	M	88	LEU
3	M	100	ARG
3	M	146	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	16	GLN
1	A	74	ASN
1	A	182	ASN
1	A	465	ASN
1	A	467	ASN
1	A	493	GLN
1	A	534	GLN
2	B	75	GLN
2	B	121	ASN
2	B	167	GLN
2	B	190	GLN
3	G	58	ASN
3	G	68	ASN
3	G	148	GLN
1	L	15	ASN
1	L	72	ASN
1	L	74	ASN
1	L	334	ASN
1	L	452	ASN
1	L	465	ASN
1	L	487	GLN

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Mol	Chain	Res	Type
1	L	513	GLN
2	E	84	HIS
2	E	142	GLN
2	E	150	ASN
2	E	190	GLN
2	E	216	ASN
3	M	68	ASN
3	M	77	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
6	B12	B	601	-	80,101,101	1.36	9 (11%)	101,166,166	1.88	26 (25%)
6	B12	E	601	-	80,101,101	1.10	7 (8%)	101,166,166	1.81	27 (26%)
5	PGO	L	602	4	3,4,4	0.46	0	1,4,4	2.56	1 (100%)
5	PGO	A	602	4	3,4,4	0.24	0	1,4,4	1.18	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
6	B12	B	601	-	-	8/51/223/223	0/3/11/11
6	B12	E	601	-	-	8/51/223/223	0/3/11/11
5	PGO	L	602	4	-	2/2/2/2	-
5	PGO	A	602	4	-	2/2/2/2	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	B12	CO-N24	-4.92	1.76	1.89
6	B	601	B12	C17-C18	3.58	1.59	1.54
6	B	601	B12	O58-C57	3.52	1.30	1.23
6	E	601	B12	O58-C57	3.32	1.30	1.23
6	E	601	B12	C17-C18	3.30	1.58	1.54
6	E	601	B12	CO-N21	-3.06	1.81	1.89
6	E	601	B12	C2R-C1R	2.85	1.58	1.53
6	B	601	B12	C2R-C1R	2.78	1.58	1.53
6	E	601	B12	P-O5	-2.68	1.42	1.55
6	B	601	B12	CO-N23	-2.53	1.82	1.94
6	E	601	B12	C48-C49	2.28	1.59	1.52
6	E	601	B12	C1-C19	2.24	1.60	1.55
6	B	601	B12	C20-C1	-2.18	1.49	1.53
6	B	601	B12	P-O5	-2.06	1.45	1.55
6	B	601	B12	CO-N22	2.03	2.04	1.94
6	B	601	B12	C60-C18	-2.01	1.49	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	B12	O58-C57-C56	-6.43	110.25	122.02
6	E	601	B12	O58-C57-C56	-5.02	112.84	122.02
6	B	601	B12	C1-C19-N24	-4.75	100.89	106.24
6	E	601	B12	C1-C19-N24	-4.62	101.03	106.24
6	B	601	B12	C7B-C8B-C9B	-4.61	115.98	120.54
6	B	601	B12	C25-C2-C1	-4.40	107.26	113.80
6	B	601	B12	C26-C2-C1	4.39	116.84	110.02
6	E	601	B12	C55-C17-C16	4.32	124.31	109.92
6	E	601	B12	O3-C2P-C1P	-4.22	98.50	106.92
6	B	601	B12	O5-P-O2	4.14	123.11	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	601	B12	C20-C1-C19	3.98	113.19	109.36
6	E	601	B12	C2-C3-C4	3.63	105.48	101.67
6	E	601	B12	C26-C2-C1	3.63	115.66	110.02
6	E	601	B12	C7B-C8B-C9B	-3.54	117.05	120.54
6	B	601	B12	C6-C5-C4	-3.49	118.83	124.27
6	B	601	B12	C56-C57-N59	3.39	122.13	116.42
6	B	601	B12	C3P-C2P-C1P	3.37	117.92	111.39
6	B	601	B12	C4B-C9B-C8B	3.30	124.49	121.10
6	B	601	B12	C55-C17-C16	3.29	120.88	109.92
6	E	601	B12	O5-P-O2	3.10	119.02	106.78
6	B	601	B12	C1-C19-C18	-3.08	116.84	121.93
6	B	601	B12	C36-C7-C37	3.07	116.06	110.83
6	E	601	B12	C56-C57-N59	3.02	121.51	116.42
6	B	601	B12	C2-C26-C27	2.93	123.45	115.22
6	E	601	B12	O5-P-O3	2.89	118.18	106.78
6	B	601	B12	C3-C4-C5	-2.80	121.52	131.68
6	E	601	B12	C16-C15-C14	-2.78	119.93	124.27
6	E	601	B12	C36-C7-C37	2.78	115.58	110.83
6	E	601	B12	C13-C14-C15	-2.77	121.64	131.68
6	B	601	B12	C54-C17-C18	-2.71	108.98	112.98
6	E	601	B12	O44-C43-C42	-2.70	113.13	121.07
6	E	601	B12	C47-C12-C46	-2.68	104.11	109.73
6	B	601	B12	O44-C43-C42	-2.67	113.22	121.07
5	L	602	PGO	O2-C2-C3	2.56	120.45	109.38
6	E	601	B12	C25-C2-C3	-2.55	111.69	115.58
6	E	601	B12	C1-C19-C18	-2.48	117.82	121.93
6	E	601	B12	C6-C5-C4	-2.47	120.42	124.27
6	B	601	B12	O58-C57-N59	2.43	127.61	123.01
6	B	601	B12	C17-C18-C19	-2.43	98.67	102.37
6	E	601	B12	C9-C10-C11	-2.43	122.42	130.91
6	E	601	B12	O51-C50-N52	2.40	129.06	122.50
6	E	601	B12	C42-C43-N45	2.40	123.99	116.51
6	E	601	B12	C54-C17-C18	-2.35	109.52	112.98
6	B	601	B12	C55-C17-C18	-2.26	106.78	111.14
6	E	601	B12	C26-C2-C3	2.25	111.61	107.47
6	E	601	B12	C5-C6-N22	-2.19	120.82	124.81
6	B	601	B12	C3R-C2R-C1R	-2.17	95.07	99.89
6	E	601	B12	C20-C1-C2	-2.07	109.90	113.32
6	E	601	B12	C15-C14-N23	2.06	128.12	124.64
6	B	601	B12	C9-C10-C11	-2.06	123.74	130.91
6	B	601	B12	C36-C7-C8	-2.05	108.41	112.11
6	B	601	B12	C47-C12-C46	-2.04	105.46	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	B12	C5B-C4B-C9B	-2.01	118.37	121.22
6	B	601	B12	O6R-C4R-C5R	-2.01	104.87	109.21

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	602	PGO	O1-C1-C2-O2
5	A	602	PGO	O1-C1-C2-O2
6	B	601	B12	C12-C13-C48-C49
6	E	601	B12	C12-C13-C48-C49
6	E	601	B12	C30-C31-C32-O34
6	B	601	B12	C30-C31-C32-O34
6	E	601	B12	C30-C31-C32-N33
6	B	601	B12	C30-C31-C32-N33
6	B	601	B12	C8-C41-C42-C43
6	E	601	B12	C1-C2-C26-C27
6	E	601	B12	C25-C2-C26-C27
6	B	601	B12	C1-C2-C26-C27
6	B	601	B12	C25-C2-C26-C27
5	L	602	PGO	O1-C1-C2-C3
5	A	602	PGO	O1-C1-C2-C3
6	E	601	B12	C17-C18-C60-C61
6	B	601	B12	C17-C18-C60-C61
6	E	601	B12	C19-C18-C60-C61
6	B	601	B12	C19-C18-C60-C61
6	E	601	B12	C1P-C2P-O3-P

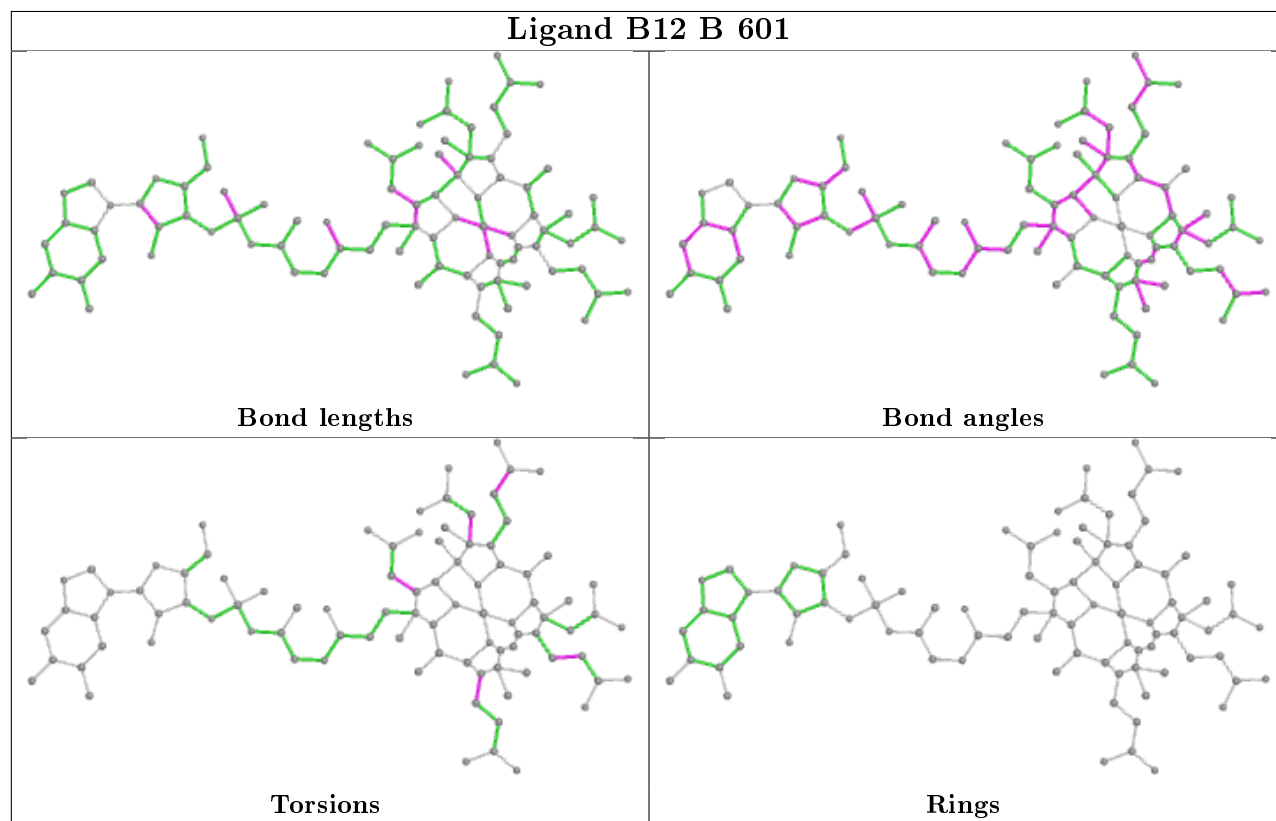
There are no ring outliers.

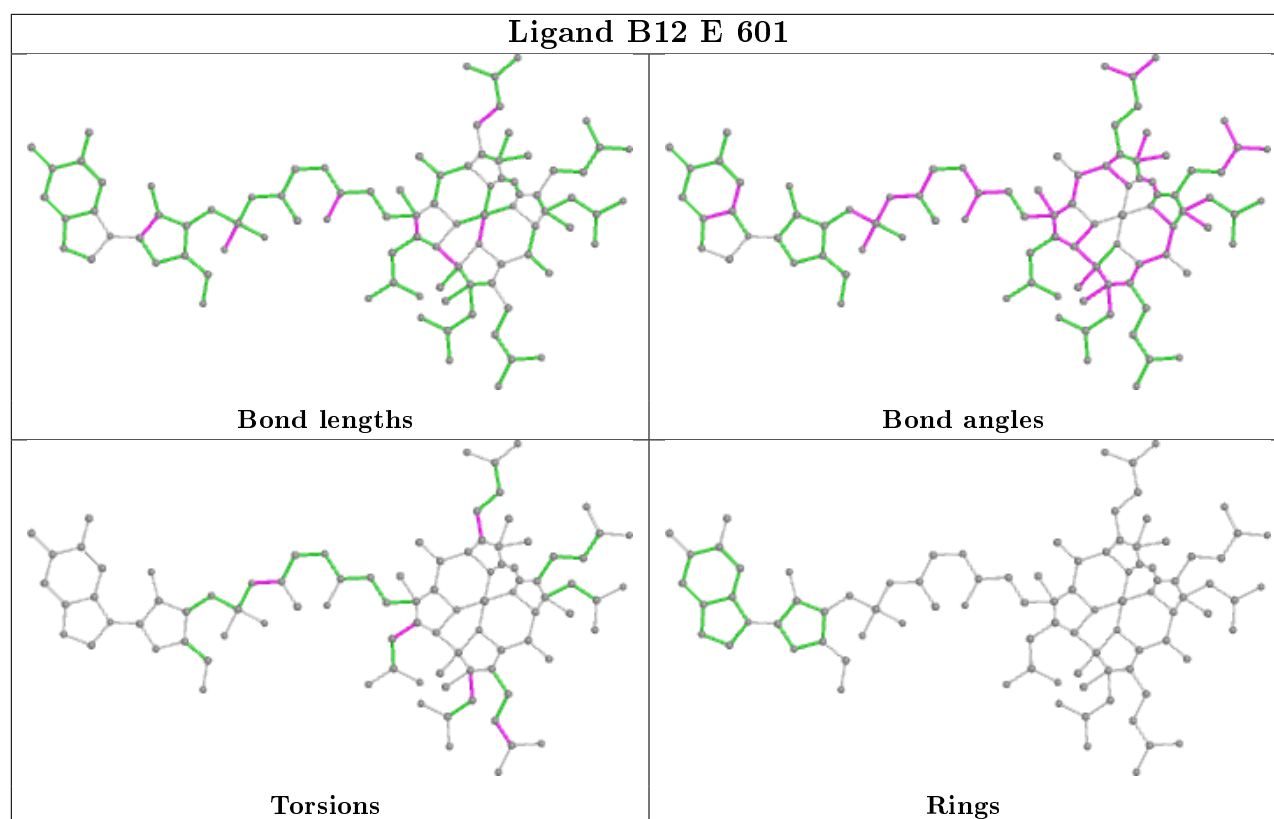
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	B12	6	0
6	E	601	B12	9	0
5	L	602	PGO	1	0
5	A	602	PGO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/554 (99%)	-0.63	1 (0%) 95 94	13, 24, 52, 90	0
1	L	551/554 (99%)	-0.54	1 (0%) 95 94	11, 27, 54, 76	0
2	B	179/224 (79%)	-0.71	1 (0%) 89 88	18, 37, 64, 99	0
2	E	179/224 (79%)	0.23	12 (6%) 17 16	21, 45, 82, 117	0
3	G	137/173 (79%)	-0.60	0 100 100	24, 35, 65, 78	0
3	M	137/173 (79%)	-0.43	4 (2%) 51 49	25, 37, 73, 86	0
All	All	1734/1902 (91%)	-0.50	19 (1%) 80 79	11, 31, 62, 117	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	58	ASN	4.2
2	E	224	LEU	3.7
2	E	58	THR	3.6
2	E	222	VAL	3.5
1	L	1	MET	3.4
1	A	1	MET	3.4
2	E	59	GLN	3.3
2	E	101	LYS	3.2
2	E	223	ALA	3.2
2	B	224	LEU	3.2
2	E	92	ILE	2.7
3	M	63	ASP	2.7
2	E	60	GLN	2.4
3	M	57	THR	2.3
2	E	57	GLY	2.3
3	M	37	SER	2.1
2	E	91	VAL	2.0
2	E	99	GLY	2.0
2	E	122	ARG	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](#)

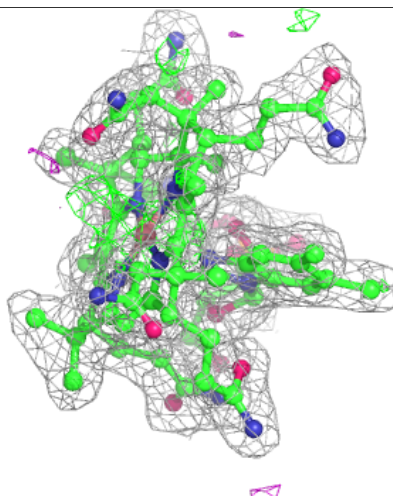
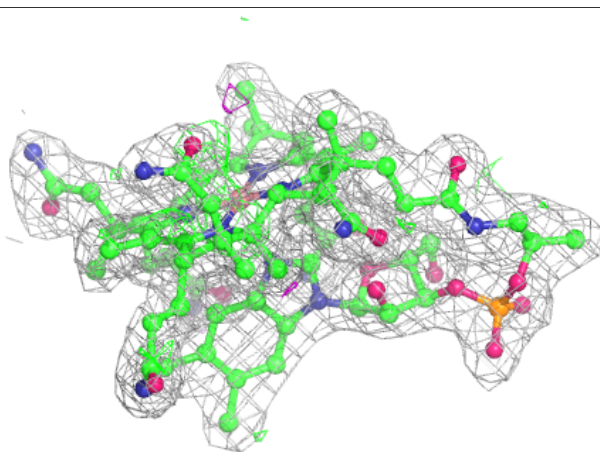
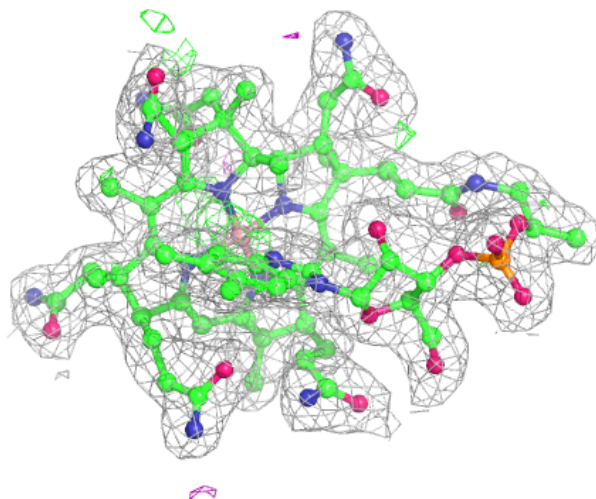
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PGO	A	602	5/5	0.95	0.26	23,23,24,25	0
5	PGO	L	602	5/5	0.97	0.27	21,23,25,25	0
6	B12	B	601	91/91	0.97	0.14	17,23,27,40	0
6	B12	E	601	91/91	0.97	0.13	22,28,31,38	0
4	K	A	603	1/1	0.98	0.10	18,18,18,18	0
4	K	L	603	1/1	0.98	0.10	19,19,19,19	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 B12 B 601:**

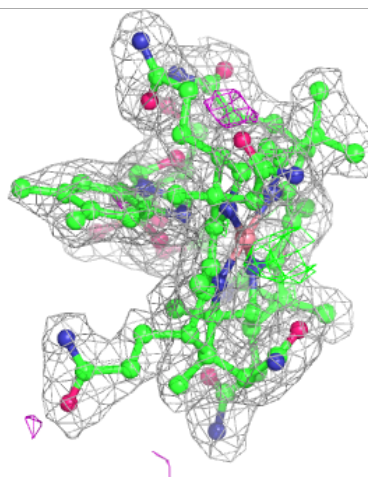
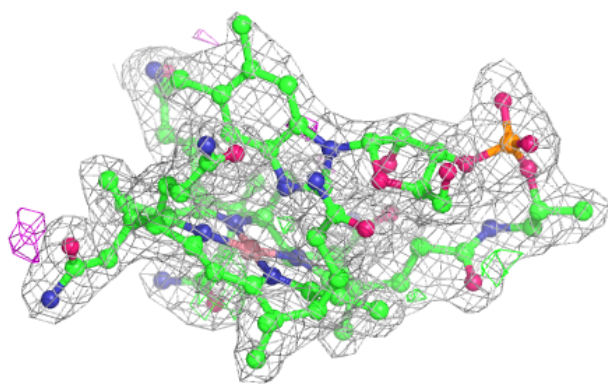
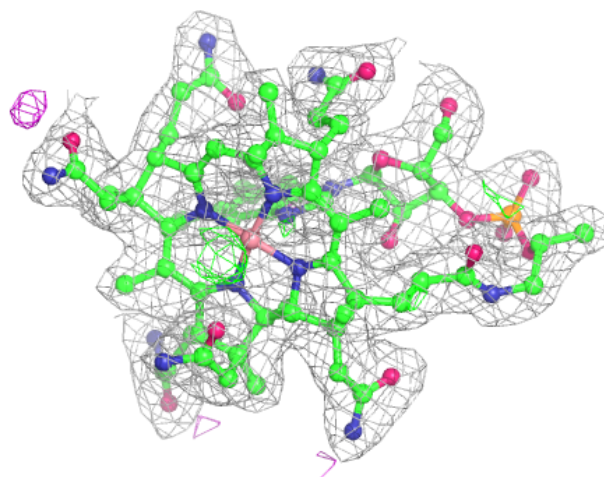
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around B12 E 601:**

$2mF_o-DF_c$  (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.