



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:26 pm BST

PDB ID : 1REQ  
Title : METHYLMALONYL-COA MUTASE  
Authors : Evans, P.R.; Mancina, F.  
Deposited on : 1996-01-19  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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

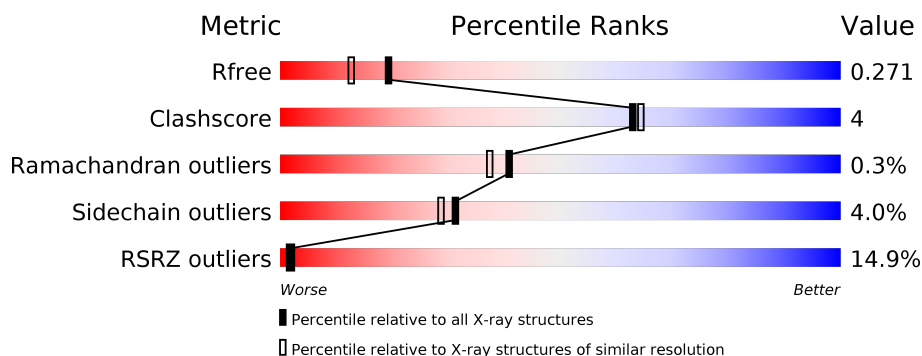
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	727	 7% 71% 26% •
1	C	727	 9% 69% 26% 5% •
2	B	637	 14% 70% 23% • • •
2	D	637	 31% 70% 22% 5% •

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22372 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	727	Total	C	N	O	S	0	0	0
			5563	3514	960	1065	24			
1	C	727	Total	C	N	O	S	0	0	0
			5560	3515	960	1061	24			

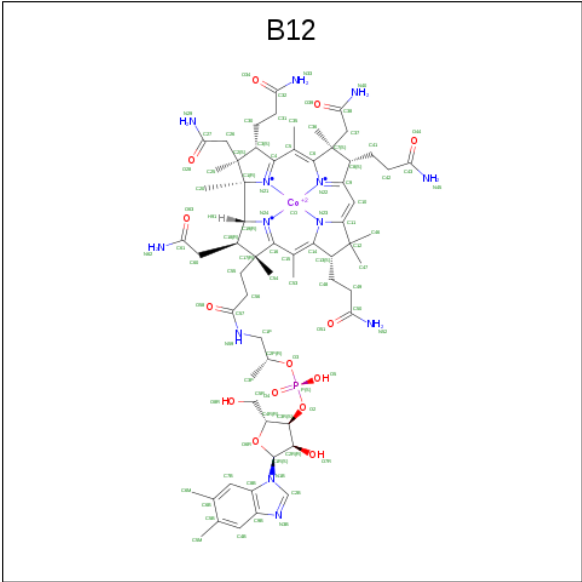
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			
2	D	622	Total	C	N	O	S	0	0	0
			4692	2958	818	903	13			

There are 6 discrepancies between the modelled and reference sequences:

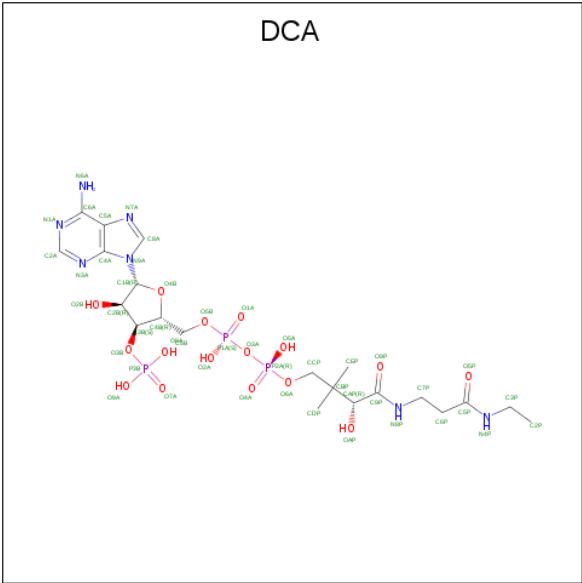
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	CONFLICT	UNP P11652
B	330	GLU	ASP	CONFLICT	UNP P11652
B	331	LEU	VAL	CONFLICT	UNP P11652
D	203	GLY	ALA	CONFLICT	UNP P11652
D	330	GLU	ASP	CONFLICT	UNP P11652
D	331	LEU	VAL	CONFLICT	UNP P11652

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).



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

- Molecule 4 is DESULFO-COENZYME A (three-letter code: DCA) (formula:  $C_{21}H_{36}N_7O_{16}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			47	21	7	16	3		
4	C	1	Total	C	N	O	P	0	0
			47	21	7	16	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	457	Total	O	0	0
			457	457		
6	B	318	Total	O	0	0
			318	318		

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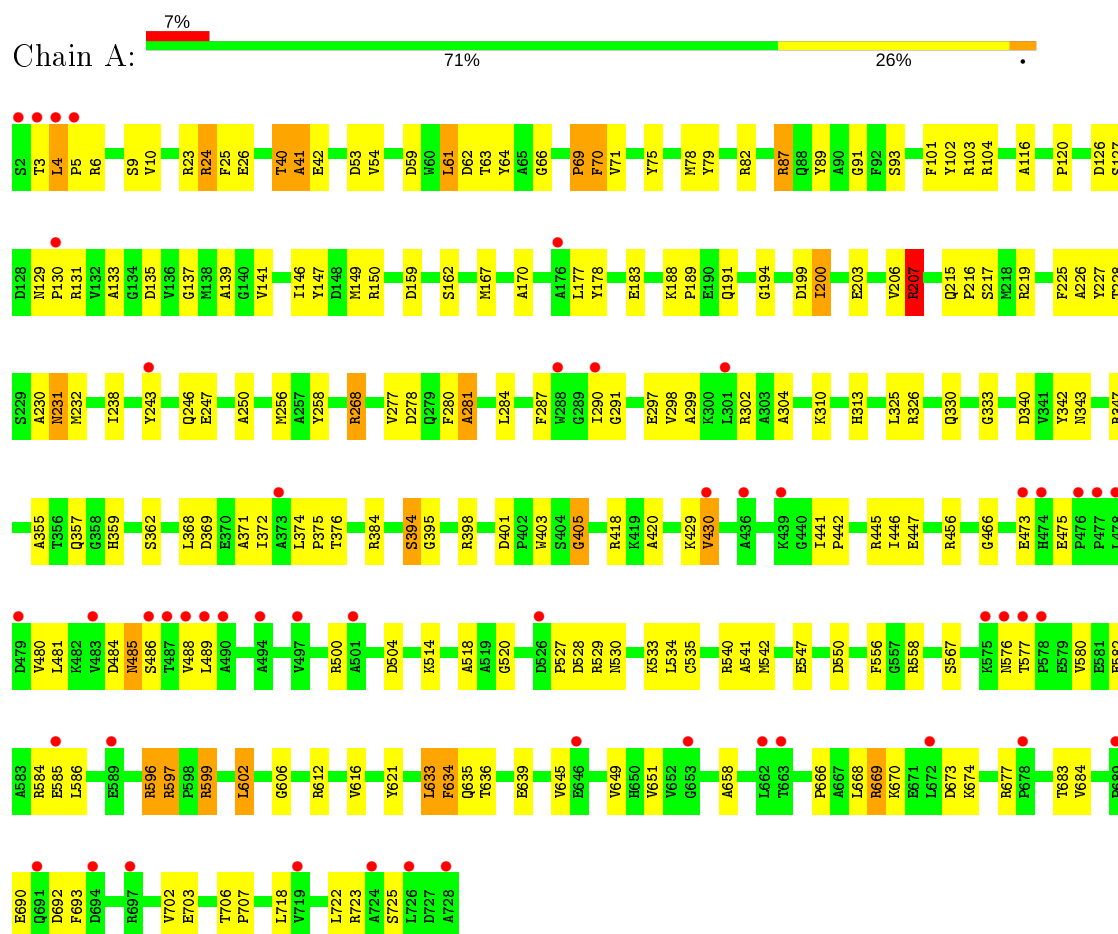
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	493	Total 493	O 493	0	0
6	D	264	Total 264	O 264	0	0

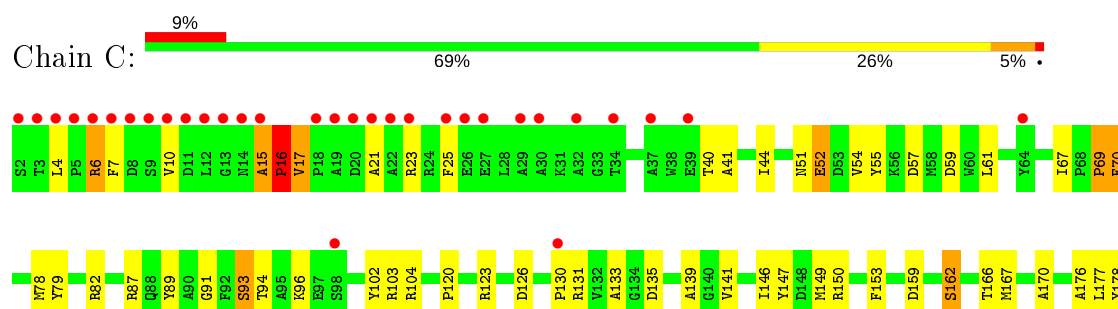
### 3 Residue-property plots

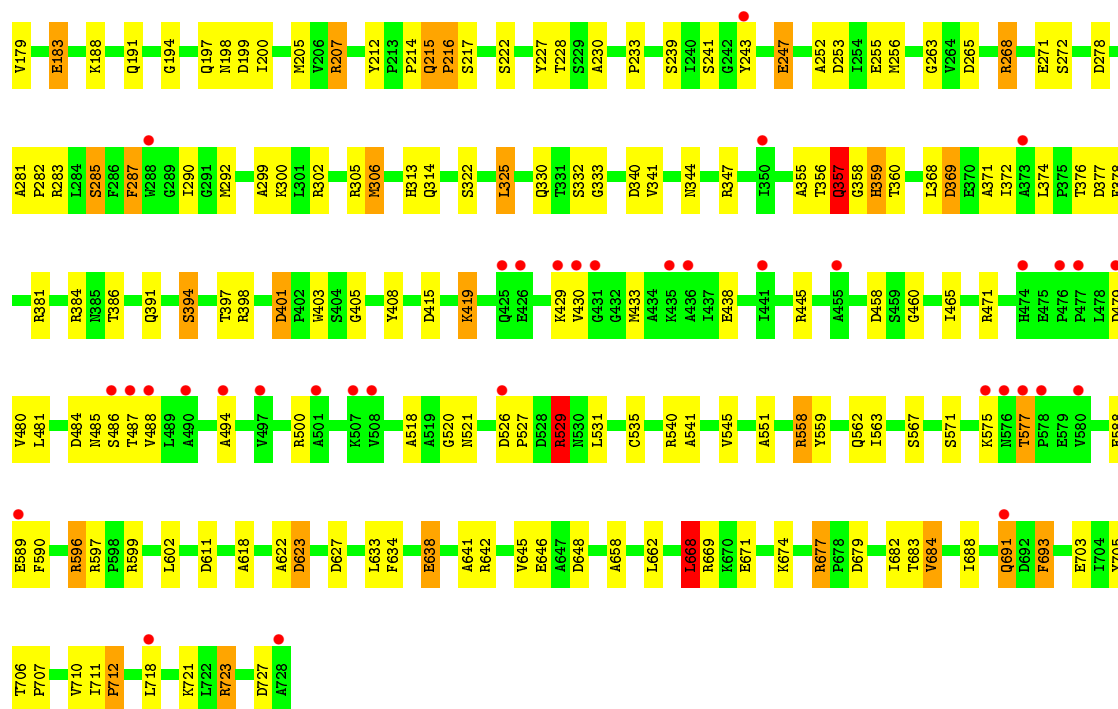
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

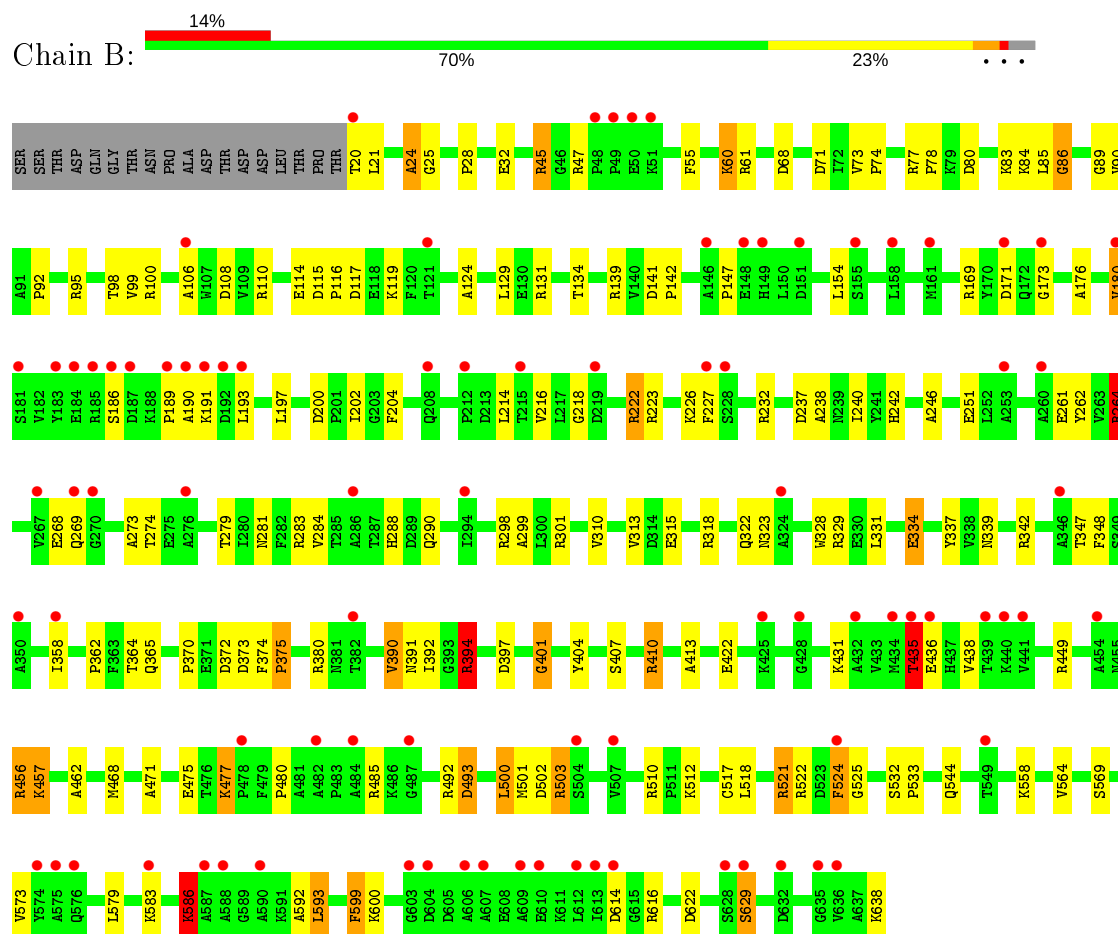


#### • Molecule 1: METHYLMALONYL-COA MUTASE



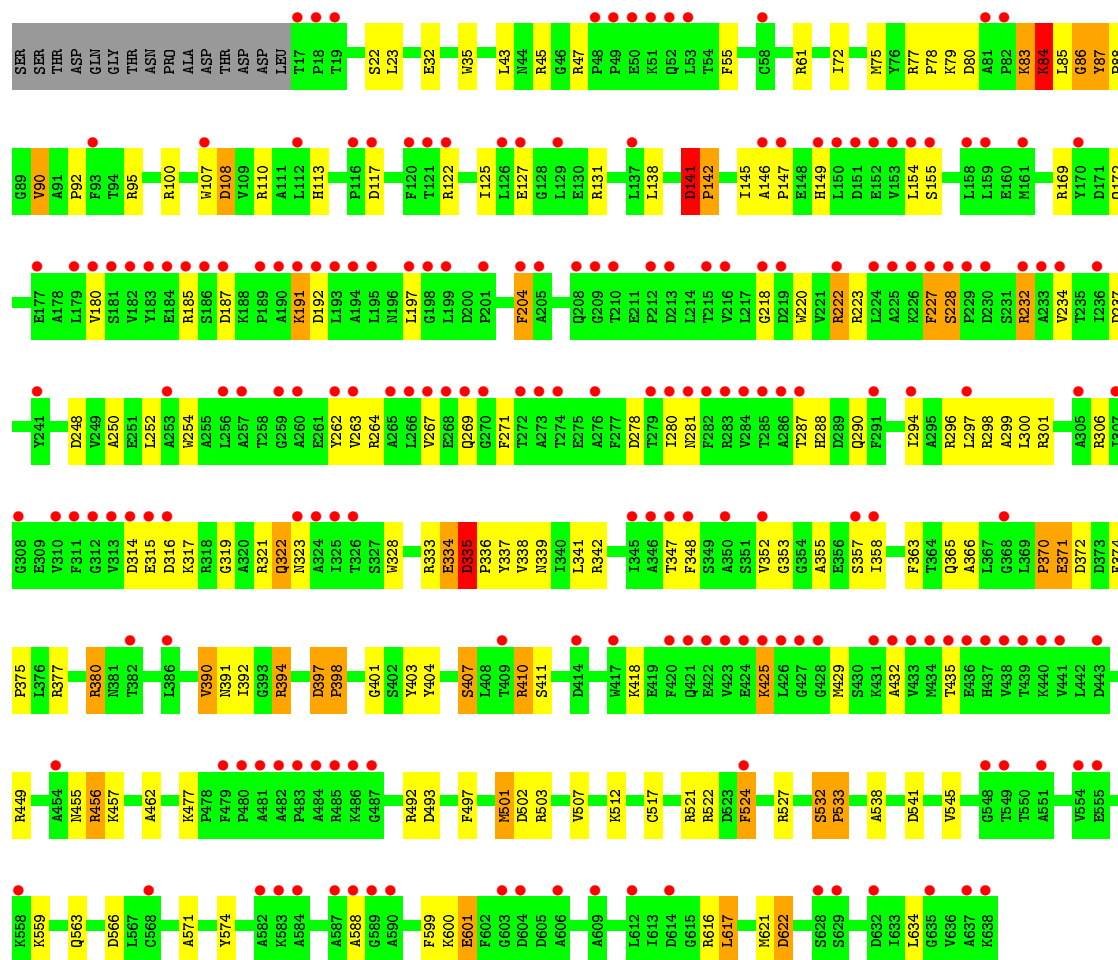


- Molecule 2: METHYLMALONYL-COA MUTASE



- Molecule 2: METHYLMALONYL-COA MUTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.80 Å   161.30 Å   88.40 Å 90.00°   105.10°   90.00°	Depositor
Resolution (Å)	20.00 – 2.00 39.62 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 96.0 (39.62-1.97)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.28 (at 1.98 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220   ,   0.275 0.252   ,   0.271	Depositor DCC
$R_{free}$ test set	10942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: GOL, B12, DCA

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	0.91	0/5679	2.03	166/7718 (2.2%)
1	C	0.95	1/5676 (0.0%)	2.14	199/7711 (2.6%)
2	B	0.82	0/4785	2.04	136/6499 (2.1%)
2	D	0.76	0/4783	2.06	143/6503 (2.2%)
All	All	0.87	1/20923 (0.0%)	2.07	644/28431 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	C	0	37
2	B	0	21
2	D	0	17
All	All	0	100

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	558	ARG	NE-CZ	5.04	1.39	1.33

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	264	ARG	CD-NE-CZ	38.96	178.14	123.60
2	D	169	ARG	CD-NE-CZ	30.40	166.16	123.60
1	C	384	ARG	CD-NE-CZ	25.54	159.35	123.60
1	A	384	ARG	CD-NE-CZ	24.99	158.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	ARG	NE-CZ-NH1	21.19	130.90	120.30
2	B	95	ARG	NE-CZ-NH2	-20.37	110.11	120.30
1	C	596	ARG	CD-NE-CZ	19.99	151.59	123.60
2	B	77	ARG	NE-CZ-NH2	-19.88	110.36	120.30
2	D	333	ARG	NE-CZ-NH2	19.67	130.14	120.30
1	A	268	ARG	NE-CZ-NH2	-18.81	110.90	120.30
2	D	321	ARG	NE-CZ-NH2	-18.46	111.07	120.30
1	A	597	ARG	NE-CZ-NH1	18.04	129.32	120.30
2	B	77	ARG	NE-CZ-NH1	17.98	129.29	120.30
2	B	410	ARG	NE-CZ-NH1	17.72	129.16	120.30
2	B	410	ARG	NE-CZ-NH2	-17.21	111.69	120.30
1	A	23	ARG	CD-NE-CZ	16.10	146.13	123.60
1	C	23	ARG	NE-CZ-NH1	15.26	127.93	120.30
2	B	342	ARG	NE-CZ-NH1	15.03	127.81	120.30
1	C	268	ARG	NE-CZ-NH2	-14.91	112.85	120.30
2	B	222	ARG	NE-CZ-NH1	13.77	127.19	120.30
1	A	597	ARG	NE-CZ-NH2	-13.76	113.42	120.30
2	B	77	ARG	CD-NE-CZ	13.59	142.63	123.60
1	C	159	ASP	CB-CG-OD1	13.36	130.33	118.30
1	C	278	ASP	CB-CG-OD1	13.32	130.29	118.30
1	C	597	ARG	NE-CZ-NH1	13.20	126.90	120.30
2	D	100	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	A	24	ARG	NE-CZ-NH2	-12.95	113.83	120.30
1	C	677	ARG	NE-CZ-NH2	12.86	126.73	120.30
2	D	110	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	C	669	ARG	NE-CZ-NH1	12.57	126.58	120.30
1	A	485	ASN	N-CA-CB	12.51	133.11	110.60
1	C	82	ARG	CD-NE-CZ	12.49	141.09	123.60
1	A	103	ARG	CD-NE-CZ	12.41	140.98	123.60
2	D	169	ARG	NE-CZ-NH2	12.35	126.48	120.30
1	C	243	TYR	CB-CG-CD2	12.35	128.41	121.00
1	A	79	TYR	CB-CG-CD2	-12.27	113.64	121.00
1	C	597	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	C	103	ARG	CD-NE-CZ	12.04	140.46	123.60
2	B	169	ARG	NE-CZ-NH1	12.03	126.31	120.30
2	D	169	ARG	NE-CZ-NH1	-12.00	114.30	120.30
1	C	135	ASP	CB-CG-OD1	11.69	128.82	118.30
1	C	596	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	C	723	ARG	NE-CZ-NH2	-11.59	114.50	120.30
2	B	47	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	C	82	ARG	NE-CZ-NH1	11.55	126.08	120.30
2	B	169	ARG	CD-NE-CZ	11.49	139.68	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASP	CB-CG-OD2	11.48	128.64	118.30
2	B	100	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	D	404	TYR	CB-CG-CD1	11.32	127.79	121.00
1	C	596	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	C	597	ARG	CD-NE-CZ	11.11	139.15	123.60
2	D	77	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	A	199	ASP	CB-CG-OD1	10.89	128.10	118.30
1	A	596	ARG	NE-CZ-NH2	-10.83	114.89	120.30
2	D	298	ARG	NE-CZ-NH1	10.79	125.69	120.30
2	B	301	ARG	NE-CZ-NH1	10.58	125.59	120.30
2	B	410	ARG	CD-NE-CZ	10.56	138.39	123.60
1	C	623	ASP	CB-CG-OD1	10.31	127.58	118.30
1	C	23	ARG	NE-CZ-NH2	-10.27	115.17	120.30
2	B	223	ARG	NE-CZ-NH2	-10.18	115.21	120.30
2	B	380	ARG	NE-CZ-NH1	10.15	125.38	120.30
2	B	622	ASP	CB-CG-OD1	10.13	127.42	118.30
2	D	95	ARG	NE-CZ-NH2	-10.12	115.24	120.30
2	B	86	GLY	O-C-N	-10.11	106.52	122.70
2	B	222	ARG	CD-NE-CZ	10.04	137.66	123.60
1	C	500	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	C	377	ASP	CB-CG-OD1	9.94	127.25	118.30
2	B	616	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	A	596	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	207	ARG	NE-CZ-NH2	-9.66	115.47	120.30
2	B	524	PHE	CB-CG-CD1	9.65	127.55	120.80
1	A	147	TYR	CB-CG-CD1	9.63	126.78	121.00
2	D	622	ASP	CB-CG-OD1	9.55	126.89	118.30
1	A	159	ASP	CB-CG-OD1	9.53	126.88	118.30
1	C	340	ASP	CB-CG-OD1	9.51	126.86	118.30
2	D	77	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	147	TYR	CB-CG-CD2	-9.43	115.34	121.00
1	A	79	TYR	CB-CG-CD1	9.35	126.61	121.00
2	B	100	ARG	NE-CZ-NH2	-9.31	115.64	120.30
2	D	110	ARG	CD-NE-CZ	9.29	136.61	123.60
2	B	95	ARG	NH1-CZ-NH2	9.26	129.59	119.40
1	C	642	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	599	ARG	NE-CZ-NH2	-9.21	115.70	120.30
2	D	524	PHE	CB-CG-CD1	9.20	127.24	120.80
1	A	207	ARG	CB-CG-CD	9.19	135.48	111.60
2	D	397	ASP	CB-CG-OD2	9.12	126.50	118.30
1	C	369	ASP	CB-CG-OD1	9.06	126.45	118.30
1	A	219	ARG	NE-CZ-NH1	-9.05	115.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	NE-CZ-NH2	9.03	124.82	120.30
1	C	243	TYR	CB-CG-CD1	-8.94	115.64	121.00
1	A	597	ARG	CD-NE-CZ	8.94	136.11	123.60
2	B	298	ARG	NE-CZ-NH1	8.92	124.76	120.30
2	D	353	GLY	C-N-CA	8.83	140.85	122.30
1	C	59	ASP	CB-CG-OD1	8.81	126.23	118.30
2	D	333	ARG	NE-CZ-NH1	-8.80	115.90	120.30
2	D	372	ASP	CB-CG-OD2	-8.78	110.40	118.30
2	D	95	ARG	CG-CD-NE	8.76	130.19	111.80
1	C	131	ARG	CD-NE-CZ	8.75	135.85	123.60
1	C	283	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	430	VAL	O-C-N	-8.68	108.45	123.20
1	A	150	ARG	NE-CZ-NH1	-8.59	116.00	120.30
1	C	265	ASP	CB-CG-OD1	8.59	126.03	118.30
2	B	131	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	C	79	TYR	CB-CG-CD2	-8.48	115.91	121.00
2	D	87	TYR	CB-CG-CD2	8.46	126.07	121.00
1	C	131	ARG	NE-CZ-NH2	8.42	124.51	120.30
2	D	232	ARG	CD-NE-CZ	8.42	135.39	123.60
1	C	347	ARG	NE-CZ-NH2	-8.37	116.12	120.30
2	B	521	ARG	NE-CZ-NH2	-8.36	116.12	120.30
2	B	95	ARG	CG-CD-NE	8.35	129.33	111.80
1	A	150	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	70	PHE	CB-CG-CD1	8.33	126.63	120.80
1	A	529	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	C	693	PHE	CB-CG-CD1	8.33	126.63	120.80
2	B	262	TYR	CB-CG-CD1	8.28	125.97	121.00
2	D	117	ASP	CB-CG-OD1	8.27	125.75	118.30
2	B	110	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	485	ASN	CA-CB-CG	8.21	131.46	113.40
1	C	150	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	C	347	ARG	NE-CZ-NH1	8.09	124.35	120.30
2	B	264	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	456	ARG	CD-NE-CZ	8.08	134.91	123.60
2	B	404	TYR	CB-CG-CD2	-8.04	116.17	121.00
2	B	422	GLU	CA-CB-CG	8.01	131.03	113.40
2	B	435	THR	CA-CB-CG2	8.01	123.62	112.40
2	D	377	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	55	TYR	CB-CG-CD1	8.00	125.80	121.00
2	B	117	ASP	CB-CG-OD1	7.98	125.48	118.30
2	D	337	TYR	CB-CG-CD1	7.96	125.77	121.00
2	D	404	TYR	CB-CG-CD2	-7.91	116.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	ARG	NE-CZ-NH2	-7.87	116.37	120.30
2	D	237	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	302	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	C	401	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	225	PHE	CB-CG-CD1	7.82	126.28	120.80
2	B	301	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	642	ARG	NE-CZ-NH2	-7.75	116.43	120.30
2	D	306	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	485	ASN	CB-CA-C	-7.74	94.92	110.40
1	C	590	PHE	CB-CG-CD1	7.74	126.22	120.80
1	A	150	ARG	NH1-CZ-NH2	7.70	127.87	119.40
1	A	485	ASN	CA-CB-CG	7.69	130.31	113.40
1	C	398	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	C	398	ARG	NE-CZ-NH1	-7.63	116.48	120.30
2	B	262	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	C	41	ALA	O-C-N	-7.60	110.54	122.70
1	A	394	SER	O-C-N	-7.59	110.29	123.20
1	A	340	ASP	CB-CG-OD1	7.59	125.13	118.30
1	C	599	ARG	CG-CD-NE	7.58	127.72	111.80
1	A	723	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	61	LEU	O-C-N	-7.56	110.61	122.70
1	A	6	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	679	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	520	GLY	O-C-N	-7.48	110.73	122.70
2	B	89	GLY	O-C-N	-7.48	110.74	122.70
1	C	147	TYR	CB-CG-CD1	7.44	125.47	121.00
1	A	445	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	C	679	ASP	CB-CG-OD1	7.42	124.98	118.30
2	D	86	GLY	O-C-N	-7.41	110.84	122.70
2	B	457	LYS	C-N-CA	7.41	140.22	121.70
2	D	492	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	B	169	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	B	390	VAL	O-C-N	-7.38	110.89	122.70
1	C	57	ASP	CB-CG-OD1	-7.37	111.66	118.30
1	C	356	THR	CA-CB-CG2	-7.37	102.08	112.40
2	D	337	TYR	CB-CG-CD2	-7.37	116.58	121.00
2	D	45	ARG	CA-C-N	7.37	130.94	116.20
1	A	41	ALA	O-C-N	-7.35	110.94	122.70
1	C	287	PHE	CB-CG-CD1	7.33	125.93	120.80
1	C	333	GLY	O-C-N	-7.32	110.99	122.70
1	A	70	PHE	CB-CG-CD2	-7.31	115.69	120.80
1	A	78	MET	O-C-N	-7.31	111.01	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	627	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	227	TYR	CB-CG-CD1	7.26	125.36	121.00
2	B	422	GLU	OE1-CD-OE2	-7.26	114.59	123.30
2	D	321	ARG	NH1-CZ-NH2	7.25	127.37	119.40
2	B	457	LYS	O-C-N	-7.25	111.11	122.70
1	A	59	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	556	PHE	CB-CG-CD1	7.21	125.85	120.80
1	A	692	ASP	CB-CG-OD2	7.20	124.78	118.30
2	B	373	ASP	CB-CG-OD2	7.19	124.77	118.30
2	D	90	VAL	CA-CB-CG2	7.18	121.68	110.90
2	D	403	TYR	CB-CG-CD1	7.17	125.30	121.00
1	A	53	ASP	CB-CG-OD1	7.17	124.75	118.30
1	C	357	GLN	O-C-N	-7.17	111.02	123.20
2	B	337	TYR	O-C-N	-7.16	111.25	122.70
2	B	404	TYR	CB-CG-CD1	7.15	125.29	121.00
2	D	84	LYS	CB-CG-CD	7.13	130.13	111.60
1	C	199	ASP	OD1-CG-OD2	-7.12	109.76	123.30
1	A	64	TYR	CB-CG-CD2	7.10	125.26	121.00
2	D	262	TYR	CB-CG-CD1	7.10	125.26	121.00
2	B	89	GLY	C-N-CA	7.09	139.41	121.70
2	D	339	ASN	O-C-N	-7.08	111.37	122.70
1	A	62	ASP	CB-CG-OD1	7.08	124.67	118.30
2	B	24	ALA	CB-CA-C	-7.08	99.49	110.10
1	C	87	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	102	TYR	CB-CG-CD1	7.07	125.24	121.00
1	C	198	ASN	O-C-N	-7.06	111.40	122.70
2	D	100	ARG	NE-CZ-NH1	7.05	123.83	120.30
2	B	510	ARG	NE-CZ-NH1	7.05	123.83	120.30
2	D	527	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	C	207	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	D	47	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	228	THR	O-C-N	-6.96	111.56	122.70
1	C	398	ARG	NH1-CZ-NH2	6.95	127.04	119.40
1	A	633	LEU	O-C-N	-6.95	111.59	122.70
1	C	332	SER	O-C-N	-6.94	111.40	123.20
2	D	456	ARG	O-C-N	-6.94	111.60	122.70
2	B	558	LYS	O-C-N	-6.93	111.61	122.70
2	D	410	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	D	501	MET	CG-SD-CE	6.87	111.20	100.20
2	B	329	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	D	404	TYR	CG-CD1-CE1	6.86	126.79	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	B	78	PRO	O-C-N	-6.83	111.78	122.70
1	C	150	ARG	NH1-CZ-NH2	6.82	126.91	119.40
1	C	150	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	C	183	GLU	O-C-N	-6.81	111.80	122.70
2	D	342	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	A	535	CYS	O-C-N	-6.78	111.85	122.70
1	A	89	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	B	616	ARG	CD-NE-CZ	6.76	133.07	123.60
2	D	616	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	B	45	ARG	CA-C-N	6.76	129.72	116.20
2	B	223	ARG	NH1-CZ-NH2	6.76	126.83	119.40
1	C	535	CYS	O-C-N	-6.75	111.91	122.70
1	A	369	ASP	O-C-N	-6.72	111.94	122.70
1	C	302	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	D	127	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	C	141	VAL	CA-CB-CG1	6.69	120.94	110.90
2	D	462	ALA	O-C-N	-6.67	112.03	122.70
2	D	533	PRO	N-CA-CB	6.66	111.30	103.30
1	A	82	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	183	GLU	O-C-N	-6.66	112.05	122.70
1	C	126	ASP	CB-CG-OD1	6.65	124.29	118.30
1	C	227	TYR	CB-CG-CD1	6.64	124.99	121.00
1	A	500	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	B	422	GLU	O-C-N	-6.63	112.09	122.70
1	C	485	ASN	CB-CA-C	-6.62	97.16	110.40
2	B	25	GLY	O-C-N	-6.62	112.11	122.70
1	A	634	PHE	CB-CG-CD2	-6.62	116.17	120.80
2	B	342	ARG	CD-NE-CZ	-6.62	114.34	123.60
1	C	559	TYR	CG-CD2-CE2	6.62	126.59	121.30
2	D	296	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	B	485	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	C	313	HIS	O-C-N	-6.60	112.14	122.70
1	C	727	ASP	C-N-CA	6.60	138.19	121.70
2	B	318	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	430	VAL	CA-CB-CG1	6.59	120.79	110.90
2	B	339	ASN	O-C-N	-6.58	112.18	122.70
2	D	371	GLU	CA-CB-CG	6.57	127.84	113.40
1	A	66	GLY	O-C-N	-6.56	112.20	122.70
2	D	457	LYS	O-C-N	-6.56	112.20	122.70
1	C	527	PRO	N-CA-CB	6.56	111.17	103.30
1	A	225	PHE	CB-CG-CD2	-6.54	116.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	PRO	O-C-N	-6.53	112.25	122.70
1	A	298	VAL	O-C-N	-6.53	112.26	122.70
1	C	147	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	C	357	GLN	C-N-CA	6.50	135.96	122.30
1	A	23	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	347	ARG	CD-NE-CZ	6.50	132.69	123.60
2	D	192	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	258	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	C	693	PHE	CB-CG-CD2	-6.46	116.27	120.80
2	B	131	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	232	MET	CA-CB-CG	6.45	124.27	113.30
2	D	315	GLU	C-N-CA	6.45	137.82	121.70
2	D	449	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	215	GLN	CA-C-O	6.42	133.59	120.10
2	D	298	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
2	D	397	ASP	OD1-CG-OD2	-6.42	111.11	123.30
1	C	397	THR	O-C-N	-6.40	112.46	122.70
2	D	456	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	A	256	MET	CG-SD-CE	-6.36	90.03	100.20
1	A	677	ARG	CA-CB-CG	6.33	127.33	113.40
2	D	248	ASP	CB-CG-OD2	-6.33	112.61	118.30
2	B	599	PHE	O-C-N	-6.32	112.59	122.70
2	D	141	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	272	SER	CA-C-N	6.31	131.08	117.20
1	C	78	MET	O-C-N	-6.30	112.62	122.70
2	D	355	ALA	N-CA-CB	6.30	118.92	110.10
1	C	677	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	226	ALA	O-C-N	-6.28	112.65	122.70
1	A	398	ARG	O-C-N	-6.28	112.65	122.70
1	C	368	LEU	O-C-N	-6.28	112.66	122.70
1	A	170	ALA	O-C-N	-6.27	112.66	122.70
1	C	408	TYR	CB-CG-CD1	6.27	124.76	121.00
2	B	502	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	D	425	LYS	CA-CB-CG	6.27	127.19	113.40
2	B	298	ARG	NH1-CZ-NH2	-6.26	112.51	119.40
2	B	600	LYS	O-C-N	-6.26	112.68	122.70
1	C	430	VAL	CA-CB-CG1	6.26	120.29	110.90
1	A	723	ARG	NE-CZ-NH2	-6.25	117.18	120.30
2	D	541	ASP	O-C-N	-6.24	112.72	122.70
1	C	611	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	333	GLY	O-C-N	-6.19	112.79	122.70
1	A	368	LEU	O-C-N	-6.19	112.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	72	ILE	CB-CG1-CD1	6.19	131.22	113.90
2	D	222	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	375	PRO	N-CA-CB	6.17	110.71	103.30
2	B	147	PRO	O-C-N	-6.17	112.83	122.70
1	C	299	ALA	N-CA-CB	-6.17	101.47	110.10
2	B	55	PHE	CB-CG-CD1	-6.14	116.50	120.80
1	A	466	GLY	O-C-N	-6.13	112.89	122.70
1	A	131	ARG	CD-NE-CZ	6.12	132.16	123.60
1	A	612	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	B	24	ALA	N-CA-CB	6.12	118.66	110.10
2	D	264	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	A	621	TYR	CB-CG-CD1	6.11	124.67	121.00
1	A	150	ARG	CD-NE-CZ	6.10	132.14	123.60
2	D	512	LYS	CB-CA-C	-6.09	98.22	110.40
2	D	634	LEU	C-N-CA	6.09	135.09	122.30
2	B	586	LYS	CA-CB-CG	6.09	126.79	113.40
1	C	102	TYR	CB-CG-CD1	6.08	124.65	121.00
2	D	507	VAL	C-N-CA	6.08	136.90	121.70
1	C	559	TYR	CZ-CE2-CD2	-6.08	114.33	119.80
1	A	206	VAL	CA-CB-CG1	6.07	120.01	110.90
2	B	269	GLN	O-C-N	-6.07	112.88	123.20
2	D	574	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	C	377	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	104	ARG	CG-CD-NE	6.04	124.49	111.80
1	A	530	ASN	OD1-CG-ND2	6.04	135.80	121.90
2	B	337	TYR	CA-C-N	6.04	130.49	117.20
2	B	86	GLY	C-N-CA	6.04	136.79	121.70
1	C	378	PHE	O-C-N	-6.03	113.06	122.70
2	D	131	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	110	ARG	CD-NE-CZ	6.01	132.02	123.60
1	C	67	ILE	CA-CB-CG1	5.99	122.39	111.00
2	B	503	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	C	633	LEU	C-N-CA	5.99	136.67	121.70
1	A	690	GLU	O-C-N	-5.98	113.13	122.70
1	C	325	LEU	CB-CG-CD2	5.98	121.17	111.00
2	B	372	ASP	CB-CG-OD1	5.98	123.68	118.30
2	B	200	ASP	CB-CG-OD2	5.97	123.68	118.30
2	D	204	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	A	26	GLU	OE1-CD-OE2	5.96	130.46	123.30
1	A	54	VAL	CA-C-N	5.96	130.32	117.20
1	C	214	PRO	N-CA-CB	5.96	110.46	103.30
1	C	215	GLN	O-C-N	-5.96	109.78	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	394	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	A	91	GLY	N-CA-C	-5.94	98.24	113.10
2	B	204	PHE	CB-CG-CD1	-5.94	116.64	120.80
2	B	268	GLU	CA-CB-CG	5.93	126.44	113.40
1	A	238	ILE	O-C-N	5.92	132.18	122.70
1	A	268	ARG	NH1-CZ-NH2	5.92	125.92	119.40
2	D	390	VAL	O-C-N	-5.92	113.23	122.70
2	D	497	PHE	CB-CG-CD1	5.92	124.94	120.80
2	B	328	TRP	O-C-N	-5.92	113.23	122.70
1	A	616	VAL	CA-CB-CG1	5.91	119.77	110.90
1	A	71	VAL	O-C-N	-5.91	113.25	122.70
1	C	300	LYS	O-C-N	-5.91	113.25	122.70
1	C	255	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	215	GLN	N-CA-CB	5.89	121.21	110.60
1	A	403	TRP	O-C-N	-5.89	113.28	122.70
2	D	223	ARG	C-N-CA	5.89	136.42	121.70
1	C	17	VAL	N-CA-CB	5.88	124.44	111.50
2	D	269	GLN	C-N-CA	5.88	134.64	122.30
1	C	281	ALA	N-CA-CB	5.87	118.32	110.10
1	A	299	ALA	CB-CA-C	-5.87	101.30	110.10
2	B	28	PRO	N-CA-CB	5.87	110.34	103.30
2	D	328	TRP	O-C-N	-5.86	113.33	122.70
2	B	264	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	297	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	C	322	SER	O-C-N	-5.85	113.34	122.70
2	D	204	PHE	CB-CG-CD1	5.85	124.90	120.80
1	C	253	ASP	CB-CG-OD1	5.84	123.56	118.30
2	B	60	LYS	O-C-N	-5.84	113.36	122.70
1	C	141	VAL	CG1-CB-CG2	-5.83	101.57	110.90
1	C	394	SER	C-N-CA	5.83	134.54	122.30
2	D	407	SER	O-C-N	-5.83	113.38	122.70
2	B	397	ASP	CB-CG-OD1	5.82	123.54	118.30
2	D	88	PRO	N-CA-CB	5.81	110.28	103.30
1	A	189	PRO	N-CA-CB	5.81	110.27	103.30
1	A	584	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	360	THR	O-C-N	-5.80	113.41	122.70
2	D	425	LYS	C-N-CA	5.79	136.17	121.70
1	A	636	THR	CA-CB-CG2	-5.78	104.31	112.40
2	B	493	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	82	ARG	CD-NE-CZ	5.76	131.66	123.60
1	A	69	PRO	O-C-N	-5.75	113.50	122.70
2	B	342	ARG	NE-CZ-NH2	-5.75	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	230	ALA	O-C-N	-5.74	113.52	122.70
1	A	102	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	684	VAL	C-N-CA	-5.72	110.30	122.30
1	C	642	ARG	CD-NE-CZ	5.72	131.60	123.60
2	D	78	PRO	N-CA-CB	5.71	110.16	103.30
1	C	61	LEU	C-N-CA	5.71	135.98	121.70
1	C	146	ILE	O-C-N	-5.71	113.56	122.70
2	B	171	ASP	CB-CG-OD1	5.71	123.44	118.30
2	B	525	GLY	C-N-CA	5.71	134.28	122.30
2	D	147	PRO	C-N-CA	5.70	135.96	121.70
1	C	484	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	520	GLY	O-C-N	-5.70	113.58	122.70
1	C	559	TYR	CA-CB-CG	5.70	124.22	113.40
1	A	635	GLN	CA-CB-CG	5.69	125.93	113.40
2	B	268	GLU	CA-C-N	5.69	129.72	117.20
1	A	216	PRO	N-CA-CB	5.69	110.12	103.30
1	C	54	VAL	O-C-N	-5.68	113.61	122.70
1	C	93	SER	N-CA-CB	-5.68	101.98	110.50
2	B	318	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	216	PRO	N-CA-CB	5.68	110.12	103.30
1	C	541	ALA	O-C-N	-5.67	113.62	122.70
2	D	278	ASP	CA-C-N	5.67	129.68	117.20
2	D	237	ASP	O-C-N	-5.67	113.64	122.70
1	C	545	VAL	O-C-N	-5.66	113.58	123.20
2	B	456	ARG	O-C-N	-5.65	113.66	122.70
2	D	299	ALA	N-CA-CB	5.65	118.01	110.10
2	B	500	LEU	O-C-N	-5.62	113.70	122.70
1	C	494	ALA	O-C-N	-5.61	113.73	122.70
1	A	558	ARG	CB-CG-CD	5.60	126.17	111.60
2	B	492	ARG	CD-NE-CZ	5.60	131.44	123.60
1	A	304	ALA	O-C-N	-5.60	113.75	122.70
1	C	727	ASP	CB-CG-OD2	5.59	123.33	118.30
2	D	250	ALA	N-CA-CB	5.59	117.93	110.10
2	D	43	LEU	O-C-N	-5.59	113.76	122.70
1	A	347	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	42	GLU	O-C-N	-5.58	113.77	122.70
2	B	614	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	551	ALA	O-C-N	-5.57	113.80	122.70
2	B	501	MET	CA-CB-CG	5.56	122.76	113.30
1	C	89	TYR	N-CA-CB	-5.56	100.58	110.60
2	B	47	ARG	NH1-CZ-NH2	-5.56	113.29	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	TYR	CB-CG-CD1	5.56	124.33	121.00
1	C	684	VAL	CA-CB-CG2	5.55	119.23	110.90
1	A	405	GLY	O-C-N	-5.55	113.82	122.70
2	D	538	ALA	O-C-N	-5.55	113.77	123.20
1	A	343	ASN	O-C-N	-5.54	113.83	122.70
1	C	677	ARG	CA-CB-CG	5.54	125.60	113.40
1	A	693	PHE	CB-CG-CD1	5.54	124.68	120.80
2	B	375	PRO	N-CA-CB	5.53	109.94	103.30
2	D	335	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	488	VAL	CB-CA-C	-5.52	100.91	111.40
2	B	462	ALA	O-C-N	-5.52	113.87	122.70
1	A	362	SER	N-CA-CB	5.52	118.78	110.50
2	D	507	VAL	O-C-N	-5.52	113.87	122.70
1	A	227	TYR	CG-CD1-CE1	5.52	125.71	121.30
2	D	366	ALA	N-CA-CB	5.51	117.82	110.10
1	C	268	ARG	CA-C-N	5.51	129.33	117.20
1	C	227	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	C	344	ASN	O-C-N	-5.51	113.88	122.70
1	C	268	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	C	484	ASP	CA-C-N	5.50	129.29	117.20
2	B	85	LEU	C-N-CA	-5.49	110.77	122.30
2	D	541	ASP	CA-C-O	5.49	131.63	120.10
2	D	524	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	A	658	ALA	O-C-N	-5.49	113.87	123.20
1	A	302	ARG	CD-NE-CZ	5.49	131.28	123.60
2	D	394	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	C	126	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	C	668	LEU	CB-CG-CD2	5.47	120.30	111.00
1	C	684	VAL	CG1-CB-CG2	-5.47	102.14	110.90
1	A	684	VAL	CA-CB-CG2	5.47	119.11	110.90
2	B	68	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	484	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	703	GLU	CG-CD-OE2	-5.46	107.39	118.30
1	A	658	ALA	C-N-CA	5.45	133.74	122.30
2	D	322	GLN	CA-C-O	5.45	131.54	120.10
1	A	178	TYR	O-C-N	-5.45	113.99	122.70
1	A	586	LEU	O-C-N	-5.44	113.99	122.70
1	C	120	PRO	O-C-N	-5.44	113.99	122.70
1	C	703	GLU	CA-CB-CG	5.44	125.37	113.40
1	C	263	GLY	O-C-N	-5.43	114.01	122.70
1	C	599	ARG	NH1-CZ-NH2	5.43	125.37	119.40
1	C	691	GLN	CG-CD-OE1	-5.43	110.74	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	705	TYR	CB-CG-CD2	-5.42	117.75	121.00
2	D	599	PHE	O-C-N	-5.42	114.02	122.70
1	A	63	THR	O-C-N	-5.42	114.02	122.70
1	C	589	GLU	O-C-N	-5.42	114.03	122.70
1	C	429	LYS	O-C-N	-5.42	114.03	122.70
1	C	104	ARG	CG-CD-NE	5.41	123.17	111.80
2	B	600	LYS	C-N-CA	5.41	135.23	121.70
1	C	93	SER	O-C-N	-5.41	114.05	122.70
1	C	285	SER	O-C-N	-5.41	114.05	122.70
1	A	550	ASP	CB-CG-OD2	5.41	123.16	118.30
2	D	79	LYS	O-C-N	-5.40	114.06	122.70
2	D	142	PRO	N-CA-CB	5.40	109.78	103.30
2	B	477	LYS	CA-CB-CG	5.40	125.27	113.40
1	C	166	THR	O-C-N	5.39	131.32	122.70
2	B	78	PRO	N-CA-CB	5.39	109.77	103.30
2	B	329	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
2	D	75	MET	CG-SD-CE	-5.39	91.58	100.20
2	B	147	PRO	C-N-CA	5.39	135.17	121.70
1	C	102	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	C	634	PHE	CB-CG-CD2	-5.38	117.03	120.80
2	D	418	LYS	CA-C-N	5.38	129.03	117.20
1	C	577	THR	CA-CB-CG2	5.37	119.92	112.40
2	B	108	ASP	N-CA-CB	-5.37	100.94	110.60
2	B	438	VAL	CA-CB-CG2	-5.37	102.85	110.90
2	D	84	LYS	CA-CB-CG	5.37	125.21	113.40
1	A	703	GLU	CA-CB-CG	5.36	125.19	113.40
2	D	223	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	B	524	PHE	CB-CG-CD2	-5.35	117.05	120.80
2	D	600	LYS	O-C-N	-5.34	114.15	122.70
2	D	497	PHE	CB-CG-CD2	-5.33	117.07	120.80
2	B	544	GLN	CA-CB-CG	5.33	125.13	113.40
2	D	521	ARG	O-C-N	-5.33	114.17	122.70
2	D	541	ASP	CB-CG-OD1	5.33	123.09	118.30
2	B	283	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	176	ALA	N-CA-CB	-5.32	102.65	110.10
1	C	278	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	590	PHE	CB-CG-CD2	-5.32	117.08	120.80
2	B	512	LYS	CA-CB-CG	5.32	125.10	113.40
2	D	337	TYR	C-N-CA	5.31	134.98	121.70
1	C	222	SER	O-C-N	-5.31	114.20	122.70
2	D	90	VAL	CG1-CB-CG2	-5.31	102.40	110.90
2	B	364	THR	O-C-N	-5.31	114.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	C	91	GLY	N-CA-C	-5.31	99.83	113.10
1	C	438	GLU	O-C-N	-5.31	114.21	122.70
1	C	344	ASN	CA-C-N	5.30	128.87	117.20
1	A	369	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	348	PHE	CB-CG-CD1	5.29	124.50	120.80
1	C	529	ARG	N-CA-CB	-5.29	101.07	110.60
1	A	61	LEU	CA-C-N	5.29	128.83	117.20
1	C	471	ARG	CA-CB-CG	5.28	125.03	113.40
2	D	403	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	646	GLU	O-C-N	-5.28	114.25	122.70
2	D	347	THR	O-C-N	-5.28	114.25	122.70
2	D	502	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	313	HIS	O-C-N	-5.28	114.26	122.70
1	A	429	LYS	C-N-CA	5.27	134.88	121.70
1	A	200	ILE	O-C-N	-5.27	114.27	122.70
1	C	133	ALA	C-N-CA	5.26	133.35	122.30
2	B	232	ARG	CD-NE-CZ	5.26	130.97	123.60
1	C	123	ARG	C-N-CA	5.25	133.33	122.30
1	C	282	PRO	O-C-N	-5.25	114.29	122.70
2	B	99	VAL	CA-CB-CG1	5.25	118.78	110.90
2	D	301	ARG	CA-C-N	5.25	128.75	117.20
1	A	120	PRO	O-C-N	-5.25	114.31	122.70
2	D	425	LYS	O-C-N	-5.25	114.31	122.70
1	A	6	ARG	CD-NE-CZ	5.25	130.94	123.60
2	B	90	VAL	CA-CB-CG2	5.24	118.77	110.90
1	C	70	PHE	CD1-CE1-CZ	5.24	126.39	120.10
2	B	242	HIS	O-C-N	-5.24	114.32	122.70
1	A	445	ARG	CD-NE-CZ	5.23	130.93	123.60
1	A	669	ARG	CB-CG-CD	5.23	125.21	111.60
1	A	333	GLY	CA-C-O	5.23	130.01	120.60
2	B	449	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	D	503	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	75	TYR	O-C-N	-5.22	114.34	122.70
2	B	92	PRO	O-C-N	-5.22	114.34	122.70
1	C	485	ASN	N-CA-CB	5.22	120.00	110.60
1	A	87	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	B	190	ALA	O-C-N	-5.22	114.35	122.70
1	A	24	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	465	ILE	CA-C-O	5.21	131.04	120.10
1	C	529	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	D	398	PRO	O-C-N	-5.21	114.37	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	PRO	N-CA-CB	5.21	109.55	103.30
1	A	25	PHE	O-C-N	-5.20	114.38	122.70
1	A	87	ARG	CD-NE-CZ	5.20	130.88	123.60
1	C	170	ALA	O-C-N	-5.20	114.38	122.70
1	A	325	LEU	CB-CG-CD2	5.20	119.83	111.00
1	A	674	LYS	CA-CB-CG	5.20	124.83	113.40
1	C	662	LEU	CA-C-N	5.19	128.62	117.20
1	A	528	ASP	C-N-CA	5.19	134.67	121.70
1	A	101	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	A	326	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	D	588	ALA	CA-C-N	5.18	126.57	116.20
1	A	639	GLU	OE1-CD-OE2	-5.18	117.09	123.30
2	B	124	ALA	O-C-N	-5.18	114.42	122.70
1	C	341	VAL	O-C-N	-5.17	114.42	122.70
1	A	669	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	20	THR	CA-C-N	5.17	128.57	117.20
1	C	529	ARG	CB-CG-CD	-5.17	98.17	111.60
1	A	447	GLU	O-C-N	-5.16	114.44	122.70
2	B	299	ALA	N-CA-CB	5.16	117.33	110.10
2	D	617	LEU	CA-CB-CG	5.16	127.18	115.30
2	D	377	ARG	NH1-CZ-NH2	5.16	125.08	119.40
2	D	380	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	702	VAL	CA-CB-CG2	5.15	118.62	110.90
1	A	547	GLU	O-C-N	-5.15	114.47	122.70
1	A	690	GLU	C-N-CA	5.14	134.56	121.70
1	A	673	ASP	O-C-N	-5.14	114.48	122.70
1	C	247	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	A	527	PRO	N-CA-CB	5.14	109.47	103.30
1	C	500	ARG	CD-NE-CZ	5.14	130.79	123.60
1	A	178	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	B	298	ARG	CD-NE-CZ	5.13	130.79	123.60
2	D	117	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	B	401	GLY	O-C-N	-5.13	114.49	122.70
2	D	370	PRO	N-CA-CB	5.13	109.45	103.30
1	C	433	MET	CA-CB-CG	-5.12	104.59	113.30
1	C	381	ARG	CG-CD-NE	-5.12	101.04	111.80
2	B	218	GLY	O-C-N	-5.12	114.50	122.70
1	A	602	LEU	CB-CG-CD2	5.12	119.70	111.00
2	D	337	TYR	CA-C-N	5.12	128.46	117.20
2	D	147	PRO	N-CA-CB	5.12	109.44	103.30
2	D	127	GLU	O-C-N	-5.11	114.51	123.20
2	D	314	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	ASP	O-C-N	-5.11	114.53	122.70
1	C	419	LYS	N-CA-CB	5.11	119.79	110.60
1	A	226	ALA	N-CA-CB	-5.11	102.95	110.10
1	A	231	ASN	O-C-N	-5.10	114.54	122.70
2	B	176	ALA	O-C-N	-5.10	114.54	122.70
2	D	191	LYS	C-N-CA	5.10	134.45	121.70
2	D	223	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	130	PRO	CA-C-N	5.10	128.42	117.20
2	D	23	LEU	O-C-N	-5.10	114.55	122.70
2	D	566	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	456	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	268	ARG	O-C-N	-5.09	114.55	122.70
1	A	582	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	137	GLY	CA-C-N	5.09	128.39	117.20
1	C	212	TYR	CA-C-O	5.09	130.78	120.10
1	A	146	ILE	O-C-N	-5.07	114.58	122.70
1	C	241	SER	C-N-CA	5.07	132.95	122.30
1	A	40	THR	O-C-N	-5.07	114.58	122.70
1	C	139	ALA	C-N-CA	5.07	132.95	122.30
2	B	362	PRO	N-CA-CB	5.07	109.38	103.30
1	C	16	PRO	O-C-N	-5.07	114.59	122.70
1	A	475	GLU	CA-CB-CG	5.06	124.53	113.40
1	C	306	MET	CG-SD-CE	5.05	108.29	100.20
1	C	518	ALA	CB-CA-C	-5.05	102.52	110.10
2	D	315	GLU	O-C-N	-5.05	114.61	122.70
1	C	178	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	518	ALA	O-C-N	-5.05	114.62	122.70
2	D	32	GLU	O-C-N	-5.05	114.62	122.70
2	D	601	GLU	O-C-N	-5.05	114.62	122.70
2	B	261	GLU	O-C-N	-5.04	114.63	122.70
2	B	573	VAL	CA-C-N	5.04	128.29	117.20
1	C	633	LEU	O-C-N	-5.04	114.64	122.70
1	C	79	TYR	CB-CG-CD1	5.04	124.02	121.00
2	D	363	PHE	C-N-CA	5.03	134.28	121.70
2	D	503	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	126	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	313	HIS	C-N-CA	5.03	134.28	121.70
2	D	108	ASP	CB-CG-OD1	5.03	122.82	118.30
2	B	413	ALA	CA-C-N	5.03	128.25	117.20
1	C	658	ALA	O-C-N	-5.03	114.66	123.20
2	D	77	ARG	CA-C-O	5.03	130.66	120.10
2	D	254	TRP	O-C-N	-5.03	114.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	189	PRO	N-CA-CB	5.02	109.32	103.30
1	C	314	GLN	CA-CB-CG	5.02	124.44	113.40
2	D	55	PHE	CG-CD1-CE1	-5.02	115.28	120.80
2	D	493	ASP	CB-CG-OD1	5.02	122.81	118.30
2	B	32	GLU	O-C-N	-5.01	114.68	122.70
1	C	648	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	302	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	D	333	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	C	222	SER	N-CA-CB	-5.00	103.00	110.50
1	C	233	PRO	N-CA-CB	5.00	109.30	103.30

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	MET	Mainchain
1	A	194	GLY	Mainchain
1	A	231	ASN	Mainchain
1	A	268	ARG	Mainchain
1	A	277	VAL	Mainchain
1	A	278	ASP	Mainchain
1	A	280	PHE	Mainchain
1	A	281	ALA	Mainchain
1	A	342	TYR	Mainchain
1	A	371	ALA	Mainchain
1	A	376	THR	Mainchain
1	A	394	SER	Mainchain
1	A	395	GLY	Mainchain
1	A	40	THR	Mainchain
1	A	405	GLY	Mainchain
1	A	41	ALA	Mainchain
1	A	420	ALA	Mainchain
1	A	504	ASP	Mainchain
1	A	540	ARG	Mainchain
1	A	61	LEU	Mainchain
1	A	633	LEU	Mainchain
1	A	645	VAL	Mainchain
1	A	670	LYS	Mainchain
1	A	70	PHE	Mainchain
1	A	87	ARG	Mainchain
2	B	106	ALA	Mainchain
2	B	129	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	154	LEU	Mainchain
2	B	173	GLY	Mainchain
2	B	222	ARG	Mainchain
2	B	246	ALA	Mainchain
2	B	264	ARG	Mainchain
2	B	273	ALA	Mainchain
2	B	334	GLU	Mainchain
2	B	394	ARG	Mainchain
2	B	401	GLY	Mainchain
2	B	456	ARG	Mainchain
2	B	457	LYS	Mainchain
2	B	500	LEU	Mainchain
2	B	521	ARG	Mainchain
2	B	522	ARG	Mainchain
2	B	599	PHE	Mainchain
2	B	629	SER	Mainchain
2	B	71	ASP	Mainchain
2	B	84	LYS	Mainchain
2	B	86	GLY	Mainchain
1	C	162	SER	Mainchain
1	C	167	MET	Mainchain
1	C	179	VAL	Mainchain
1	C	183	GLU	Mainchain
1	C	194	GLY	Mainchain
1	C	205	MET	Mainchain
1	C	228	THR	Mainchain
1	C	230	ALA	Mainchain
1	C	268	ARG	Mainchain
1	C	271	GLU	Mainchain
1	C	285	SER	Mainchain
1	C	292	MET	Mainchain
1	C	357	GLN	Mainchain
1	C	359	HIS	Mainchain
1	C	369	ASP	Mainchain
1	C	371	ALA	Mainchain
1	C	376	THR	Mainchain
1	C	391	GLN	Mainchain
1	C	394	SER	Mainchain
1	C	40	THR	Mainchain
1	C	403	TRP	Mainchain
1	C	405	GLY	Mainchain
1	C	460	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	C	479	ASP	Mainchain
1	C	51	ASN	Mainchain
1	C	526	ASP	Mainchain
1	C	531	LEU	Mainchain
1	C	540	ARG	Mainchain
1	C	588	GLU	Mainchain
1	C	622	ALA	Mainchain
1	C	638	GLU	Mainchain
1	C	645	VAL	Mainchain
1	C	674	LYS	Mainchain
1	C	677	ARG	Mainchain
1	C	693	PHE	Mainchain
1	C	70	PHE	Mainchain
1	C	723	ARG	Mainchain
2	D	154	LEU	Mainchain
2	D	220	TRP	Mainchain
2	D	228	SER	Mainchain
2	D	287	THR	Mainchain
2	D	319	GLY	Mainchain
2	D	334	GLU	Mainchain
2	D	335	ASP	Mainchain
2	D	336	PRO	Mainchain
2	D	338	VAL	Mainchain
2	D	348	PHE	Mainchain
2	D	35	TRP	Mainchain
2	D	401	GLY	Mainchain
2	D	456	ARG	Mainchain
2	D	563	GLN	Mainchain
2	D	61	ARG	Mainchain
2	D	622	ASP	Mainchain
2	D	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	5563	0	5443	41	0
1	C	5560	0	5456	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4695	0	4610	40	0
2	D	4692	0	4580	48	0
3	A	91	0	88	11	0
3	C	91	0	88	10	0
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	12	0	16	3	0
5	B	18	0	24	2	0
5	C	12	0	16	3	0
5	D	12	0	15	1	0
6	A	457	0	0	0	0
6	B	318	0	0	1	0
6	C	493	0	0	2	0
6	D	264	0	0	1	0
All	All	22372	0	20400	178	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 4.

All (178) 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:A:800:B12:H363	3:A:800:B12:C42	1.54	1.29
3:A:800:B12:C36	3:A:800:B12:H421	1.67	1.23
3:A:800:B12:H531	3:A:800:B12:H552	1.24	1.10
3:A:800:B12:H372	3:A:800:B12:H351	1.51	0.90
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.20	0.89
1:C:330:GLN:HE22	5:C:802:GOL:H31	1.39	0.88
3:A:800:B12:H531	3:A:800:B12:C55	2.02	0.84
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.25	0.83
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.62	0.80
3:C:800:B12:H372	3:C:800:B12:H351	1.64	0.80
3:A:800:B12:H363	3:A:800:B12:H421	0.80	0.76
1:A:330:GLN:HE22	5:A:802:GOL:H31	1.53	0.73
1:C:638:GLU:HA	1:C:671:GLU:HG3	1.70	0.72
3:C:800:B12:H531	3:C:800:B12:H552	1.71	0.72
1:A:24:ARG:HH22	2:B:315:GLU:HG3	1.57	0.70
2:D:180:VAL:HG13	2:D:197:LEU:HD21	1.72	0.69
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.75	0.68
2:B:586:LYS:HD3	2:B:593:LEU:HD12	1.74	0.68
3:C:800:B12:H301	3:C:800:B12:H203	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.79	0.65
3:A:800:B12:H372	3:A:800:B12:C35	2.26	0.65
1:C:247:GLU:HB3	3:C:800:B12:H532	1.78	0.64
1:C:374:LEU:HB2	1:C:481:LEU:HD23	1.78	0.64
1:C:706:THR:HB	1:C:707:PRO:CD	2.27	0.64
1:A:706:THR:HB	1:A:707:PRO:HD2	1.79	0.64
1:A:247:GLU:HB3	3:A:800:B12:H532	1.78	0.64
2:B:98:THR:HB	5:B:639:GOL:H11	1.80	0.63
1:A:359:HIS:CE1	1:A:401:ASP:H	2.16	0.63
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.81	0.63
2:D:83:LYS:H	2:D:84:LYS:NZ	1.96	0.62
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.45	0.62
1:C:188:LYS:H	1:C:191:GLN:HE21	1.48	0.61
1:C:188:LYS:H	1:C:191:GLN:NE2	1.98	0.61
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.83	0.61
1:A:188:LYS:H	1:A:191:GLN:HE21	1.49	0.61
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.48	0.61
2:D:191:LYS:HA	2:D:227:PHE:HA	1.82	0.61
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.84	0.60
2:B:468:MET:HE3	2:B:471:ALA:HA	1.85	0.59
2:B:391:ASN:ND2	2:B:394:ARG:HE	2.01	0.58
2:D:108:ASP:HB3	2:D:357:SER:HA	1.85	0.58
1:A:706:THR:HB	1:A:707:PRO:CD	2.33	0.58
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.85	0.58
1:C:706:THR:HB	1:C:707:PRO:HD2	1.85	0.57
1:C:330:GLN:NE2	5:C:802:GOL:H31	2.16	0.57
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.87	0.57
1:A:188:LYS:H	1:A:191:GLN:NE2	2.02	0.56
2:D:138:LEU:HD23	2:D:145:ILE:HD13	1.88	0.56
1:A:374:LEU:HB2	1:A:481:LEU:HD23	1.87	0.56
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.88	0.56
1:C:357:GLN:HE22	2:D:290:GLN:NE2	2.01	0.56
3:C:800:B12:C35	3:C:800:B12:H372	2.36	0.56
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.87	0.55
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.89	0.55
2:D:172:GLN:NE2	2:D:204:PHE:HB2	2.21	0.54
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.05	0.54
2:D:297:LEU:HA	2:D:322:GLN:HE22	1.72	0.54
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.55	0.54
1:C:359:HIS:CE1	1:C:401:ASP:H	2.25	0.54
2:D:83:LYS:HB2	2:D:84:LYS:HZ1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:THR:HG22	1:A:580:VAL:H	1.72	0.54
2:B:493:ASP:HA	5:B:640:GOL:H31	1.90	0.53
3:A:800:B12:H601	3:A:800:B12:H252	1.91	0.53
2:D:83:LYS:H	2:D:84:LYS:HZ2	1.56	0.53
1:A:651:VAL:HB	1:A:722:LEU:HD21	1.91	0.52
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.92	0.52
1:A:359:HIS:HE1	1:A:401:ASP:H	1.57	0.52
1:C:571:SER:HB3	1:C:623:ASP:HB3	1.91	0.52
1:A:357:GLN:HE22	2:B:290:GLN:NE2	2.00	0.52
1:C:602:LEU:HD12	1:C:618:ALA:HB2	1.92	0.51
1:C:372:ILE:HG22	1:C:480:VAL:HG11	1.91	0.51
1:A:683:THR:HG21	1:A:718:LEU:HD13	1.94	0.50
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.93	0.50
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.94	0.50
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.58	0.50
2:B:579:LEU:HD11	2:B:583:LYS:HE3	1.92	0.50
1:A:133:ALA:HB1	1:A:489:LEU:HD21	1.93	0.50
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.93	0.50
1:C:372:ILE:HG23	6:C:1277:HOH:O	2.12	0.50
1:C:372:ILE:CG2	1:C:480:VAL:HG11	2.41	0.49
3:C:800:B12:H531	3:C:800:B12:C55	2.40	0.49
2:D:532:SER:CB	2:D:533:PRO:HD3	2.43	0.49
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.94	0.49
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.95	0.49
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.37	0.49
2:B:202:ILE:HG13	2:B:214:LEU:HD11	1.94	0.49
2:D:122:ARG:HH11	2:D:122:ARG:HB3	1.77	0.49
3:C:800:B12:H492	3:C:800:B12:C47	2.43	0.49
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.95	0.48
1:C:7:PHE:HA	1:C:10:VAL:HG23	1.95	0.48
1:A:149:MET:HG3	1:A:177:LEU:HB3	1.94	0.48
1:A:330:GLN:NE2	5:A:802:GOL:H31	2.26	0.48
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.94	0.47
1:C:15:ALA:HA	1:C:16:PRO:HD2	1.57	0.47
2:B:468:MET:HE1	6:B:646:HOH:O	2.15	0.47
2:B:503:ARG:NE	2:B:638:LYS:HB3	2.30	0.47
2:B:284:VAL:HG11	2:B:322:GLN:HE21	1.79	0.47
1:C:69:PRO:HB2	1:C:306:MET:HG2	1.96	0.47
1:A:541:ALA:O	1:A:542:MET:HB2	2.15	0.46
1:C:94:THR:HG22	1:C:488:VAL:HG13	1.97	0.46
1:C:149:MET:HG3	1:C:177:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.96	0.46
2:D:234:VAL:HB	2:D:280:ILE:HG12	1.97	0.46
1:C:52:GLU:HG3	2:D:85:LEU:HG	1.97	0.46
1:C:15:ALA:HB1	2:D:92:PRO:HG3	1.98	0.46
1:A:602:LEU:HD22	3:A:800:B12:HM52	1.97	0.45
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.98	0.45
1:C:44:ILE:HD11	1:C:419:LYS:HD2	1.98	0.45
2:D:107:TRP:CD1	2:D:358:ILE:HD12	2.51	0.45
2:B:80:ASP:HB3	2:B:407:SER:HB2	1.97	0.45
2:B:431:LYS:O	2:B:435:THR:HB	2.16	0.45
1:A:606:GLY:O	1:A:634:PHE:HA	2.16	0.45
1:A:310:LYS:HE2	2:B:21:LEU:HD11	1.98	0.45
1:A:599:ARG:HG2	1:A:649:VAL:HA	1.99	0.45
1:C:215:GLN:N	1:C:216:PRO:HD2	2.31	0.45
1:C:415:ASP:O	1:C:419:LYS:HG3	2.17	0.45
2:B:116:PRO:HG3	2:B:480:PRO:HG3	1.99	0.45
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.51	0.45
1:C:305:ARG:HG2	1:C:325:LEU:HB3	1.99	0.45
1:C:458:ASP:HB3	1:C:710:VAL:HG13	1.99	0.45
1:A:188:LYS:N	1:A:191:GLN:HE21	2.12	0.44
1:C:17:VAL:N	2:D:92:PRO:HD3	2.32	0.44
1:C:197:GLN:HA	1:C:239:SER:HB3	1.99	0.44
1:C:358:GLY:O	1:C:359:HIS:HB2	2.17	0.44
2:D:397:ASP:N	2:D:398:PRO:HD3	2.32	0.44
1:A:372:ILE:HG22	1:A:480:VAL:HG11	2.00	0.44
1:A:514:LYS:HD3	1:A:534:LEU:HD22	2.00	0.44
2:D:113:HIS:HB2	2:D:138:LEU:HG	2.00	0.44
2:D:501:MET:HE3	6:D:1463:HOH:O	2.17	0.44
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.99	0.44
2:D:252:LEU:HD11	2:D:300:LEU:HA	1.99	0.44
1:A:69:PRO:HG3	2:B:24:ALA:HA	2.01	0.43
2:B:518:LEU:HB2	2:B:569:SER:HB2	2.00	0.43
1:C:711:ILE:N	1:C:712:PRO:HD2	2.33	0.43
3:C:800:B12:H363	3:C:800:B12:C42	2.48	0.43
1:A:129:ASN:HA	1:A:130:PRO:HD2	1.88	0.43
2:D:370:PRO:HB3	2:D:375:PRO:HG2	2.01	0.43
2:D:218:GLY:O	2:D:222:ARG:HG3	2.18	0.43
2:D:365:GLN:HE21	5:D:1:GOL:H31	1.83	0.43
1:A:4:LEU:HD13	2:B:264:ARG:HG2	2.01	0.43
1:A:4:LEU:HA	1:A:5:PRO:HD2	1.89	0.43
2:D:390:VAL:HG12	2:D:392:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.54	0.43
2:B:193:LEU:O	2:B:227:PHE:HB3	2.19	0.43
2:D:429:MET:HA	2:D:432:ALA:HB3	2.01	0.43
1:C:6:ARG:HA	1:C:6:ARG:HD3	1.89	0.42
2:B:331:LEU:HD13	2:B:365:GLN:HB3	2.01	0.42
1:C:330:GLN:HE22	5:C:802:GOL:C3	2.21	0.42
2:D:146:ALA:HB3	2:D:149:HIS:ND1	2.34	0.42
2:B:114:GLU:HG2	2:B:139:ARG:HB2	2.01	0.42
2:B:274:THR:HA	2:B:313:VAL:HG13	2.01	0.42
1:C:641:ALA:CB	1:C:671:GLU:HB3	2.49	0.42
1:C:521:ASN:O	1:C:529:ARG:HD3	2.20	0.42
2:D:294:ILE:HG12	2:D:352:VAL:HB	2.02	0.42
2:D:517:CYS:HB2	2:D:545:VAL:O	2.20	0.42
2:D:267:VAL:HA	2:D:271:PHE:O	2.20	0.41
1:A:281:ALA:HA	1:A:284:LEU:HG	2.01	0.41
1:A:116:ALA:O	1:A:141:VAL:HG12	2.20	0.41
1:A:139:ALA:HB1	3:A:800:B12:H362	2.02	0.41
2:D:80:ASP:HB3	2:D:407:SER:HB2	2.02	0.41
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.49	0.41
2:B:115:ASP:OD2	2:B:477:LYS:HE3	2.21	0.41
1:A:203:GLU:HA	1:A:207:ARG:HB3	2.02	0.41
2:D:125:ILE:HD11	2:D:138:LEU:HD21	2.02	0.41
1:C:602:LEU:HD22	3:C:800:B12:HM52	2.03	0.41
2:D:263:VAL:O	2:D:267:VAL:HG23	2.20	0.41
1:C:16:PRO:HD2	2:D:92:PRO:HB3	2.01	0.41
1:A:246:GLN:HE22	1:A:291:GLY:HA3	1.86	0.41
2:D:532:SER:HB3	2:D:533:PRO:HD3	2.02	0.41
1:C:252:ALA:O	1:C:256:MET:HG3	2.21	0.41
1:C:563:ILE:HD11	6:C:1048:HOH:O	2.21	0.41
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.51	0.41
2:D:455:ASN:HA	2:D:621:MET:O	2.20	0.41
1:A:243:TYR:HE2	5:A:802:GOL:H2	1.86	0.40
3:C:800:B12:H203	3:C:800:B12:C30	2.47	0.40
1:C:386:THR:HA	2:D:341:LEU:HD13	2.02	0.40
1:A:10:VAL:HG11	2:B:310:VAL:HG21	2.03	0.40
2:D:571:ALA:HA	2:D:601:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/727 (100%)	698 (96%)	26 (4%)	1 (0%)	51	49
1	C	725/727 (100%)	685 (94%)	37 (5%)	3 (0%)	34	30
2	B	617/637 (97%)	595 (96%)	21 (3%)	1 (0%)	47	44
2	D	620/637 (97%)	580 (94%)	38 (6%)	2 (0%)	41	37
All	All	2687/2728 (98%)	2558 (95%)	122 (4%)	7 (0%)	41	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ALA
1	C	16	PRO
2	D	228	SER
1	A	486	SER
1	C	486	SER
2	B	45	ARG
2	D	435	THR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/590 (97%)	550 (96%)	21 (4%)	34	32
1	C	571/590 (97%)	551 (96%)	20 (4%)	36	35
2	B	474/509 (93%)	455 (96%)	19 (4%)	31	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	472/509 (93%)	448 (95%)	24 (5%)	24	19
All	All	2088/2198 (95%)	2004 (96%)	84 (4%)	31	29

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	LEU
1	A	9	SER
1	A	93	SER
1	A	127	SER
1	A	162	SER
1	A	207	ARG
1	A	287	PHE
1	A	430	VAL
1	A	473	GLU
1	A	485	ASN
1	A	533	LYS
1	A	567	SER
1	A	576	ASN
1	A	585	GLU
1	A	596	ARG
1	A	597	ARG
1	A	599	ARG
1	A	668	LEU
1	A	669	ARG
1	A	725	SER
2	B	60	LYS
2	B	83	LYS
2	B	119	LYS
2	B	134	THR
2	B	180	VAL
2	B	186	SER
2	B	191	LYS
2	B	216	VAL
2	B	226	LYS
2	B	279	THR
2	B	288	HIS
2	B	334	GLU
2	B	410	ARG
2	B	435	THR
2	B	436	GLU

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Mol	Chain	Res	Type
2	B	475	GLU
2	B	586	LYS
2	B	593	LEU
2	B	629	SER
1	C	4	LEU
1	C	6	ARG
1	C	52	GLU
1	C	93	SER
1	C	96	LYS
1	C	162	SER
1	C	207	ARG
1	C	287	PHE
1	C	487	THR
1	C	529	ARG
1	C	558	ARG
1	C	562	GLN
1	C	567	SER
1	C	575	LYS
1	C	577	THR
1	C	596	ARG
1	C	668	LEU
1	C	691	GLN
1	C	712	PRO
1	C	721	LYS
2	D	22	SER
2	D	83	LYS
2	D	84	LYS
2	D	141	ASP
2	D	155	SER
2	D	185	ARG
2	D	187	ASP
2	D	227	PHE
2	D	232	ARG
2	D	288	HIS
2	D	316	ASP
2	D	317	LYS
2	D	334	GLU
2	D	335	ASP
2	D	371	GLU
2	D	380	ARG
2	D	410	ARG
2	D	411	SER

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Mol	Chain	Res	Type
2	D	425	LYS
2	D	477	LYS
2	D	522	ARG
2	D	532	SER
2	D	559	LYS
2	D	617	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	198	ASN
1	A	246	GLN
1	A	330	GLN
1	A	359	HIS
1	A	366	ASN
1	A	385	ASN
1	A	454	GLN
1	A	485	ASN
1	A	492	GLN
1	A	592	GLN
1	A	635	GLN
1	A	643	GLN
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	391	ASN
1	C	14	ASN
1	C	191	GLN
1	C	198	ASN
1	C	246	GLN
1	C	330	GLN
1	C	359	HIS
1	C	366	ASN
1	C	385	ASN
1	C	454	GLN
1	C	492	GLN
1	C	635	GLN
1	C	643	GLN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN

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Mol	Chain	Res	Type
2	D	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 ⓘ

13 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	$\# Z  > 2$
5	GOL	B	1	-	5,5,5	0.66	0	5,5,5	0.25	0
4	DCA	C	801	-	41,49,49	1.36	6 (14%)	51,74,74	1.67	12 (23%)
4	DCA	A	801	-	41,49,49	1.28	4 (9%)	51,74,74	1.27	4 (7%)
5	GOL	C	803	-	5,5,5	0.50	0	5,5,5	0.59	0
3	B12	C	800	1,6	80,101,101	1.95	7 (8%)	101,166,166	2.41	40 (39%)
5	GOL	D	1	-	5,5,5	0.58	0	5,5,5	2.03	1 (20%)
5	GOL	A	803	-	5,5,5	0.80	0	5,5,5	0.62	0
3	B12	A	800	1	80,101,101	2.01	9 (11%)	101,166,166	2.22	33 (32%)
5	GOL	C	802	-	5,5,5	1.05	0	5,5,5	2.77	1 (20%)
5	GOL	A	802	-	5,5,5	0.76	0	5,5,5	1.68	1 (20%)
5	GOL	B	640	-	5,5,5	0.44	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	D	639	-	5,5,5	0.21	0	5,5,5	0.86	0
5	GOL	B	639	-	5,5,5	0.29	0	5,5,5	0.55	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
5	GOL	B	1	-	-	0/4/4/4	-
4	DCA	C	801	-	-	2/43/63/63	0/3/3/3
4	DCA	A	801	-	-	2/43/63/63	0/3/3/3
5	GOL	C	803	-	-	0/4/4/4	-
3	B12	C	800	1,6	-	6/51/223/223	0/3/11/11
5	GOL	D	1	-	-	3/4/4/4	-
5	GOL	A	803	-	-	0/4/4/4	-
3	B12	A	800	1	-	10/51/223/223	0/3/11/11
5	GOL	C	802	-	-	0/4/4/4	-
5	GOL	A	802	-	-	0/4/4/4	-
5	GOL	B	640	-	-	4/4/4/4	-
5	GOL	D	639	-	-	2/4/4/4	-
5	GOL	B	639	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	CO-N21	-13.18	1.56	1.89
3	A	800	B12	CO-N21	-13.04	1.57	1.89
3	A	800	B12	CO-N23	-5.73	1.66	1.94
3	C	800	B12	CO-N23	-4.90	1.70	1.94
4	A	801	DCA	P3B-O3B	4.71	1.68	1.59
3	A	800	B12	P-O2	3.54	1.69	1.60
3	C	800	B12	P-O2	3.39	1.69	1.60
3	A	800	B12	C17-C18	-3.12	1.50	1.54
3	A	800	B12	C55-C56	3.09	1.60	1.53
3	C	800	B12	CO-N22	2.95	2.08	1.94
4	C	801	DCA	P3B-O3B	2.85	1.64	1.59
3	C	800	B12	C3R-C4R	2.59	1.59	1.52
4	C	801	DCA	C7P-N8P	2.52	1.51	1.46
4	C	801	DCA	O5P-C5P	2.52	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	801	DCA	P1A-O1A	-2.45	1.42	1.50
4	C	801	DCA	CDP-CBP	-2.25	1.48	1.53
3	A	800	B12	C3R-C4R	2.20	1.58	1.52
4	A	801	DCA	P2A-O5A	-2.19	1.45	1.55
3	A	800	B12	O58-C57	-2.19	1.18	1.23
3	A	800	B12	C6M-C6B	-2.17	1.46	1.51
4	C	801	DCA	P3B-O8A	-2.09	1.46	1.54
3	C	800	B12	P-O4	-2.08	1.43	1.50
3	A	800	B12	C56-C57	2.04	1.55	1.51
4	A	801	DCA	C8A-N7A	-2.02	1.31	1.34
4	A	801	DCA	C2A-N3A	2.01	1.35	1.32
3	C	800	B12	P-O5	-2.01	1.45	1.55

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C16-C15-C14	-7.25	112.96	124.27
3	C	800	B12	C7B-C8B-C9B	6.30	126.77	120.54
5	C	802	GOL	O3-C3-C2	6.03	139.09	110.20
3	C	800	B12	C16-C15-C14	-5.81	115.20	124.27
3	C	800	B12	C41-C42-C43	5.41	130.93	112.59
3	A	800	B12	C12-C11-C10	-5.29	115.68	124.64
3	C	800	B12	C2P-C1P-N59	-5.28	105.15	112.93
4	C	801	DCA	C7P-N8P-C9P	-5.23	113.26	122.59
3	A	800	B12	C7B-C8B-C9B	5.10	125.58	120.54
3	A	800	B12	C55-C56-C57	-5.03	100.25	111.23
3	C	800	B12	C13-C14-C15	-4.93	113.80	131.68
3	A	800	B12	C2P-C1P-N59	-4.83	105.81	112.93
3	C	800	B12	C25-C2-C1	4.54	120.55	113.80
3	A	800	B12	C1-C19-N24	-4.52	101.15	106.24
3	C	800	B12	C1P-N59-C57	-4.52	112.84	122.69
3	A	800	B12	C1P-N59-C57	-4.47	112.96	122.69
3	A	800	B12	C13-C14-C15	-4.45	115.54	131.68
3	A	800	B12	C25-C2-C1	4.45	120.41	113.80
3	C	800	B12	O44-C43-N45	-4.38	110.53	122.50
3	C	800	B12	C30-C31-C32	4.37	127.40	112.59
3	A	800	B12	C55-C17-C18	4.35	119.54	111.14
3	C	800	B12	C36-C7-C8	-4.26	104.43	112.11
3	A	800	B12	C56-C55-C17	-4.23	107.32	115.50
4	A	801	DCA	CEP-CBP-CCP	4.08	114.89	108.23
3	C	800	B12	O44-C43-C42	4.02	132.87	121.07
3	A	800	B12	O6R-C1R-C2R	-3.91	101.21	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801	DCA	C4A-C5A-N7A	3.90	113.47	109.40
3	C	800	B12	C49-C50-N52	3.89	128.63	116.51
3	C	800	B12	C55-C17-C18	3.85	118.58	111.14
3	C	800	B12	C20-C1-C19	3.77	112.99	109.36
3	C	800	B12	C5B-C4B-C9B	-3.77	115.89	121.22
3	C	800	B12	C1-C2-C3	-3.76	96.87	101.59
5	D	1	GOL	C3-C2-C1	3.68	126.01	111.70
3	C	800	B12	C2-C1-C19	-3.68	112.80	118.60
4	A	801	DCA	C7P-N8P-C9P	-3.67	116.04	122.59
3	C	800	B12	C37-C7-C8	3.64	118.11	108.37
3	C	800	B12	O6R-C1R-C2R	-3.61	101.65	106.93
4	C	801	DCA	C5A-C6A-N6A	3.61	125.84	120.35
3	A	800	B12	O5-P-O4	3.57	129.87	112.24
3	C	800	B12	C55-C17-C16	3.51	121.60	109.92
3	A	800	B12	C36-C7-C8	-3.50	105.80	112.11
3	C	800	B12	C25-C2-C3	-3.42	110.36	115.58
3	C	800	B12	O51-C50-C49	-3.42	111.03	121.07
3	C	800	B12	C12-C11-C10	-3.41	118.85	124.64
3	A	800	B12	C5B-C4B-C9B	-3.29	116.57	121.22
3	C	800	B12	O28-C27-N29	-3.21	113.75	122.50
5	A	802	GOL	O3-C3-C2	3.18	125.45	110.20
3	C	800	B12	C56-C55-C17	-3.13	109.44	115.50
4	A	801	DCA	CDP-CBP-CAP	-3.09	103.46	108.82
3	C	800	B12	O5-P-O4	3.09	127.51	112.24
4	C	801	DCA	O9P-C9P-N8P	3.00	129.43	122.99
3	A	800	B12	O51-C50-C49	-2.99	112.27	121.07
3	A	800	B12	C37-C7-C8	2.99	116.37	108.37
3	A	800	B12	C9-C10-C11	-2.79	121.17	130.91
3	C	800	B12	C3-C4-C5	-2.78	121.59	131.68
3	A	800	B12	O63-C61-C60	-2.76	115.06	120.87
4	C	801	DCA	O8A-P3B-O7A	2.70	121.23	110.68
3	A	800	B12	C3-C4-C5	-2.63	122.14	131.68
3	C	800	B12	C9-C10-C11	-2.57	121.92	130.91
3	C	800	B12	C15-C14-N23	2.56	128.97	124.64
3	C	800	B12	C6-C5-C4	-2.55	120.30	124.27
3	A	800	B12	C2-C1-C19	-2.54	114.59	118.60
3	A	800	B12	O58-C57-C56	-2.49	117.47	122.02
3	A	800	B12	C26-C27-N29	2.47	124.34	116.52
3	C	800	B12	C55-C56-C57	-2.38	106.03	111.23
4	C	801	DCA	C1B-N9A-C4A	-2.33	122.54	126.64
4	C	801	DCA	O6A-CCP-CBP	-2.33	106.80	110.55
3	A	800	B12	C48-C13-C12	-2.32	110.15	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C4B-C5B-C6B	2.30	123.79	119.91
4	C	801	DCA	O9P-C9P-CAP	-2.28	114.12	121.06
3	C	800	B12	C26-C27-N29	2.28	123.73	116.52
3	A	800	B12	C55-C17-C16	2.27	117.49	109.92
3	A	800	B12	C4B-C5B-C6B	2.27	123.73	119.91
3	A	800	B12	C36-C7-C37	2.24	114.66	110.83
4	A	801	DCA	O8A-P3B-O7A	2.24	119.44	110.68
3	C	800	B12	C56-C57-N59	-2.24	112.65	116.42
4	C	801	DCA	O5B-C5B-C4B	2.23	116.65	108.99
3	A	800	B12	O28-C27-N29	-2.21	116.46	122.50
3	C	800	B12	C31-C32-N33	2.20	123.37	116.51
3	A	800	B12	C60-C18-C17	2.20	121.06	115.74
3	A	800	B12	C8-C9-N22	2.20	113.87	111.12
3	C	800	B12	C30-C3-C2	-2.19	114.50	119.13
4	C	801	DCA	CDP-CBP-CAP	-2.14	105.10	108.82
3	A	800	B12	C6-C5-C4	-2.14	120.94	124.27
3	C	800	B12	C54-C17-C55	-2.13	105.74	109.26
3	C	800	B12	C18-C60-C61	-2.12	108.68	113.97
3	C	800	B12	C5M-C5B-C6B	-2.10	116.43	120.74
4	C	801	DCA	OAP-CAP-CBP	-2.10	105.31	110.25
3	A	800	B12	O2-C3R-C2R	2.08	119.22	111.68
4	C	801	DCA	C6P-C5P-N4P	2.08	119.92	116.42
3	A	800	B12	O3-C2P-C1P	-2.06	102.80	106.92
3	C	800	B12	C2-C3-C4	2.01	103.78	101.67

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	800	B12	C42-C41-C8-C9
5	D	1	GOL	O1-C1-C2-C3
5	D	1	GOL	C1-C2-C3-O3
5	B	640	GOL	C1-C2-C3-O3
5	D	639	GOL	C1-C2-C3-O3
5	B	639	GOL	C1-C2-C3-O3
3	A	800	B12	C42-C41-C8-C7
3	C	800	B12	C8-C41-C42-C43
3	A	800	B12	C16-C17-C55-C56
5	B	640	GOL	O1-C1-C2-C3
3	C	800	B12	C30-C31-C32-O34
5	B	640	GOL	O2-C2-C3-O3
5	B	639	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	801	DCA	P2A-O3A-P1A-O1A
3	C	800	B12	C30-C31-C32-N33
3	A	800	B12	C41-C42-C43-O44
3	C	800	B12	C2P-O3-P-O2
3	A	800	B12	C4-C3-C30-C31
3	A	800	B12	C41-C42-C43-N45
3	A	800	B12	C2P-O3-P-O2
4	C	801	DCA	P2A-O3A-P1A-O2A
4	A	801	DCA	P2A-O3A-P1A-O2A
3	A	800	B12	C18-C60-C61-O63
3	A	800	B12	C30-C31-C32-N33
4	A	801	DCA	P2A-O3A-P1A-O1A
5	D	1	GOL	O1-C1-C2-O2
5	B	640	GOL	O1-C1-C2-O2
3	A	800	B12	C3-C30-C31-C32
3	A	800	B12	C30-C31-C32-O34
3	C	800	B12	C55-C56-C57-O58
5	D	639	GOL	O2-C2-C3-O3

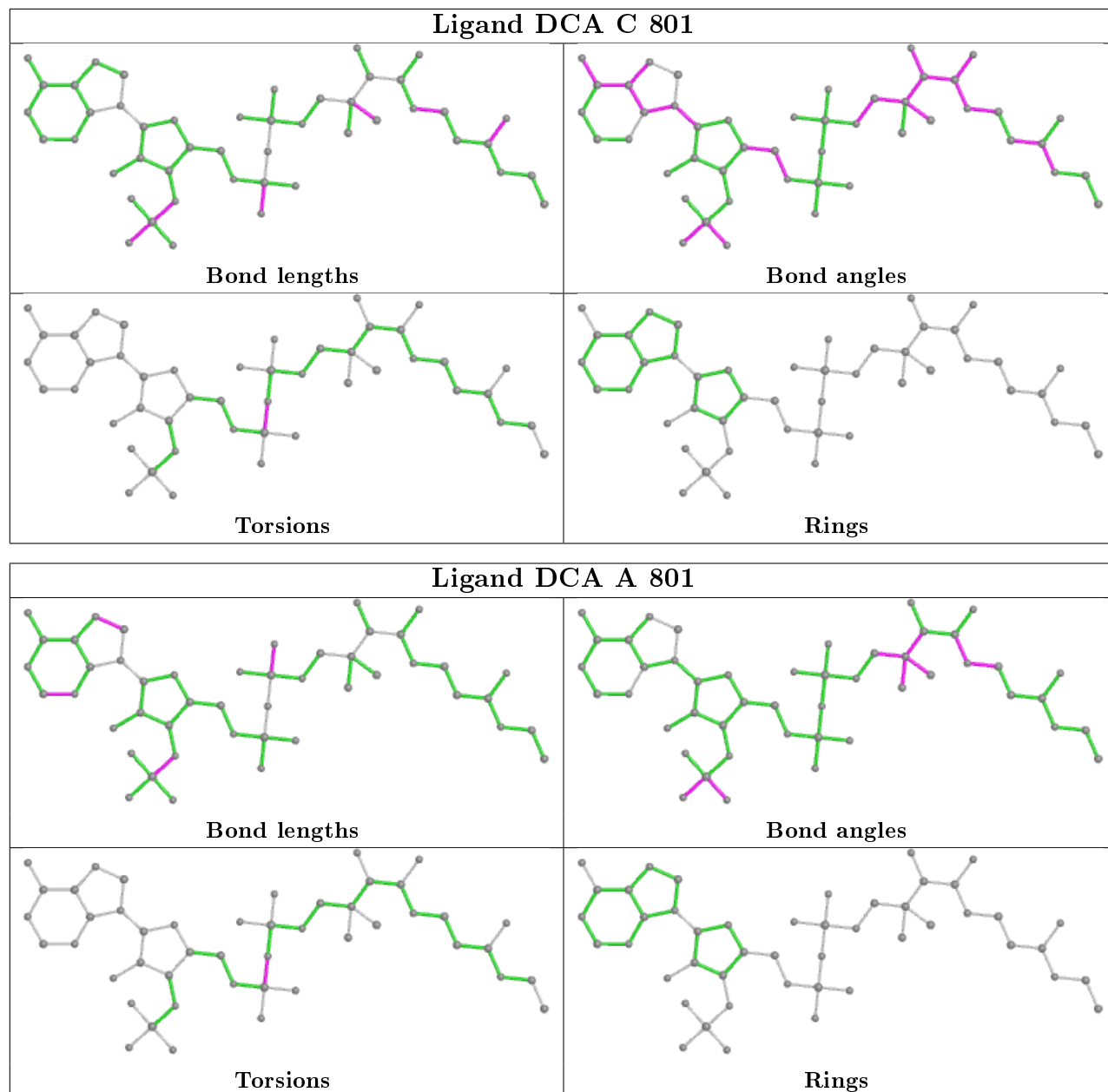
There are no ring outliers.

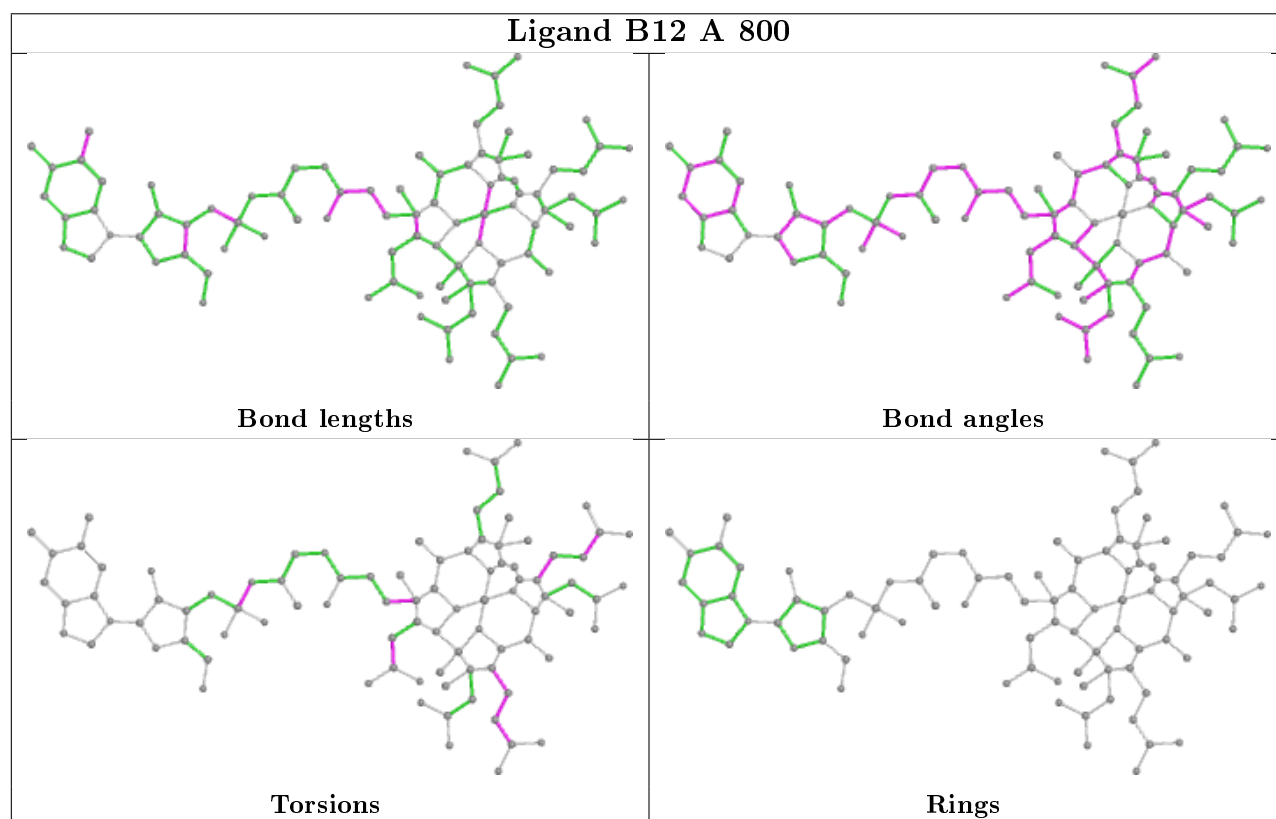
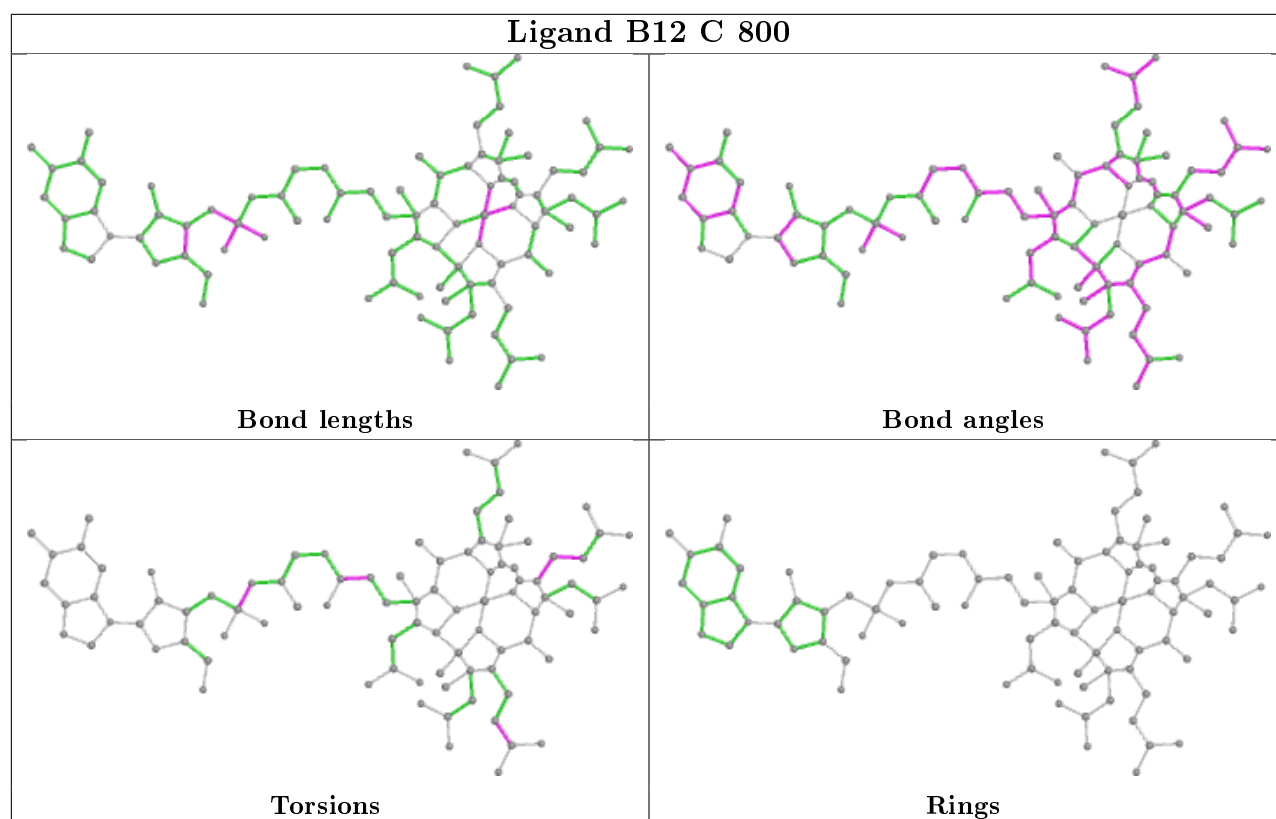
7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	800	B12	10	0
5	D	1	GOL	1	0
3	A	800	B12	11	0
5	C	802	GOL	3	0
5	A	802	GOL	3	0
5	B	640	GOL	1	0
5	B	639	GOL	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	727/727 (100%)	0.97	50 (6%) 16 16	19, 35, 61, 89	0
1	C	727/727 (100%)	1.07	68 (9%) 8 8	18, 34, 60, 105	0
2	B	619/637 (97%)	1.10	86 (13%) 2 2	23, 41, 61, 82	0
2	D	622/637 (97%)	1.60	197 (31%) 0 0	23, 50, 75, 103	0
All	All	2695/2728 (98%)	1.17	401 (14%) 2 2	18, 39, 67, 105	0

All (401) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	428	GLY	8.2
1	C	3	THR	8.0
1	C	30	ALA	7.0
2	D	190	ALA	6.9
1	C	2	SER	6.7
1	A	3	THR	6.5
2	D	158	LEU	6.4
1	C	10	VAL	6.4
2	D	225	ALA	6.3
1	A	728	ALA	6.2
1	C	9	SER	6.0
1	A	2	SER	5.8
2	D	270	GLY	5.3
2	D	434	MET	5.2
2	D	432	ALA	5.1
2	D	193	LEU	5.1
1	A	487	THR	5.1
1	C	23	ARG	5.1
2	D	265	ALA	5.0
1	A	501	ALA	5.0
2	D	253	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	181	SER	4.9
2	D	441	VAL	4.8
2	D	187	ASP	4.8
1	A	477	PRO	4.8
2	D	146	ALA	4.8
2	D	161	MET	4.8
2	D	439	THR	4.6
2	D	422	GLU	4.5
1	A	578	PRO	4.5
2	D	183	TYR	4.5
2	B	609	ALA	4.5
1	C	32	ALA	4.5
2	B	185	ARG	4.5
1	C	27	GLU	4.5
1	C	474	HIS	4.4
2	B	590	ALA	4.4
2	D	226	LYS	4.4
2	B	49	PRO	4.4
2	D	260	ALA	4.4
2	D	224	LEU	4.3
2	D	487	GLY	4.3
2	D	192	ASP	4.2
2	D	122	ARG	4.2
1	C	15	ALA	4.1
1	C	501	ALA	4.1
2	B	587	ALA	4.1
2	D	267	VAL	4.1
2	D	205	ALA	4.1
2	D	51	LYS	4.1
2	D	310	VAL	4.1
2	D	151	ASP	4.1
1	A	577	THR	4.0
2	D	421	GLN	4.0
2	D	638	LYS	4.0
2	D	189	PRO	4.0
2	D	307	ILE	4.0
2	B	161	MET	4.0
1	A	724	ALA	3.9
2	D	179	LEU	3.9
1	A	476	PRO	3.8
1	C	476	PRO	3.8
2	D	590	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	578	PRO	3.8
2	D	272	THR	3.8
1	C	575	LYS	3.8
2	B	613	ILE	3.8
2	D	425	LYS	3.8
2	D	147	PRO	3.8
2	B	51	LYS	3.8
2	B	612	LEU	3.7
1	A	497	VAL	3.7
2	B	606	ALA	3.7
2	D	227	PHE	3.7
2	D	431	LYS	3.7
2	D	181	SER	3.7
2	D	230	ASP	3.7
2	B	190	ALA	3.7
1	C	486	SER	3.7
2	D	194	ALA	3.6
2	B	158	LEU	3.6
2	D	424	GLU	3.6
2	D	276	ALA	3.6
2	D	588	ALA	3.6
2	D	191	LYS	3.6
2	D	186	SER	3.6
2	D	19	THR	3.6
1	C	430	VAL	3.6
2	D	312	GLY	3.6
1	C	477	PRO	3.6
2	B	183	TYR	3.5
1	C	7	PHE	3.5
1	C	13	GLY	3.5
2	D	215	THR	3.5
1	C	5	PRO	3.5
2	D	49	PRO	3.5
1	C	508	VAL	3.5
2	D	433	VAL	3.5
1	A	436	ALA	3.5
2	D	423	VAL	3.5
2	D	484	ALA	3.5
2	B	155	SER	3.5
1	C	14	ASN	3.4
1	A	691	GLN	3.4
2	D	154	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	305	ALA	3.4
2	B	187	ASP	3.4
1	A	486	SER	3.4
2	B	20	THR	3.4
2	B	192	ASP	3.4
2	D	180	VAL	3.4
2	D	440	LYS	3.4
1	C	494	ALA	3.4
1	C	487	THR	3.4
1	A	576	ASN	3.3
2	D	50	GLU	3.3
2	B	148	GLU	3.3
2	D	184	GLU	3.3
2	D	155	SER	3.3
2	D	324	ALA	3.3
2	D	551	ALA	3.3
1	C	6	ARG	3.2
1	A	5	PRO	3.2
1	C	25	PHE	3.2
1	C	436	ALA	3.2
2	D	17	THR	3.2
2	D	583	LYS	3.2
2	B	629	SER	3.2
1	A	474	HIS	3.2
2	D	486	LYS	3.2
2	D	350	ALA	3.2
1	C	4	LEU	3.2
2	B	632	ASP	3.2
2	D	280	ILE	3.2
2	D	435	THR	3.2
2	D	213	ASP	3.2
2	D	587	ALA	3.2
2	D	93	PHE	3.2
2	D	311	PHE	3.2
1	C	34	THR	3.1
2	D	426	LEU	3.1
2	B	189	PRO	3.1
1	C	20	ASP	3.1
2	D	438	VAL	3.1
2	B	575	ALA	3.1
2	D	427	GLY	3.1
1	C	576	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	610	GLU	3.1
2	B	180	VAL	3.1
2	B	607	ALA	3.1
1	C	18	PRO	3.1
2	D	269	GLN	3.1
2	D	185	ARG	3.1
2	D	218	GLY	3.0
2	B	50	GLU	3.0
2	D	121	THR	3.0
2	D	274	THR	3.0
2	B	193	LEU	3.0
2	D	308	GLY	3.0
1	C	488	VAL	3.0
2	D	358	ILE	3.0
1	A	663	THR	3.0
2	D	257	ALA	3.0
2	D	262	TYR	3.0
2	D	549	THR	3.0
2	B	603	GLY	3.0
2	D	589	GLY	3.0
2	B	48	PRO	3.0
2	B	484	ALA	3.0
2	D	177	GLU	3.0
2	B	507	VAL	3.0
2	D	48	PRO	3.0
2	D	629	SER	3.0
2	D	263	VAL	2.9
2	D	281	ASN	2.9
2	B	432	ALA	2.9
2	D	273	ALA	2.9
2	D	482	ALA	2.9
2	D	632	ASP	2.9
2	D	209	GLY	2.9
2	D	204	PHE	2.9
2	D	325	ILE	2.9
2	D	229	PRO	2.9
2	B	253	ALA	2.9
1	A	4	LEU	2.9
2	D	170	TYR	2.9
1	C	37	ALA	2.9
2	D	149	HIS	2.9
2	D	606	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	614	ASP	2.9
2	D	284	VAL	2.9
1	C	22	ALA	2.9
2	B	588	ALA	2.9
1	C	577	THR	2.9
2	D	228	SER	2.9
2	D	558	LYS	2.9
2	D	182	VAL	2.8
2	B	276	ALA	2.8
2	D	107	TRP	2.8
2	D	112	LEU	2.8
2	B	439	THR	2.8
2	D	436	GLU	2.8
2	D	117	ASP	2.8
2	D	315	GLU	2.8
1	C	12	LEU	2.8
2	D	584	ALA	2.8
1	C	589	GLU	2.7
1	C	8	ASP	2.7
1	A	494	ALA	2.7
1	A	646	GLU	2.7
2	B	428	GLY	2.7
2	D	316	ASP	2.7
2	D	116	PRO	2.7
2	D	197	LEU	2.7
2	B	270	GLY	2.7
2	B	487	GLY	2.7
1	C	497	VAL	2.7
2	D	382	THR	2.7
2	B	434	MET	2.7
1	C	39	GLU	2.7
2	B	636	VAL	2.7
2	D	216	VAL	2.7
1	C	441	ILE	2.7
2	D	628	SER	2.7
2	D	120	PHE	2.7
1	C	455	ALA	2.7
2	B	191	LYS	2.7
2	B	574	TYR	2.7
2	B	227	PHE	2.7
2	D	368	GLY	2.7
2	D	614	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	212	PRO	2.6
2	D	443	ASP	2.6
2	D	357	SER	2.6
2	D	612	LEU	2.6
2	D	346	ALA	2.6
2	B	425	LYS	2.6
2	D	409	THR	2.6
2	D	603	GLY	2.6
2	D	266	LEU	2.6
2	D	637	ALA	2.6
2	B	186	SER	2.6
2	B	435	THR	2.6
2	D	195	LEU	2.6
1	A	473	GLU	2.6
1	C	490	ALA	2.6
1	C	64	TYR	2.5
1	A	575	LYS	2.5
1	C	425	GLN	2.5
2	D	53	LEU	2.5
1	A	483	VAL	2.5
1	A	585	GLU	2.5
2	D	241	TYR	2.5
2	D	18	PRO	2.5
2	D	524	PHE	2.5
1	A	672	LEU	2.5
2	D	635	GLY	2.5
2	B	504	SER	2.5
2	D	352	VAL	2.5
2	D	555	GLU	2.5
2	B	440	LYS	2.5
2	B	208	GLN	2.5
2	D	282	PHE	2.5
1	C	26	GLU	2.5
2	B	350	ALA	2.5
2	D	152	GLU	2.5
2	D	52	GLN	2.5
2	D	483	PRO	2.4
2	D	554	VAL	2.4
2	D	417	TRP	2.4
1	C	431	GLY	2.4
2	D	548	GLY	2.4
1	C	11	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	526	ASP	2.4
2	D	201	PRO	2.4
2	B	219	ASP	2.4
1	C	19	ALA	2.4
1	C	373	ALA	2.4
2	B	146	ALA	2.4
2	D	150	LEU	2.4
1	A	176	ALA	2.4
2	D	609	ALA	2.4
1	C	507	LYS	2.4
2	D	386	LEU	2.3
2	B	454	ALA	2.3
2	D	279	THR	2.3
1	C	479	ASP	2.3
1	C	350	ILE	2.3
1	A	301	LEU	2.3
2	D	259	GLY	2.3
2	D	485	ARG	2.3
2	D	159	LEU	2.3
2	B	635	GLY	2.3
2	D	234	VAL	2.3
2	D	313	VAL	2.3
1	C	426	GLU	2.3
2	D	437	HIS	2.3
1	A	130	PRO	2.3
2	D	256	LEU	2.3
1	A	430	VAL	2.3
1	A	678	PRO	2.3
2	B	358	ILE	2.3
2	B	106	ALA	2.3
2	B	524	PHE	2.3
1	A	488	VAL	2.3
1	A	719	VAL	2.3
1	C	435	LYS	2.3
1	A	526	ASP	2.3
2	D	414	ASP	2.3
2	D	285	THR	2.2
2	D	153	VAL	2.2
2	D	127	GLU	2.2
2	D	294	ILE	2.2
2	D	345	ILE	2.2
2	D	126	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	286	ALA	2.2
2	D	582	ALA	2.2
1	C	691	GLN	2.2
2	D	283	ARG	2.2
2	B	628	SER	2.2
2	D	82	PRO	2.2
1	A	290	ILE	2.2
2	D	232	ARG	2.2
1	A	662	LEU	2.2
2	D	199	LEU	2.2
1	C	728	ALA	2.2
2	B	260	ALA	2.2
2	D	210	THR	2.2
2	D	604	ASP	2.2
2	D	297	LEU	2.2
1	A	697	ARG	2.2
1	C	580	VAL	2.2
2	D	323	ASN	2.2
1	A	243	TYR	2.1
2	D	291	PHE	2.1
2	B	121	THR	2.1
2	D	347	THR	2.1
1	A	478	LEU	2.1
1	A	726	LEU	2.1
2	B	173	GLY	2.1
2	D	568	CYS	2.1
1	A	373	ALA	2.1
2	D	326	THR	2.1
2	D	481	ALA	2.1
2	B	478	PRO	2.1
2	D	129	LEU	2.1
2	D	137	LEU	2.1
2	D	208	GLN	2.1
1	A	589	GLU	2.1
2	B	441	VAL	2.1
2	D	198	GLY	2.1
2	D	479	PHE	2.1
1	C	29	ALA	2.1
1	C	243	TYR	2.1
2	B	215	THR	2.1
2	D	81	ALA	2.1
2	D	454	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	480	PRO	2.1
1	A	694	ASP	2.1
2	B	151	ASP	2.1
2	B	184	GLU	2.1
2	B	436	GLU	2.1
2	B	576	GLN	2.1
2	D	233	ALA	2.1
1	C	288	TRP	2.1
2	D	58	CYS	2.1
1	A	439	LYS	2.1
1	C	718	LEU	2.1
1	A	689	PRO	2.1
1	C	21	ALA	2.1
2	D	222	ARG	2.1
1	A	653	GLY	2.1
2	B	228	SER	2.0
2	B	294	ILE	2.0
2	B	604	ASP	2.0
2	D	314	ASP	2.0
2	B	212	PRO	2.0
1	C	429	LYS	2.0
2	B	267	VAL	2.0
2	B	286	ALA	2.0
2	B	324	ALA	2.0
2	B	346	ALA	2.0
2	B	382	THR	2.0
2	D	348	PHE	2.0
1	A	288	TRP	2.0
1	C	98	SER	2.0
2	B	583	LYS	2.0
1	A	489	LEU	2.0
1	A	490	ALA	2.0
2	B	149	HIS	2.0
2	B	549	THR	2.0
2	D	287	THR	2.0
2	D	268	GLU	2.0
2	D	420	PHE	2.0
1	A	479	ASP	2.0
2	B	269	GLN	2.0
2	D	219	ASP	2.0
1	C	130	PRO	2.0
2	B	482	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	236	ILE	2.0
2	B	171	ASP	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](#)

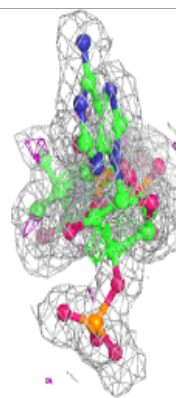
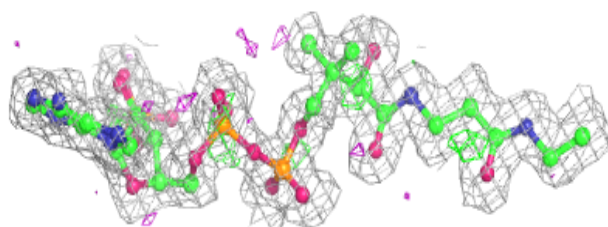
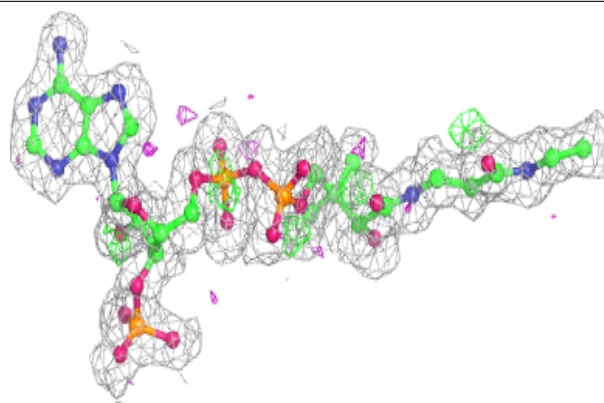
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	GOL	B	1	6/6	0.50	0.38	54,59,61,61	0
5	GOL	D	1	6/6	0.58	0.29	61,62,64,68	0
5	GOL	B	640	6/6	0.68	0.29	50,60,62,68	0
5	GOL	D	639	6/6	0.73	0.29	53,61,64,70	0
5	GOL	B	639	6/6	0.77	0.23	44,48,53,53	0
5	GOL	A	802	6/6	0.85	0.24	29,41,45,48	0
5	GOL	C	802	6/6	0.86	0.21	21,32,43,45	0
5	GOL	C	803	6/6	0.87	0.20	38,39,41,45	0
5	GOL	A	803	6/6	0.90	0.18	34,38,42,46	0
4	DCA	C	801	47/47	0.93	0.17	14,23,30,32	0
4	DCA	A	801	47/47	0.93	0.17	20,25,28,31	0
3	B12	A	800	91/91	0.94	0.18	17,29,48,68	0
3	B12	C	800	91/91	0.95	0.19	15,26,40,53	0

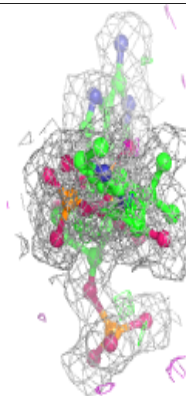
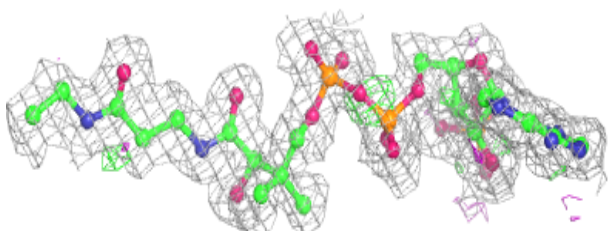
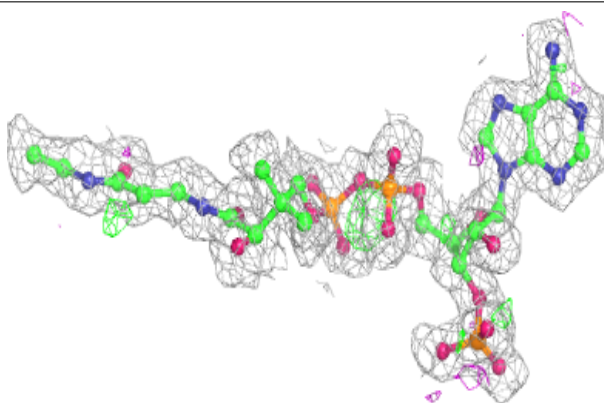
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DCA C 801:**

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

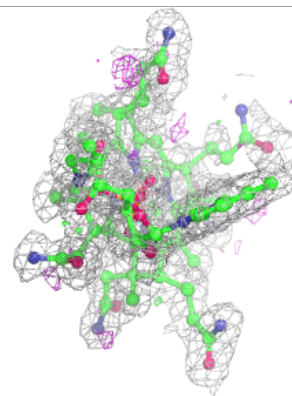
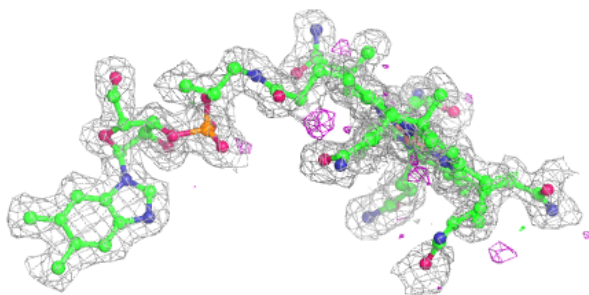
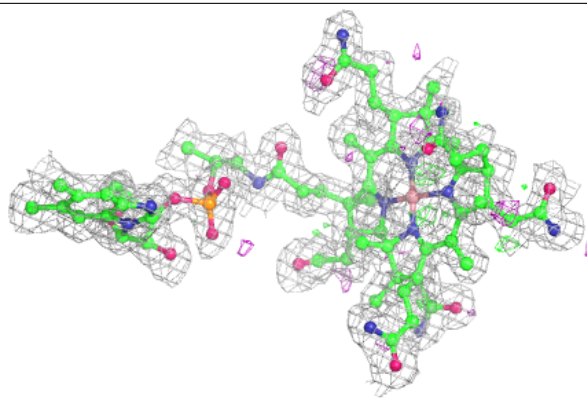
**Electron density around DCA A 801:**

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

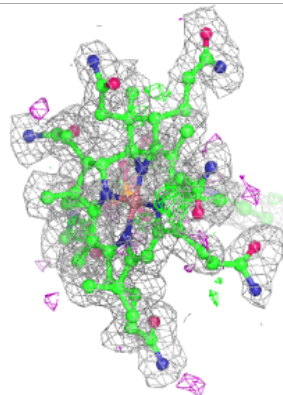
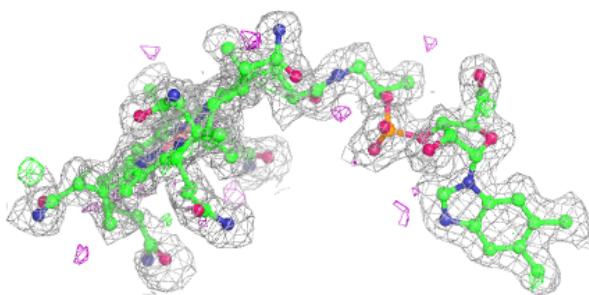
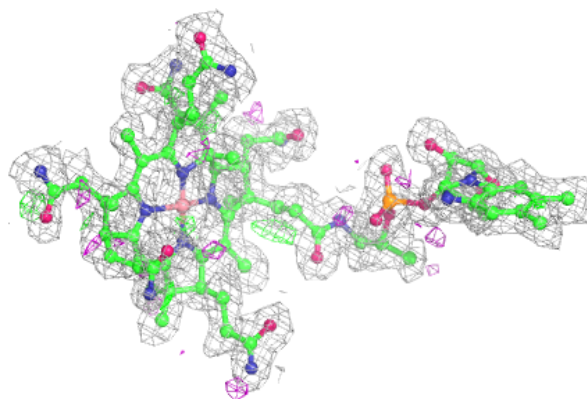


**Electron density around B12 A 800:**

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

**Electron density around B12 C 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.