



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 PM GMT

PDB ID : 4REQ  
Title : Methylmalonyl-CoA Mutase substrate complex  
Authors : Evans, P.R.; Mancina, F.  
Deposited on : 1998-06-17  
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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

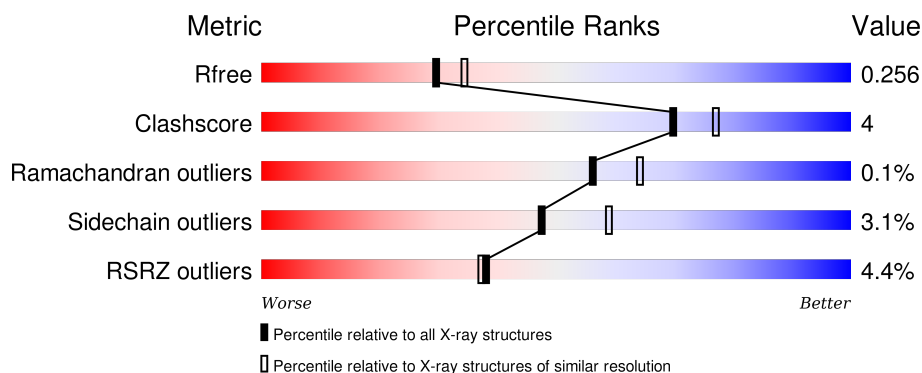
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	C	727	<div> <div>3%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	B	637	<div> <div>5%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
2	D	637	<div> <div>9%</div> <div>75%</div> <div>20%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	5AD	A	803	-	-	-	X
6	5AD	C	803	-	-	X	X
7	GOL	A	1	-	-	-	X
7	GOL	B	639	-	-	-	X
7	GOL	C	1	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22334 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	726	Total	C	N	O	S	0	0	0
			5575	3526	966	1059	24			
1	C	726	Total	C	N	O	S	0	0	0
			5575	3526	966	1059	24			

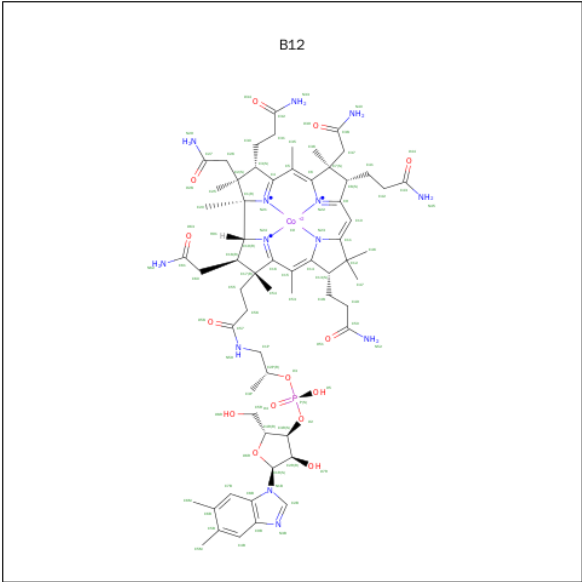
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4718	2977	826	902	13			
2	D	619	Total	C	N	O	S	0	0	0
			4718	2977	826	902	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	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).



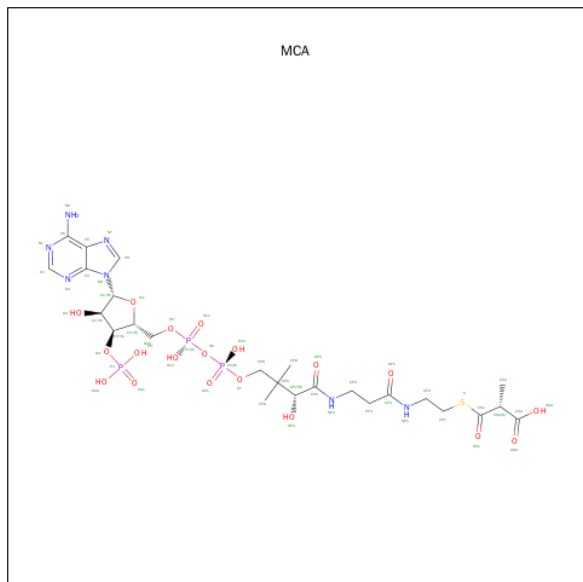
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is SUCCINYL-COENZYME A (three-letter code: SCA) (formula: C<sub>25</sub>H<sub>40</sub>N<sub>7</sub>O<sub>19</sub>P<sub>3</sub>S).



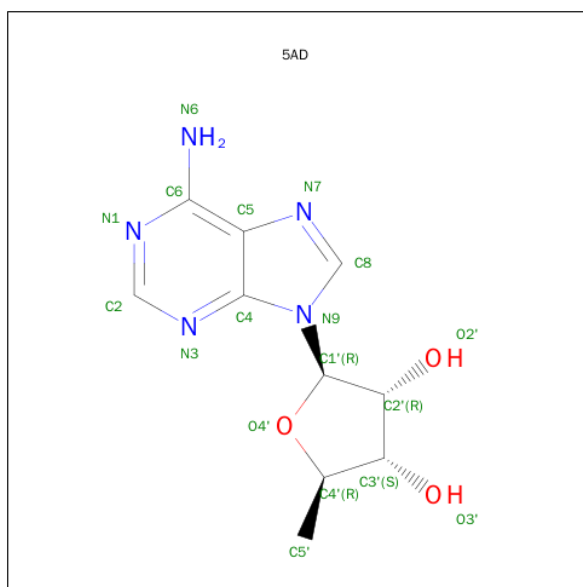
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	1
			55	25	7	19	3	1		
4	C	1	Total	C	N	O	P	S	0	1
			55	25	7	19	3	1		

- Molecule 5 is METHYLMALONYL-COENZYME A (three-letter code: MCA) (formula:  $C_{25}H_{40}N_7O_{19}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	1
			55	25	7	19	3	1		
5	C	1	Total	C	N	O	P	S	0	1
			55	25	7	19	3	1		

- Molecule 6 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

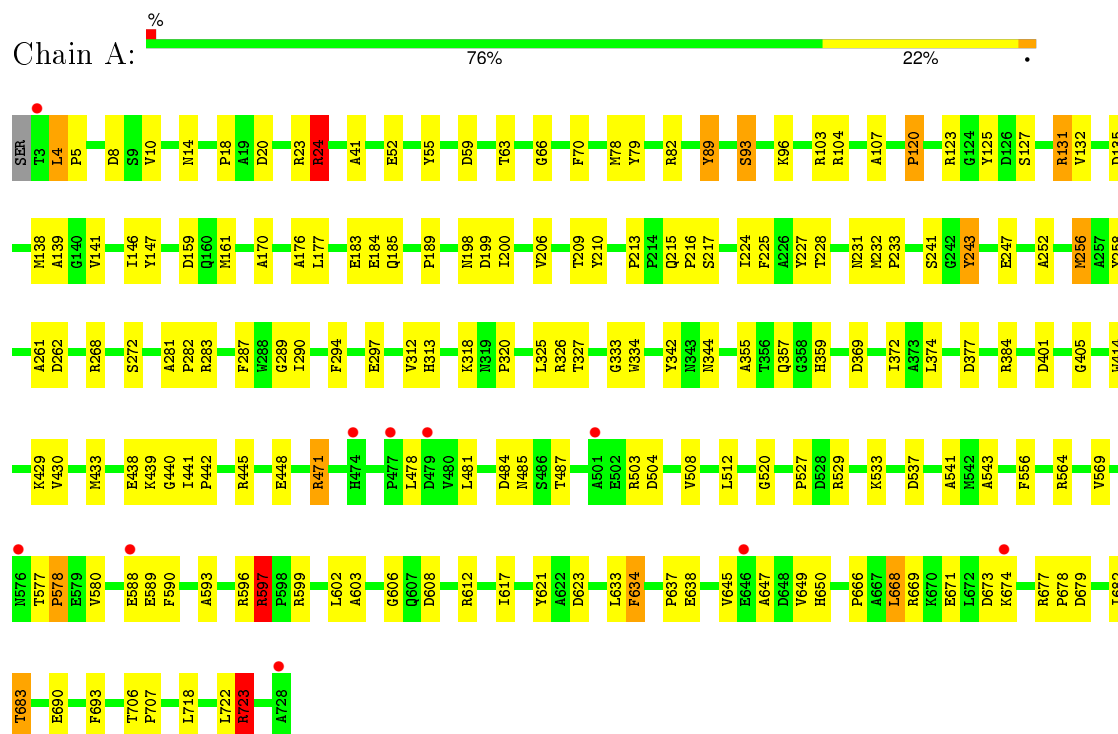
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	404	Total	O	0	0
			404	404		
8	B	239	Total	O	0	0
			239	239		
8	C	400	Total	O	0	0
			400	400		
8	D	243	Total	O	0	0
			243	243		

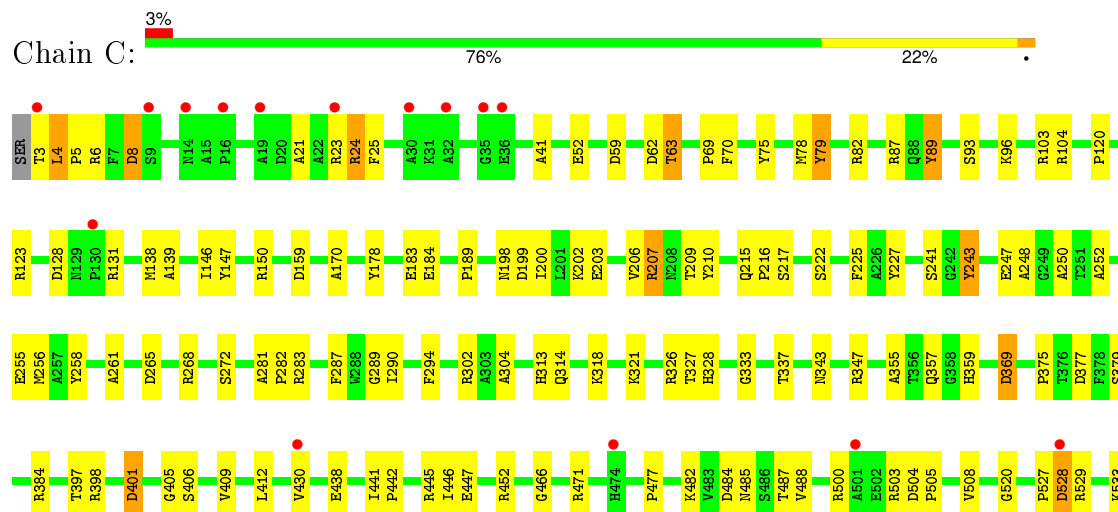
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

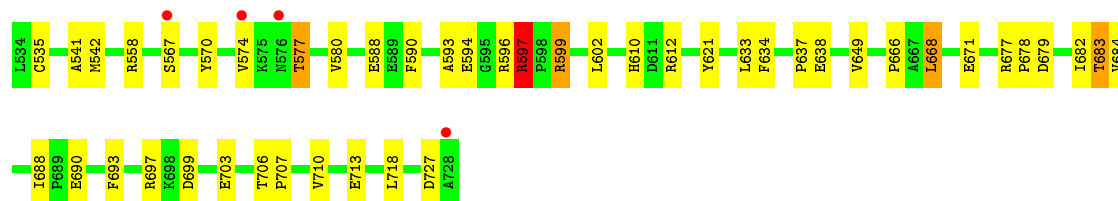
#### • Molecule 1: METHYLMALONYL-COA MUTASE



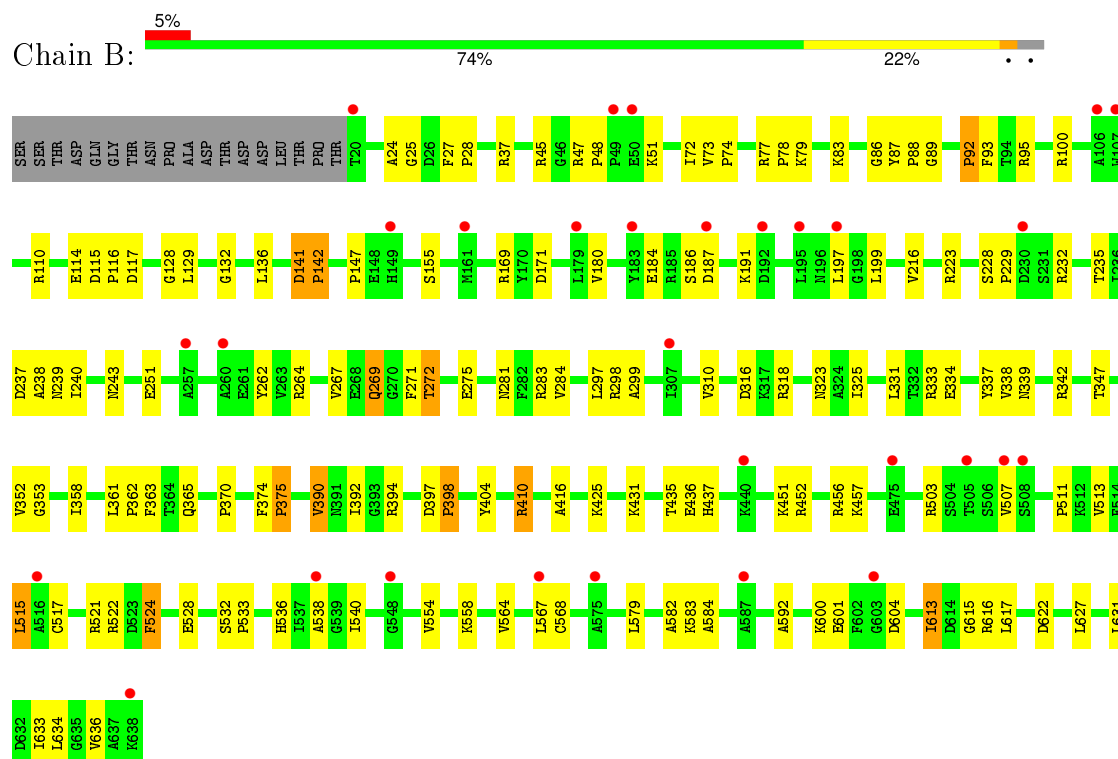
#### • Molecule 1: METHYLMALONYL-COA MUTASE



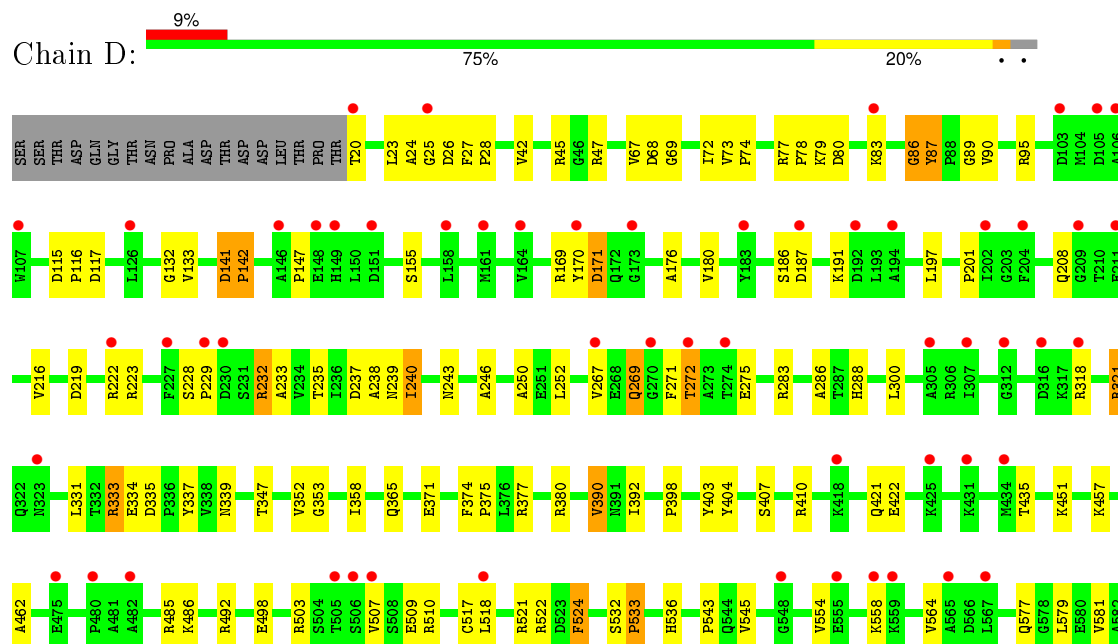


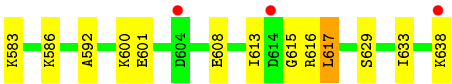


- Molecule 2: METHYLMALONYL-COA MUTASE



- 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, $\alpha$ , $\beta$ , $\gamma$	120.13 Å   160.90 Å   88.50 Å 90.00°   104.64°   90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.9 (19.98-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.19 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.222   ,   0.277 0.215   ,   0.256	Depositor DCC
$R_{free}$ test set	8306 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 322250 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: B12, GOL, SCA, 5AD, MCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.66	1/5692 (0.0%)	1.93	152/7730 (2.0%)
1	C	0.67	0/5692	1.93	155/7730 (2.0%)
2	B	0.59	0/4808	1.80	104/6521 (1.6%)
2	D	0.58	0/4808	1.80	93/6521 (1.4%)
All	All	0.63	1/21000 (0.0%)	1.87	504/28502 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	GLY	N-CA	-5.05	1.38	1.46

All (504) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	ARG	CD-NE-CZ	21.09	153.12	123.60
1	A	384	ARG	CD-NE-CZ	19.56	150.99	123.60
1	A	268	ARG	NE-CZ-NH2	-15.29	112.65	120.30
1	C	79	TYR	CB-CG-CD2	-12.76	113.35	121.00
1	C	597	ARG	CD-NE-CZ	12.61	141.25	123.60
2	B	95	ARG	NE-CZ-NH2	-12.54	114.03	120.30
1	A	596	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	597	ARG	CD-NE-CZ	12.34	140.87	123.60
1	A	79	TYR	CB-CG-CD2	-11.71	113.97	121.00
2	D	269	GLN	C-N-CA	11.71	146.88	122.30
1	C	597	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	C	268	ARG	NE-CZ-NH2	-11.56	114.52	120.30
2	D	524	PHE	CB-CG-CD1	10.66	128.27	120.80
2	D	503	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	A	131	ARG	CD-NE-CZ	10.58	138.41	123.60
2	D	333	ARG	NE-CZ-NH2	10.56	125.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	597	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	384	ARG	NE-CZ-NH2	-10.12	115.24	120.30
2	D	404	TYR	CB-CG-CD1	9.88	126.93	121.00
2	D	169	ARG	CD-NE-CZ	9.84	137.38	123.60
2	B	524	PHE	CB-CG-CD1	9.58	127.51	120.80
1	C	41	ALA	C-N-CA	9.58	145.65	121.70
2	B	77	ARG	CD-NE-CZ	9.57	137.00	123.60
2	D	435	THR	CA-CB-CG2	9.52	125.73	112.40
1	C	24	ARG	CD-NE-CZ	9.41	136.78	123.60
1	C	287	PHE	CB-CG-CD1	9.37	127.36	120.80
1	A	678	PRO	C-N-CA	9.36	145.09	121.70
1	A	723	ARG	CD-NE-CZ	9.33	136.66	123.60
2	D	377	ARG	CD-NE-CZ	9.31	136.64	123.60
2	B	77	ARG	NE-CZ-NH1	9.21	124.91	120.30
2	B	435	THR	CA-CB-CG2	9.21	125.29	112.40
1	C	384	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	C	79	TYR	CB-CG-CD1	9.10	126.46	121.00
2	B	397	ASP	CB-CG-OD1	9.07	126.47	118.30
2	B	262	TYR	CB-CG-CD1	9.07	126.44	121.00
2	B	269	GLN	C-N-CA	9.03	141.27	122.30
2	B	616	ARG	NE-CZ-NH2	-8.93	115.83	120.30
2	D	169	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	C	377	ASP	CB-CG-OD1	8.89	126.30	118.30
2	B	394	ARG	NE-CZ-NH2	-8.88	115.86	120.30
2	D	77	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	C	302	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	C	104	ARG	NE-CZ-NH2	8.79	124.69	120.30
2	B	87	TYR	CB-CG-CD2	8.68	126.21	121.00
1	A	24	ARG	CD-NE-CZ	8.55	135.56	123.60
1	A	679	ASP	CB-CG-OD2	8.51	125.95	118.30
2	B	232	ARG	CD-NE-CZ	8.51	135.51	123.60
2	D	601	GLU	C-N-CA	8.50	142.95	121.70
2	D	45	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	287	PHE	CB-CG-CD1	8.37	126.66	120.80
1	A	79	TYR	CB-CG-CD1	8.37	126.02	121.00
2	B	457	LYS	C-N-CA	8.21	142.22	121.70
2	B	298	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	A	258	TYR	CB-CG-CD2	-8.16	116.10	121.00
2	B	115	ASP	CB-CG-OD1	8.14	125.62	118.30
2	B	601	GLU	C-N-CA	8.10	141.96	121.70
1	C	123	ARG	NE-CZ-NH2	-8.10	116.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	258	TYR	CB-CG-CD1	8.04	125.82	121.00
1	C	621	TYR	CB-CG-CD1	8.03	125.82	121.00
1	A	82	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	D	403	TYR	CB-CG-CD1	7.94	125.76	121.00
2	B	339	ASN	O-C-N	-7.92	110.03	122.70
1	A	439	LYS	C-N-CA	7.91	138.91	122.30
1	A	104	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	C	41	ALA	O-C-N	-7.86	110.12	122.70
1	C	255	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	A	377	ASP	CB-CG-OD1	7.83	125.35	118.30
2	B	117	ASP	CB-CG-OD1	7.83	125.35	118.30
1	C	384	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	159	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	677	ARG	CA-CB-CG	7.74	130.43	113.40
1	A	24	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	C	452	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	C	326	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	D	352	VAL	C-N-CA	7.65	138.36	122.30
2	D	601	GLU	O-C-N	-7.64	110.47	122.70
1	C	294	PHE	CB-CG-CD2	-7.62	115.47	120.80
2	D	616	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	147	TYR	CB-CG-CD1	7.58	125.55	121.00
2	B	37	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	B	262	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	C	24	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	596	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	471	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	75	TYR	CB-CG-CD2	7.48	125.49	121.00
1	A	282	PRO	O-C-N	-7.47	110.74	122.70
1	C	52	GLU	O-C-N	-7.46	110.75	122.70
1	A	723	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	445	ARG	NE-CZ-NH2	-7.43	116.59	120.30
2	D	318	ARG	NE-CZ-NH1	7.41	124.01	120.30
2	B	333	ARG	NE-CZ-NH2	7.38	123.99	120.30
2	B	318	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	287	PHE	CB-CG-CD2	-7.34	115.66	120.80
2	B	536	HIS	O-C-N	-7.33	110.97	122.70
1	C	697	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	D	269	GLN	O-C-N	-7.32	110.75	123.20
1	C	621	TYR	CB-CG-CD2	-7.28	116.63	121.00
2	B	86	GLY	O-C-N	-7.27	111.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	ALA	CA-C-N	7.27	133.19	117.20
1	A	52	GLU	O-C-N	-7.26	111.08	122.70
1	A	326	ARG	NE-CZ-NH1	7.26	123.93	120.30
2	D	232	ARG	CD-NE-CZ	7.26	133.76	123.60
1	C	430	VAL	CA-CB-CG1	7.24	121.76	110.90
2	D	95	ARG	CG-CD-NE	7.22	126.97	111.80
1	A	430	VAL	CA-CB-CG1	7.20	121.70	110.90
2	D	457	LYS	C-N-CA	7.17	139.64	121.70
2	D	24	ALA	C-N-CA	7.16	137.33	122.30
1	C	209	THR	N-CA-CB	7.15	123.89	110.30
1	A	281	ALA	N-CA-CB	7.14	120.10	110.10
1	A	41	ALA	C-N-CA	7.13	139.52	121.70
1	C	690	GLU	O-C-N	-7.08	111.38	122.70
2	B	45	ARG	NE-CZ-NH2	-7.07	116.77	120.30
2	D	521	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	590	PHE	CB-CG-CD1	7.04	125.73	120.80
2	D	72	ILE	CB-CG1-CD1	7.02	133.56	113.90
2	D	117	ASP	CB-CG-OD1	6.99	124.59	118.30
1	C	321	LYS	O-C-N	-6.99	111.51	122.70
1	C	558	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	D	87	TYR	CB-CG-CD2	6.98	125.19	121.00
2	D	243	ASN	C-N-CA	6.97	139.13	121.70
1	A	131	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	D	503	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	D	524	PHE	CB-CG-CD2	-6.95	115.93	120.80
1	C	89	TYR	CA-CB-CG	6.90	126.52	113.40
2	B	352	VAL	C-N-CA	6.89	136.76	122.30
2	B	521	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	D	115	ASP	CB-CG-OD1	6.88	124.49	118.30
2	B	522	ARG	CD-NE-CZ	6.86	133.20	123.60
1	A	241	SER	N-CA-C	6.86	129.51	111.00
2	D	132	GLY	N-CA-C	6.86	130.24	113.10
1	A	633	LEU	O-C-N	-6.85	111.73	122.70
2	B	363	PHE	C-N-CA	6.84	138.79	121.70
1	A	637	PRO	C-N-CA	6.83	138.78	121.70
2	D	24	ALA	O-C-N	-6.83	111.58	123.20
1	A	326	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	B	601	GLU	O-C-N	-6.83	111.77	122.70
2	B	298	ARG	CD-NE-CZ	6.82	133.15	123.60
2	D	339	ASN	O-C-N	-6.82	111.78	122.70
2	D	243	ASN	O-C-N	-6.82	111.79	122.70
1	C	241	SER	N-CA-C	6.82	129.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	ASN	O-C-N	-6.81	111.80	122.70
1	C	206	VAL	CA-CB-CG1	6.79	121.09	110.90
1	C	6	ARG	CD-NE-CZ	6.79	133.10	123.60
2	D	600	LYS	O-C-N	-6.78	111.85	122.70
1	A	261	ALA	O-C-N	-6.78	111.85	122.70
1	A	63	THR	O-C-N	-6.75	111.90	122.70
1	A	283	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	674	LYS	C-N-CA	6.72	138.50	121.70
1	C	633	LEU	O-C-N	-6.72	111.95	122.70
1	A	147	TYR	CB-CG-CD1	6.70	125.02	121.00
1	A	206	VAL	CB-CA-C	-6.68	98.71	111.40
1	C	227	TYR	CB-CG-CD2	6.68	125.01	121.00
1	A	82	ARG	CD-NE-CZ	6.66	132.92	123.60
1	C	82	ARG	CD-NE-CZ	6.65	132.91	123.60
1	C	258	TYR	CB-CG-CD1	6.62	124.97	121.00
2	D	335	ASP	CB-CG-OD1	6.61	124.25	118.30
2	D	223	ARG	CD-NE-CZ	6.60	132.84	123.60
1	C	243	TYR	CB-CG-CD2	6.58	124.95	121.00
1	A	334	TRP	O-C-N	-6.57	112.18	122.70
2	B	269	GLN	O-C-N	-6.57	112.03	123.20
2	B	398	PRO	O-C-N	-6.57	112.19	122.70
2	D	337	TYR	O-C-N	-6.56	112.21	122.70
2	D	47	ARG	CD-NE-CZ	6.56	132.78	123.60
1	A	690	GLU	C-N-CA	6.55	138.07	121.70
2	B	95	ARG	CG-CD-NE	6.55	125.55	111.80
2	B	243	ASN	C-N-CA	6.53	138.01	121.70
1	C	369	ASP	O-C-N	-6.51	112.28	122.70
1	A	287	PHE	CB-CG-CD2	-6.51	116.25	120.80
1	C	59	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	727	ASP	CB-CG-OD1	6.49	124.14	118.30
2	D	238	ALA	C-N-CA	6.48	137.91	121.70
2	B	72	ILE	CB-CG1-CD1	6.48	132.04	113.90
1	C	690	GLU	C-N-CA	6.47	137.88	121.70
1	A	369	ASP	O-C-N	-6.46	112.36	122.70
1	C	679	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	8	ASP	C-N-CA	6.45	137.82	121.70
2	D	321	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	D	353	GLY	C-N-CA	6.43	135.80	122.30
1	C	593	ALA	CA-C-N	6.41	131.29	117.20
2	B	37	ARG	CD-NE-CZ	6.39	132.54	123.60
2	D	45	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	D	89	GLY	C-N-CA	6.34	137.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	357	GLN	C-N-CA	6.33	135.59	122.30
1	A	66	GLY	O-C-N	-6.32	112.59	122.70
2	D	404	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	C	87	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	123	ARG	CD-NE-CZ	6.27	132.38	123.60
1	A	184	GLU	O-C-N	-6.27	112.66	122.70
1	A	608	ASP	CB-CG-OD1	6.27	123.95	118.30
1	A	294	PHE	CB-CG-CD1	-6.27	116.41	120.80
1	A	185	GLN	C-N-CA	6.27	135.46	122.30
2	B	47	ARG	CD-NE-CZ	6.26	132.36	123.60
1	C	699	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	C	207	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	103	ARG	CD-NE-CZ	6.24	132.34	123.60
1	C	23	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	D	78	PRO	O-C-N	-6.24	112.72	122.70
2	B	78	PRO	O-C-N	-6.21	112.76	122.70
1	C	282	PRO	O-C-N	-6.21	112.76	122.70
2	B	77	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	4	LEU	CA-CB-CG	6.21	129.57	115.30
2	B	622	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	693	PHE	CB-CG-CD1	6.20	125.14	120.80
1	C	666	PRO	N-CA-CB	6.20	110.73	103.30
2	D	533	PRO	N-CA-CB	6.19	110.73	103.30
1	A	637	PRO	O-C-N	-6.18	112.81	122.70
1	A	325	LEU	CB-CG-CD2	6.17	121.48	111.00
1	C	504	ASP	CB-CG-OD1	6.17	123.85	118.30
2	B	404	TYR	CB-CG-CD1	6.16	124.70	121.00
2	B	89	GLY	C-N-CA	6.16	137.10	121.70
1	A	24	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	683	THR	N-CA-CB	6.15	121.99	110.30
2	D	26	ASP	CB-CA-C	-6.14	98.11	110.40
2	B	600	LYS	O-C-N	-6.13	112.89	122.70
1	C	131	ARG	CD-NE-CZ	6.13	132.18	123.60
1	A	123	ARG	C-N-CA	6.12	135.14	122.30
1	A	262	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	169	ARG	CD-NE-CZ	6.11	132.15	123.60
1	C	198	ASN	N-CA-CB	-6.11	99.61	110.60
1	A	170	ALA	O-C-N	-6.10	112.94	122.70
2	B	243	ASN	O-C-N	-6.09	112.95	122.70
1	C	527	PRO	N-CA-CB	6.08	110.59	103.30
1	A	59	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	674	LYS	O-C-N	-6.06	113.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	425	LYS	C-N-CA	6.06	136.86	121.70
1	C	528	ASP	C-N-CA	6.06	136.85	121.70
1	A	125	TYR	CB-CG-CD2	-6.04	117.37	121.00
1	A	228	THR	O-C-N	-6.03	113.05	122.70
1	C	594	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	A	590	PHE	CB-CG-CD2	-6.02	116.59	120.80
2	D	232	ARG	NE-CZ-NH1	6.01	123.30	120.30
2	D	600	LYS	C-N-CA	6.01	136.72	121.70
2	D	390	VAL	O-C-N	-6.00	113.09	122.70
1	A	357	GLN	O-C-N	-6.00	113.00	123.20
1	A	529	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	466	GLY	O-C-N	-6.00	113.10	122.70
2	B	634	LEU	C-N-CA	6.00	134.89	122.30
2	D	223	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	B	503	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	673	ASP	O-C-N	-5.99	113.12	122.70
1	C	183	GLU	O-C-N	-5.99	113.12	122.70
1	C	697	ARG	CD-NE-CZ	5.98	131.98	123.60
1	A	272	SER	O-C-N	-5.97	113.14	122.70
1	A	206	VAL	CA-CB-CG1	5.97	119.85	110.90
1	A	227	TYR	CB-CG-CD2	5.97	124.58	121.00
2	B	47	ARG	NE-CZ-NH1	5.97	123.28	120.30
2	B	25	GLY	O-C-N	-5.96	113.17	122.70
1	C	281	ALA	N-CA-CB	5.93	118.40	110.10
1	C	590	PHE	CB-CG-CD1	5.92	124.94	120.80
2	B	110	ARG	CD-NE-CZ	5.89	131.85	123.60
2	B	437	HIS	CA-CB-CG	-5.89	103.59	113.60
2	B	24	ALA	C-N-CA	5.89	134.66	122.30
1	C	75	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	C	63	THR	C-N-CA	5.88	136.41	121.70
1	A	41	ALA	O-C-N	-5.87	113.30	122.70
2	B	316	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	209	THR	N-CA-CB	5.87	121.45	110.30
2	B	337	TYR	CA-C-N	5.87	130.11	117.20
2	D	398	PRO	O-C-N	-5.87	113.31	122.70
1	C	225	PHE	CB-CG-CD1	5.86	124.91	120.80
1	A	24	ARG	CG-CD-NE	5.86	124.11	111.80
1	A	333	GLY	O-C-N	-5.83	113.37	122.70
1	C	634	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	283	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	314	GLN	C-N-CA	5.82	136.24	121.70
1	C	210	TYR	CB-CG-CD1	5.81	124.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	TYR	CB-CG-CD1	5.80	124.48	121.00
1	C	333	GLY	O-C-N	-5.80	113.41	122.70
2	D	95	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	8	ASP	C-N-CA	5.79	136.17	121.70
1	C	314	GLN	O-C-N	-5.77	113.46	122.70
2	B	511	PRO	N-CA-CB	5.76	110.21	103.30
2	B	375	PRO	N-CA-CB	5.75	110.20	103.30
1	A	520	GLY	O-C-N	-5.75	113.50	122.70
1	A	369	ASP	CB-CG-OD1	5.75	123.47	118.30
2	B	352	VAL	O-C-N	-5.73	113.46	123.20
2	D	485	ARG	CD-NE-CZ	5.73	131.62	123.60
1	A	232	MET	CA-CB-CG	5.73	123.04	113.30
2	D	229	PRO	C-N-CA	5.72	136.01	121.70
1	C	447	GLU	O-C-N	-5.72	113.55	122.70
2	B	100	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	D	371	GLU	CA-CB-CG	5.71	125.97	113.40
1	A	527	PRO	N-CA-CB	5.70	110.14	103.30
1	C	272	SER	O-C-N	-5.70	113.58	122.70
2	D	25	GLY	C-N-CA	5.70	135.96	121.70
1	A	537	ASP	CB-CG-OD1	5.70	123.43	118.30
2	D	457	LYS	O-C-N	-5.69	113.59	122.70
2	B	78	PRO	N-CA-CB	5.68	110.12	103.30
1	C	103	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	326	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	B	452	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	C	6	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	261	ALA	O-C-N	-5.66	113.65	122.70
1	C	633	LEU	CA-C-O	5.65	131.97	120.10
1	C	500	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	B	524	PHE	CB-CG-CD2	-5.65	116.85	120.80
2	B	503	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	439	LYS	O-C-N	-5.64	113.61	123.20
2	D	147	PRO	C-N-CA	5.64	135.79	121.70
2	B	613	ILE	CA-C-O	5.63	131.93	120.10
1	A	693	PHE	CB-CG-CD1	5.63	124.74	120.80
2	B	79	LYS	O-C-N	-5.62	113.71	122.70
2	B	604	ASP	C-N-CA	5.60	135.71	121.70
2	D	333	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	C	282	PRO	C-N-CA	5.59	135.69	121.70
2	D	69	GLY	N-CA-C	5.59	127.08	113.10
1	C	558	ARG	CD-NE-CZ	5.59	131.42	123.60
1	C	430	VAL	O-C-N	-5.59	113.70	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	297	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	C	369	ASP	C-N-CA	5.58	135.66	121.70
2	D	462	ALA	O-C-N	-5.58	113.77	122.70
2	D	283	ARG	N-CA-CB	5.58	120.64	110.60
1	A	70	PHE	O-C-N	-5.58	113.78	122.70
2	D	321	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	304	ALA	CA-C-N	5.57	129.46	117.20
1	C	170	ALA	O-C-N	-5.57	113.79	122.70
1	C	683	THR	N-CA-CB	5.57	120.87	110.30
1	A	429	LYS	C-N-CA	5.55	135.59	121.70
2	D	337	TYR	C-N-CA	5.55	135.59	121.70
2	D	462	ALA	C-N-CA	5.55	135.58	121.70
1	C	241	SER	CB-CA-C	-5.55	99.56	110.10
1	C	189	PRO	N-CA-CB	5.55	109.96	103.30
1	A	184	GLU	C-N-CA	5.54	135.55	121.70
2	B	353	GLY	C-N-CA	5.54	133.93	122.30
1	A	369	ASP	C-N-CA	5.54	135.54	121.70
2	B	456	ARG	O-C-N	-5.54	113.84	122.70
1	C	184	GLU	O-C-N	-5.52	113.86	122.70
1	C	637	PRO	C-N-CA	5.51	135.48	121.70
1	A	634	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	C	70	PHE	O-C-N	-5.51	113.88	122.70
1	C	63	THR	O-C-N	-5.50	113.89	122.70
2	D	23	LEU	O-C-N	-5.50	113.90	122.70
2	D	79	LYS	O-C-N	-5.50	113.91	122.70
1	C	199	ASP	CB-CG-OD1	5.49	123.24	118.30
2	B	435	THR	O-C-N	-5.49	113.92	122.70
1	A	320	PRO	N-CA-CB	5.49	109.88	103.30
1	A	4	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	69	PRO	O-C-N	-5.47	113.94	122.70
1	A	225	PHE	CB-CG-CD1	5.47	124.63	120.80
1	A	233	PRO	N-CA-CB	5.47	109.86	103.30
2	B	92	PRO	O-C-N	-5.46	113.95	122.70
1	A	342	TYR	O-C-N	-5.46	113.97	122.70
1	C	313	HIS	O-C-N	-5.46	113.97	122.70
1	A	93	SER	N-CA-CB	-5.46	102.32	110.50
2	B	617	LEU	N-CA-CB	5.45	121.31	110.40
1	C	535	CYS	O-C-N	-5.45	113.97	122.70
1	A	612	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	690	GLU	O-C-N	-5.45	113.98	122.70
1	A	603	ALA	N-CA-CB	-5.45	102.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	645	VAL	O-C-N	-5.44	114.00	122.70
1	C	5	PRO	N-CA-CB	5.43	109.82	103.30
2	D	339	ASN	C-N-CA	5.43	135.28	121.70
1	C	347	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	159	ASP	CB-CG-OD1	5.43	123.18	118.30
1	C	78	MET	C-N-CA	5.42	135.26	121.70
1	C	248	ALA	C-N-CA	5.42	133.68	122.30
2	B	229	PRO	C-N-CA	5.41	135.23	121.70
2	B	338	VAL	O-C-N	-5.41	114.04	122.70
1	A	199	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	678	PRO	C-N-CA	5.40	135.20	121.70
1	A	89	TYR	CA-CB-CG	5.40	123.66	113.40
1	A	183	GLU	O-C-N	-5.39	114.07	122.70
2	B	338	VAL	CA-C-N	5.39	129.07	117.20
1	C	398	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	23	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	20	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	231	ASN	CB-CA-C	-5.38	99.64	110.40
1	A	438	GLU	O-C-N	-5.38	114.09	122.70
2	D	492	ARG	CD-NE-CZ	5.38	131.13	123.60
1	A	5	PRO	N-CA-CB	5.38	109.75	103.30
1	A	161	MET	CA-CB-CG	5.38	122.44	113.30
1	C	268	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	617	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	504	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	93	SER	N-CA-CB	-5.36	102.45	110.50
1	A	633	LEU	C-N-CA	5.36	135.10	121.70
1	C	52	GLU	C-N-CA	5.36	135.10	121.70
1	C	150	ARG	CA-CB-CG	5.36	125.19	113.40
2	D	403	TYR	CB-CG-CD2	-5.36	117.79	121.00
2	B	410	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	313	HIS	O-C-N	-5.35	114.14	122.70
1	A	578	PRO	N-CA-CB	5.35	109.72	103.30
1	A	405	GLY	CA-C-N	5.34	128.96	117.20
1	C	677	ARG	CA-CB-CG	5.34	125.16	113.40
1	C	401	ASP	CB-CG-OD1	5.34	123.10	118.30
1	C	412	LEU	O-C-N	-5.33	114.17	122.70
1	C	128	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	621	TYR	CB-CG-CD1	5.33	124.19	121.00
2	B	142	PRO	N-CA-CB	5.32	109.68	103.30
2	B	132	GLY	N-CA-C	5.32	126.40	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	52	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	C	120	PRO	O-C-N	-5.31	114.20	122.70
1	C	123	ARG	C-N-CA	5.31	133.46	122.30
1	C	438	GLU	O-C-N	-5.31	114.20	122.70
2	B	86	GLY	CA-C-O	5.31	130.16	120.60
2	B	147	PRO	C-N-CA	5.31	134.97	121.70
2	B	397	ASP	OD1-CG-OD2	-5.31	113.21	123.30
1	C	178	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	A	135	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	D	522	ARG	CD-NE-CZ	5.30	131.03	123.60
1	A	433	MET	CB-CG-SD	5.30	128.31	112.40
2	B	116	PRO	N-CA-CB	5.30	109.66	103.30
1	A	384	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	B	457	LYS	O-C-N	-5.30	114.22	122.70
1	A	107	ALA	O-C-N	-5.29	114.23	122.70
1	C	337	THR	CA-C-O	5.29	131.20	120.10
2	D	67	VAL	C-N-CA	5.28	134.91	121.70
2	B	600	LYS	C-N-CA	5.27	134.88	121.70
2	D	68	ASP	CB-CG-OD1	5.27	123.05	118.30
2	D	337	TYR	CA-C-N	5.27	128.80	117.20
1	A	146	ILE	C-N-CA	5.26	134.86	121.70
1	C	679	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	184	GLU	C-N-CA	5.26	134.85	121.70
1	C	529	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	327	THR	N-CA-C	5.25	125.17	111.00
2	D	86	GLY	O-C-N	-5.25	114.30	122.70
2	B	79	LYS	C-N-CA	5.24	134.80	121.70
2	D	142	PRO	N-CA-CB	5.24	109.59	103.30
1	A	268	ARG	NH1-CZ-NH2	5.23	125.16	119.40
1	A	120	PRO	O-C-N	-5.22	114.34	122.70
1	C	62	ASP	CB-CG-OD1	5.22	123.00	118.30
2	D	485	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	235	THR	N-CA-CB	5.22	120.22	110.30
1	A	282	PRO	CA-C-N	5.22	128.68	117.20
1	A	177	LEU	O-C-N	-5.21	114.36	122.70
2	B	223	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	D	239	ASN	C-N-CA	5.21	134.74	121.70
2	B	88	PRO	N-CA-CB	5.21	109.55	103.30
1	C	146	ILE	C-N-CA	5.21	134.72	121.70
2	D	235	THR	N-CA-CB	5.21	120.19	110.30
2	D	510	ARG	CD-NE-CZ	5.21	130.89	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	543	PRO	N-CA-CB	5.21	109.55	103.30
1	A	674	LYS	CA-CB-CG	5.20	124.85	113.40
1	C	375	PRO	N-CA-CB	5.20	109.54	103.30
1	A	176	ALA	CB-CA-C	-5.19	102.32	110.10
1	C	147	TYR	CB-CG-CD2	-5.19	117.89	121.00
2	B	342	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	128	GLY	CA-C-N	5.18	128.59	117.20
1	A	256	MET	CB-CA-C	-5.17	100.05	110.40
2	B	264	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	633	LEU	CA-C-O	5.17	130.96	120.10
1	A	564	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	477	PRO	N-CA-CB	5.17	109.50	103.30
2	B	604	ASP	O-C-N	-5.17	114.43	122.70
2	D	286	ALA	N-CA-C	-5.17	97.05	111.00
2	B	87	TYR	CG-CD1-CE1	5.16	125.43	121.30
1	A	312	VAL	O-C-N	-5.16	114.44	122.70
1	A	357	GLN	C-N-CA	5.16	133.14	122.30
1	A	78	MET	O-C-N	-5.15	114.46	122.70
1	C	612	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	D	536	HIS	O-C-N	-5.14	114.47	122.70
1	C	222	SER	O-C-N	-5.14	114.47	122.70
1	C	520	GLY	O-C-N	-5.14	114.47	122.70
2	D	86	GLY	CA-C-O	5.14	129.85	120.60
1	C	637	PRO	O-C-N	-5.14	114.48	122.70
1	A	593	ALA	O-C-N	-5.14	114.48	122.70
1	A	63	THR	N-CA-CB	5.13	120.05	110.30
1	C	357	GLN	O-C-N	-5.13	114.48	123.20
1	C	82	ARG	NH1-CZ-NH2	-5.12	113.76	119.40
1	C	131	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	574	VAL	N-CA-CB	5.12	122.77	111.50
2	B	390	VAL	O-C-N	-5.12	114.51	122.70
2	B	339	ASN	C-N-CA	5.12	134.49	121.70
1	A	18	PRO	N-CA-CB	5.11	109.44	103.30
1	A	198	ASN	N-CA-CB	-5.11	101.40	110.60
1	C	445	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	B	25	GLY	C-N-CA	5.10	134.46	121.70
1	C	488	VAL	CB-CA-C	-5.10	101.70	111.40
1	C	570	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	272	SER	C-N-CA	5.08	134.41	121.70
1	A	344	ASN	O-C-N	-5.08	114.57	122.70
1	C	146	ILE	O-C-N	-5.08	114.57	122.70
2	B	114	GLU	CA-CB-CG	5.08	124.57	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	ASP	CB-CG-OD1	5.08	122.87	118.30
2	D	201	PRO	N-CA-CB	5.08	109.39	103.30
2	B	299	ALA	N-CA-CB	5.08	117.21	110.10
2	B	633	ILE	O-C-N	-5.07	114.59	122.70
2	B	283	ARG	N-CA-CB	5.07	119.72	110.60
2	B	239	ASN	O-C-N	-5.07	114.59	122.70
2	D	521	ARG	O-C-N	-5.06	114.60	122.70
1	A	666	PRO	N-CA-CB	5.06	109.37	103.30
1	A	541	ALA	C-N-CA	5.05	134.33	121.70
1	A	189	PRO	O-C-N	-5.05	114.62	122.70
1	A	141	VAL	CA-CB-CG1	5.05	118.47	110.90
2	B	362	PRO	N-CA-CB	5.04	109.35	103.30
1	C	505	PRO	N-CA-CB	5.04	109.35	103.30
1	A	243	TYR	CB-CG-CD2	5.04	124.02	121.00
2	D	422	GLU	O-C-N	-5.04	114.64	122.70
2	D	78	PRO	C-N-CA	5.03	134.28	121.70
1	A	327	THR	N-CA-C	5.03	124.58	111.00
1	C	379	SER	O-C-N	-5.02	114.67	122.70
2	D	116	PRO	N-CA-CB	5.02	109.32	103.30
1	A	210	TYR	CB-CG-CD1	5.02	124.01	121.00
1	C	202	LYS	CA-C-N	5.01	128.23	117.20
2	B	416	ALA	N-CA-CB	5.01	117.12	110.10
2	D	79	LYS	C-N-CA	5.01	134.23	121.70
1	A	224	ILE	O-C-N	-5.01	114.69	122.70
2	B	184	GLU	C-N-CA	5.01	134.23	121.70
1	A	669	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5575	0	5481	41	0
1	C	5575	0	5481	40	0
2	B	4718	0	4672	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4718	0	4670	38	0
3	A	91	0	88	16	0
3	C	91	0	88	11	0
4	A	55	0	35	2	0
4	C	55	0	35	5	0
5	A	55	0	35	1	0
5	C	55	0	35	1	0
6	A	18	0	13	1	0
6	C	18	0	13	7	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	D	6	0	8	0	0
8	A	404	0	0	0	0
8	B	239	0	0	1	0
8	C	400	0	0	2	0
8	D	243	0	0	1	0
All	All	22334	0	20678	186	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 (186) 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)
6:C:803:5AD:H5'2	6:C:803:5AD:C8	1.45	1.45
6:C:803:5AD:H8	6:C:803:5AD:C5'	1.61	1.30
3:C:800:B12:H531	3:C:800:B12:H552	1.35	1.09
3:A:800:B12:H531	3:A:800:B12:H552	1.31	1.07
4:C:801[A]:SCA:NP2	4:C:801[A]:SCA:H92	1.88	0.85
1:A:638:GLU:HA	1:A:671:GLU:HG2	1.60	0.81
3:A:800:B12:C55	3:A:800:B12:H531	2.07	0.81
6:C:803:5AD:C8	6:C:803:5AD:C5'	2.35	0.81
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.63	0.80
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.66	0.76
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.66	0.76
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.68	0.76
3:C:800:B12:H531	3:C:800:B12:C55	2.08	0.74
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.70	0.73
1:A:650:HIS:HB3	1:A:722:LEU:HD11	1.68	0.73
2:D:237:ASP:HB3	2:D:240:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:THR:HB	1:C:707:PRO:HD2	1.71	0.71
2:B:554:VAL:HG12	2:B:558:LYS:HD2	1.72	0.70
3:A:800:B12:H302	3:A:800:B12:H353	1.73	0.70
1:A:706:THR:HB	1:A:707:PRO:HD2	1.73	0.70
6:C:803:5AD:H5'2	6:C:803:5AD:H8	0.73	0.70
1:C:503:ARG:HD2	1:C:508:VAL:HG21	1.74	0.69
1:A:247:GLU:HB3	3:A:800:B12:H532	1.74	0.68
2:B:579:LEU:HG	2:B:583:LYS:HD2	1.74	0.68
3:C:800:B12:H353	3:C:800:B12:H302	1.75	0.67
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.43	0.67
2:D:564:VAL:HG22	2:D:592:ALA:HB3	1.78	0.65
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.79	0.64
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.80	0.64
2:D:579:LEU:HG	2:D:583:LYS:HD2	1.80	0.64
2:B:507:VAL:HG21	2:B:636:VAL:HG22	1.81	0.62
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.82	0.61
1:C:247:GLU:HB3	3:C:800:B12:H532	1.82	0.61
4:A:801[A]:SCA:NP2	4:A:801[A]:SCA:H92	2.15	0.61
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.83	0.60
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.84	0.60
1:C:599:ARG:HG2	1:C:649:VAL:HA	1.83	0.60
4:C:801[A]:SCA:CP9	4:C:801[A]:SCA:NP2	2.63	0.60
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.84	0.59
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.84	0.59
2:D:554:VAL:HG12	2:D:558:LYS:HD2	1.84	0.58
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.84	0.57
2:D:532:SER:HB3	2:D:533:PRO:HD3	1.87	0.57
1:A:599:ARG:HG2	1:A:649:VAL:HG12	1.86	0.56
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.88	0.56
2:D:197:LEU:HB2	2:D:233:ALA:HA	1.88	0.56
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.87	0.56
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.87	0.56
3:C:800:B12:H353	3:C:800:B12:C30	2.37	0.55
1:C:139:ALA:HB1	3:C:800:B12:H362	1.89	0.55
1:A:359:HIS:CE1	1:A:401:ASP:H	2.24	0.55
1:C:359:HIS:CE1	1:C:401:ASP:H	2.23	0.55
3:A:800:B12:H372	3:A:800:B12:H351	1.89	0.55
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.87	0.55
1:A:599:ARG:HG2	1:A:649:VAL:HA	1.89	0.54
3:A:800:B12:H362	3:A:800:B12:H351	1.89	0.54
1:A:120:PRO:HG3	1:A:132:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:800:B12:H261	6:C:803:5AD:H3'	1.90	0.53
2:D:390:VAL:HG12	2:D:392:ILE:HG23	1.90	0.53
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.73	0.53
1:C:577:THR:HG22	1:C:580:VAL:H	1.74	0.53
1:A:706:THR:HB	1:A:707:PRO:CD	2.37	0.53
2:B:513:VAL:HG13	2:B:564:VAL:HG12	1.90	0.53
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.91	0.52
2:D:272:THR:HB	2:D:275:GLU:H	1.75	0.52
2:D:507:VAL:HG12	2:D:509:GLU:H	1.75	0.52
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.92	0.52
6:C:803:5AD:C8	6:C:803:5AD:C4'	2.87	0.52
2:D:27:PHE:HB3	2:D:28:PRO:HD2	1.91	0.52
1:A:139:ALA:HB1	3:A:800:B12:H362	1.92	0.52
1:A:89:TYR:CE2	5:A:802[B]:MCA:HS2	2.45	0.51
2:D:180:VAL:HG13	2:D:197:LEU:HD21	1.93	0.51
2:B:513:VAL:HG23	2:B:540:ILE:HG21	1.93	0.50
2:D:80:ASP:HB3	2:D:407:SER:HB2	1.92	0.50
2:D:518:LEU:HD22	2:D:581:VAL:HG21	1.93	0.50
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.94	0.50
1:A:512:LEU:HD21	1:A:543:ALA:HB1	1.94	0.49
1:C:138:MET:SD	1:C:485:ASN:HB2	2.52	0.49
2:B:613:ILE:HG22	2:B:615:GLY:H	1.77	0.49
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.95	0.49
1:A:683:THR:HG21	1:A:718:LEU:HD13	1.93	0.49
3:A:800:B12:H2B	3:A:800:B12:O7R	2.13	0.49
1:C:610:HIS:NE2	3:C:800:B12:H202	2.28	0.48
1:A:484:ASP:HB3	1:A:487:THR:HG22	1.96	0.48
2:D:219:ASP:HA	2:D:222:ARG:NH2	2.27	0.48
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.95	0.48
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.78	0.48
2:D:331:LEU:HD13	2:D:365:GLN:HB3	1.95	0.48
1:C:484:ASP:HB3	1:C:487:THR:HG22	1.94	0.48
1:C:79:TYR:HB3	1:C:397:THR:HB	1.95	0.48
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.96	0.47
6:C:803:5AD:H8	6:C:803:5AD:C4'	2.39	0.47
3:A:800:B12:H261	6:A:803:5AD:H3'	1.97	0.47
3:A:800:B12:H252	3:A:800:B12:H601	1.97	0.47
4:A:801[A]:SCA:OS1	4:A:801[A]:SCA:CS4	2.60	0.47
1:A:602:LEU:HD22	3:A:800:B12:HM52	1.96	0.47
1:C:638:GLU:HA	1:C:671:GLU:HG2	1.96	0.47
1:A:599:ARG:HH21	1:A:647:ALA:HB1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.97	0.47
1:A:374:LEU:HB2	1:A:481:LEU:HD23	1.97	0.47
4:C:801[A]:SCA:H92	4:C:801[A]:SCA:HN2	1.77	0.47
1:C:706:THR:HB	1:C:707:PRO:CD	2.44	0.46
1:C:528:ASP:HA	1:C:533:LYS:HE3	1.97	0.46
2:B:538:ALA:HB2	2:B:627:LEU:HD13	1.96	0.46
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.50	0.46
1:A:372:ILE:HD13	1:A:478:LEU:HD23	1.96	0.46
1:C:252:ALA:O	1:C:256:MET:HG3	2.16	0.46
3:A:800:B12:H2B	3:A:800:B12:O2	2.16	0.46
2:B:281:ASN:ND2	2:B:323:ASN:HD21	2.11	0.45
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.51	0.45
1:A:577:THR:HG22	1:A:580:VAL:H	1.81	0.45
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.98	0.45
2:D:232:ARG:HD2	2:D:321:ARG:HH21	1.81	0.45
1:C:89:TYR:CE2	5:C:802[B]:MCA:HS2	2.51	0.45
2:D:176:ALA:HB1	2:D:197:LEU:HD22	1.98	0.45
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.47	0.45
1:A:503:ARG:HD2	1:A:508:VAL:HG21	1.98	0.45
8:C:807:HOH:O	2:D:42:VAL:HG21	2.16	0.45
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.48	0.44
2:D:133:VAL:HG23	2:D:380:ARG:HD2	1.99	0.44
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.99	0.44
1:A:138:MET:SD	1:A:485:ASN:HB2	2.58	0.44
2:B:92:PRO:O	2:B:93:PHE:HB2	2.18	0.44
2:D:252:LEU:HD11	2:D:300:LEU:HA	1.99	0.44
2:D:267:VAL:HA	2:D:271:PHE:O	2.18	0.44
2:D:333:ARG:HH21	2:D:498:GLU:HB3	1.82	0.44
2:B:515:LEU:HD12	2:B:528:GLU:HG2	2.00	0.44
1:A:589:GLU:HG3	1:A:723:ARG:NH1	2.33	0.44
1:A:448:GLU:HG2	1:A:569:VAL:HG21	1.99	0.43
3:C:800:B12:H543	3:C:800:B12:C53	2.47	0.43
1:C:215:GLN:HB3	1:C:216:PRO:CD	2.47	0.43
1:C:441:ILE:HB	1:C:442:PRO:HD3	2.00	0.43
3:A:800:B12:H372	3:A:800:B12:C35	2.49	0.43
1:C:250:ALA:HB2	1:C:446:ILE:HG12	2.00	0.43
1:A:589:GLU:HG3	1:A:723:ARG:HH12	1.84	0.43
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.39	0.43
2:D:208:GLN:O	2:D:486:LYS:HB2	2.19	0.43
4:C:801[A]:SCA:OS1	4:C:801[A]:SCA:CS4	2.66	0.43
1:C:602:LEU:HD22	3:C:800:B12:HM52	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:THR:HA	1:A:578:PRO:HD3	1.90	0.43
1:C:406:SER:HB3	1:C:409:VAL:HB	2.01	0.42
1:A:597:ARG:HG2	1:A:597:ARG:HH11	1.84	0.42
1:C:597:ARG:HG2	1:C:597:ARG:HH11	1.84	0.42
1:A:252:ALA:O	1:A:256:MET:HG3	2.20	0.42
1:A:606:GLY:O	1:A:634:PHE:HA	2.19	0.42
1:C:541:ALA:O	1:C:542:MET:HB2	2.19	0.42
2:D:170:TYR:O	2:D:171:ASP:HB2	2.20	0.42
2:B:331:LEU:HD13	2:B:365:GLN:HB3	2.02	0.42
3:A:800:B12:C30	3:A:800:B12:H353	2.45	0.42
2:B:272:THR:HB	2:B:275:GLU:H	1.84	0.42
2:B:325:ILE:HD11	2:B:361:LEU:HD21	2.02	0.42
2:B:631:LEU:HD22	2:B:636:VAL:HG11	2.02	0.41
1:C:63:THR:HB	8:C:908:HOH:O	2.19	0.41
1:C:25:PHE:HB2	2:D:87:TYR:HB3	2.02	0.41
2:D:613:ILE:HG22	2:D:615:GLY:H	1.85	0.41
1:A:10:VAL:HG11	2:B:310:VAL:HG21	2.03	0.41
1:A:668:LEU:HD13	1:A:682:ILE:HG12	2.02	0.41
2:B:517:CYS:HA	2:B:568:CYS:O	2.21	0.41
1:A:602:LEU:HD11	1:A:617:ILE:HG22	2.03	0.41
1:C:668:LEU:HD13	1:C:682:ILE:HG12	2.02	0.41
2:D:86:GLY:HA3	8:D:648:HOH:O	2.20	0.41
1:A:213:PRO:HD2	1:A:216:PRO:HG2	2.02	0.41
1:A:215:GLN:HB3	1:A:216:PRO:CD	2.50	0.41
1:C:683:THR:HG22	1:C:703:GLU:HB2	2.03	0.41
1:C:405:GLY:O	1:C:406:SER:C	2.59	0.41
2:B:567:LEU:HD11	2:B:582:ALA:HB2	2.02	0.41
2:B:267:VAL:HA	2:B:271:PHE:O	2.21	0.41
2:B:48:PRO:HG2	2:B:51:LYS:HB2	2.03	0.41
1:C:203:GLU:OE2	1:C:207:ARG:HD3	2.21	0.41
1:C:710:VAL:HB	1:C:713:GLU:HB2	2.03	0.41
1:A:216:PRO:HB3	1:A:556:PHE:CD1	2.55	0.40
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.86	0.40
1:C:8:ASP:HA	2:D:421:GLN:HG2	2.03	0.40
1:C:243:TYR:CE2	1:C:247:GLU:HG3	2.56	0.40
3:A:800:B12:H363	3:A:800:B12:C42	2.52	0.40
1:C:328:HIS:HB2	4:C:801[A]:SCA:H52	2.04	0.40
1:A:638:GLU:HG3	1:A:671:GLU:OE2	2.20	0.40
2:D:592:ALA:HB2	2:D:633:ILE:HG21	2.03	0.40
2:B:272:THR:HG22	8:B:863:HOH:O	2.20	0.40
2:B:284:VAL:HG21	2:B:297:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LEU:HD21	2:B:136:LEU:HD21	2.04	0.40
3:C:800:B12:H372	3:C:800:B12:H351	2.03	0.40
3:A:800:B12:H362	3:A:800:B12:C35	2.52	0.40
2:B:554:VAL:HG21	2:B:584:ALA:HB1	2.03	0.40
2:D:517:CYS:HB2	2:D:545:VAL:O	2.22	0.40
2:B:431:LYS:HD2	2:B:431:LYS:HA	1.98	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	724/727 (100%)	697 (96%)	27 (4%)	0	100	100
1	C	724/727 (100%)	687 (95%)	37 (5%)	0	100	100
2	B	617/637 (97%)	591 (96%)	24 (4%)	2 (0%)	46	50
2	D	617/637 (97%)	584 (95%)	31 (5%)	2 (0%)	46	50
All	All	2682/2728 (98%)	2559 (95%)	119 (4%)	4 (0%)	56	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	171	ASP
2	D	269	GLN
2	B	269	GLN
2	B	171	ASP

### 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	572/590 (97%)	557 (97%)	15 (3%)	54	66
1	C	572/590 (97%)	558 (98%)	14 (2%)	57	69
2	B	481/509 (94%)	465 (97%)	16 (3%)	45	56
2	D	481/509 (94%)	460 (96%)	21 (4%)	35	42
All	All	2106/2198 (96%)	2040 (97%)	66 (3%)	47	59

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	14	ASN
1	A	24	ARG
1	A	93	SER
1	A	96	LYS
1	A	127	SER
1	A	131	ARG
1	A	318	LYS
1	A	414	TRP
1	A	471	ARG
1	A	533	LYS
1	A	588	GLU
1	A	597	ARG
1	A	668	LEU
1	A	723	ARG
2	B	83	LYS
2	B	141	ASP
2	B	155	SER
2	B	186	SER
2	B	187	ASP
2	B	191	LYS
2	B	199	LEU
2	B	216	VAL
2	B	228	SER
2	B	272	THR
2	B	334	GLU
2	B	398	PRO
2	B	410	ARG

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Mol	Chain	Res	Type
2	B	436	GLU
2	B	451	LYS
2	B	515	LEU
1	C	3	THR
1	C	4	LEU
1	C	24	ARG
1	C	96	LYS
1	C	265	ASP
1	C	318	LYS
1	C	369	ASP
1	C	471	ARG
1	C	482	LYS
1	C	567	SER
1	C	577	THR
1	C	588	GLU
1	C	597	ARG
1	C	668	LEU
2	D	20	THR
2	D	83	LYS
2	D	141	ASP
2	D	155	SER
2	D	186	SER
2	D	187	ASP
2	D	191	LYS
2	D	216	VAL
2	D	228	SER
2	D	240	ILE
2	D	272	THR
2	D	288	HIS
2	D	334	GLU
2	D	410	ARG
2	D	451	LYS
2	D	577	GLN
2	D	586	LYS
2	D	608	GLU
2	D	617	LEU
2	D	629	SER
2	D	638	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	14	ASN
1	A	359	HIS
1	A	385	ASN
1	A	635	GLN
1	A	643	GLN
2	B	323	ASN
1	C	359	HIS
1	C	385	ASN
1	C	635	GLN
1	C	643	GLN
2	D	322	GLN
2	D	323	ASN

### 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](#)

12 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	$\# Z  > 2$
7	GOL	A	1	-	5,5,5	0.66	0	5,5,5	1.09	1 (20%)
3	B12	A	800	1	74,101,101	1.17	7 (9%)	111,166,166	1.67	21 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SCA	A	801[A]	-	44,57,57	0.86	0	57,84,84	1.84	7 (12%)
5	MCA	A	802[B]	-	42,57,57	0.82	0	53,85,85	1.44	6 (11%)
6	5AD	A	803	-	15,20,20	0.78	0	14,30,30	2.64	5 (35%)
7	GOL	B	639	-	5,5,5	0.29	0	5,5,5	0.59	0
7	GOL	C	1	-	5,5,5	0.71	0	5,5,5	0.96	0
3	B12	C	800	1	74,101,101	1.14	5 (6%)	111,166,166	1.74	25 (22%)
4	SCA	C	801[A]	-	44,57,57	0.80	1 (2%)	57,84,84	1.62	11 (19%)
5	MCA	C	802[B]	-	42,57,57	0.77	0	53,85,85	1.32	7 (13%)
6	5AD	C	803	-	15,20,20	0.90	0	14,30,30	3.17	4 (28%)
7	GOL	D	639	-	5,5,5	0.50	0	5,5,5	0.67	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
7	GOL	A	1	-	-	0/4/4/4	0/0/0/0
3	B12	A	800	1	-	0/51/223/223	0/3/11/11
4	SCA	A	801[A]	-	-	0/50/72/72	0/3/3/3
5	MCA	A	802[B]	-	-	0/51/75/75	0/3/3/3
6	5AD	A	803	-	-	0/0/20/20	0/3/3/3
7	GOL	B	639	-	-	0/4/4/4	0/0/0/0
7	GOL	C	1	-	-	0/4/4/4	0/0/0/0
3	B12	C	800	1	-	0/51/223/223	0/3/11/11
4	SCA	C	801[A]	-	-	0/50/72/72	0/3/3/3
5	MCA	C	802[B]	-	-	0/51/75/75	0/3/3/3
6	5AD	C	803	-	-	0/0/20/20	0/3/3/3
7	GOL	D	639	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	C11-C10	-2.77	1.36	1.41
3	A	800	B12	C11-C10	-2.58	1.36	1.41
4	C	801[A]	SCA	P1-O11	-2.14	1.45	1.54
3	A	800	B12	C55-C56	2.09	1.58	1.53
3	A	800	B12	P-O2	2.27	1.66	1.59
3	A	800	B12	C54-C17	2.29	1.58	1.54
3	C	800	B12	C54-C17	2.48	1.59	1.54
3	C	800	B12	C30-C3	2.52	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C30-C3	2.53	1.58	1.54
3	A	800	B12	C41-C8	2.71	1.58	1.54
3	C	800	B12	C41-C8	2.94	1.58	1.54
3	C	800	B12	C48-C13	3.28	1.59	1.54
3	A	800	B12	C48-C13	4.43	1.61	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	803	5AD	C5'-C4'-C3'	-6.04	109.49	115.80
4	A	801[A]	SCA	OS1-CS1-CS2	-5.35	120.25	123.94
3	A	800	B12	C4R-O6R-C1R	-5.21	104.00	109.72
6	A	803	5AD	C5'-C4'-C3'	-4.95	110.62	115.80
4	C	801[A]	SCA	CP9-CPA-CP7	-4.83	100.53	109.34
5	A	802[B]	MCA	CP1-CP2-NP1	-4.75	102.85	112.36
4	C	801[A]	SCA	CP1-CP2-NP1	-4.26	103.84	112.36
3	A	800	B12	C55-C56-C57	-4.26	102.46	111.06
5	A	802[B]	MCA	CP2-NP1-CP3	-4.20	114.53	122.79
6	A	803	5AD	C4'-O4'-C1'	-3.94	105.39	109.72
5	C	802[B]	MCA	CP2-NP1-CP3	-3.84	115.23	122.79
3	A	800	B12	C9-C10-C11	-3.83	122.68	132.28
3	A	800	B12	C13-C14-C15	-3.70	119.41	131.88
3	C	800	B12	C35-C5-C4	-3.61	111.79	118.25
4	A	801[A]	SCA	CP1-CP2-NP1	-3.56	105.25	112.36
5	C	802[B]	MCA	CP1-CP2-NP1	-3.55	105.27	112.36
3	A	800	B12	C3-C4-C5	-3.41	120.38	131.88
5	C	802[B]	MCA	C2'-C1'-N9	-3.31	109.23	114.29
3	C	800	B12	C3-C4-C5	-3.19	121.12	131.88
5	A	802[B]	MCA	OP3-CP7-CP6	-3.16	103.13	110.38
4	A	801[A]	SCA	CS2-CS1-S	-3.15	110.52	113.36
4	A	801[A]	SCA	CP9-CPA-CP7	-3.05	103.77	109.34
4	C	801[A]	SCA	OS1-CS1-CS2	-2.96	121.90	123.94
6	A	803	5AD	C1'-N9-C4	-2.85	122.63	126.94
6	C	803	5AD	C1'-N9-C4	-2.81	122.70	126.94
3	C	800	B12	C2P-C1P-N59	-2.81	108.77	112.92
3	C	800	B12	C9-C10-C11	-2.70	125.51	132.28
3	A	800	B12	C2-C1-C19	-2.69	113.91	118.56
3	C	800	B12	C2-C1-C19	-2.69	113.91	118.56
3	C	800	B12	C25-C2-C3	-2.60	111.17	115.56
5	C	802[B]	MCA	OP3-CP7-CP6	-2.60	104.42	110.38
3	C	800	B12	C55-C56-C57	-2.58	105.85	111.06
3	C	800	B12	O51-C50-C49	-2.53	113.68	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	803	5AD	C4'-O4'-C1'	-2.53	106.94	109.72
5	A	802[B]	MCA	OP1-CP3-NP1	-2.50	117.98	122.94
3	C	800	B12	C5B-C4B-C9B	-2.48	116.87	120.92
3	A	800	B12	C1P-N59-C57	-2.43	116.59	122.68
3	C	800	B12	C5M-C5B-C6B	-2.42	115.41	120.73
3	A	800	B12	C48-C13-C12	-2.41	109.92	116.53
3	C	800	B12	C56-C57-N59	-2.41	112.27	116.46
3	A	800	B12	C56-C55-C17	-2.41	110.53	115.57
3	C	800	B12	C13-C14-C15	-2.40	123.79	131.88
3	C	800	B12	O58-C57-C56	-2.37	117.89	121.98
3	C	800	B12	C54-C17-C55	-2.36	105.35	109.27
3	A	800	B12	C5M-C5B-C6B	-2.35	115.56	120.73
3	A	800	B12	C5B-C4B-C9B	-2.32	117.13	120.92
3	C	800	B12	C56-C55-C17	-2.28	110.79	115.57
4	C	801[A]	SCA	CS2-CS1-S	-2.27	111.31	113.36
3	A	800	B12	C31-C30-C3	-2.24	108.10	114.80
7	A	1	GOL	C3-C2-C1	-2.22	102.40	111.12
4	C	801[A]	SCA	CP5-NP2-CP6	-2.22	118.14	122.53
3	C	800	B12	O44-C43-N45	-2.08	116.48	122.46
4	A	801[A]	SCA	CS2-CS3-CS4	-2.07	108.96	112.75
3	C	800	B12	C4B-C9B-C8B	-2.07	118.99	121.10
6	A	803	5AD	O4'-C1'-N9	-2.06	103.79	108.10
4	C	801[A]	SCA	CP2-NP1-CP3	-2.02	118.81	122.79
3	A	800	B12	O51-C50-C49	-2.00	115.22	121.05
5	C	802[B]	MCA	CP2-CP1-S	2.03	116.79	111.36
3	C	800	B12	C18-C17-C16	2.04	103.30	100.54
4	C	801[A]	SCA	CP4-CP5-NP2	2.06	116.39	111.88
5	A	802[B]	MCA	CP2-CP1-S	2.09	116.95	111.36
3	A	800	B12	C30-C31-C32	2.10	119.18	112.53
5	C	802[B]	MCA	O22-P2-O21	2.25	124.71	112.53
5	C	802[B]	MCA	CP8-CPA-CPB	2.30	111.48	108.50
4	C	801[A]	SCA	CP8-CPA-CP9	2.31	113.92	109.28
3	A	800	B12	C31-C32-N33	2.32	123.82	116.53
3	A	800	B12	C18-C17-C16	2.33	103.69	100.54
3	C	800	B12	C25-C2-C1	2.38	117.56	113.79
3	A	800	B12	C20-C1-C19	2.46	111.79	109.38
4	C	801[A]	SCA	CP8-CPA-CPB	2.68	111.98	108.50
5	A	802[B]	MCA	CP8-CPA-CPB	2.70	112.00	108.50
3	A	800	B12	C35-C5-C6	2.91	123.46	118.25
3	C	800	B12	C20-C1-C19	2.96	112.28	109.38
3	C	800	B12	O58-C57-N59	3.48	129.84	122.94
3	A	800	B12	C55-C17-C18	3.56	118.12	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801[A]	SCA	CP9-CPA-CPB	3.68	113.27	108.50
3	C	800	B12	C55-C17-C18	3.79	118.59	110.97
3	C	800	B12	C53-C15-C14	4.10	125.58	118.25
3	A	800	B12	C53-C15-C14	4.41	126.15	118.25
3	A	800	B12	C7B-C8B-C9B	4.67	125.17	120.54
4	A	801[A]	SCA	CP8-CPA-CPB	4.75	114.66	108.50
4	C	801[A]	SCA	OS1-CS1-S	4.98	126.78	122.83
3	C	800	B12	C7B-C8B-C9B	5.96	126.44	120.54
3	C	800	B12	C35-C5-C6	6.18	129.32	118.25
6	A	803	5AD	N3-C2-N1	6.34	133.75	128.89
4	A	801[A]	SCA	OS1-CS1-S	8.06	129.22	122.83
6	C	803	5AD	N3-C2-N1	8.89	135.70	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	16	0
4	A	801[A]	SCA	2	0
5	A	802[B]	MCA	1	0
6	A	803	5AD	1	0
3	C	800	B12	11	0
4	C	801[A]	SCA	5	0
5	C	802[B]	MCA	1	0
6	C	803	5AD	7	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	726/727 (99%)	-0.09	10 (1%) 78 77	12, 30, 54, 90	0
1	C	726/727 (99%)	-0.02	19 (2%) 59 58	11, 30, 54, 90	0
2	B	619/637 (97%)	0.31	30 (4%) 34 34	16, 42, 71, 103	0
2	D	619/637 (97%)	0.58	59 (9%) 10 9	18, 43, 71, 103	0
All	All	2690/2728 (98%)	0.17	118 (4%) 38 37	11, 35, 66, 103	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	728	ALA	7.3
1	C	728	ALA	7.1
1	A	3	THR	5.5
1	C	3	THR	5.4
2	D	107	TRP	5.3
1	A	576	ASN	5.2
1	C	23	ARG	5.1
1	C	576	ASN	5.1
2	D	567	LEU	4.8
2	D	173	GLY	4.7
2	D	192	ASP	4.3
2	D	146	ALA	4.2
2	D	270	GLY	4.1
1	C	474	HIS	4.1
2	B	567	LEU	4.1
2	D	267	VAL	3.9
2	D	161	MET	3.8
2	D	183	TYR	3.8
2	B	587	ALA	3.8
2	D	638	LYS	3.7
1	A	477	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	482	ALA	3.7
2	B	107	TRP	3.7
1	A	474	HIS	3.7
2	B	106	ALA	3.6
2	B	508	SER	3.5
2	B	230	ASP	3.5
2	D	548	GLY	3.5
2	D	20	THR	3.5
2	B	20	THR	3.4
2	D	555	GLU	3.3
1	C	528	ASP	3.2
2	D	170	TYR	3.2
2	D	230	ASP	3.2
2	D	158	LEU	3.2
2	D	151	ASP	3.1
2	B	192	ASP	3.1
2	B	307	ILE	3.1
1	C	9	SER	3.0
2	B	179	LEU	3.0
2	B	161	MET	3.0
2	D	106	ALA	3.0
2	D	565	ALA	2.9
1	C	16	PRO	2.9
2	D	148	GLU	2.9
2	D	316	ASP	2.9
2	D	187	ASP	2.9
1	C	130	PRO	2.9
2	D	425	LYS	2.9
2	D	318	ARG	2.8
1	C	36	GLU	2.7
2	B	548	GLY	2.7
1	C	32	ALA	2.7
2	D	274	THR	2.6
2	D	505	THR	2.6
1	C	14	ASN	2.6
2	D	559	LYS	2.6
1	C	501	ALA	2.6
2	B	260	ALA	2.6
2	D	323	ASN	2.6
2	B	187	ASP	2.5
2	B	507	VAL	2.5
2	D	227	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	149	HIS	2.5
1	A	501	ALA	2.5
2	D	307	ILE	2.5
2	D	480	PRO	2.5
2	B	195	LEU	2.5
1	A	479	ASP	2.5
2	D	418	LYS	2.5
2	D	507	VAL	2.5
2	B	638	LYS	2.4
2	B	516	ALA	2.4
2	D	614	ASP	2.4
2	B	197	LEU	2.4
2	D	518	LEU	2.4
2	D	272	THR	2.4
2	B	603	GLY	2.4
1	C	35	GLY	2.3
2	B	149	HIS	2.3
2	B	505	THR	2.3
2	D	431	LYS	2.3
2	D	558	LYS	2.3
2	D	604	ASP	2.2
2	D	164	VAL	2.2
2	D	126	LEU	2.2
1	C	30	ALA	2.2
2	B	538	ALA	2.2
2	B	50	GLU	2.2
1	C	567	SER	2.2
2	B	183	TYR	2.2
2	D	506	SER	2.2
2	D	211	GLU	2.2
2	D	475	GLU	2.2
2	B	49	PRO	2.2
2	D	312	GLY	2.1
2	D	83	LYS	2.1
2	B	475	GLU	2.1
2	D	202	ILE	2.1
2	D	103	ASP	2.1
2	D	229	PRO	2.1
1	C	430	VAL	2.1
2	D	105	ASP	2.1
2	D	434	MET	2.1
1	A	588	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	204	PHE	2.1
1	A	646	GLU	2.1
2	B	257	ALA	2.1
2	D	222	ARG	2.1
1	A	674	LYS	2.1
2	D	209	GLY	2.0
2	B	440	LYS	2.0
2	B	575	ALA	2.0
2	D	305	ALA	2.0
2	D	25	GLY	2.0
1	C	574	VAL	2.0
1	C	19	ALA	2.0
2	D	194	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	5AD	C	803	18/18	0.76	0.45	15.21	17,30,37,37	18
6	5AD	A	803	18/18	0.80	0.47	13.96	27,32,35,38	18
7	GOL	C	1	6/6	0.82	0.18	11.49	30,36,38,41	0
7	GOL	A	1	6/6	0.84	0.21	9.61	28,35,38,42	0
7	GOL	B	639	6/6	0.79	0.27	4.40	37,47,49,49	0
7	GOL	D	639	6/6	0.82	0.29	0.98	50,53,56,58	0
4	SCA	C	801[A]	55/55	0.97	0.10	-0.40	7,19,24,26	55
5	MCA	C	802[B]	55/55	0.97	0.10	-0.57	12,21,25,26	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SCA	A	801[A]	55/55	0.97	0.09	-0.75	6,20,27,30	55
3	B12	A	800	91/91	0.98	0.09	-0.76	11,20,28,29	0
5	MCA	A	802[B]	55/55	0.97	0.09	-0.79	10,20,25,25	55
3	B12	C	800	91/91	0.98	0.09	-0.94	10,18,26,30	0

## 6.5 Other polymers

There are no such residues in this entry.