



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:01 AM GMT

PDB ID : 7REQ
Title : METHYLMALONYL-COA MUTASE, 2-CARBOXYPROPYL-COA INHIBITOR COMPLEX
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1998-09-10
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

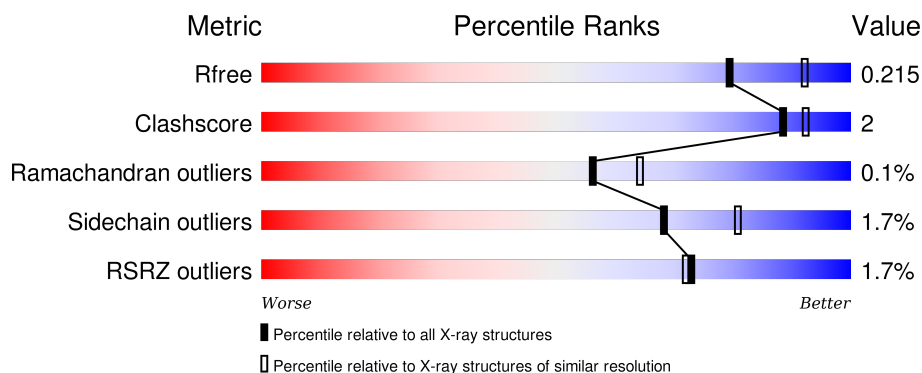
1 Overall quality at a glance

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 ≥ 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>2%</div> <div>81% 17% .</div> </div>
1	C	727	<div> <div>2%</div> <div>80% 18% .</div> </div>
2	B	637	<div> <div>2%</div> <div>81% 15% ..</div> </div>
2	D	637	<div> <div>2%</div> <div>82% 15% ..</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
5	GOL	B	3002	-	-	-	X
5	GOL	D	3004	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5539	3507	952	1056	24			
1	C	725	Total	C	N	O	S	0	0	0
			5539	3507	952	1056	24			

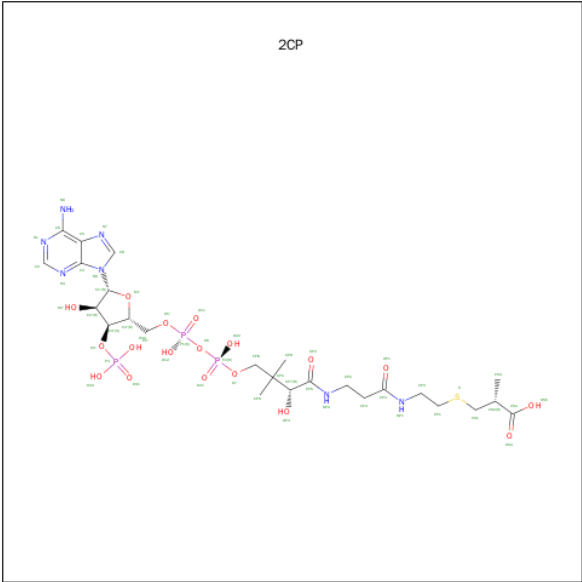
- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	623	Total	C	N	O	S	0	0	0
			4744	2992	823	916	13			
2	D	623	Total	C	N	O	S	0	0	0
			4744	2992	823	916	13			

There are 6 discrepancies between the modelled and reference sequences:

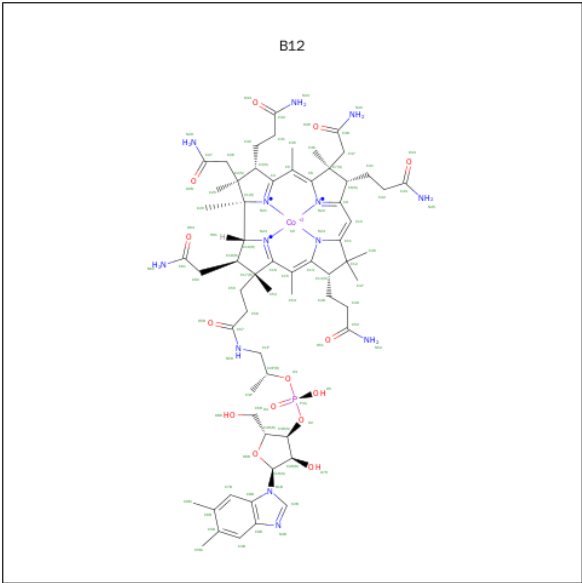
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is 2-CARBOXYPROPYL-COENZYME A (three-letter code: 2CP) (formula: C₂₅H₄₂N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	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
			3	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	420	Total	O	0	0
			420	420		
6	B	243	Total	O	0	0
			243	243		
6	C	421	Total	O	0	0
			421	421		
6	D	242	Total	O	0	0
			242	242		

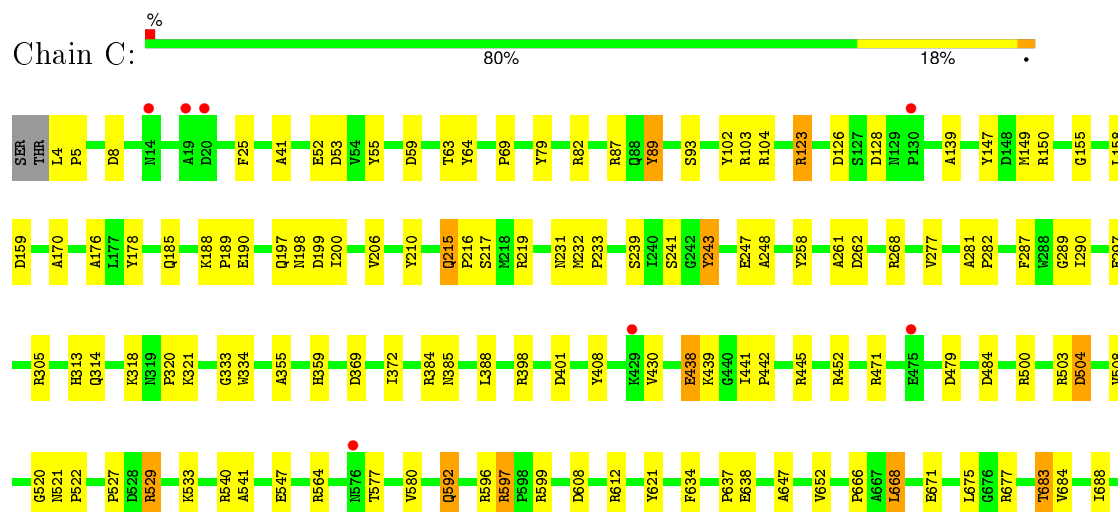
3 Residue-property plots [i](#)

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: PROTEIN (METHYLMALONYL-COA MUTASE)

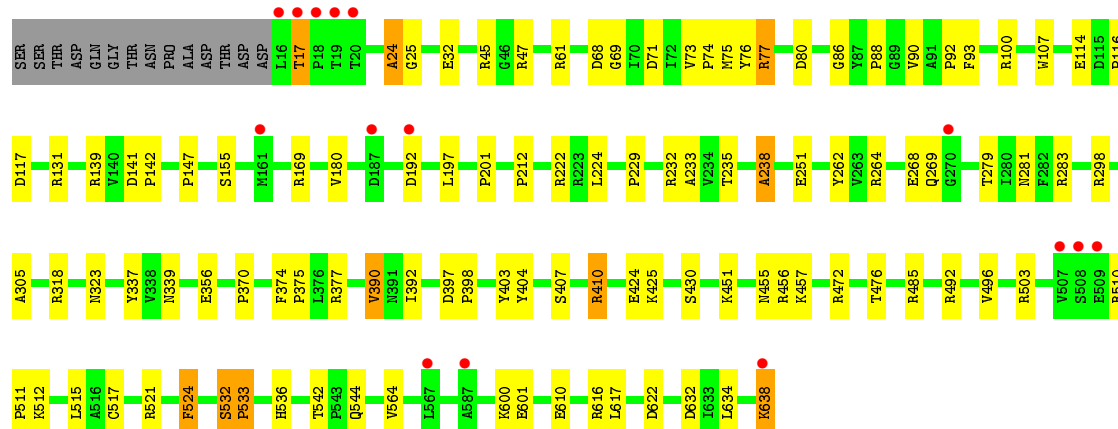
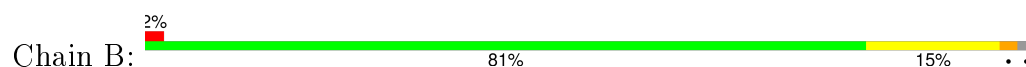


• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE)

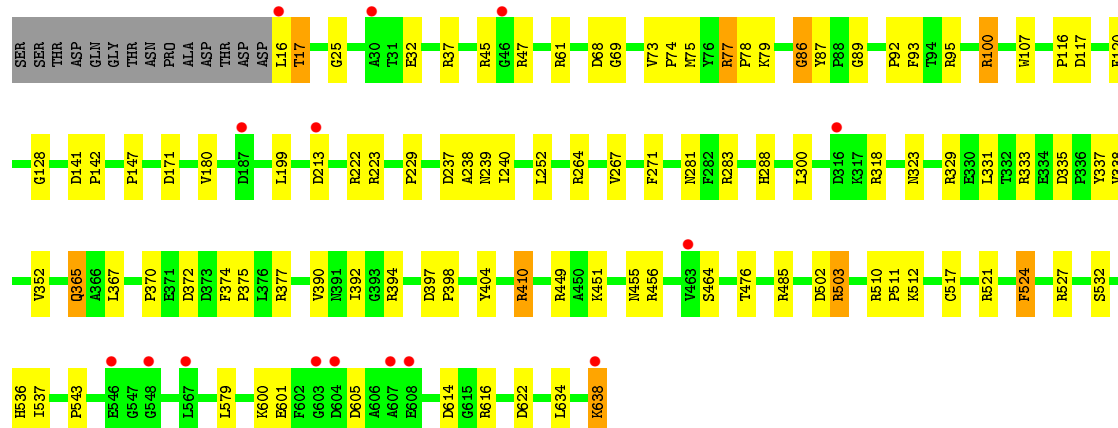
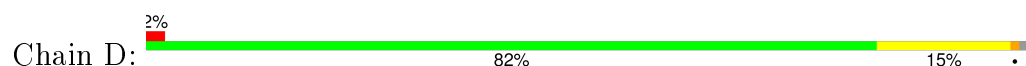




• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)



• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.53 Å 161.40 Å 86.97 Å 90.00° 104.81° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-2.20) 95.4 (19.96-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.19 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.229 0.176 , 0.215	Depositor DCC
R_{free} test set	7983 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 157423 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22203	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: GOL, 2CP, B12

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/5655	1.92	136/7686 (1.8%)
1	C	0.63	0/5655	1.86	126/7686 (1.6%)
2	B	0.58	0/4835	1.84	102/6569 (1.6%)
2	D	0.58	0/4835	1.84	89/6569 (1.4%)
All	All	0.61	0/20980	1.87	453/28510 (1.6%)

There are no bond length outliers.

All (453) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ARG	CD-NE-CZ	39.80	179.32	123.60
2	B	410	ARG	CD-NE-CZ	38.44	177.41	123.60
2	D	410	ARG	CD-NE-CZ	36.73	175.03	123.60
1	C	103	ARG	CD-NE-CZ	25.43	159.21	123.60
1	A	103	ARG	CD-NE-CZ	21.78	154.09	123.60
2	D	264	ARG	NE-CZ-NH2	-20.97	109.82	120.30
1	A	452	ARG	NE-CZ-NH2	-17.77	111.41	120.30
1	C	452	ARG	NE-CZ-NH2	-17.42	111.59	120.30
2	D	264	ARG	CD-NE-CZ	14.54	143.96	123.60
1	A	597	ARG	NE-CZ-NH1	14.12	127.36	120.30
1	C	596	ARG	CD-NE-CZ	14.00	143.21	123.60
1	C	597	ARG	CD-NE-CZ	13.61	142.65	123.60
2	D	77	ARG	CD-NE-CZ	13.42	142.39	123.60
1	A	677	ARG	NE-CZ-NH2	-12.50	114.05	120.30
2	D	264	ARG	NE-CZ-NH1	12.23	126.42	120.30
2	B	77	ARG	CD-NE-CZ	12.12	140.56	123.60
1	C	597	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	597	ARG	CD-NE-CZ	11.20	139.29	123.60
2	B	77	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	384	ARG	CD-NE-CZ	10.88	138.83	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	452	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	103	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	A	596	ARG	NE-CZ-NH1	10.06	125.33	120.30
2	B	616	ARG	NE-CZ-NH2	-10.01	115.29	120.30
2	B	169	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	C	82	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	C	500	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	C	287	PHE	CB-CG-CD1	9.79	127.65	120.80
1	C	452	ARG	CD-NE-CZ	9.73	137.23	123.60
1	A	82	ARG	CD-NE-CZ	9.72	137.21	123.60
1	A	147	TYR	CB-CG-CD2	9.64	126.79	121.00
2	D	524	PHE	CB-CG-CD1	9.57	127.50	120.80
1	C	210	TYR	CB-CG-CD1	9.55	126.73	121.00
2	B	264	ARG	CD-NE-CZ	9.52	136.93	123.60
2	B	622	ASP	CB-CG-OD1	9.45	126.80	118.30
2	D	283	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	C	471	ARG	NE-CZ-NH1	9.14	124.87	120.30
2	D	77	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	C	484	ASP	CB-CG-OD1	9.03	126.42	118.30
1	A	23	ARG	NE-CZ-NH2	9.01	124.80	120.30
1	A	369	ASP	CB-CG-OD2	8.97	126.38	118.30
1	A	599	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	283	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	B	298	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	B	222	ARG	NE-CZ-NH1	8.79	124.70	120.30
2	D	616	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	723	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	C	82	ARG	NE-CZ-NH2	-8.64	115.98	120.30
2	D	223	ARG	NE-CZ-NH1	8.60	124.60	120.30
2	B	264	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	C	445	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	C	55	TYR	CB-CG-CD1	-8.38	115.97	121.00
2	B	404	TYR	CB-CG-CD1	8.31	125.99	121.00
2	D	622	ASP	CB-CG-OD1	8.29	125.76	118.30
1	A	102	TYR	CB-CG-CD1	8.29	125.97	121.00
1	A	268	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	258	TYR	CB-CG-CD2	8.27	125.96	121.00
1	C	63	THR	O-C-N	-8.22	109.55	122.70
1	A	523	ASP	CB-CG-OD1	8.17	125.65	118.30
1	A	147	TYR	CB-CG-CD1	-8.12	116.13	121.00
2	D	229	PRO	C-N-CA	8.11	141.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ASP	CB-CG-OD1	8.07	125.57	118.30
1	C	150	ARG	NE-CZ-NH2	8.06	124.33	120.30
2	D	318	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	484	ASP	CB-CG-OD1	7.97	125.48	118.30
1	C	55	TYR	CB-CG-CD2	7.97	125.78	121.00
1	A	597	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	232	MET	CA-CB-CG	7.87	126.68	113.30
2	D	329	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	262	ASP	CB-CG-OD2	7.85	125.36	118.30
1	C	384	ARG	CD-NE-CZ	7.83	134.56	123.60
1	C	727	ASP	C-N-CA	7.80	141.20	121.70
1	A	283	ARG	NE-CZ-NH2	-7.73	116.44	120.30
2	B	229	PRO	C-N-CA	7.72	141.00	121.70
2	B	17	THR	CA-C-O	7.71	136.29	120.10
2	B	616	ARG	CD-NE-CZ	7.66	134.33	123.60
1	C	529	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	55	TYR	CB-CG-CD2	7.66	125.59	121.00
1	C	408	TYR	CB-CG-CD2	7.63	125.58	121.00
2	B	318	ARG	CD-NE-CZ	7.61	134.25	123.60
1	C	637	PRO	O-C-N	-7.59	110.56	122.70
2	D	510	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	452	ARG	CD-NE-CZ	7.56	134.18	123.60
1	A	471	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	103	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	C	102	TYR	CB-CG-CD1	7.51	125.51	121.00
2	D	17	THR	CA-C-O	7.50	135.86	120.10
1	A	103	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	104	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	A	326	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	C	597	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	D	47	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	D	527	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	439	LYS	C-N-CA	7.33	137.69	122.30
2	B	76	TYR	CB-CG-CD1	-7.32	116.61	121.00
2	D	600	LYS	O-C-N	-7.31	111.00	122.70
1	C	599	ARG	CD-NE-CZ	7.23	133.72	123.60
2	B	536	HIS	O-C-N	-7.18	111.21	122.70
2	D	117	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	255	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	C	89	TYR	CA-CB-CG	7.09	126.88	113.40
1	A	206	VAL	CA-CB-CG1	7.09	121.53	110.90
1	C	243	TYR	CB-CG-CD2	7.07	125.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	521	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	B	68	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	683	THR	N-CA-CB	7.06	123.72	110.30
2	D	318	ARG	CD-NE-CZ	7.04	133.45	123.60
1	C	281	ALA	N-CA-CB	7.04	119.95	110.10
1	A	541	ALA	O-C-N	-7.03	111.45	122.70
1	A	258	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	C	634	PHE	CB-CG-CD1	-6.99	115.90	120.80
1	C	41	ALA	O-C-N	-6.99	111.52	122.70
1	C	199	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	243	TYR	CB-CG-CD2	6.98	125.19	121.00
1	C	268	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	287	PHE	CB-CG-CD2	-6.95	115.94	120.80
2	B	76	TYR	CB-CG-CD2	6.89	125.14	121.00
1	C	82	ARG	CD-NE-CZ	6.89	133.25	123.60
2	D	502	ASP	CB-CG-OD1	6.87	124.48	118.30
2	D	455	ASN	O-C-N	-6.86	111.73	122.70
2	B	492	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	500	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	634	PHE	CB-CG-CD1	-6.83	116.02	120.80
2	B	90	VAL	CA-CB-CG2	6.81	121.12	110.90
1	C	170	ALA	O-C-N	-6.81	111.81	122.70
1	C	693	PHE	CB-CG-CD1	6.80	125.56	120.80
1	C	59	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	41	ALA	C-N-CA	6.76	138.60	121.70
1	C	438	GLU	O-C-N	-6.74	111.92	122.70
2	B	264	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	621	TYR	CB-CG-CD1	6.68	125.01	121.00
2	D	25	GLY	C-N-CA	6.67	138.38	121.70
2	B	229	PRO	O-C-N	-6.67	112.03	122.70
1	C	398	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	B	616	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	504	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	384	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	100	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	B	339	ASN	O-C-N	-6.62	112.11	122.70
1	C	541	ALA	O-C-N	-6.61	112.13	122.70
2	B	222	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	D	222	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	B	404	TYR	CB-CG-CD2	-6.58	117.05	121.00
2	D	92	PRO	O-C-N	-6.58	112.18	122.70
1	C	79	TYR	CB-CG-CD2	-6.58	117.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	95	ARG	CG-CD-NE	6.57	125.59	111.80
2	B	169	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	D	394	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	723	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	305	ARG	NE-CZ-NH2	6.53	123.57	120.30
1	A	320	PRO	O-C-N	-6.53	112.25	122.70
1	C	503	ARG	NE-CZ-NH2	-6.51	117.04	120.30
2	B	397	ASP	CB-CG-OD2	6.50	124.15	118.30
2	D	600	LYS	C-N-CA	6.50	137.94	121.70
1	A	93	SER	N-CA-CB	-6.49	100.77	110.50
1	A	150	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	C	93	SER	N-CA-CB	-6.47	100.80	110.50
2	D	352	VAL	O-C-N	-6.46	112.23	123.20
1	C	540	ARG	O-C-N	-6.42	112.43	122.70
2	D	521	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	D	229	PRO	O-C-N	-6.40	112.47	122.70
2	D	614	ASP	CB-CG-OD1	6.39	124.05	118.30
2	B	139	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	678	PRO	O-C-N	-6.38	112.49	122.70
1	C	198	ASN	N-CA-CB	-6.37	99.13	110.60
2	B	476	THR	CA-CB-CG2	6.36	121.31	112.40
1	A	63	THR	O-C-N	-6.34	112.55	122.70
1	A	693	PHE	CB-CG-CD1	6.34	125.24	120.80
2	D	536	HIS	O-C-N	-6.34	112.56	122.70
1	A	159	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	727	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	564	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	B	155	SER	CB-CA-C	-6.32	98.10	110.10
2	B	403	TYR	CB-CG-CD2	6.31	124.79	121.00
1	A	198	ASN	N-CA-CB	-6.30	99.25	110.60
1	C	297	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	A	357	GLN	C-N-CA	6.29	135.51	122.30
2	B	632	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	64	TYR	CB-CG-CD2	6.27	124.76	121.00
2	D	89	GLY	C-N-CA	6.27	137.38	121.70
2	D	171	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	79	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	D	68	ASP	CB-CG-OD1	6.24	123.91	118.30
2	D	456	ARG	NE-CZ-NH2	-6.23	117.18	120.30
2	D	86	GLY	C-N-CA	6.23	137.27	121.70
2	B	600	LYS	C-N-CA	6.23	137.27	121.70
1	C	313	HIS	O-C-N	-6.21	112.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	277	VAL	O-C-N	-6.20	112.78	122.70
1	C	541	ALA	C-N-CA	6.20	137.19	121.70
2	D	449	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	B	131	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	B	117	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	527	PRO	N-CA-CB	6.18	110.72	103.30
1	C	41	ALA	C-N-CA	6.17	137.13	121.70
1	A	703	GLU	CA-CB-CG	6.17	126.97	113.40
2	B	337	TYR	C-N-CA	6.16	137.09	121.70
1	C	206	VAL	CB-CA-C	-6.14	99.74	111.40
2	B	24	ALA	C-N-CA	6.13	135.18	122.30
2	B	24	ALA	O-C-N	-6.13	112.77	123.20
2	B	69	GLY	N-CA-C	6.13	128.44	113.10
2	B	377	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	520	GLY	O-C-N	-6.12	112.90	122.70
1	A	500	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	500	ARG	CD-NE-CZ	6.10	132.13	123.60
1	A	241	SER	N-CA-C	6.08	127.42	111.00
1	A	429	LYS	C-N-CA	6.08	136.89	121.70
1	C	210	TYR	CB-CG-CD2	-6.08	117.36	121.00
1	C	268	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	215	GLN	N-CA-CB	6.06	121.50	110.60
1	A	637	PRO	O-C-N	-6.05	113.03	122.70
1	C	199	ASP	OD1-CG-OD2	-6.05	111.81	123.30
2	D	333	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	C	408	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	A	41	ALA	O-C-N	-6.02	113.06	122.70
1	C	231	ASN	O-C-N	-6.01	113.08	122.70
1	C	520	GLY	O-C-N	-6.00	113.10	122.70
1	A	287	PHE	CB-CG-CD1	6.00	125.00	120.80
2	B	524	PHE	CB-CG-CD1	5.99	124.99	120.80
1	C	147	TYR	CB-CG-CD2	5.98	124.59	121.00
1	A	666	PRO	O-C-N	-5.98	113.13	122.70
1	C	333	GLY	O-C-N	-5.98	113.13	122.70
2	D	337	TYR	O-C-N	-5.98	113.14	122.70
2	B	147	PRO	O-C-N	-5.96	113.16	122.70
1	A	678	PRO	C-N-CA	5.95	136.58	121.70
1	C	232	MET	CA-CB-CG	5.93	123.39	113.30
1	C	693	PHE	CB-CG-CD2	-5.93	116.65	120.80
1	C	261	ALA	O-C-N	-5.92	113.23	122.70
2	D	476	THR	CA-CB-CG2	5.92	120.68	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	342	TYR	O-C-N	-5.90	113.26	122.70
1	A	677	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	D	397	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	206	VAL	CG1-CB-CG2	-5.90	101.47	110.90
1	A	418	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	C	199	ASP	CB-CG-OD1	5.88	123.59	118.30
2	B	305	ALA	N-CA-CB	5.86	118.30	110.10
1	C	128	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	D	601	GLU	C-N-CA	5.84	136.31	121.70
2	D	86	GLY	O-C-N	-5.84	113.36	122.70
2	D	352	VAL	C-N-CA	5.84	134.56	122.30
1	A	199	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	372	ILE	CB-CG1-CD1	5.82	130.18	113.90
1	A	62	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	269	GLN	C-N-CA	5.79	134.47	122.30
1	C	258	TYR	CB-CG-CD2	5.79	124.47	121.00
2	D	32	GLU	C-N-CA	5.78	136.14	121.70
1	A	146	ILE	O-C-N	-5.77	113.47	122.70
1	C	158	LEU	O-C-N	-5.76	113.48	122.70
1	A	727	ASP	C-N-CA	5.75	136.08	121.70
1	A	556	PHE	CB-CG-CD2	5.74	124.82	120.80
1	C	262	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	159	ASP	CB-CG-OD1	5.74	123.47	118.30
2	B	377	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	D	318	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	621	TYR	CB-CG-CD1	5.74	124.44	121.00
1	A	529	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	B	71	ASP	CB-CG-OD1	5.73	123.46	118.30
1	C	683	THR	N-CA-CB	5.73	121.18	110.30
2	B	456	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	334	TRP	O-C-N	-5.71	113.56	122.70
1	A	52	GLU	O-C-N	-5.71	113.56	122.70
1	C	178	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	A	130	PRO	N-CA-CB	5.71	110.15	103.30
1	C	206	VAL	CA-CB-CG1	5.71	119.46	110.90
2	B	337	TYR	O-C-N	-5.70	113.58	122.70
2	B	600	LYS	O-C-N	-5.69	113.60	122.70
1	A	64	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	A	102	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	297	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	A	313	HIS	O-C-N	-5.66	113.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100	ARG	CD-NE-CZ	5.66	131.53	123.60
2	D	338	VAL	O-C-N	-5.66	113.64	122.70
2	B	238	ALA	C-N-CA	5.66	135.84	121.70
1	C	621	TYR	CB-CG-CD2	-5.66	117.61	121.00
2	B	45	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	B	617	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	622	ALA	O-C-N	-5.65	113.66	122.70
1	A	282	PRO	O-C-N	-5.64	113.67	122.70
1	A	540	ARG	O-C-N	-5.63	113.69	122.70
2	D	512	LYS	CB-CA-C	-5.63	99.14	110.40
1	C	666	PRO	N-CA-CB	5.61	110.04	103.30
2	B	192	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	410	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	C	321	LYS	O-C-N	-5.60	113.74	122.70
1	A	253	ASP	CB-CG-OD1	5.59	123.34	118.30
2	D	17	THR	N-CA-C	5.59	126.11	111.00
1	A	527	PRO	O-C-N	-5.59	113.75	122.70
2	B	86	GLY	CA-C-O	5.59	130.66	120.60
1	C	176	ALA	CB-CA-C	-5.59	101.72	110.10
1	C	596	ARG	CG-CD-NE	5.58	123.53	111.80
1	A	261	ALA	CB-CA-C	5.58	118.47	110.10
2	B	472	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	D	37	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	698	LYS	O-C-N	-5.57	113.80	122.70
2	D	398	PRO	N-CA-CB	5.57	109.98	103.30
2	D	521	ARG	O-C-N	-5.56	113.80	122.70
1	A	554	LYS	CA-CB-CG	5.55	125.61	113.40
2	B	601	GLU	C-N-CA	5.55	135.57	121.70
2	D	543	PRO	N-CA-CB	5.55	109.96	103.30
2	D	25	GLY	O-C-N	-5.55	113.83	122.70
2	D	116	PRO	N-CA-CB	5.55	109.96	103.30
1	A	302	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	D	45	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	B	390	VAL	O-C-N	-5.53	113.85	122.70
1	A	89	TYR	CA-CB-CG	5.52	123.89	113.40
1	C	79	TYR	CB-CG-CD1	5.52	124.31	121.00
2	B	47	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	522	PRO	N-CA-CB	5.51	109.92	103.30
1	A	553	GLU	O-C-N	-5.51	113.88	122.70
1	A	118	ASP	CB-CG-OD1	5.51	123.26	118.30
2	B	25	GLY	O-C-N	-5.51	113.88	122.70
2	D	128	GLY	O-C-N	-5.50	113.89	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	LEU	C-N-CA	5.50	133.84	122.30
1	C	128	ASP	CB-CG-OD1	5.49	123.24	118.30
2	D	372	ASP	CB-CG-OD1	5.49	123.24	118.30
2	B	283	ARG	N-CA-CB	5.49	120.48	110.60
1	C	320	PRO	N-CA-CB	5.48	109.88	103.30
1	A	449	ALA	O-C-N	-5.47	113.94	122.70
2	D	17	THR	CA-C-N	-5.47	101.78	117.10
1	C	612	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	612	ARG	CD-NE-CZ	5.47	131.25	123.60
2	B	61	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	541	ALA	C-N-CA	5.45	135.33	121.70
2	B	232	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	D	222	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	510	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	647	ALA	O-C-N	-5.44	113.99	122.70
1	C	697	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	379	SER	O-C-N	-5.44	114.00	122.70
1	C	64	TYR	CB-CG-CD2	5.44	124.27	121.00
1	A	690	GLU	O-C-N	-5.44	114.00	122.70
1	A	70	PHE	CB-CG-CD2	5.43	124.60	120.80
1	C	8	ASP	C-N-CA	5.43	135.27	121.70
1	C	87	ARG	CD-NE-CZ	5.41	131.17	123.60
2	B	114	GLU	CA-CB-CG	5.40	125.29	113.40
2	B	425	LYS	C-N-CA	5.40	135.20	121.70
1	C	126	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	D	78	PRO	O-C-N	-5.40	114.06	122.70
2	D	601	GLU	O-C-N	-5.40	114.06	122.70
2	B	93	PHE	O-C-N	-5.39	114.07	122.70
1	A	677	ARG	CA-CB-CG	5.38	125.24	113.40
1	C	123	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	D	329	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	A	79	TYR	CB-CG-CD1	5.37	124.22	121.00
1	A	271	GLU	O-C-N	-5.37	114.11	122.70
1	C	190	GLU	O-C-N	-5.37	114.11	122.70
2	D	120	PHE	CB-CG-CD2	5.37	124.56	120.80
2	D	78	PRO	N-CA-CB	5.37	109.74	103.30
1	C	52	GLU	O-C-N	-5.36	114.12	122.70
1	A	277	VAL	O-C-N	-5.36	114.12	122.70
1	A	634	PHE	CB-CG-CD2	5.35	124.55	120.80
2	B	75	MET	CA-CB-CG	-5.35	104.20	113.30
1	C	219	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	673	ASP	C-N-CA	5.35	135.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	SER	N-CA-C	5.34	125.43	111.00
2	B	235	THR	N-CA-CB	5.34	120.44	110.30
1	C	675	LEU	C-N-CA	5.34	133.51	122.30
2	B	262	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	133	ALA	O-C-N	-5.33	114.15	123.20
2	B	533	PRO	N-CA-CB	5.32	109.69	103.30
1	A	261	ALA	O-C-N	-5.32	114.20	122.70
2	D	335	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	69	PRO	O-C-N	-5.29	114.23	122.70
2	D	79	LYS	O-C-N	-5.29	114.23	122.70
2	B	511	PRO	N-CA-CB	5.29	109.65	103.30
1	A	176	ALA	CB-CA-C	-5.29	102.17	110.10
2	B	512	LYS	CA-CB-CG	5.29	125.03	113.40
1	A	407	ALA	CB-CA-C	5.28	118.03	110.10
1	A	215	GLN	CB-CG-CD	5.28	125.32	111.60
2	B	496	VAL	O-C-N	-5.28	114.25	122.70
2	D	61	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	185	GLN	C-N-CA	5.26	133.36	122.30
1	A	697	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	17	THR	CA-C-N	-5.25	102.41	117.10
2	B	86	GLY	O-C-N	-5.25	114.31	122.70
2	B	116	PRO	N-CA-CB	5.24	109.59	103.30
2	B	77	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	369	ASP	O-C-N	-5.24	114.32	122.70
1	A	320	PRO	N-CA-CB	5.23	109.58	103.30
1	C	215	GLN	CB-CG-CD	5.23	125.20	111.60
1	A	281	ALA	N-CA-CB	5.22	117.41	110.10
1	C	547	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	A	578	PRO	N-CA-CB	5.22	109.56	103.30
2	D	503	ARG	CD-NE-CZ	5.22	130.91	123.60
1	C	677	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	155	GLY	O-C-N	-5.21	114.37	122.70
2	B	601	GLU	O-C-N	-5.20	114.38	122.70
1	A	547	GLU	OE1-CD-OE2	-5.19	117.07	123.30
2	D	377	ARG	CD-NE-CZ	5.19	130.87	123.60
2	D	213	ASP	CB-CG-OD1	5.19	122.97	118.30
2	B	222	ARG	O-C-N	-5.18	114.41	122.70
2	D	367	LEU	CB-CA-C	-5.18	100.36	110.20
2	B	542	THR	CA-CB-CG2	5.17	119.64	112.40
1	A	199	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	199	ASP	OD1-CG-OD2	-5.17	113.48	123.30
1	A	430	VAL	CA-CB-CG1	5.16	118.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	634	LEU	O-C-N	-5.16	114.43	123.20
1	C	703	GLU	CA-CB-CG	5.16	124.75	113.40
2	B	232	ARG	CD-NE-CZ	5.16	130.82	123.60
2	D	485	ARG	CG-CD-NE	-5.15	100.98	111.80
1	C	248	ALA	CA-C-N	5.15	126.50	116.20
2	B	88	PRO	N-CA-CB	5.15	109.48	103.30
1	C	53	ASP	CB-CG-OD1	5.14	122.93	118.30
2	D	238	ALA	C-N-CA	5.14	134.55	121.70
1	C	522	PRO	N-CA-CB	5.14	109.47	103.30
1	A	20	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	233	PRO	N-CA-CB	5.14	109.47	103.30
2	D	370	PRO	N-CA-CB	5.13	109.46	103.30
1	C	320	PRO	O-C-N	-5.12	114.50	122.70
2	D	86	GLY	CA-C-O	5.12	129.82	120.60
2	D	239	ASN	O-C-N	-5.12	114.50	122.70
2	B	456	ARG	O-C-N	-5.12	114.51	122.70
2	D	93	PHE	O-C-N	-5.12	114.51	122.70
2	B	201	PRO	N-CA-CB	5.11	109.43	103.30
2	B	268	GLU	C-N-CA	5.11	134.47	121.70
1	C	170	ALA	C-N-CA	5.11	134.46	121.70
1	C	438	GLU	CA-C-N	5.10	128.42	117.20
2	D	47	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	405	GLY	O-C-N	-5.10	114.55	122.70
1	A	152	LEU	O-C-N	-5.10	114.55	122.70
2	B	238	ALA	O-C-N	-5.09	114.55	122.70
2	D	69	GLY	N-CA-C	5.09	125.83	113.10
2	B	147	PRO	N-CA-CB	5.08	109.40	103.30
1	A	241	SER	N-CA-CB	-5.08	102.88	110.50
1	A	590	PHE	CB-CG-CD2	5.08	124.36	120.80
2	B	457	LYS	C-N-CA	5.08	134.40	121.70
2	D	283	ARG	N-CA-CB	5.08	119.75	110.60
1	C	647	ALA	O-C-N	-5.08	114.57	122.70
2	B	455	ASN	O-C-N	-5.07	114.58	122.70
2	D	147	PRO	N-CA-CB	5.07	109.38	103.30
1	A	625	GLY	CA-C-O	-5.06	111.49	120.60
1	A	527	PRO	N-CA-CB	5.06	109.37	103.30
2	B	485	ARG	CD-NE-CZ	5.05	130.68	123.60
2	B	398	PRO	N-CA-CB	5.05	109.36	103.30
1	C	282	PRO	N-CA-CB	5.04	109.35	103.30
1	A	408	TYR	CB-CG-CD2	5.04	124.03	121.00
1	C	314	GLN	O-C-N	-5.04	114.63	122.70
2	D	222	ARG	O-C-N	-5.04	114.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	GLU	C-N-CA	5.03	134.27	121.70
1	A	320	PRO	C-N-CA	5.02	134.26	121.70
1	A	471	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	B	564	VAL	CA-CB-CG2	5.02	118.43	110.90
1	A	222	SER	O-C-N	-5.02	114.67	122.70
2	B	100	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	608	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	712	PRO	N-CA-CB	5.01	109.32	103.30
2	D	404	TYR	CA-CB-CG	5.01	122.93	113.40
2	D	365	GLN	O-C-N	-5.01	114.69	122.70
2	B	100	ARG	CD-NE-CZ	5.01	130.61	123.60
1	A	5	PRO	N-CA-CB	5.00	109.30	103.30
2	B	92	PRO	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5539	0	5413	22	0
1	C	5539	0	5413	27	0
2	B	4744	0	4648	20	0
2	D	4744	0	4648	20	0
3	A	54	0	37	2	0
3	C	54	0	37	2	0
4	A	91	0	88	9	0
4	C	91	0	88	8	0
5	B	12	0	16	2	0
5	D	9	0	11	2	0
6	A	420	0	0	0	0
6	B	243	0	0	0	0
6	C	421	0	0	0	0
6	D	242	0	0	1	0
All	All	22203	0	20399	101	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 2.

All (101) 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)
4:C:2800:B12:H531	4:C:2800:B12:H552	1.48	0.92
1:A:638:GLU:HA	1:A:671:GLU:HG2	1.52	0.90
4:A:1800:B12:H552	4:A:1800:B12:H531	1.61	0.82
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.29	0.81
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.71	0.72
2:D:503:ARG:HD2	2:D:638:LYS:HD3	1.71	0.72
4:A:1800:B12:H362	4:A:1800:B12:H351	1.72	0.70
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.75	0.69
2:B:356:GLU:HA	5:B:3002:GOL:H2	1.75	0.68
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.77	0.67
1:C:638:GLU:HA	1:C:671:GLU:HG2	1.76	0.67
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.77	0.67
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.44	0.65
1:A:247:GLU:HB3	4:A:1800:B12:H532	1.77	0.64
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.80	0.62
4:C:2800:B12:H531	4:C:2800:B12:C55	2.24	0.62
2:B:503:ARG:HD2	2:B:638:LYS:HD3	1.80	0.62
4:A:1800:B12:C55	4:A:1800:B12:H531	2.30	0.61
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.84	0.59
2:B:515:LEU:HB2	2:B:544:GLN:HB3	1.84	0.59
1:C:706:THR:HB	1:C:707:PRO:HD2	1.84	0.58
1:A:706:THR:HB	1:A:707:PRO:HD2	1.85	0.58
1:C:706:THR:HB	1:C:707:PRO:CD	2.34	0.57
1:A:706:THR:HB	1:A:707:PRO:CD	2.35	0.57
3:C:2801:2CP:HB1	3:C:2801:2CP:OP2	2.04	0.56
2:D:141:ASP:HB3	2:D:142:PRO:HD2	1.86	0.56
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.87	0.56
1:C:359:HIS:CE1	1:C:401:ASP:H	2.24	0.56
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.88	0.56
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.88	0.55
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.89	0.55
4:A:1800:B12:H372	4:A:1800:B12:H351	1.88	0.54
1:C:247:GLU:HB3	4:C:2800:B12:H532	1.90	0.54
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.90	0.54
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.90	0.54
1:A:139:ALA:HB1	4:A:1800:B12:H362	1.91	0.53
4:C:2800:B12:H351	4:C:2800:B12:H362	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:TRP:HB3	5:B:3002:GOL:H11	1.92	0.51
1:A:359:HIS:CE1	1:A:401:ASP:H	2.29	0.51
2:D:107:TRP:HB3	5:D:3004:GOL:H11	1.93	0.51
1:C:139:ALA:HB1	4:C:2800:B12:H362	1.93	0.50
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.76	0.50
2:D:237:ASP:HB3	2:D:240:ILE:HD12	1.93	0.50
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.95	0.49
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.95	0.48
3:A:1801:2CP:HB1	3:A:1801:2CP:OP2	2.13	0.48
2:D:100:ARG:HH21	5:D:3004:GOL:H12	1.78	0.48
2:D:511:PRO:HB3	2:D:634:LEU:HD13	1.96	0.48
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.95	0.48
1:A:308:TRP:HB2	1:A:325:LEU:HD12	1.96	0.47
2:B:212:PRO:HG2	2:B:430:SER:HB3	1.95	0.47
4:C:2800:B12:H353	4:C:2800:B12:H302	1.97	0.47
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.45	0.47
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.96	0.46
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.85	0.46
1:A:89:TYR:CE2	3:A:1801:2CP:HS2	2.51	0.46
1:A:69:PRO:HG3	2:B:24:ALA:HA	1.99	0.45
2:D:390:VAL:HG12	2:D:392:ILE:HG23	1.99	0.45
1:C:197:GLN:HG3	1:C:239:SER:HB3	1.99	0.44
1:C:592:GLN:HA	1:C:592:GLN:HE21	1.83	0.44
1:A:200:ILE:HG12	1:A:217:SER:HB3	1.99	0.44
2:D:579:LEU:HD22	2:D:605:ASP:HB3	1.98	0.44
1:A:489:LEU:HG	1:A:493:LYS:HE3	1.99	0.44
4:A:1800:B12:C35	4:A:1800:B12:H372	2.48	0.44
1:C:577:THR:HG22	1:C:580:VAL:H	1.81	0.44
2:B:224:LEU:HD12	2:B:233:ALA:HB2	2.00	0.44
4:A:1800:B12:C35	4:A:1800:B12:H362	2.46	0.44
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.81	0.44
2:D:331:LEU:HD13	2:D:365:GLN:HB3	1.99	0.44
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.52	0.43
4:A:1800:B12:C37	4:A:1800:B12:H351	2.47	0.43
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.99	0.43
1:A:592:GLN:HA	1:A:592:GLN:HE21	1.84	0.43
1:C:385:ASN:HD22	1:C:388:LEU:HD12	1.84	0.43
4:C:2800:B12:H421	4:C:2800:B12:H363	2.01	0.43
1:A:599:ARG:HD2	1:A:649:VAL:HA	1.99	0.43
1:C:710:VAL:HG12	1:C:712:PRO:HD2	2.00	0.43
1:A:597:ARG:HG2	1:A:597:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.48	0.43
2:B:180:VAL:HG13	2:B:197:LEU:HD21	2.00	0.43
1:C:504:ASP:O	1:C:508:VAL:HG23	2.19	0.42
2:D:86:GLY:HA3	6:D:752:HOH:O	2.18	0.42
1:A:683:THR:HG21	1:A:718:LEU:HD13	2.02	0.42
1:A:213:PRO:HD2	1:A:216:PRO:HG2	2.02	0.42
1:C:385:ASN:HA	1:C:385:ASN:HD22	1.73	0.42
2:D:464:SER:HA	2:D:537:ILE:HG12	2.02	0.42
1:C:200:ILE:HG12	1:C:217:SER:HB3	2.03	0.41
1:A:339:GLN:HG2	1:A:471:ARG:NH2	2.36	0.41
1:C:89:TYR:CE2	3:C:2801:2CP:HS2	2.55	0.41
1:C:683:THR:HG21	1:C:718:LEU:HD13	2.02	0.41
1:C:318:LYS:HD3	1:C:318:LYS:HA	1.95	0.41
2:B:80:ASP:HB3	2:B:407:SER:HB2	2.02	0.41
4:C:2800:B12:H351	4:C:2800:B12:H372	2.02	0.41
2:D:252:LEU:HD11	2:D:300:LEU:HA	2.03	0.41
1:A:7:PHE:HB2	2:B:424:GLU:HG3	2.02	0.41
1:C:521:ASN:O	1:C:529:ARG:HD3	2.20	0.40
1:C:188:LYS:HB3	1:C:189:PRO:HD2	2.03	0.40
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.56	0.40
1:C:652:VAL:HG11	1:C:668:LEU:HD11	2.03	0.40
2:D:141:ASP:HB3	2:D:142:PRO:CD	2.50	0.40
2:D:267:VAL:HA	2:D:271:PHE:O	2.20	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	723/727 (99%)	701 (97%)	22 (3%)	0	100	100
1	C	723/727 (99%)	702 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	621/637 (98%)	606 (98%)	14 (2%)	1 (0%)	52	59
2	D	621/637 (98%)	605 (97%)	15 (2%)	1 (0%)	52	59
All	All	2688/2728 (98%)	2614 (97%)	72 (3%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	THR
2	D	17	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/590 (95%)	554 (98%)	9 (2%)	70	82
1	C	563/590 (95%)	553 (98%)	10 (2%)	66	79
2	B	480/509 (94%)	473 (98%)	7 (2%)	72	84
2	D	480/509 (94%)	470 (98%)	10 (2%)	61	74
All	All	2086/2198 (95%)	2050 (98%)	36 (2%)	68	81

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

Mol	Chain	Res	Type
1	A	103	ARG
1	A	149	MET
1	A	229	SER
1	A	430	VAL
1	A	438	GLU
1	A	487	THR
1	A	592	GLN
1	A	597	ARG
1	A	668	LEU
2	B	77	ARG

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Mol	Chain	Res	Type
2	B	279	THR
2	B	410	ARG
2	B	451	LYS
2	B	532	SER
2	B	610	GLU
2	B	638	LYS
1	C	69	PRO
1	C	123	ARG
1	C	149	MET
1	C	430	VAL
1	C	438	GLU
1	C	479	ASP
1	C	533	LYS
1	C	592	GLN
1	C	597	ARG
1	C	668	LEU
2	D	16	LEU
2	D	75	MET
2	D	77	ARG
2	D	180	VAL
2	D	199	LEU
2	D	288	HIS
2	D	410	ARG
2	D	451	LYS
2	D	532	SER
2	D	638	LYS

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

Mol	Chain	Res	Type
1	A	359	HIS
1	A	385	ASN
1	A	592	GLN
1	A	635	GLN
1	A	643	GLN
2	B	323	ASN
1	C	51	ASN
1	C	359	HIS
1	C	385	ASN
1	C	592	GLN
1	C	635	GLN
1	C	643	GLN

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Mol	Chain	Res	Type
2	D	322	GLN
2	D	323	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 ⓘ

8 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$
4	B12	A	1800	1,6	74,101,101	1.11	5 (6%)	111,166,166	1.52	18 (16%)
3	2CP	A	1801	-	43,56,56	1.13	7 (16%)	53,83,83	2.01	16 (30%)
5	GOL	B	3001	-	5,5,5	0.22	0	5,5,5	0.48	0
5	GOL	B	3002	-	5,5,5	0.23	0	5,5,5	0.44	0
4	B12	C	2800	1,6	74,101,101	1.07	3 (4%)	111,166,166	1.48	17 (15%)
3	2CP	C	2801	-	43,56,56	1.20	6 (13%)	53,83,83	1.88	9 (16%)
5	GOL	D	3003	-	5,5,5	0.17	0	5,5,5	0.49	0
5	GOL	D	3004	-	2,2,5	0.48	0	1,1,5	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	B12	A	1800	1,6	-	0/51/223/223	0/3/11/11
3	2CP	A	1801	-	-	0/48/72/72	0/3/3/3
5	GOL	B	3001	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3002	-	-	0/4/4/4	0/0/0/0
4	B12	C	2800	1,6	-	0/51/223/223	0/3/11/11
3	2CP	C	2801	-	-	0/48/72/72	0/3/3/3
5	GOL	D	3003	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3004	-	-	0/0/0/4	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	B12	C11-C10	-3.23	1.35	1.41
4	A	1800	B12	C2-C3	-2.45	1.54	1.58
3	C	2801	2CP	P1-O12	-2.24	1.45	1.54
3	A	1801	2CP	P3-O32	-2.17	1.46	1.54
3	C	2801	2CP	P2-O7	-2.13	1.49	1.59
3	A	1801	2CP	CS1-CS2	-2.10	1.49	1.53
3	A	1801	2CP	P2-O22	-2.10	1.46	1.54
3	A	1801	2CP	P2-O7	-2.06	1.49	1.59
3	C	2801	2CP	P2-O22	-2.04	1.46	1.54
4	C	2800	B12	C48-C13	2.25	1.57	1.54
3	A	1801	2CP	C2-N1	2.27	1.38	1.33
4	C	2800	B12	C54-C17	2.33	1.58	1.54
4	A	1800	B12	C54-C17	2.39	1.59	1.54
3	A	1801	2CP	CP2-NP1	2.49	1.52	1.46
4	A	1800	B12	C30-C3	2.65	1.58	1.54
3	C	2801	2CP	C2-N1	2.66	1.39	1.33
3	A	1801	2CP	CP5-NP2	2.84	1.52	1.46
3	C	2801	2CP	CP5-NP2	2.85	1.52	1.46
4	C	2800	B12	C30-C3	2.88	1.58	1.54
3	C	2801	2CP	CP2-NP1	3.37	1.54	1.46
4	A	1800	B12	C48-C13	3.75	1.60	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2801	2CP	CP2-NP1-CP3	-5.74	111.50	122.79
4	A	1800	B12	C54-C17-C55	-5.09	100.83	109.27
3	A	1801	2CP	CP1-CP2-NP1	-4.20	103.96	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	2CP	CP2-NP1-CP3	-4.19	114.55	122.79
3	C	2801	2CP	CP1-CP2-NP1	-4.07	104.23	112.36
4	C	2800	B12	C13-C14-C15	-3.46	120.20	131.88
3	A	1801	2CP	CP5-NP2-CP6	-3.44	115.71	122.53
3	C	2801	2CP	O7-CPB-CPA	-3.33	105.19	110.55
4	C	2800	B12	C1P-N59-C57	-3.13	114.80	122.68
4	A	1800	B12	C55-C56-C57	-3.08	104.84	111.06
3	A	1801	2CP	O7-CPB-CPA	-3.04	105.65	110.55
4	C	2800	B12	C9-C10-C11	-2.95	124.89	132.28
3	A	1801	2CP	OP3-CP7-CP6	-2.93	103.65	110.38
3	A	1801	2CP	CP9-CPA-CP7	-2.90	104.04	109.34
3	C	2801	2CP	CP9-CPA-CP7	-2.87	104.10	109.34
4	C	2800	B12	C55-C56-C57	-2.77	105.45	111.06
4	C	2800	B12	C5M-C5B-C6B	-2.71	114.78	120.73
4	A	1800	B12	C13-C14-C15	-2.65	122.92	131.88
4	C	2800	B12	C54-C17-C18	-2.63	108.66	112.94
3	A	1801	2CP	CP8-CPA-CP9	-2.59	104.07	109.28
3	C	2801	2CP	CP5-NP2-CP6	-2.58	117.42	122.53
4	C	2800	B12	C5B-C4B-C9B	-2.56	116.74	120.92
3	A	1801	2CP	N3-C2-N1	-2.48	126.99	128.89
4	A	1800	B12	C48-C13-C12	-2.42	109.89	116.53
4	A	1800	B12	C3-C4-C5	-2.38	123.84	131.88
4	A	1800	B12	O8R-C5R-C4R	-2.36	103.54	111.33
4	C	2800	B12	C3-C4-C5	-2.34	123.99	131.88
4	C	2800	B12	C2P-C1P-N59	-2.33	109.48	112.92
3	A	1801	2CP	C2'-C1'-N9	-2.32	110.75	114.29
4	C	2800	B12	C1-C19-C18	-2.24	117.91	121.85
4	A	1800	B12	C25-C2-C3	-2.22	111.81	115.56
4	C	2800	B12	O28-C27-N29	-2.18	116.20	122.46
4	A	1800	B12	C5M-C5B-C6B	-2.14	116.04	120.73
3	A	1801	2CP	O7-P2-O21	-2.12	101.37	109.62
4	A	1800	B12	O28-C27-N29	-2.04	116.62	122.46
4	A	1800	B12	C31-C30-C3	-2.01	108.79	114.80
4	C	2800	B12	O2-P-O3	2.01	101.98	100.07
4	C	2800	B12	C31-C32-N33	2.01	122.85	116.53
3	C	2801	2CP	P3-O3'-C3'	2.02	126.41	121.56
3	A	1801	2CP	C4-C5-N7	2.05	111.37	109.48
3	A	1801	2CP	OP2-CP6-NP2	2.20	127.49	123.08
4	A	1800	B12	C20-C1-C19	2.32	111.66	109.38
3	A	1801	2CP	O6-P2-O7	2.38	109.24	102.94
3	A	1801	2CP	O33-P3-O32	2.59	117.23	107.38
4	A	1800	B12	C36-C7-C8	2.63	117.00	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	B12	C53-C15-C16	2.64	122.97	118.25
4	A	1800	B12	C18-C17-C16	2.79	104.31	100.54
4	C	2800	B12	C53-C15-C16	3.12	123.84	118.25
3	C	2801	2CP	CP9-CPA-CPB	3.17	112.61	108.50
4	C	2800	B12	C55-C17-C18	3.20	117.40	110.97
4	A	1800	B12	C55-C17-C18	3.24	117.48	110.97
3	C	2801	2CP	O6-P2-O7	3.27	111.61	102.94
4	A	1800	B12	P-O3-C2P	3.38	125.36	120.92
4	C	2800	B12	C18-C17-C16	3.39	105.12	100.54
4	A	1800	B12	O2-P-O3	3.47	103.37	100.07
3	A	1801	2CP	CP9-CPA-CPB	4.20	113.94	108.50
4	A	1800	B12	C7B-C8B-C9B	4.80	125.29	120.54
4	C	2800	B12	C7B-C8B-C9B	5.49	125.97	120.54
3	C	2801	2CP	CP8-CPA-CPB	6.81	117.33	108.50
3	A	1801	2CP	CP8-CPA-CPB	7.26	117.92	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1800	B12	9	0
3	A	1801	2CP	2	0
5	B	3002	GOL	2	0
4	C	2800	B12	8	0
3	C	2801	2CP	2	0
5	D	3004	GOL	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	725/727 (99%)	-0.46	7 (0%) 84 83	9, 19, 38, 65	0
1	C	725/727 (99%)	-0.47	9 (1%) 81 80	7, 19, 38, 66	0
2	B	623/637 (97%)	-0.07	15 (2%) 62 61	14, 29, 49, 80	0
2	D	623/637 (97%)	-0.11	15 (2%) 62 61	13, 29, 49, 79	0
All	All	2696/2728 (98%)	-0.29	46 (1%) 73 72	7, 24, 45, 80	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	16	LEU	10.2
2	B	18	PRO	7.6
1	C	728	ALA	6.7
2	D	16	LEU	6.6
2	B	19	THR	6.1
2	B	17	THR	5.6
1	A	728	ALA	5.4
2	D	638	LYS	4.2
2	B	638	LYS	4.1
2	B	509	GLU	3.3
2	B	20	THR	3.1
2	D	213	ASP	3.0
2	D	187	ASP	2.9
1	A	14	ASN	2.8
1	A	473	GLU	2.8
2	B	567	LEU	2.7
2	B	270	GLY	2.7
1	C	19	ALA	2.6
2	B	507	VAL	2.6
1	A	9	SER	2.6
1	C	475	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	187	ASP	2.5
1	A	574	VAL	2.5
2	D	567	LEU	2.4
1	C	14	ASN	2.4
1	C	20	ASP	2.4
1	C	429	LYS	2.4
2	D	603	GLY	2.3
2	D	46	GLY	2.3
2	D	604	ASP	2.2
2	D	607	ALA	2.2
1	C	694	ASP	2.2
2	D	316	ASP	2.2
1	A	576	ASN	2.2
2	B	161	MET	2.1
2	D	608	GLU	2.1
2	B	192	ASP	2.1
1	C	576	ASN	2.1
2	D	546	GLU	2.1
2	D	463	VAL	2.1
2	B	508	SER	2.1
2	D	30	ALA	2.0
1	C	130	PRO	2.0
2	D	548	GLY	2.0
2	B	587	ALA	2.0
1	A	477	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	D	3004	3/6	0.66	0.50	10.87	65,65,65,66	0
5	GOL	B	3002	6/6	0.73	0.35	7.24	64,67,68,69	0
3	2CP	C	2801	54/54	0.98	0.09	-0.43	6,13,31,33	0
4	B12	A	1800	91/91	0.99	0.08	-0.45	4,12,18,23	0
3	2CP	A	1801	54/54	0.98	0.09	-0.52	8,14,29,31	0
4	B12	C	2800	91/91	0.98	0.08	-0.83	4,13,19,24	0
5	GOL	D	3003	6/6	0.96	0.22	-	59,60,60,61	0
5	GOL	B	3001	6/6	0.92	0.10	-	57,59,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.