



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:22 PM UTC

PDB ID : 1K3T / pdb_00001k3t
Title : Structure of Glycosomal Glyceraldehyde-3-Phosphate Dehydrogenase from Trypanosoma cruzi Complexed with Chalepin, a Coumarin Derivative Inhibitor
Authors : Pavao, F.
Deposited on : 2001-10-04
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

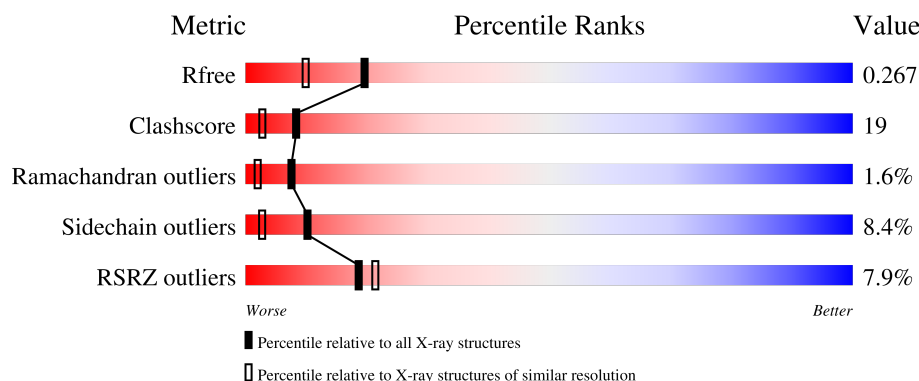
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

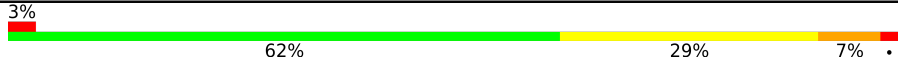
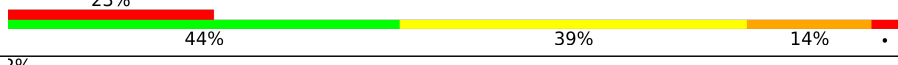
The reported resolution of this entry is 1.95 Å.

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
1	C	359	
1	D	359	

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
2	BRZ	C	960	-	X	X	-

2 Entry composition [i](#)

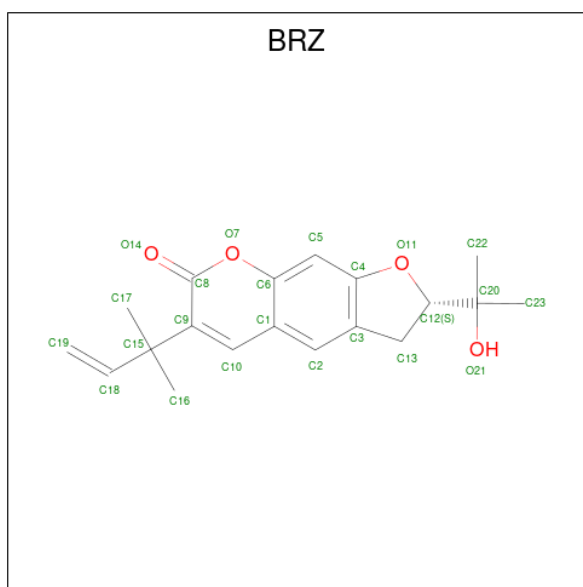
There are 3 unique types of molecules in this entry. The entry contains 11942 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2744	1725	486	519	14			
1	B	359	Total	C	N	O	S	0	0	0
			2744	1725	486	519	14			
1	C	359	Total	C	N	O	S	0	1	0
			2750	1728	487	520	15			
1	D	359	Total	C	N	O	S	0	0	0
			2744	1725	486	519	14			

- Molecule 2 is 6-(1,1-DIMETHYLALLYL)-2-(1-HYDROXY-1-METHYLETHYL)-2,3-DIHYDRO-7H-FURO[3,2-G]CHROMEN-7-ONE (CCD ID: BRZ) (formula: C₁₉H₂₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			23	19	4		

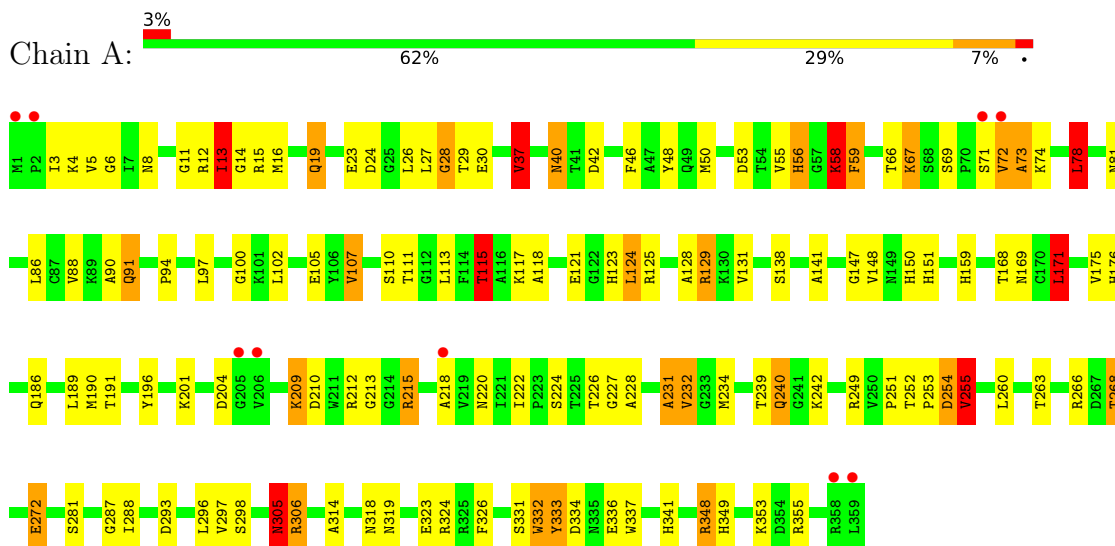
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	271	Total 271	O 271	0	0
3	B	223	Total 223	O 223	0	0
3	C	161	Total 161	O 161	0	0
3	D	282	Total 282	O 282	0	0

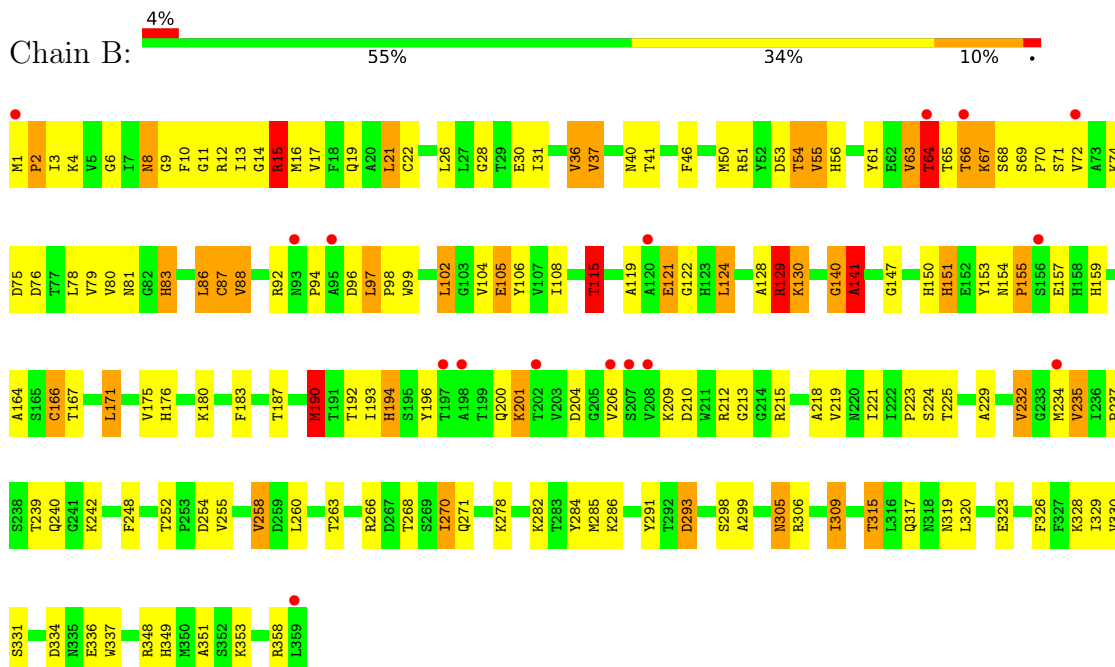
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

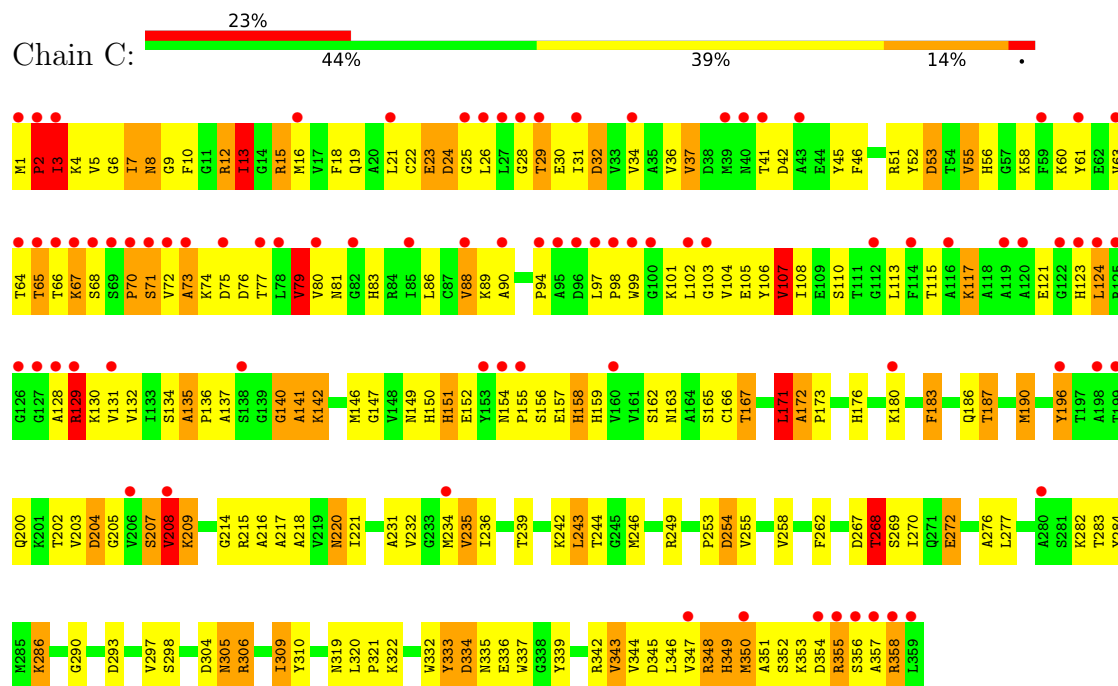
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



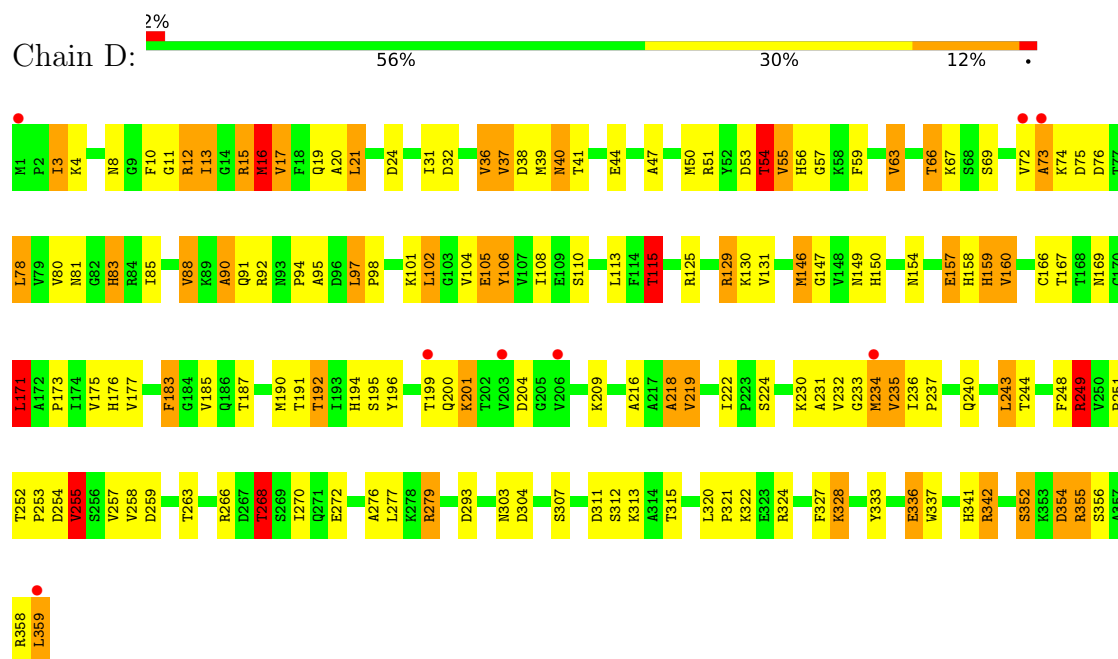
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.08Å 84.97Å 105.24Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.95) 77.7 (15.00-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.280 0.197 , 0.267	Depositor DCC
R_{free} test set	2483 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11942	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BRZ

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	1.02	1/2797 (0.0%)	2.13	107/3792 (2.8%)
1	B	0.97	2/2797 (0.1%)	2.16	122/3792 (3.2%)
1	C	0.87	1/2803 (0.0%)	1.99	98/3800 (2.6%)
1	D	1.05	1/2797 (0.0%)	2.27	125/3792 (3.3%)
All	All	0.98	5/11194 (0.0%)	2.14	452/15176 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	HIS	N-CA	-5.86	1.39	1.46
1	B	194	HIS	CA-CB	5.64	1.60	1.53
1	C	254	ASP	C-N	-5.48	1.26	1.33
1	A	6	GLY	N-CA	5.31	1.50	1.45
1	D	337	TRP	N-CA	-5.17	1.40	1.46

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	ARG	CD-NE-CZ	30.80	167.52	124.40
1	D	249	ARG	CD-NE-CZ	20.39	152.95	124.40
1	D	279	ARG	CD-NE-CZ	19.14	151.19	124.40
1	D	266	ARG	CD-NE-CZ	17.72	149.21	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	ARG	CD-NE-CZ	17.26	148.56	124.40
1	B	204	ASP	CA-CB-CG	14.63	127.23	112.60
1	B	293	ASP	CA-CB-CG	13.09	125.69	112.60
1	A	159	HIS	CA-CB-CG	-12.55	101.25	113.80
1	D	40	ASN	CA-CB-CG	12.13	124.73	112.60
1	A	125	ARG	CD-NE-CZ	11.39	140.35	124.40
1	B	193	ILE	CA-C-N	11.24	137.73	122.77
1	B	193	ILE	C-N-CA	11.24	137.73	122.77
1	B	337	TRP	N-CA-C	10.81	122.82	111.14
1	C	15	ARG	CD-NE-CZ	10.47	139.06	124.40
1	D	81	ASN	CA-CB-CG	10.32	122.92	112.60
1	B	157	GLU	N-CA-C	-9.96	100.67	113.12
1	D	204	ASP	CA-CB-CG	9.93	122.53	112.60
1	A	15	ARG	CD-NE-CZ	9.90	138.25	124.40
1	C	140	GLY	N-CA-C	-9.85	100.56	112.48
1	D	336	GLU	CA-C-N	9.71	133.84	120.63
1	D	336	GLU	C-N-CA	9.71	133.84	120.63
1	B	319	ASN	CA-CB-CG	-9.38	103.22	112.60
1	D	355	ARG	CD-NE-CZ	9.35	137.48	124.40
1	A	215	ARG	NE-CZ-NH2	9.34	127.61	119.20
1	A	254	ASP	CA-CB-CG	9.28	121.88	112.60
1	A	323	GLU	CB-CG-CD	9.01	127.92	112.60
1	D	36	VAL	N-CA-CB	8.86	123.64	111.41
1	D	146	MET	CA-C-O	8.86	131.02	120.92
1	C	355	ARG	N-CA-C	-8.81	101.37	110.97
1	C	15	ARG	NH1-CZ-NH2	-8.64	108.07	119.30
1	B	293	ASP	N-CA-CB	8.57	124.77	111.39
1	C	220	ASN	CA-CB-CG	8.52	121.12	112.60
1	D	158	HIS	CA-CB-CG	8.48	122.28	113.80
1	A	297	VAL	CA-C-O	-8.44	111.82	121.44
1	A	115	THR	N-CA-CB	-8.44	96.38	110.39
1	A	12	ARG	CD-NE-CZ	8.43	136.21	124.40
1	C	204	ASP	CA-CB-CG	8.43	121.03	112.60
1	B	221	ILE	N-CA-CB	8.42	121.06	111.21
1	D	51	ARG	CB-CA-C	-8.28	97.89	110.88
1	D	129	ARG	NE-CZ-NH1	-8.26	113.24	121.50
1	B	194	HIS	N-CA-C	8.21	122.12	108.73
1	D	312	SER	CA-C-O	-8.21	111.72	120.42
1	B	323	GLU	CB-CG-CD	8.14	126.43	112.60
1	A	13	ILE	N-CA-CB	8.11	122.75	110.58
1	B	83	HIS	CA-CB-CG	-8.06	105.74	113.80
1	B	183	PHE	CA-C-O	8.01	128.91	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	THR	N-CA-CB	-8.01	97.89	110.46
1	B	54	THR	CA-CB-OG1	7.98	121.57	109.60
1	B	70	PRO	CA-C-N	7.96	131.26	120.44
1	B	70	PRO	C-N-CA	7.96	131.26	120.44
1	B	92	ARG	CD-NE-CZ	7.89	135.44	124.40
1	D	337	TRP	CA-C-O	-7.86	112.81	120.90
1	D	234	MET	CA-C-O	7.78	127.70	119.14
1	D	159	HIS	CA-CB-CG	-7.77	106.03	113.80
1	C	216	ALA	CA-C-N	7.75	131.29	120.29
1	C	216	ALA	C-N-CA	7.75	131.29	120.29
1	D	57	GLY	O-C-N	-7.73	115.57	122.91
1	B	46	PHE	CA-CB-CG	7.70	121.50	113.80
1	D	53	ASP	CA-CB-CG	-7.67	104.93	112.60
1	B	237	PRO	O-C-N	-7.67	112.89	122.17
1	C	8	ASN	CA-CB-CG	7.67	120.27	112.60
1	B	155	PRO	CA-C-O	-7.66	106.66	120.60
1	D	336	GLU	N-CA-C	7.66	119.53	111.03
1	B	155	PRO	CA-C-N	-7.65	110.47	122.49
1	B	155	PRO	C-N-CA	-7.65	110.47	122.49
1	A	27	LEU	N-CA-CB	7.61	121.43	109.71
1	B	329	ILE	CA-C-O	7.61	128.30	120.39
1	B	268	THR	CA-C-O	-7.60	114.72	120.19
1	B	266	ARG	CG-CD-NE	7.60	128.72	112.00
1	D	15	ARG	CA-C-N	7.58	130.44	120.28
1	D	15	ARG	C-N-CA	7.58	130.44	120.28
1	A	341	HIS	CA-C-O	-7.57	112.53	120.55
1	B	121	GLU	O-C-N	-7.56	114.11	122.12
1	B	87	CYS	CA-C-O	-7.50	112.26	120.43
1	B	141	ALA	N-CA-CB	7.48	123.13	110.49
1	D	36	VAL	CA-C-N	-7.48	112.74	123.06
1	D	36	VAL	C-N-CA	-7.48	112.74	123.06
1	C	15	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	C	3	ILE	N-CA-CB	7.38	123.41	111.23
1	C	334	ASP	N-CA-C	-7.37	96.54	108.41
1	D	257	VAL	CA-C-O	7.37	128.78	120.90
1	B	305	ASN	OD1-CG-ND2	7.33	129.93	122.60
1	B	140	GLY	N-CA-C	-7.32	98.93	112.62
1	C	337	TRP	N-CA-C	7.28	118.90	110.97
1	B	309	ILE	CA-CB-CG1	7.27	122.75	110.40
1	D	342	ARG	CD-NE-CZ	7.24	134.54	124.40
1	D	101	LYS	CB-CG-CD	7.24	127.95	111.30
1	B	56	HIS	CA-CB-CG	-7.18	106.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	THR	CA-C-O	-7.18	113.25	121.58
1	A	222	ILE	N-CA-C	7.13	115.21	108.15
1	D	16	MET	CB-CA-C	7.13	122.63	110.79
1	B	54	THR	N-CA-CB	7.08	120.53	110.12
1	B	159	HIS	CA-CB-CG	-7.07	106.73	113.80
1	C	134	SER	CA-C-N	7.07	132.31	122.06
1	C	134	SER	C-N-CA	7.07	132.31	122.06
1	A	240	GLN	CB-CG-CD	7.06	124.60	112.60
1	D	66	THR	N-CA-CB	7.06	123.00	111.21
1	B	64	THR	N-CA-CB	-7.03	100.25	111.43
1	A	333	TYR	O-C-N	7.00	131.41	123.42
1	A	231	ALA	CA-C-O	6.99	127.94	119.49
1	B	151	HIS	CA-CB-CG	-6.96	106.83	113.80
1	A	332	TRP	O-C-N	-6.96	115.17	123.03
1	A	58	LYS	CA-C-O	-6.95	113.13	121.05
1	C	290	GLY	N-CA-C	-6.95	100.53	112.06
1	B	215	ARG	CA-C-N	6.91	131.25	121.02
1	B	215	ARG	C-N-CA	6.91	131.25	121.02
1	D	54	THR	N-CA-CB	6.91	120.86	110.22
1	B	8	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	D	66	THR	CA-CB-OG1	6.91	119.96	109.60
1	D	171	LEU	CB-CA-C	-6.88	100.07	110.88
1	D	336	GLU	CA-C-O	6.84	127.94	120.90
1	D	51	ARG	CD-NE-CZ	6.80	133.92	124.40
1	D	328	LYS	CA-C-N	-6.78	114.25	123.14
1	D	328	LYS	C-N-CA	-6.78	114.25	123.14
1	B	166	CYS	CA-C-O	-6.78	113.36	120.55
1	D	311	ASP	CA-C-O	-6.77	113.88	120.92
1	A	37	VAL	CB-CA-C	6.75	120.63	110.63
1	A	212	ARG	NE-CZ-NH2	-6.69	113.18	119.20
1	B	15	ARG	CB-CG-CD	6.69	126.69	111.30
1	C	9	GLY	CA-C-N	-6.68	112.64	122.86
1	C	9	GLY	C-N-CA	-6.68	112.64	122.86
1	D	11	GLY	N-CA-C	-6.67	102.40	112.41
1	A	12	ARG	N-CA-C	6.65	118.53	111.28
1	D	59	PHE	CA-CB-CG	6.64	120.44	113.80
1	A	53	ASP	CA-CB-CG	-6.62	105.98	112.60
1	D	85	ILE	O-C-N	6.61	130.06	123.18
1	A	13	ILE	O-C-N	6.57	128.60	121.83
1	B	63	VAL	N-CA-CB	6.54	120.71	111.82
1	D	20	ALA	O-C-N	-6.52	115.21	122.12
1	B	271	GLN	CA-C-O	-6.51	113.98	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	THR	CA-CB-OG1	6.51	119.37	109.60
1	B	119	ALA	CA-C-O	6.51	127.32	120.42
1	A	314	ALA	N-CA-CB	6.51	120.24	110.22
1	C	172	ALA	O-C-N	-6.49	114.61	120.71
1	A	336	GLU	N-CA-C	6.48	118.03	110.97
1	B	235	VAL	N-CA-CB	-6.43	100.85	111.98
1	A	81	ASN	CA-C-N	6.43	134.02	121.41
1	A	81	ASN	C-N-CA	6.43	134.02	121.41
1	B	224	SER	O-C-N	-6.43	116.15	123.48
1	C	234	MET	CA-CB-CG	6.43	126.96	114.10
1	C	196	TYR	N-CA-CB	6.42	120.05	110.29
1	D	83	HIS	CA-C-N	6.40	131.21	122.19
1	D	83	HIS	C-N-CA	6.40	131.21	122.19
1	D	219	VAL	N-CA-CB	6.40	120.48	112.16
1	D	253	PRO	N-CA-CB	-6.39	97.51	103.46
1	D	268	THR	CB-CA-C	-6.38	97.71	110.42
1	D	204	ASP	CB-CG-OD1	6.37	133.04	118.40
1	B	86	LEU	CA-C-O	6.35	128.22	120.92
1	D	16	MET	N-CA-CB	-6.35	100.79	110.12
1	D	20	ALA	CA-C-N	6.34	129.29	120.29
1	D	20	ALA	C-N-CA	6.34	129.29	120.29
1	D	337	TRP	N-CA-C	6.34	118.06	111.03
1	A	263	THR	CA-C-N	6.33	130.32	120.75
1	A	263	THR	C-N-CA	6.33	130.32	120.75
1	B	330	VAL	O-C-N	-6.32	116.01	123.03
1	B	252	THR	CA-C-N	6.32	126.06	119.05
1	B	252	THR	C-N-CA	6.32	126.06	119.05
1	B	6	GLY	CA-C-N	-6.30	114.92	123.12
1	B	6	GLY	C-N-CA	-6.30	114.92	123.12
1	B	331	SER	CA-C-O	6.29	128.28	120.54
1	C	8	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	C	68	SER	N-CA-C	-6.29	106.83	114.75
1	B	254	ASP	CA-C-O	-6.28	114.52	121.23
1	A	5	VAL	CA-C-N	-6.27	116.78	121.61
1	A	5	VAL	C-N-CA	-6.27	116.78	121.61
1	A	287	GLY	CA-C-N	-6.27	116.75	123.08
1	A	287	GLY	C-N-CA	-6.27	116.75	123.08
1	B	271	GLN	CB-CG-CD	6.26	123.25	112.60
1	C	309	ILE	CA-C-O	6.22	127.04	120.51
1	D	243	LEU	CA-CB-CG	6.21	138.05	116.30
1	D	183	PHE	N-CA-C	-6.19	104.45	111.14
1	D	104	VAL	CA-C-O	-6.19	113.79	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	A	148	VAL	CA-C-O	-6.17	115.46	120.70
1	C	208	VAL	N-CA-C	6.16	122.16	109.34
1	B	305	ASN	CB-CG-ND2	-6.13	107.20	116.40
1	C	262	PHE	O-C-N	6.12	129.97	123.42
1	A	23	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	319	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	128	ALA	CA-C-O	-6.11	114.79	121.87
1	A	305	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	D	146	MET	O-C-N	-6.09	115.39	122.95
1	D	236	ILE	CA-C-N	6.08	127.44	119.84
1	D	236	ILE	C-N-CA	6.08	127.44	119.84
1	D	51	ARG	CG-CD-NE	-6.08	98.62	112.00
1	B	225	THR	N-CA-C	-6.08	102.94	110.41
1	D	276	ALA	O-C-N	6.07	129.07	122.15
1	B	192	THR	CA-CB-CG2	6.07	120.82	110.50
1	D	255	VAL	N-CA-CB	6.06	121.23	111.23
1	D	176	HIS	CA-C-N	6.06	128.28	120.70
1	D	176	HIS	C-N-CA	6.06	128.28	120.70
1	D	354	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	106	TYR	CA-C-N	-6.05	115.30	122.93
1	D	106	TYR	C-N-CA	-6.05	115.30	122.93
1	D	63	VAL	CA-C-O	-6.05	114.10	120.39
1	A	337	TRP	N-CA-C	6.05	117.67	111.14
1	C	183	PHE	N-CA-C	-6.05	104.80	111.82
1	A	40	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	91	GLN	CA-C-O	-6.05	114.28	121.11
1	D	51	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	D	359	LEU	CA-CB-CG	6.04	137.43	116.30
1	C	269	SER	O-C-N	6.04	130.04	123.10
1	C	356	SER	CA-C-N	6.03	133.05	121.54
1	C	356	SER	C-N-CA	6.03	133.05	121.54
1	D	38	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	348	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	B	106	TYR	CA-C-O	6.00	126.92	120.38
1	B	115	THR	N-CA-CB	-5.99	100.63	110.40
1	A	288	ILE	N-CA-C	-5.98	106.42	111.56
1	C	163	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	320	LEU	CA-C-O	5.96	125.06	119.76
1	D	341	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	37	VAL	CA-CB-CG1	5.94	120.50	110.40
1	A	266	ARG	O-C-N	5.94	129.78	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	LEU	CA-C-N	5.94	128.16	120.44
1	C	277	LEU	C-N-CA	5.94	128.16	120.44
1	A	266	ARG	CA-C-O	-5.94	114.88	121.23
1	B	351	ALA	CA-C-O	5.93	127.05	120.82
1	B	248	PHE	N-CA-CB	5.93	120.08	110.77
1	D	248	PHE	CA-CB-CG	5.91	119.71	113.80
1	C	333	TYR	CA-C-N	-5.90	114.57	122.42
1	C	333	TYR	C-N-CA	-5.90	114.57	122.42
1	B	141	ALA	N-CA-C	-5.90	98.23	110.80
1	B	232	VAL	O-C-N	-5.89	115.34	122.06
1	A	228	ALA	N-CA-C	5.89	118.17	111.11
1	A	59	PHE	CA-CB-CG	5.88	119.68	113.80
1	D	249	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	D	194	HIS	N-CA-C	5.87	118.97	109.40
1	C	304	ASP	CA-C-N	-5.87	113.27	122.65
1	C	304	ASP	C-N-CA	-5.87	113.27	122.65
1	D	268	THR	CA-CB-OG1	5.86	118.39	109.60
1	D	342	ARG	NH1-CZ-NH2	-5.86	111.69	119.30
1	C	310	TYR	O-C-N	-5.84	115.74	122.93
1	D	272	GLU	CA-C-O	-5.84	114.36	120.55
1	B	215	ARG	O-C-N	-5.84	116.13	122.79
1	C	46	PHE	N-CA-CB	5.84	118.64	109.94
1	A	86	LEU	CA-C-N	-5.83	115.26	122.84
1	A	86	LEU	C-N-CA	-5.83	115.26	122.84
1	B	240	GLN	N-CA-CB	5.83	118.64	109.83
1	C	272	GLU	CA-C-O	5.83	126.60	120.42
1	C	358	ARG	CD-NE-CZ	-5.82	116.25	124.40
1	C	262	PHE	CA-C-N	-5.82	114.90	123.05
1	C	262	PHE	C-N-CA	-5.82	114.90	123.05
1	D	230	LYS	CA-C-O	-5.82	114.38	120.55
1	A	30	GLU	CA-C-N	-5.81	114.92	122.99
1	A	30	GLU	C-N-CA	-5.81	114.92	122.99
1	D	216	ALA	CB-CA-C	5.81	118.52	110.16
1	B	298	SER	N-CA-C	5.78	117.58	111.28
1	D	21	LEU	CA-CB-CG	5.78	136.53	116.30
1	A	209	LYS	CA-C-N	-5.78	114.33	123.23
1	A	209	LYS	C-N-CA	-5.78	114.33	123.23
1	A	336	GLU	O-C-N	-5.76	116.04	122.03
1	A	171	LEU	N-CA-C	5.76	117.36	111.14
1	B	104	VAL	CA-C-O	-5.76	114.28	120.85
1	B	6	GLY	CA-C-O	-5.75	116.46	120.94
1	D	336	GLU	N-CA-CB	-5.75	101.65	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	MET	CA-CB-CG	5.74	125.58	114.10
1	D	303	ASN	CB-CG-ND2	-5.74	107.80	116.40
1	A	37	VAL	CA-C-O	5.73	126.40	120.39
1	C	306	ARG	NH1-CZ-NH2	5.73	126.74	119.30
1	A	240	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	C	171	LEU	N-CA-C	5.71	117.31	111.14
1	B	282	LYS	CA-C-N	-5.71	114.08	121.79
1	B	282	LYS	C-N-CA	-5.71	114.08	121.79
1	B	157	GLU	N-CA-CB	5.69	119.12	110.42
1	C	2	PRO	CA-C-N	5.68	132.19	121.97
1	C	2	PRO	C-N-CA	5.68	132.19	121.97
1	D	352	SER	N-CA-CB	5.68	118.24	110.01
1	A	14	GLY	N-CA-C	-5.67	105.92	112.50
1	C	135	ALA	CB-CA-C	-5.67	103.84	110.76
1	C	343	VAL	CA-C-N	5.67	128.22	120.46
1	C	343	VAL	C-N-CA	5.67	128.22	120.46
1	A	331	SER	CA-C-O	5.65	127.49	120.54
1	A	305	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	215	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	221	ILE	N-CA-C	-5.64	99.75	107.99
1	C	53	ASP	CA-CB-CG	-5.62	106.98	112.60
1	D	90	ALA	CA-C-O	5.61	128.04	121.87
1	C	187	THR	CA-CB-OG1	-5.60	101.20	109.60
1	A	11	GLY	CA-C-O	-5.58	115.61	122.03
1	A	281	SER	CA-C-O	-5.58	113.80	120.10
1	A	296	LEU	O-C-N	5.58	129.19	122.94
1	D	11	GLY	CA-C-O	-5.57	116.71	122.28
1	A	336	GLU	CA-C-O	5.57	126.85	121.00
1	D	12	ARG	N-CA-C	5.57	117.79	111.11
1	A	141	ALA	N-CA-CB	5.55	118.13	109.97
1	B	270	ILE	O-C-N	-5.54	115.54	121.80
1	C	305	ASN	N-CA-CB	5.53	118.64	110.56
1	B	254	ASP	N-CA-CB	-5.53	102.99	111.56
1	D	66	THR	CB-CA-C	-5.53	98.79	111.95
1	D	311	ASP	O-C-N	5.53	129.70	122.68
1	B	252	THR	CB-CA-C	5.52	117.18	108.84
1	C	348	ARG	N-CA-C	-5.51	104.96	110.97
1	A	138	SER	CA-C-O	5.51	128.18	121.68
1	B	305	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	14	GLY	CA-C-N	5.50	127.59	120.44
1	B	14	GLY	C-N-CA	5.50	127.59	120.44
1	A	168	THR	CA-CB-OG1	-5.50	101.36	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	GLU	CA-C-O	-5.49	114.60	120.42
1	B	6	GLY	O-C-N	5.49	127.88	123.49
1	A	260	LEU	CA-C-N	-5.49	115.26	122.99
1	A	260	LEU	C-N-CA	-5.49	115.26	122.99
1	A	24	ASP	CA-CB-CG	-5.48	107.12	112.60
1	D	149	ASN	CA-C-O	-5.48	113.81	119.51
1	C	217	ALA	N-CA-C	5.46	117.32	111.36
1	B	334	ASP	N-CA-C	-5.46	98.07	108.17
1	C	276	ALA	CA-C-N	-5.46	112.97	120.28
1	C	276	ALA	C-N-CA	-5.46	112.97	120.28
1	A	115	THR	O-C-N	-5.45	115.13	122.43
1	A	169	ASN	CA-C-O	-5.45	113.94	120.10
1	C	269	SER	CA-C-O	-5.45	115.62	121.45
1	C	270	ILE	CA-C-O	5.44	126.13	120.25
1	D	95	ALA	O-C-N	-5.44	115.19	122.43
1	C	10	PHE	CA-CB-CG	-5.42	108.38	113.80
1	C	203	VAL	CB-CA-C	-5.42	104.33	111.70
1	D	327	PHE	N-CA-C	5.42	117.92	109.52
1	A	297	VAL	N-CA-CB	5.41	118.51	112.45
1	B	239	THR	CA-C-O	-5.41	112.74	119.28
1	C	267	ASP	CA-CB-CG	-5.40	107.20	112.60
1	C	79	VAL	N-CA-CB	5.39	118.05	112.65
1	A	268	THR	CB-CA-C	5.39	121.15	110.42
1	B	271	GLN	CG-CD-NE2	-5.38	108.32	116.40
1	B	254	ASP	CA-C-N	5.38	131.65	121.97
1	B	254	ASP	C-N-CA	5.38	131.65	121.97
1	A	333	TYR	N-CA-CB	5.38	119.66	110.57
1	D	304	ASP	CA-CB-CG	-5.37	107.23	112.60
1	C	18	PHE	CA-C-O	-5.37	115.19	120.82
1	C	236	ILE	CA-C-N	5.36	125.69	119.47
1	C	236	ILE	C-N-CA	5.36	125.69	119.47
1	D	160	VAL	O-C-N	-5.36	117.52	123.20
1	C	158	HIS	CA-C-O	5.36	126.11	120.54
1	D	192	THR	N-CA-CB	5.36	118.98	110.57
1	C	348	ARG	CA-C-O	-5.36	115.38	121.00
1	C	293	ASP	N-CA-C	-5.35	105.45	112.41
1	D	125	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	B	317	GLN	CA-CB-CG	-5.34	103.43	114.10
1	B	234	MET	CB-CA-C	-5.33	99.50	110.38
1	C	7	ILE	CA-C-O	-5.33	114.24	120.75
1	B	55	VAL	CA-C-O	-5.33	114.46	120.32
1	C	13	ILE	CA-CB-CG2	5.33	119.56	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	PRO	N-CA-C	-5.32	102.77	110.80
1	C	205	GLY	CA-C-N	5.32	130.04	123.12
1	C	205	GLY	C-N-CA	5.32	130.04	123.12
1	C	270	ILE	CA-C-N	5.32	127.41	120.28
1	C	270	ILE	C-N-CA	5.32	127.41	120.28
1	D	54	THR	CA-C-O	-5.30	114.11	120.10
1	C	244	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	272	GLU	N-CA-CB	5.30	118.00	110.16
1	A	48	TYR	CA-C-O	-5.29	115.27	120.82
1	B	8	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	285	MET	CG-SD-CE	5.27	112.49	100.90
1	D	24	ASP	CA-CB-CG	-5.26	107.34	112.60
1	C	286	LYS	CA-CB-CG	5.26	124.62	114.10
1	C	258	VAL	CA-C-O	5.25	126.19	120.57
1	D	218	ALA	CA-C-O	-5.25	113.08	119.43
1	D	248	PHE	N-CA-CB	5.25	118.84	110.65
1	A	100	GLY	CA-C-N	5.25	127.62	120.54
1	A	100	GLY	C-N-CA	5.25	127.62	120.54
1	A	186	GLN	CA-C-O	5.25	126.16	120.55
1	A	46	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	260	LEU	CA-C-O	-5.24	114.76	120.36
1	A	78	LEU	CA-CB-CG	5.23	134.62	116.30
1	C	231	ALA	N-CA-CB	5.23	118.28	110.22
1	B	9	GLY	CA-C-N	-5.23	113.93	123.34
1	B	9	GLY	C-N-CA	-5.23	113.93	123.34
1	C	207	SER	CA-C-N	5.22	131.38	121.97
1	C	207	SER	C-N-CA	5.22	131.38	121.97
1	C	297	VAL	CA-C-O	-5.22	116.14	121.67
1	B	54	THR	CA-C-O	-5.22	115.02	120.55
1	A	314	ALA	N-CA-C	-5.21	105.71	111.71
1	A	210	ASP	N-CA-CB	-5.21	101.18	110.82
1	A	306	ARG	CD-NE-CZ	5.21	131.69	124.40
1	A	69	SER	CA-C-N	5.21	125.26	119.32
1	A	69	SER	C-N-CA	5.21	125.26	119.32
1	D	270	ILE	CA-CB-CG2	5.21	119.35	110.50
1	A	56	HIS	CA-C-O	-5.20	112.99	119.28
1	D	263	THR	CA-C-O	-5.19	114.61	120.32
1	A	28	GLY	O-C-N	-5.19	115.95	122.70
1	A	129	ARG	CD-NE-CZ	5.19	131.67	124.40
1	B	187	THR	CA-CB-OG1	-5.19	101.81	109.60
1	A	53	ASP	CA-C-O	5.19	126.53	120.20
1	D	253	PRO	CB-CA-C	5.19	119.66	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	HIS	CB-CA-C	-5.18	101.80	110.19
1	B	96	ASP	CA-CB-CG	-5.18	107.42	112.60
1	C	333	TYR	N-CA-CB	5.17	120.14	110.99
1	B	129	ARG	CG-CD-NE	5.17	123.37	112.00
1	C	167	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	28	GLY	CA-C-O	-5.16	111.59	120.57
1	C	358	ARG	N-CA-C	-5.16	106.12	112.72
1	C	66	THR	N-CA-CB	5.14	118.37	110.70
1	C	173	PRO	O-C-N	-5.14	116.36	122.17
1	D	252	THR	N-CA-C	-5.14	102.23	110.10
1	A	252	THR	N-CA-C	-5.14	102.38	110.14
1	B	22	CYS	CA-C-O	5.14	125.87	120.42
1	A	305	ASN	O-C-N	5.14	128.76	122.34
1	B	40	ASN	CB-CG-ND2	5.13	124.10	116.40
1	B	53	ASP	CA-CB-CG	-5.13	107.47	112.60
1	B	130	LYS	CA-C-O	5.13	127.01	121.06
1	C	334	ASP	CA-C-O	-5.13	115.09	120.58
1	A	29	THR	CB-CA-C	5.13	119.55	111.39
1	C	268	THR	N-CA-CB	5.13	119.16	110.49
1	C	207	SER	CA-CB-OG	5.12	121.35	111.10
1	D	195	SER	CA-CB-OG	-5.12	100.86	111.10
1	C	309	ILE	CA-CB-CG1	5.12	119.09	110.40
1	D	204	ASP	OD1-CG-OD2	-5.11	110.63	122.90
1	D	115	THR	CA-CB-OG1	5.11	117.27	109.60
1	D	234	MET	O-C-N	-5.11	115.64	122.49
1	D	235	VAL	CB-CA-C	5.11	116.45	110.88
1	B	306	ARG	CG-CD-NE	-5.11	100.77	112.00
1	A	227	GLY	CA-C-N	5.10	127.43	120.54
1	A	227	GLY	C-N-CA	5.10	127.43	120.54
1	B	164	ALA	CA-C-N	5.09	131.37	122.81
1	B	164	ALA	C-N-CA	5.09	131.37	122.81
1	D	15	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	167	THR	CA-CB-CG2	5.09	119.16	110.50
1	B	224	SER	CA-C-O	5.09	126.44	120.43
1	C	107	VAL	CA-C-O	5.09	125.98	120.53
1	A	296	LEU	CA-C-N	-5.08	115.79	123.27
1	A	296	LEU	C-N-CA	-5.08	115.79	123.27
1	A	232	VAL	CA-C-N	5.08	126.49	120.14
1	A	232	VAL	C-N-CA	5.08	126.49	120.14
1	B	309	ILE	CA-CB-CG2	-5.08	101.86	110.50
1	A	255	VAL	N-CA-CB	5.08	119.61	111.23
1	D	80	VAL	N-CA-C	5.07	114.79	106.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	VAL	CB-CA-C	5.07	118.45	110.95
1	D	92	ARG	CD-NE-CZ	5.07	131.50	124.40
1	D	75	ASP	CA-C-O	-5.07	115.61	121.19
1	D	293	ASP	N-CA-C	-5.07	105.47	113.02
1	B	242	LYS	CA-CB-CG	5.05	124.20	114.10
1	C	140	GLY	CA-C-O	-5.05	117.85	122.24
1	D	293	ASP	CB-CA-C	5.05	118.92	110.44
1	A	293	ASP	N-CA-C	-5.04	105.44	112.30
1	B	105	GLU	N-CA-CB	5.04	117.83	110.47
1	A	272	GLU	CA-CB-CG	5.04	124.17	114.10
1	B	41	THR	N-CA-C	-5.03	107.12	114.12
1	D	234	MET	CA-CB-CG	5.03	124.17	114.10
1	D	191	THR	CA-C-N	-5.03	116.06	123.00
1	D	191	THR	C-N-CA	-5.03	116.06	123.00
1	D	76	ASP	CA-CB-CG	-5.03	107.57	112.60
1	B	92	ARG	CA-C-O	5.03	125.78	120.10
1	B	270	ILE	CA-C-N	5.02	126.97	120.44
1	B	270	ILE	C-N-CA	5.02	126.97	120.44
1	D	17	VAL	CA-C-O	5.02	126.49	121.17
1	C	7	ILE	CB-CA-C	-5.02	104.88	111.25
1	D	183	PHE	CA-C-O	5.02	125.87	120.70
1	B	237	PRO	CA-C-N	5.02	128.62	120.60
1	B	237	PRO	C-N-CA	5.02	128.62	120.60
1	D	160	VAL	CA-C-O	5.01	125.61	120.39
1	C	12	ARG	CD-NE-CZ	5.01	131.42	124.40
1	B	36	VAL	CA-CB-CG2	-5.01	101.88	110.40
1	D	185	VAL	CA-C-O	5.01	125.22	120.31
1	B	315	THR	CA-C-O	-5.00	115.57	120.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	GLY	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2744	0	2749	88	0
1	B	2744	0	2749	88	0
1	C	2750	0	2752	172	0
1	D	2744	0	2749	88	0
2	C	23	0	22	13	0
3	A	271	0	0	16	0
3	B	223	0	0	13	0
3	C	161	0	0	17	0
3	D	282	0	0	13	0
All	All	11942	0	11021	423	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 19.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166[A]:CYS:SG	2:C:960:BRZ:HC18	1.96	1.05
1:C:166[A]:CYS:H	2:C:960:BRZ:HC73	1.27	0.97
1:A:94:PRO:HA	1:A:97:LEU:HD23	1.46	0.97
1:B:190:MET:HE1	1:B:258:VAL:HG22	1.48	0.95
1:A:40:ASN:HD21	1:A:42:ASP:HB3	1.31	0.95
1:A:220:ASN:HD21	1:D:54:THR:HG21	1.33	0.93
1:C:107:VAL:HG13	1:C:131:VAL:HG22	1.53	0.90
1:D:190:MET:HE3	1:D:258:VAL:HG22	1.53	0.90
1:B:64:THR:HG22	1:B:79:VAL:HB	1.53	0.90
1:C:121:GLU:HA	1:C:124:LEU:HD22	1.56	0.87
1:C:176:HIS:CE1	1:C:180:LYS:HD2	2.09	0.85
1:B:66:THR:HG22	1:B:67:LYS:H	1.41	0.84
1:C:166[A]:CYS:SG	2:C:960:BRZ:C18	2.66	0.83
1:C:358:ARG:HD2	3:C:1025:HOH:O	1.77	0.83
1:A:8:ASN:ND2	1:A:37:VAL:HG22	1.94	0.82
1:A:117:LYS:O	1:A:121:GLU:HG3	1.78	0.82
1:D:190:MET:CE	1:D:192:THR:HB	2.11	0.81
1:C:70:PRO:O	1:C:71:SER:HB2	1.80	0.80
1:D:167:THR:HG21	1:D:190:MET:HE1	1.64	0.79
1:A:305:ASN:HB3	3:A:527:HOH:O	1.81	0.79
1:D:50:MET:HE1	1:D:78:LEU:HG	1.65	0.79
1:A:196:TYR:HB3	3:A:538:HOH:O	1.80	0.79
1:D:50:MET:HG2	3:D:530:HOH:O	1.82	0.79
1:C:154:ASN:HD22	1:C:157:GLU:H	1.30	0.78
1:C:8:ASN:HD22	1:C:37:VAL:HG13	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HB	1:B:88:VAL:HG22	1.66	0.76
1:C:115:THR:HG23	1:C:137:ALA:HA	1.68	0.75
1:C:239:THR:HB	1:C:243:LEU:HD22	1.68	0.74
1:A:55:VAL:HG23	1:A:56:HIS:CD2	2.23	0.74
1:D:3:ILE:HG22	1:D:355:ARG:NH2	2.02	0.74
1:A:8:ASN:HD22	1:A:37:VAL:HG22	1.51	0.73
1:B:68:SER:HB3	1:B:86:LEU:HD21	1.69	0.73
1:B:12:ARG:HG2	1:B:16:MET:HE2	1.70	0.73
1:C:8:ASN:HA	1:C:37:VAL:HG13	1.72	0.72
1:C:146:MET:HE3	1:C:346:LEU:HB2	1.71	0.72
1:B:190:MET:HG2	1:B:229:ALA:HB2	1.71	0.72
1:C:1:MET:HB3	1:C:2:PRO:CD	2.19	0.72
1:D:47:ALA:HA	1:D:50:MET:HE3	1.71	0.71
1:A:305:ASN:C	1:A:305:ASN:HD22	1.97	0.71
1:A:13:ILE:HG23	1:A:110:SER:HB2	1.72	0.71
1:C:61:TYR:HD2	1:C:81:ASN:HB2	1.55	0.71
1:A:115:THR:HB	3:A:376:HOH:O	1.91	0.71
1:C:183:PHE:CD1	1:C:268:THR:HG21	2.26	0.71
1:B:54:THR:HG21	1:C:220:ASN:HD21	1.53	0.70
1:B:115:THR:HG22	3:B:498:HOH:O	1.91	0.70
1:B:10:PHE:CG	1:B:36:VAL:HG21	2.25	0.70
1:A:105:GLU:HG3	1:A:129:ARG:HD2	1.73	0.70
1:B:196:TYR:HB3	3:B:485:HOH:O	1.91	0.70
1:D:39:MET:HE2	1:D:90:ALA:HB3	1.72	0.70
1:C:154:ASN:HD22	1:C:157:GLU:N	1.89	0.70
1:D:166:CYS:HB3	3:D:533:HOH:O	1.90	0.70
1:B:166:CYS:HB3	3:B:525:HOH:O	1.91	0.69
1:C:106:TYR:OH	1:C:351:ALA:HA	1.91	0.69
1:A:40:ASN:ND2	1:A:42:ASP:H	1.90	0.69
1:A:3:ILE:HG23	1:A:355:ARG:NH2	2.08	0.69
1:D:167:THR:CG2	1:D:190:MET:HE1	2.22	0.68
1:A:218:ALA:HA	1:A:251:PRO:HB3	1.75	0.68
1:A:324:ARG:HG3	3:A:610:HOH:O	1.93	0.68
1:A:40:ASN:HD21	1:A:42:ASP:CB	2.07	0.67
1:B:129:ARG:HH21	1:B:358:ARG:HH21	1.43	0.67
1:C:349:HIS:CE1	1:C:353:LYS:HZ2	2.14	0.66
1:C:354:ASP:O	1:C:358:ARG:HG3	1.96	0.66
1:D:8:ASN:ND2	1:D:37:VAL:HG22	2.10	0.66
1:C:147:GLY:H	1:C:150:HIS:CD2	2.13	0.66
1:A:115:THR:HG21	3:A:467:HOH:O	1.94	0.66
1:A:215:ARG:HH21	1:D:54:THR:HG22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HD12	1:D:106:TYR:CD1	2.31	0.66
1:D:115:THR:HB	3:D:522:HOH:O	1.96	0.66
1:D:336:GLU:HA	3:D:516:HOH:O	1.96	0.66
1:C:355:ARG:HG2	3:C:1058:HOH:O	1.96	0.65
1:D:130:LYS:NZ	1:D:159:HIS:HD2	1.94	0.65
1:C:34:VAL:HG12	1:C:102:LEU:HD23	1.78	0.65
1:C:28:GLY:HA2	1:C:32:ASP:OD2	1.97	0.65
1:D:201:LYS:HE2	3:D:527:HOH:O	1.97	0.64
1:C:1:MET:HB3	1:C:2:PRO:HD2	1.78	0.64
1:D:3:ILE:HG22	1:D:355:ARG:HH22	1.61	0.64
1:B:10:PHE:CD1	1:B:36:VAL:HG21	2.32	0.64
1:C:208:VAL:HG13	1:C:209:LYS:HG2	1.80	0.63
1:B:8:ASN:HD22	1:B:37:VAL:HG22	1.63	0.63
1:C:305:ASN:HB3	3:C:1055:HOH:O	1.98	0.63
1:A:3:ILE:HG23	1:A:355:ARG:HH21	1.63	0.63
1:D:50:MET:HE3	1:D:63:VAL:HG11	1.80	0.63
1:B:54:THR:HG23	1:C:204:ASP:OD1	1.99	0.63
1:C:166[A]:CYS:HB2	2:C:960:BRZ:O14	1.98	0.62
1:B:171:LEU:HD13	1:B:232:VAL:HG21	1.82	0.62
3:C:1018:HOH:O	1:D:187:THR:HG22	2.00	0.62
1:C:7:ILE:HB	1:C:36:VAL:HG12	1.82	0.62
1:D:4:LYS:NZ	1:D:32:ASP:OD1	2.34	0.61
1:D:13:ILE:HG22	1:D:110:SER:HB2	1.82	0.61
1:C:31:ILE:HD11	1:C:348:ARG:HD3	1.81	0.61
1:C:221:ILE:HD12	3:D:439:HOH:O	2.00	0.61
1:D:234:MET:HE2	3:D:571:HOH:O	2.00	0.61
1:C:51:ARG:HG2	1:C:52:TYR:CE2	2.36	0.60
1:C:176:HIS:NE2	1:C:180:LYS:HD2	2.15	0.60
1:C:335:ASN:HB2	2:C:960:BRZ:HC92	1.82	0.60
1:A:37:VAL:HG23	1:A:90:ALA:HA	1.83	0.60
1:A:204:ASP:OD1	1:D:54:THR:HG23	2.01	0.60
1:B:129:ARG:HD2	3:B:535:HOH:O	2.01	0.60
1:A:318:ASN:HB3	3:A:585:HOH:O	2.02	0.59
1:C:51:ARG:HG3	3:C:1014:HOH:O	2.02	0.59
1:B:51:ARG:HD3	3:B:444:HOH:O	2.01	0.59
1:A:213:GLY:HA2	1:A:249:ARG:HH12	1.68	0.59
1:C:129:ARG:HD2	1:C:358:ARG:NH1	2.17	0.59
1:A:118:ALA:HA	1:A:121:GLU:CD	2.27	0.59
1:A:37:VAL:HG21	1:A:97:LEU:HD11	1.85	0.59
1:B:219:VAL:HG11	1:C:253:PRO:HG3	1.84	0.59
1:A:220:ASN:ND2	1:D:54:THR:HG21	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLY:H	1:A:150:HIS:HD2	1.48	0.59
1:C:15:ARG:O	1:C:19:GLN:HG3	2.03	0.59
1:C:26:LEU:HD13	1:C:348:ARG:HD3	1.84	0.59
1:C:154:ASN:ND2	1:C:157:GLU:H	1.99	0.59
1:C:166[A]:CYS:SG	2:C:960:BRZ:C17	2.91	0.59
1:D:222:ILE:O	1:D:249:ARG:HD3	2.03	0.59
1:B:190:MET:O	1:B:190:MET:HG3	2.03	0.59
1:C:167:THR:HG22	1:C:190:MET:HE1	1.85	0.59
1:A:107:VAL:HG13	1:A:131:VAL:HG22	1.83	0.58
1:C:147:GLY:H	1:C:150:HIS:HD2	1.50	0.58
1:C:339:TYR:O	1:C:343:VAL:HG23	2.03	0.58
1:D:47:ALA:HA	1:D:50:MET:CE	2.32	0.58
1:B:200:GLN:O	1:B:201:LYS:HE3	2.04	0.58
1:B:11:GLY:O	1:B:15:ARG:HB2	2.03	0.58
1:A:67:LYS:HB2	1:A:72:VAL:HB	1.84	0.57
1:C:166[A]:CYS:H	2:C:960:BRZ:C17	2.11	0.57
1:C:348:ARG:O	1:C:349:HIS:C	2.47	0.57
1:C:129:ARG:HD2	1:C:358:ARG:HH12	1.68	0.57
1:C:348:ARG:O	1:C:351:ALA:N	2.36	0.57
1:B:140:GLY:O	1:B:141:ALA:CB	2.50	0.57
1:A:19:GLN:OE1	1:A:50:MET:HG2	2.05	0.57
1:A:147:GLY:H	1:A:150:HIS:CD2	2.22	0.57
1:C:320:LEU:HG	1:D:244:THR:HG22	1.85	0.57
1:C:55:VAL:HG13	1:C:56:HIS:CD2	2.40	0.57
1:B:28:GLY:HA3	1:B:83:HIS:CE1	2.39	0.57
1:D:17:VAL:HG11	1:D:108:ILE:HD13	1.87	0.57
1:A:215:ARG:NH2	1:D:54:THR:HG22	2.20	0.57
1:B:98:PRO:HG2	1:B:102:LEU:HD22	1.86	0.57
1:D:12:ARG:CZ	1:D:16:MET:HE1	2.35	0.56
1:A:224:SER:HB2	1:A:249:ARG:HH21	1.70	0.56
1:B:54:THR:HG22	1:C:215:ARG:HH21	1.70	0.56
1:C:16:MET:HE1	1:C:336:GLU:HG2	1.86	0.56
1:C:110:SER:HA	3:C:983:HOH:O	2.06	0.56
1:C:72:VAL:O	1:C:73:ALA:HB2	2.06	0.56
1:B:176:HIS:HE1	3:B:471:HOH:O	1.88	0.56
1:D:171:LEU:HD22	1:D:175:VAL:HG23	1.87	0.56
1:C:3:ILE:HD11	1:C:355:ARG:HH21	1.70	0.56
1:C:6:GLY:HA3	1:C:99:TRP:CZ3	2.41	0.56
1:C:22:CYS:O	1:C:23:GLU:C	2.49	0.56
1:C:142:LYS:NZ	1:C:152:GLU:OE1	2.38	0.56
1:C:183:PHE:CE1	1:C:268:THR:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:MET:HE3	1:C:346:LEU:CB	2.35	0.56
1:B:8:ASN:ND2	1:B:37:VAL:HG22	2.21	0.55
1:C:186:GLN:HG2	1:C:187:THR:HG23	1.89	0.55
1:A:111:THR:HB	1:A:113:LEU:HD13	1.88	0.55
1:C:183:PHE:HD1	1:C:268:THR:HG21	1.70	0.55
1:C:298:SER:HB3	1:C:332:TRP:CZ3	2.42	0.55
1:B:129:ARG:HH21	1:B:358:ARG:NH2	2.05	0.55
1:D:131:VAL:HB	1:D:160:VAL:HG22	1.89	0.55
1:B:78:LEU:HD23	1:B:87:CYS:SG	2.47	0.55
1:C:98:PRO:HB2	1:C:101:LYS:HB2	1.89	0.55
1:D:224:SER:HB2	1:D:249:ARG:NH1	2.21	0.55
1:A:107:VAL:HG11	1:A:123:HIS:HB3	1.89	0.54
1:A:349:HIS:NE2	1:A:353:LYS:HE2	2.21	0.54
1:B:129:ARG:O	1:B:130:LYS:HD3	2.07	0.54
1:B:105:GLU:HB3	1:B:129:ARG:HD3	1.89	0.54
1:A:71:SER:O	1:A:73:ALA:N	2.40	0.54
1:C:3:ILE:CG1	1:C:355:ARG:HH21	2.20	0.54
1:A:176:HIS:HD2	3:A:487:HOH:O	1.89	0.54
1:A:150:HIS:HE1	3:A:536:HOH:O	1.90	0.54
1:C:12:ARG:O	1:C:16:MET:HG3	2.08	0.54
1:C:108:ILE:HD11	1:C:347:VAL:HG21	1.90	0.54
1:A:115:THR:HG22	3:A:462:HOH:O	2.08	0.54
1:B:218:ALA:HB3	3:B:400:HOH:O	2.07	0.54
1:C:5:VAL:HG22	1:C:106:TYR:HB2	1.90	0.54
1:C:132:VAL:HG22	1:C:350:MET:HE1	1.90	0.54
1:A:220:ASN:HD21	1:D:54:THR:CG2	2.15	0.53
1:B:3:ILE:HB	1:B:31:ILE:HD13	1.90	0.53
1:C:358:ARG:HB2	3:C:1103:HOH:O	2.07	0.53
1:B:21:LEU:HD13	1:B:26:LEU:HB2	1.89	0.53
1:B:130:LYS:NZ	1:B:155:PRO:O	2.41	0.53
2:C:960:BRZ:C18	2:C:960:BRZ:O14	2.56	0.53
1:C:121:GLU:O	1:C:124:LEU:HB2	2.09	0.53
2:C:960:BRZ:C19	2:C:960:BRZ:C8	2.85	0.53
1:C:155:PRO:HB3	1:C:354:ASP:CB	2.39	0.53
1:B:99:TRP:HA	1:B:99:TRP:CE3	2.43	0.53
1:C:207:SER:HB3	1:C:214:GLY:CA	2.39	0.53
1:B:54:THR:HG22	1:C:215:ARG:NH2	2.24	0.53
1:B:147:GLY:H	1:B:150:HIS:CD2	2.27	0.53
1:B:153:TYR:HD2	1:B:353:LYS:HD3	1.74	0.53
1:C:130:LYS:CD	1:C:159:HIS:HA	2.39	0.53
1:D:328:LYS:NZ	3:D:437:HOH:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LYS:HB2	1:C:140:GLY:O	2.10	0.52
1:C:154:ASN:HB3	1:C:157:GLU:HB2	1.92	0.52
1:A:13:ILE:CG2	1:A:110:SER:HB2	2.38	0.52
1:D:8:ASN:HD22	1:D:37:VAL:HG22	1.73	0.52
1:A:226:THR:HB	3:A:557:HOH:O	2.09	0.52
1:C:12:ARG:HG2	1:C:16:MET:HE2	1.92	0.52
1:C:344:VAL:O	1:C:348:ARG:HG3	2.10	0.52
1:A:19:GLN:HG3	1:A:59:PHE:CE1	2.45	0.51
1:A:26:LEU:HD13	1:A:348:ARG:HD2	1.92	0.51
1:A:305:ASN:C	1:A:305:ASN:ND2	2.66	0.51
1:C:104:VAL:O	1:C:128:ALA:HA	2.09	0.51
1:A:13:ILE:HD12	1:A:13:ILE:O	2.10	0.51
1:A:171:LEU:HD13	1:A:232:VAL:HG21	1.93	0.51
1:B:151:HIS:HB2	3:B:414:HOH:O	2.10	0.51
1:D:105:GLU:OE1	1:D:129:ARG:NH2	2.43	0.51
1:C:61:TYR:CD2	1:C:81:ASN:HB2	2.42	0.51
1:D:21:LEU:HD11	1:D:31:ILE:HD13	1.93	0.51
1:A:72:VAL:O	1:A:73:ALA:C	2.54	0.51
1:A:26:LEU:HD21	1:A:348:ARG:NH2	2.25	0.51
1:B:105:GLU:CB	1:B:129:ARG:HD3	2.41	0.51
1:D:94:PRO:HA	1:D:97:LEU:HD22	1.92	0.51
1:A:239:THR:HA	1:A:242:LYS:HD2	1.93	0.51
1:B:328:LYS:NZ	3:B:451:HOH:O	2.37	0.51
1:C:166[A]:CYS:SG	1:C:335:ASN:O	2.62	0.51
1:C:166[A]:CYS:SG	1:C:339:TYR:HB2	2.52	0.50
1:A:3:ILE:HG12	3:A:617:HOH:O	2.10	0.50
1:A:305:ASN:HD22	1:A:306:ARG:N	2.09	0.50
1:D:50:MET:CE	1:D:63:VAL:HG11	2.41	0.50
1:C:321:PRO:O	1:C:322:LYS:HB2	2.10	0.50
1:C:89:LYS:HG2	1:C:90:ALA:H	1.77	0.50
1:A:176:HIS:HE1	3:A:430:HOH:O	1.95	0.50
1:C:28:GLY:N	1:C:31:ILE:O	2.44	0.50
1:C:239:THR:HA	1:C:242:LYS:HD2	1.93	0.50
1:D:354:ASP:O	1:D:358:ARG:HG3	2.12	0.50
1:C:166[A]:CYS:SG	1:C:339:TYR:CB	3.00	0.50
1:D:183:PHE:CD1	1:D:268:THR:HG21	2.47	0.50
1:A:50:MET:HE1	1:A:78:LEU:HG	1.92	0.50
1:A:91:GLN:HB2	1:A:97:LEU:HD22	1.94	0.49
1:C:21:LEU:HD11	1:C:31:ILE:HG21	1.94	0.49
1:B:13:ILE:HD11	3:B:443:HOH:O	2.10	0.49
1:C:146:MET:CE	1:C:346:LEU:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:HB	1:D:88:VAL:HG22	1.94	0.49
1:B:349:HIS:NE2	1:B:353:LYS:HD2	2.27	0.49
1:B:121:GLU:O	1:B:122:GLY:C	2.55	0.49
1:D:268:THR:O	1:D:324:ARG:HA	2.12	0.49
1:B:124:LEU:HA	1:B:128:ALA:O	2.13	0.49
1:C:172:ALA:HB2	1:C:232:VAL:HG22	1.94	0.49
1:D:130:LYS:HZ2	1:D:159:HIS:HD2	1.61	0.49
1:C:283:THR:OG1	1:C:284:TYR:N	2.38	0.49
1:C:342:ARG:HA	1:C:345:ASP:HB2	1.94	0.49
1:C:3:ILE:CD1	1:C:355:ARG:HH21	2.25	0.49
1:C:4:LYS:HD3	1:C:103:GLY:O	2.13	0.48
1:C:306:ARG:HD2	3:C:1086:HOH:O	2.13	0.48
1:A:196:TYR:CD2	1:A:251:PRO:HA	2.48	0.48
1:D:259:ASP:OD1	1:D:328:LYS:NZ	2.35	0.48
1:A:326:PHE:CE1	1:B:263:THR:HG23	2.48	0.48
1:B:1:MET:HB3	1:B:4:LYS:NZ	2.28	0.48
1:B:66:THR:HG22	1:B:67:LYS:N	2.20	0.48
1:C:154:ASN:ND2	1:C:157:GLU:HG3	2.28	0.48
1:D:91:GLN:HB2	1:D:97:LEU:HD13	1.95	0.48
1:A:253:PRO:HG3	3:A:481:HOH:O	2.12	0.48
1:D:146:MET:HB2	1:D:342:ARG:HD3	1.94	0.48
1:B:65:THR:HG22	1:B:78:LEU:HD13	1.96	0.48
1:B:206:VAL:HG13	1:C:45:TYR:HE2	1.77	0.48
1:C:355:ARG:HA	3:C:1058:HOH:O	2.14	0.47
1:D:218:ALA:HA	1:D:251:PRO:HB3	1.96	0.47
1:D:231:ALA:O	1:D:234:MET:HG2	2.14	0.47
1:D:355:ARG:NH1	3:D:482:HOH:O	2.45	0.47
1:D:130:LYS:HZ3	1:D:159:HIS:HD2	1.59	0.47
1:D:233:GLY:O	1:D:240:GLN:HG3	2.14	0.47
1:B:176:HIS:HD2	3:B:402:HOH:O	1.97	0.47
1:B:210:ASP:OD2	1:B:213:GLY:HA3	2.15	0.47
1:B:278:LYS:HE2	1:B:291:TYR:CE2	2.49	0.47
1:C:346:LEU:O	1:C:349:HIS:HB3	2.14	0.47
1:A:231:ALA:HB1	1:A:234:MET:HE2	1.95	0.47
1:A:254:ASP:OD2	1:A:334:ASP:OD1	2.32	0.46
1:B:154:ASN:HD22	1:B:154:ASN:HA	1.63	0.46
1:C:42:ASP:HA	3:C:1026:HOH:O	2.14	0.46
1:D:10:PHE:CE1	1:D:36:VAL:HG11	2.50	0.46
1:C:149:ASN:ND2	1:C:235:VAL:HG22	2.30	0.46
1:C:351:ALA:O	1:C:355:ARG:HG3	2.16	0.46
1:A:190:MET:HG2	1:A:191:THR:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:CD1	1:B:81:ASN:HB2	2.51	0.46
1:B:69:SER:O	1:B:72:VAL:HG23	2.15	0.46
1:D:173:PRO:O	1:D:177:VAL:HG23	2.15	0.46
3:A:481:HOH:O	1:D:219:VAL:HG11	2.16	0.46
1:D:358:ARG:O	1:D:359:LEU:HD23	2.15	0.46
1:B:270:ILE:HD11	1:B:315:THR:CG2	2.46	0.46
1:D:15:ARG:O	1:D:19:GLN:HG3	2.15	0.46
1:D:21:LEU:HD11	1:D:31:ILE:CD1	2.45	0.46
1:B:270:ILE:HD11	1:B:315:THR:HG22	1.98	0.46
1:B:129:ARG:HE	1:B:358:ARG:NH2	2.14	0.46
1:C:136:PRO:HG3	1:C:165:SER:HB3	1.97	0.46
1:C:146:MET:HE3	1:C:346:LEU:HA	1.98	0.45
1:D:196:TYR:CD2	1:D:251:PRO:HA	2.52	0.45
1:D:224:SER:HB2	1:D:249:ARG:CZ	2.46	0.45
1:A:254:ASP:O	1:A:255:VAL:HB	2.16	0.45
1:C:70:PRO:O	1:C:71:SER:CB	2.57	0.45
1:A:118:ALA:HA	1:A:121:GLU:OE1	2.17	0.45
1:C:140:GLY:O	1:C:141:ALA:HB2	2.17	0.45
1:A:268:THR:OG1	1:A:272:GLU:HG3	2.15	0.45
1:C:89:LYS:HG2	1:C:90:ALA:N	2.31	0.45
1:C:154:ASN:ND2	1:C:157:GLU:N	2.62	0.45
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.32	0.45
1:A:151:HIS:HD2	3:A:452:HOH:O	1.98	0.45
1:C:53:ASP:HB2	3:C:986:HOH:O	2.17	0.45
1:C:166[A]:CYS:SG	2:C:960:BRZ:HC71	2.56	0.45
1:C:218:ALA:HB3	3:C:1027:HOH:O	2.17	0.45
1:B:180:LYS:HD3	1:B:284:TYR:CE2	2.52	0.44
1:C:149:ASN:HB2	1:C:152:GLU:CD	2.43	0.44
1:D:32:ASP:OD2	1:D:83:HIS:HE1	2.01	0.44
1:D:67:LYS:HE3	1:D:73:ALA:O	2.18	0.44
1:B:12:ARG:HD3	3:B:539:HOH:O	2.16	0.44
1:B:212:ARG:NH1	1:B:223:PRO:HG2	2.32	0.44
1:D:356:SER:HB2	3:D:627:HOH:O	2.16	0.44
1:C:8:ASN:HD22	1:C:37:VAL:CG1	2.25	0.44
1:C:41:THR:O	1:C:42:ASP:C	2.60	0.44
1:C:137:ALA:HB2	1:C:162:SER:HB2	1.98	0.44
1:B:190:MET:HE3	1:B:190:MET:HB2	1.83	0.44
1:C:37:VAL:HG21	1:C:97:LEU:HD11	2.00	0.44
1:D:98:PRO:O	1:D:102:LEU:HD22	2.18	0.44
1:A:58:LYS:HE3	3:C:977:HOH:O	2.18	0.44
1:D:147:GLY:H	1:D:150:HIS:CD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:MET:HE3	1:A:234:MET:HB2	1.80	0.44
1:B:67:LYS:NZ	1:B:67:LYS:HB3	2.33	0.44
1:C:298:SER:HB3	1:C:332:TRP:HZ3	1.83	0.44
2:C:960:BRZ:HC32	2:C:960:BRZ:HC11	1.70	0.44
1:A:298:SER:HB3	1:A:332:TRP:HZ3	1.83	0.43
1:C:129:ARG:HD2	1:C:358:ARG:NH2	2.33	0.43
1:D:190:MET:HG3	1:D:258:VAL:HG13	1.99	0.43
1:C:155:PRO:HB3	1:C:354:ASP:HB2	1.99	0.43
1:A:19:GLN:HE22	1:A:50:MET:HA	1.83	0.43
1:B:12:ARG:HG2	1:B:16:MET:CE	2.44	0.43
1:A:305:ASN:ND2	1:A:306:ARG:HD3	2.33	0.43
1:B:76:ASP:HA	3:B:521:HOH:O	2.17	0.43
1:A:224:SER:CB	1:A:249:ARG:HE	2.32	0.43
1:D:55:VAL:HG13	1:D:56:HIS:CD2	2.54	0.43
1:D:169:ASN:O	1:D:307:SER:HB3	2.19	0.43
1:D:177:VAL:HG11	1:D:277:LEU:HD23	2.00	0.43
1:A:4:LYS:NZ	3:A:496:HOH:O	2.49	0.43
1:B:69:SER:OG	1:B:71:SER:HB3	2.19	0.43
1:C:8:ASN:ND2	1:C:37:VAL:HG13	2.27	0.43
1:C:55:VAL:HG21	1:C:254:ASP:CB	2.49	0.43
1:C:86:LEU:CD2	1:C:88:VAL:HG12	2.48	0.43
1:C:135:ALA:HB1	1:C:136:PRO:CD	2.49	0.43
1:C:166[A]:CYS:SG	2:C:960:BRZ:C15	3.06	0.43
1:A:224:SER:HB2	1:A:249:ARG:HE	1.82	0.43
1:B:99:TRP:HA	1:B:99:TRP:HE3	1.82	0.43
1:C:171:LEU:HD13	1:C:232:VAL:HG21	2.01	0.43
1:D:50:MET:HE1	1:D:78:LEU:CG	2.43	0.43
1:C:130:LYS:HD3	1:C:159:HIS:HA	2.00	0.43
1:A:171:LEU:HD22	1:A:175:VAL:HG23	2.01	0.43
1:C:99:TRP:HE3	1:C:104:VAL:HB	1.84	0.43
1:C:21:LEU:C	1:C:21:LEU:HD23	2.43	0.42
1:C:98:PRO:HG2	1:C:102:LEU:HD13	2.01	0.42
1:C:129:ARG:HD2	1:C:358:ARG:CZ	2.49	0.42
1:B:299:ALA:CB	1:D:54:THR:HB	2.49	0.42
1:D:254:ASP:O	1:D:255:VAL:HB	2.19	0.42
1:A:218:ALA:CA	1:A:251:PRO:HB3	2.48	0.42
1:B:17:VAL:HG11	1:B:108:ILE:HD13	2.02	0.42
1:C:29:THR:OG1	1:C:30:GLU:N	2.47	0.42
1:C:63:VAL:HG22	1:C:80:VAL:HG22	2.01	0.42
1:C:207:SER:HB3	1:C:214:GLY:HA3	2.01	0.42
1:D:171:LEU:HD13	1:D:232:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:MET:HE3	1:B:50:MET:HB2	1.90	0.42
1:C:151:HIS:HD2	1:C:353:LYS:NZ	2.17	0.42
1:C:246:MET:HE3	1:C:246:MET:HB2	1.87	0.42
1:C:282:LYS:O	1:C:286:LYS:HD3	2.19	0.42
1:A:91:GLN:HB2	1:A:97:LEU:CD2	2.49	0.42
1:B:54:THR:CG2	1:C:215:ARG:HH21	2.31	0.42
1:C:3:ILE:HG13	1:C:355:ARG:HH21	1.84	0.42
1:C:107:VAL:HG11	1:C:123:HIS:HB3	2.02	0.42
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.92	0.42
1:C:28:GLY:HA3	1:C:83:HIS:CE1	2.54	0.42
1:C:142:LYS:HG3	1:C:158:HIS:NE2	2.34	0.42
1:C:319:ASN:HB3	3:C:1096:HOH:O	2.18	0.42
1:D:183:PHE:HD1	1:D:268:THR:HG21	1.84	0.42
1:C:268:THR:HG22	1:C:272:GLU:OE1	2.20	0.42
1:D:44:GLU:CD	1:D:74:LYS:HE2	2.45	0.42
1:D:320:LEU:HA	1:D:321:PRO:HD3	1.84	0.42
1:B:4:LYS:HA	1:B:4:LYS:HD2	1.94	0.42
1:A:189:LEU:HG	1:B:326:PHE:HE2	1.85	0.42
1:B:1:MET:HA	1:B:2:PRO:HD2	1.91	0.42
1:D:313:LYS:HD2	3:D:638:HOH:O	2.18	0.42
1:B:105:GLU:OE1	1:B:129:ARG:CZ	2.68	0.41
1:C:67:LYS:HG2	3:C:1120:HOH:O	2.19	0.41
1:C:196:TYR:HA	1:C:200:GLN:NE2	2.34	0.41
1:C:146:MET:HB2	1:C:342:ARG:HD3	2.01	0.41
1:C:105:GLU:OE1	1:C:129:ARG:NH2	2.54	0.41
1:C:166[A]:CYS:SG	1:C:339:TYR:CG	3.13	0.41
1:B:12:ARG:NE	1:B:336:GLU:OE2	2.50	0.41
1:B:171:LEU:HD22	1:B:175:VAL:HG23	2.02	0.41
1:C:6:GLY:HA3	1:C:99:TRP:HZ3	1.84	0.41
1:D:15:ARG:HG3	1:D:15:ARG:HH11	1.86	0.41
1:D:199:THR:HA	3:D:518:HOH:O	2.19	0.41
1:A:196:TYR:HD2	1:A:251:PRO:HA	1.85	0.41
1:C:209:LYS:HG2	1:C:209:LYS:H	1.57	0.41
1:D:209:LYS:HE2	1:D:209:LYS:HB3	1.89	0.41
1:B:74:LYS:O	1:B:75:ASP:C	2.64	0.41
1:B:129:ARG:NH2	1:B:358:ARG:HH21	2.15	0.41
1:C:58:LYS:HB2	1:C:60:LYS:NZ	2.36	0.41
1:C:107:VAL:HG21	1:C:123:HIS:ND1	2.36	0.41
1:A:213:GLY:HA2	1:A:249:ARG:NH1	2.34	0.41
1:C:107:VAL:CG1	1:C:131:VAL:HG22	2.37	0.41
1:D:222:ILE:HB	1:D:249:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:O	1:A:124:LEU:HB2	2.20	0.41
1:C:23:GLU:O	1:C:24:ASP:C	2.64	0.41
1:A:40:ASN:HD21	1:A:42:ASP:H	1.65	0.41
1:B:15:ARG:O	1:B:19:GLN:HG3	2.20	0.41
1:B:30:GLU:OE2	1:B:348:ARG:NH1	2.53	0.41
1:B:94:PRO:HA	1:B:97:LEU:CD2	2.51	0.41
1:C:1:MET:HB2	1:C:29:THR:O	2.21	0.41
1:C:25:GLY:HA2	3:C:1110:HOH:O	2.21	0.41
1:D:154:ASN:ND2	1:D:157:GLU:OE1	2.54	0.41
1:C:13:ILE:HA	1:C:13:ILE:HD13	1.78	0.41
1:C:99:TRP:O	1:C:103:GLY:N	2.53	0.41
1:C:105:GLU:HG3	1:C:106:TYR:H	1.87	0.41
1:C:286:LYS:HE2	1:C:286:LYS:HB3	1.78	0.41
2:C:960:BRZ:O14	2:C:960:BRZ:C19	2.69	0.41
1:C:60:LYS:HD3	1:C:60:LYS:HA	1.96	0.40
1:C:75:ASP:OD1	1:C:75:ASP:N	2.54	0.40
1:C:115:THR:HB	3:C:1075:HOH:O	2.21	0.40
1:D:315:THR:HG23	1:D:328:LYS:O	2.21	0.40
1:A:209:LYS:HD2	1:A:209:LYS:O	2.21	0.40
1:A:298:SER:HB3	1:A:332:TRP:CZ3	2.57	0.40
1:B:63:VAL:HG13	1:B:80:VAL:HG22	2.03	0.40
1:C:94:PRO:O	1:C:97:LEU:HD23	2.21	0.40
1:C:135:ALA:HB1	1:C:136:PRO:HD2	2.03	0.40
1:D:150:HIS:HE1	3:D:587:HOH:O	2.04	0.40
1:C:65:THR:HA	1:C:77:THR:O	2.21	0.40
1:C:86:LEU:HD23	1:C:88:VAL:HG12	2.04	0.40
1:A:19:GLN:CD	1:A:50:MET:HG2	2.47	0.40
1:B:190:MET:HE3	1:B:258:VAL:HG13	2.03	0.40
1:C:64:THR:OG1	1:C:79:VAL:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/359 (99%)	346 (97%)	8 (2%)	3 (1%)	16	8
1	B	357/359 (99%)	336 (94%)	18 (5%)	3 (1%)	16	8
1	C	358/359 (100%)	320 (89%)	24 (7%)	14 (4%)	2	0
1	D	357/359 (99%)	340 (95%)	14 (4%)	3 (1%)	16	8
All	All	1429/1436 (100%)	1342 (94%)	64 (4%)	23 (2%)	7	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	C	3	ILE
1	C	73	ALA
1	C	141	ALA
1	A	255	VAL
1	B	141	ALA
1	B	255	VAL
1	C	29	THR
1	C	74	LYS
1	C	208	VAL
1	C	255	VAL
1	C	357	ALA
1	D	73	ALA
1	D	255	VAL
1	B	2	PRO
1	C	71	SER
1	C	151	HIS
1	C	349	HIS
1	A	73	ALA
1	C	23	GLU
1	C	76	ASP
1	C	2	PRO
1	D	72	VAL

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	296/296 (100%)	278 (94%)	18 (6%)	17	7
1	B	296/296 (100%)	272 (92%)	24 (8%)	11	3
1	C	297/296 (100%)	268 (90%)	29 (10%)	7	2
1	D	296/296 (100%)	267 (90%)	29 (10%)	7	2
All	All	1185/1184 (100%)	1085 (92%)	100 (8%)	10	3

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	16	MET
1	A	19	GLN
1	A	37	VAL
1	A	58	LYS
1	A	66	THR
1	A	67	LYS
1	A	74	LYS
1	A	78	LEU
1	A	88	VAL
1	A	102	LEU
1	A	107	VAL
1	A	115	THR
1	A	124	LEU
1	A	171	LEU
1	A	240	GLN
1	A	305	ASN
1	A	333	TYR
1	B	15	ARG
1	B	21	LEU
1	B	37	VAL
1	B	55	VAL
1	B	64	THR
1	B	66	THR
1	B	67	LYS
1	B	88	VAL
1	B	97	LEU
1	B	102	LEU
1	B	115	THR
1	B	124	LEU
1	B	129	ARG
1	B	171	LEU
1	B	190	MET

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Mol	Chain	Res	Type
1	B	194	HIS
1	B	201	LYS
1	B	209	LYS
1	B	235	VAL
1	B	258	VAL
1	B	286	LYS
1	B	293	ASP
1	B	305	ASN
1	B	309	ILE
1	C	13	ILE
1	C	24	ASP
1	C	32	ASP
1	C	37	VAL
1	C	55	VAL
1	C	65	THR
1	C	67	LYS
1	C	79	VAL
1	C	88	VAL
1	C	107	VAL
1	C	113	LEU
1	C	117	LYS
1	C	124	LEU
1	C	129	ARG
1	C	142	LYS
1	C	156	SER
1	C	171	LEU
1	C	190	MET
1	C	202	THR
1	C	209	LYS
1	C	235	VAL
1	C	243	LEU
1	C	249	ARG
1	C	268	THR
1	C	309	ILE
1	C	333	TYR
1	C	334	ASP
1	C	350	MET
1	C	352	SER
1	D	3	ILE
1	D	13	ILE
1	D	16	MET
1	D	37	VAL

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Mol	Chain	Res	Type
1	D	40	ASN
1	D	41	THR
1	D	54	THR
1	D	55	VAL
1	D	66	THR
1	D	69	SER
1	D	78	LEU
1	D	88	VAL
1	D	97	LEU
1	D	102	LEU
1	D	105	GLU
1	D	113	LEU
1	D	115	THR
1	D	157	GLU
1	D	171	LEU
1	D	201	LYS
1	D	235	VAL
1	D	237	PRO
1	D	243	LEU
1	D	249	ARG
1	D	268	THR
1	D	279	ARG
1	D	322	LYS
1	D	333	TYR
1	D	352	SER

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	GLN
1	A	40	ASN
1	A	150	HIS
1	A	151	HIS
1	A	159	HIS
1	A	176	HIS
1	A	200	GLN
1	A	220	ASN
1	A	240	GLN
1	A	305	ASN
1	B	8	ASN
1	B	49	GLN

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Mol	Chain	Res	Type
1	B	83	HIS
1	B	150	HIS
1	B	154	ASN
1	B	176	HIS
1	B	186	GLN
1	B	271	GLN
1	B	305	ASN
1	C	8	ASN
1	C	83	HIS
1	C	91	GLN
1	C	150	HIS
1	C	151	HIS
1	C	154	ASN
1	C	200	GLN
1	C	349	HIS
1	D	8	ASN
1	D	19	GLN
1	D	159	HIS
1	D	176	HIS
1	D	200	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	BRZ	C	960	-	24,25,25	1.96	6 (25%)	36,40,40	5.43	25 (69%)

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
2	BRZ	C	960	-	-	11/13/23/23	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	960	BRZ	C8-C9	4.69	1.55	1.47
2	C	960	BRZ	C1-C10	3.91	1.51	1.43
2	C	960	BRZ	O14-C8	3.60	1.28	1.21
2	C	960	BRZ	O7-C8	3.24	1.42	1.38
2	C	960	BRZ	O7-C6	2.76	1.42	1.38
2	C	960	BRZ	C13-C12	2.27	1.56	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	960	BRZ	O7-C8-C9	-13.76	106.71	117.56
2	C	960	BRZ	C10-C9-C8	12.86	130.40	119.33
2	C	960	BRZ	O7-C8-O14	12.74	133.01	116.22
2	C	960	BRZ	O11-C12-C20	10.38	120.08	108.13
2	C	960	BRZ	C2-C1-C6	8.10	129.19	119.42
2	C	960	BRZ	C17-C15-C18	7.11	129.36	109.40
2	C	960	BRZ	C1-C2-C3	-6.85	112.39	122.25
2	C	960	BRZ	O21-C20-C12	6.55	123.30	107.93
2	C	960	BRZ	C23-C20-C12	-5.59	100.77	110.58
2	C	960	BRZ	C18-C15-C9	-5.18	99.62	109.89
2	C	960	BRZ	C6-C1-C10	-4.89	114.46	118.05
2	C	960	BRZ	C6-O7-C8	4.36	126.42	122.26
2	C	960	BRZ	O11-C12-C13	4.24	108.67	106.18
2	C	960	BRZ	C2-C1-C10	-3.73	116.36	122.73
2	C	960	BRZ	C1-C10-C9	-3.28	118.05	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	960	BRZ	O7-C6-C5	3.25	120.43	115.83
2	C	960	BRZ	C3-C13-C12	-3.23	100.36	102.52
2	C	960	BRZ	O7-C6-C1	3.05	123.94	120.51
2	C	960	BRZ	C23-C20-C22	-2.71	106.56	110.52
2	C	960	BRZ	O14-C8-C9	-2.66	120.21	125.60
2	C	960	BRZ	C13-C12-C20	2.60	119.47	116.05
2	C	960	BRZ	C15-C18-C19	2.33	139.47	127.90
2	C	960	BRZ	C13-C3-C4	2.16	110.26	108.10
2	C	960	BRZ	C5-C6-C1	-2.15	115.63	120.15
2	C	960	BRZ	C2-C3-C4	2.05	121.19	119.59

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	960	BRZ	O11-C12-C20-O21
2	C	960	BRZ	O11-C12-C20-C22
2	C	960	BRZ	O11-C12-C20-C23
2	C	960	BRZ	C13-C12-C20-O21
2	C	960	BRZ	C13-C12-C20-C22
2	C	960	BRZ	C13-C12-C20-C23
2	C	960	BRZ	C17-C15-C9-C8
2	C	960	BRZ	C17-C15-C9-C10
2	C	960	BRZ	C16-C15-C9-C8
2	C	960	BRZ	C16-C15-C9-C10
2	C	960	BRZ	C9-C15-C18-C19

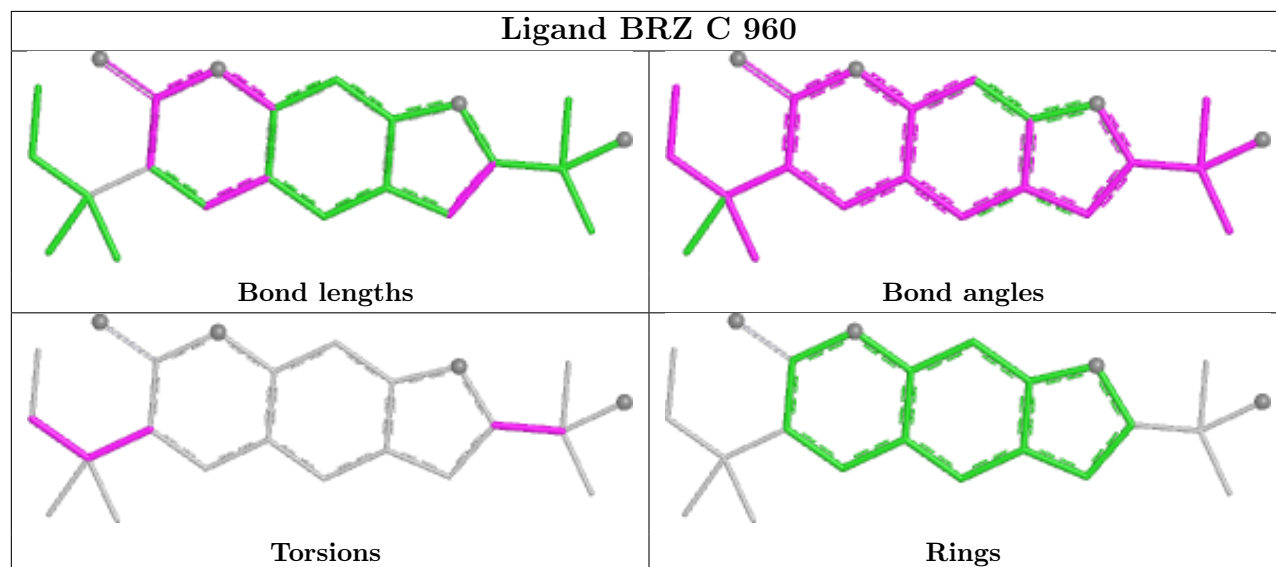
There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	960	BRZ	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	359/359 (100%)	-0.08	9 (2%) 58 65	13, 23, 41, 65	0
1	B	359/359 (100%)	0.27	16 (4%) 38 44	12, 28, 51, 64	0
1	C	359/359 (100%)	1.01	81 (22%) 2 2	13, 38, 81, 104	1 (0%)
1	D	359/359 (100%)	-0.00	8 (2%) 62 69	14, 24, 41, 55	0
All	All	1436/1436 (100%)	0.30	114 (7%) 18 21	12, 27, 63, 104	1 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	THR	6.4
1	C	357	ALA	6.3
1	B	156	SER	5.4
1	C	99	TRP	5.3
1	C	72	VAL	4.9
1	C	1	MET	4.9
1	C	122	GLY	4.6
1	D	359	LEU	4.5
1	C	95	ALA	4.4
1	C	358	ARG	4.2
1	C	70	PRO	4.2
1	C	123	HIS	4.0
1	C	359	LEU	4.0
1	C	90	ALA	3.9
1	D	73	ALA	3.9
1	A	72	VAL	3.8
1	C	102	LEU	3.8
1	C	67	LYS	3.8
1	B	206	VAL	3.8
1	D	72	VAL	3.8
1	D	1	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	100	GLY	3.7
1	C	206	VAL	3.6
1	C	120	ALA	3.6
1	D	199	THR	3.5
1	C	94	PRO	3.5
1	C	68	SER	3.5
1	C	61	TYR	3.5
1	C	3	ILE	3.5
1	C	63	VAL	3.4
1	C	97	LEU	3.4
1	A	1	MET	3.4
1	C	78	LEU	3.4
1	C	131	VAL	3.4
1	B	95	ALA	3.3
1	B	202	THR	3.3
1	C	124	LEU	3.3
1	A	71	SER	3.3
1	A	206	VAL	3.3
1	B	1	MET	3.2
1	C	31	ILE	3.1
1	C	41	THR	3.1
1	C	116	ALA	3.1
1	C	26	LEU	3.1
1	C	160	VAL	3.1
1	A	218	ALA	3.1
1	C	71	SER	3.1
1	C	128	ALA	3.1
1	C	198	ALA	3.1
1	C	127	GLY	3.1
1	C	80	VAL	3.1
1	C	129	ARG	3.0
1	C	40	ASN	2.9
1	C	356	SER	2.9
1	B	208	VAL	2.9
1	C	34	VAL	2.8
1	C	180	LYS	2.8
1	B	198	ALA	2.8
1	C	73	ALA	2.8
1	C	69	SER	2.8
1	C	77	THR	2.8
1	D	203	VAL	2.8
1	C	155	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	234	MET	2.7
1	C	126	GLY	2.6
1	B	197	THR	2.6
1	C	138	SER	2.6
1	C	355	ARG	2.6
1	C	65	THR	2.6
1	D	234	MET	2.5
1	C	75	ASP	2.5
1	C	103	GLY	2.5
1	C	43	ALA	2.5
1	C	153	TYR	2.5
1	A	358	ARG	2.5
1	A	2	PRO	2.5
1	B	72	VAL	2.4
1	D	206	VAL	2.4
1	C	28	GLY	2.4
1	C	59	PHE	2.4
1	C	154	ASN	2.4
1	C	29	THR	2.4
1	B	120	ALA	2.4
1	B	93	ASN	2.3
1	C	39	MET	2.3
1	C	25	GLY	2.3
1	C	2	PRO	2.3
1	B	207	SER	2.3
1	C	114	PHE	2.3
1	B	66	THR	2.3
1	C	16	MET	2.3
1	C	125	ARG	2.2
1	A	205	GLY	2.2
1	A	359	LEU	2.2
1	C	27	LEU	2.2
1	C	82	GLY	2.2
1	C	354	ASP	2.2
1	C	21	LEU	2.2
1	C	96	ASP	2.1
1	C	88	VAL	2.1
1	C	347	VAL	2.1
1	B	359	LEU	2.1
1	C	208	VAL	2.1
1	C	64	THR	2.1
1	C	98	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	280	ALA	2.1
1	C	196	TYR	2.0
1	B	64	THR	2.0
1	C	199	THR	2.0
1	C	112	GLY	2.0
1	C	119	ALA	2.0
1	B	234	MET	2.0
1	C	350	MET	2.0
1	C	85	ILE	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](#)

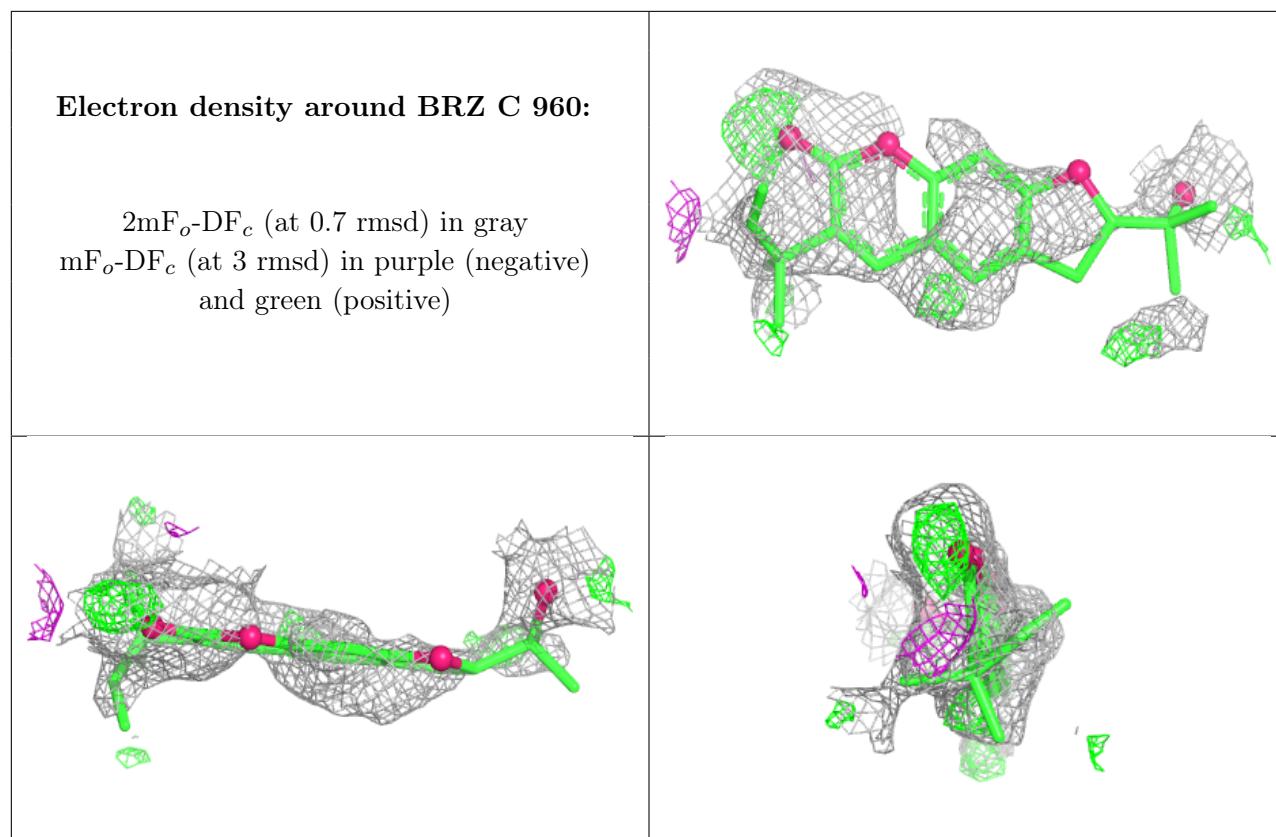
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BRZ	C	960	23/23	0.67	0.21	68,70,71,71	23

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



6.5 Other polymers [i](#)

There are no such residues in this entry.