



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:38 AM UTC

PDB ID : 1QAK / pdb_00001qak
Title : THE ACTIVE SITE BASE CONTROLS COFACTOR REACTIVITY IN ES-
CHERICHIA COLI AMINE OXIDASE : X-RAY CRYSTALLOGRAPHIC
STUDIES WITH MUTATIONAL VARIANTS
Authors : Murray, J.M.; Wilmot, C.M.; Saysell, C.G.; Jaeger, J.; Knowles, P.F.; Phillips,
S.E.; McPherson, M.J.
Deposited on : 1999-03-15
Resolution : 2.00 Å(reported)

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

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

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
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

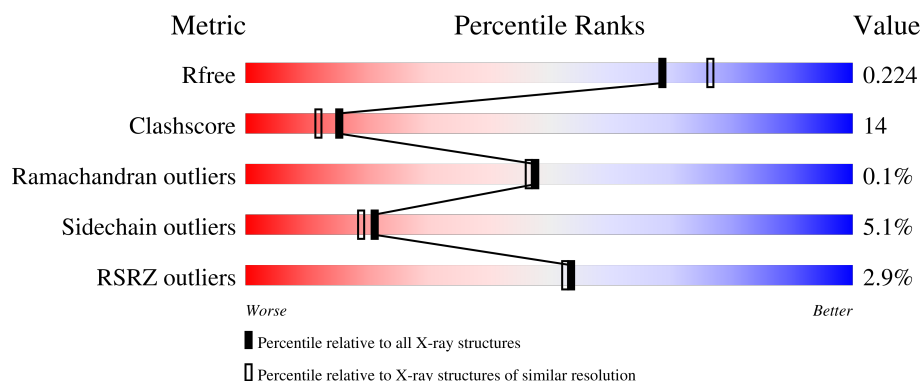
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

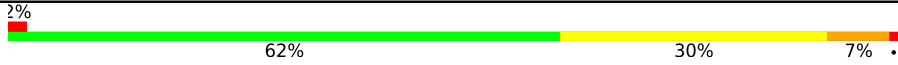
The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	722	
1	B	722	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12895 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	1	1
			5686	3616	969	1079	22			
1	B	722	Total	C	N	O	S	0	1	0
			5712	3632	973	1085	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	ASP	engineered mutation	UNP P46883
A	466	TPQ	TYR	modified residue	UNP P46883
B	383	ALA	ASP	engineered mutation	UNP P46883
B	466	TPQ	TYR	modified residue	UNP P46883

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

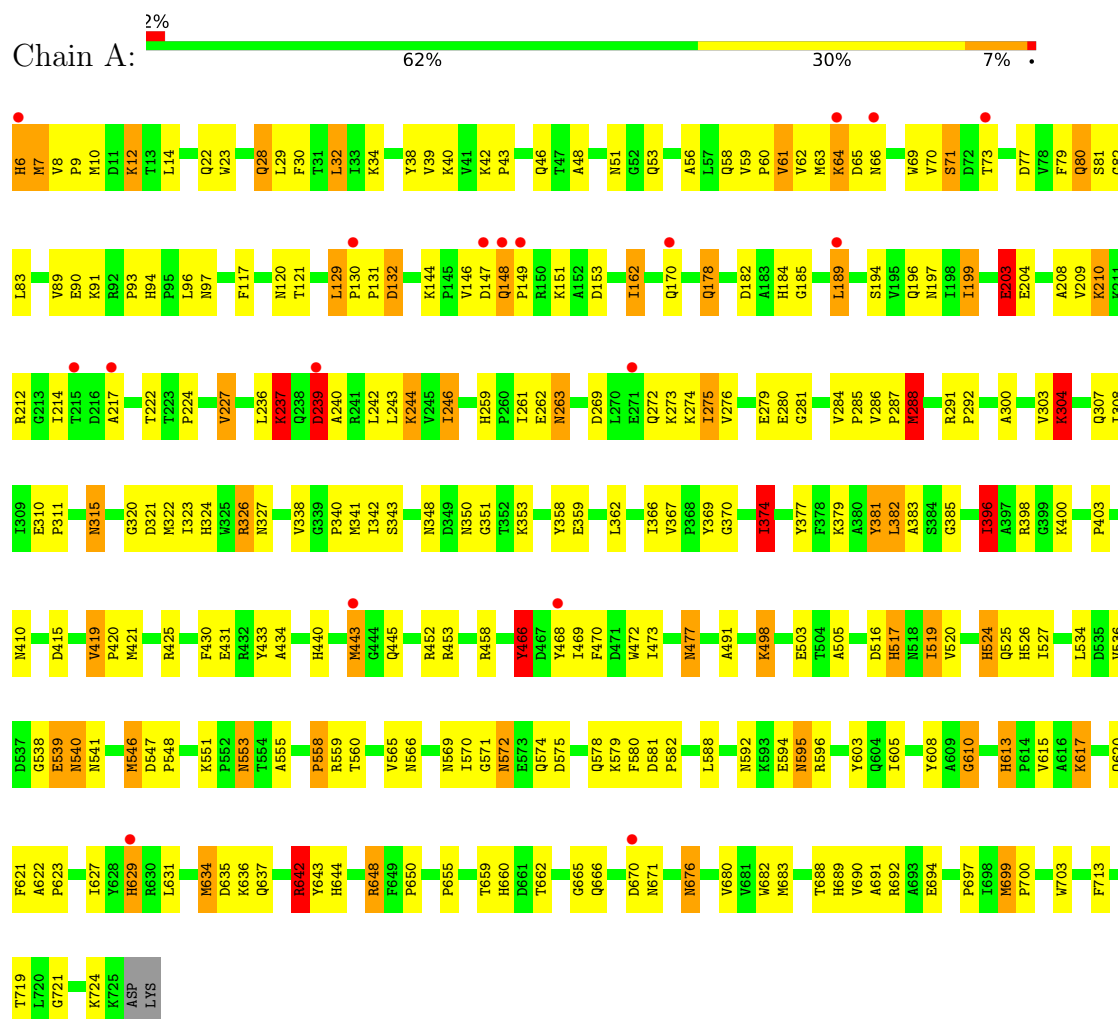
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	791	Total 791	O 791	0	0
4	B	700	Total 700	O 700	0	0

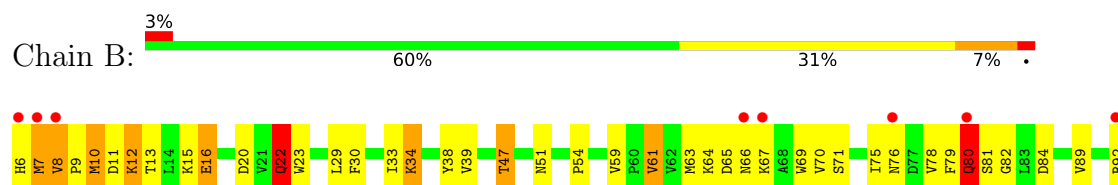
3 Residue-property plots

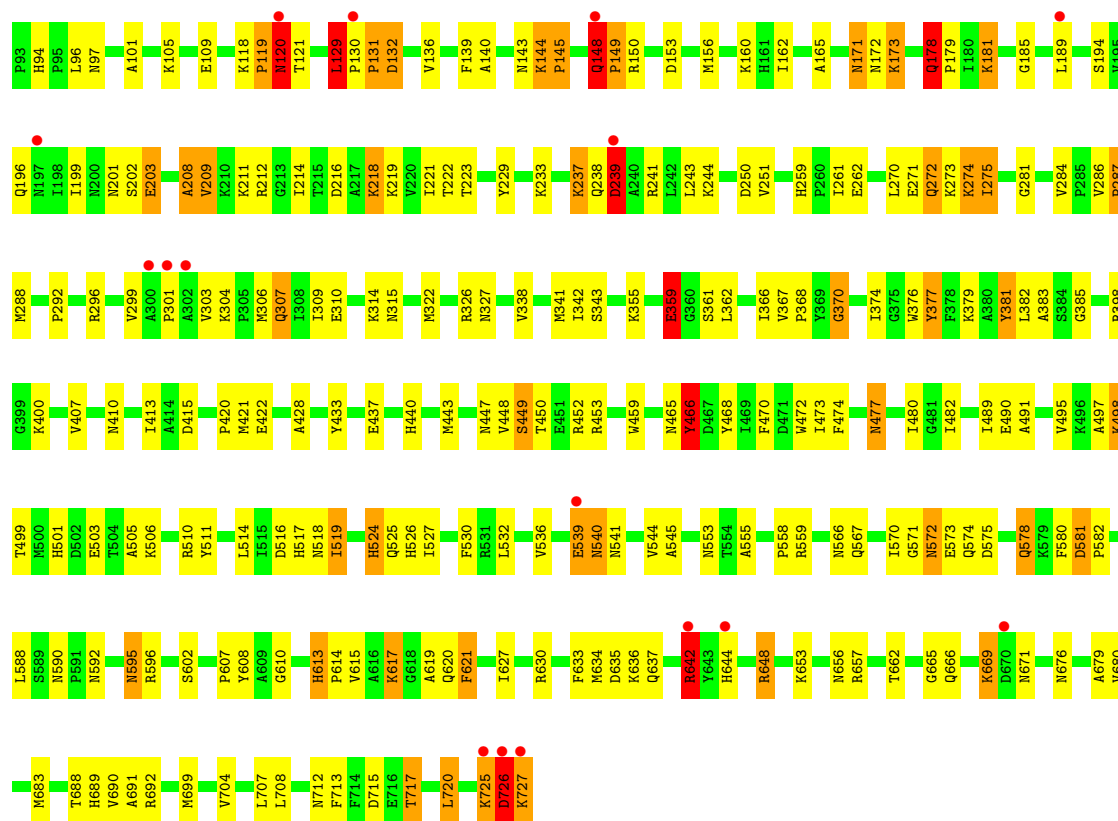
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: COPPER AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.66Å 166.17Å 79.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.00) 90.9 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 1.99Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.176 , 0.244 0.170 , 0.224	Depositor DCC
R_{free} test set	3766 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12895	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPQ, CU, CA

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	0.70	1/5802 (0.0%)	2.13	215/7899 (2.7%)
1	B	0.66	0/5828	2.07	219/7930 (2.8%)
All	All	0.68	1/11630 (0.0%)	2.10	434/15829 (2.7%)

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
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	724	LYS	C-N	-5.40	1.25	1.33

All (434) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ASN	OD1-CG-ND2	24.29	146.89	122.60
1	A	596	ARG	CD-NE-CZ	18.84	150.78	124.40
1	A	130	PRO	O-C-N	18.21	129.71	121.15
1	B	120	ASN	CA-CB-CG	12.78	125.38	112.60
1	A	629	HIS	CA-CB-CG	-12.33	101.47	113.80
1	A	129	LEU	CA-C-N	12.07	128.35	119.66
1	A	129	LEU	C-N-CA	12.07	128.35	119.66
1	A	571	GLY	N-CA-C	11.74	129.22	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	CD-NE-CZ	10.79	139.50	124.40
1	A	539	GLU	CB-CG-CD	10.50	130.45	112.60
1	A	642	ARG	CD-NE-CZ	10.20	138.68	124.40
1	B	359	GLU	CA-CB-CG	10.01	134.11	114.10
1	B	692	ARG	NE-CZ-NH2	-9.94	110.25	119.20
1	B	22	GLN	CB-CG-CD	9.84	129.32	112.60
1	A	692	ARG	CD-NE-CZ	9.70	137.98	124.40
1	A	130	PRO	N-CA-CB	9.64	108.23	103.22
1	A	130	PRO	CB-CA-C	-9.63	102.12	111.17
1	A	713	PHE	N-CA-C	-9.60	99.88	111.69
1	A	676	ASN	OD1-CG-ND2	-9.55	113.05	122.60
1	B	526	HIS	CA-CB-CG	-9.53	104.27	113.80
1	A	440	HIS	N-CA-CB	9.46	125.19	110.71
1	A	129	LEU	N-CA-C	-9.34	91.87	108.69
1	B	81	SER	N-CA-C	9.33	121.45	111.28
1	A	566	ASN	CB-CG-OD1	-9.28	102.24	120.80
1	A	666	GLN	OE1-CD-NE2	-9.21	113.39	122.60
1	B	82	GLY	N-CA-C	-9.18	103.56	114.48
1	B	8	VAL	N-CA-CB	-9.14	103.90	111.67
1	B	524	HIS	CE1-NE2-CD2	9.07	118.08	109.00
1	A	691	ALA	N-CA-C	8.87	121.31	110.41
1	B	144	LYS	CA-C-O	8.76	127.56	119.76
1	B	129	LEU	N-CA-C	-8.72	98.82	109.72
1	B	148	GLN	CB-CA-C	8.60	121.00	108.87
1	B	259	HIS	CA-CB-CG	-8.56	105.24	113.80
1	B	437	GLU	N-CA-C	-8.56	102.03	111.36
1	A	304	LYS	CA-CB-CG	8.55	131.21	114.10
1	B	691	ALA	N-CA-C	8.49	121.49	110.53
1	A	526	HIS	CE1-NE2-CD2	8.44	117.44	109.00
1	B	571	GLY	N-CA-C	8.43	125.12	114.66
1	B	590	ASN	OD1-CG-ND2	8.39	130.99	122.60
1	A	324	HIS	CA-CB-CG	-8.32	105.48	113.80
1	A	7	MET	N-CA-C	8.30	121.49	110.53
1	B	7	MET	N-CA-C	8.28	122.48	109.81
1	B	377	TYR	N-CA-C	8.27	121.34	111.33
1	A	239	ASP	CA-CB-CG	8.20	120.80	112.60
1	A	189	LEU	CB-CA-C	8.13	124.50	110.68
1	B	566	ASN	OD1-CG-ND2	8.02	130.62	122.60
1	B	440	HIS	N-CA-CB	8.01	122.96	110.71
1	B	505	ALA	N-CA-C	8.00	120.71	111.11
1	A	64	LYS	CA-C-O	7.90	129.01	120.32
1	A	132	ASP	CA-CB-CG	-7.89	104.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	VAL	CA-C-O	7.87	126.44	118.96
1	A	28	GLN	OE1-CD-NE2	7.84	130.44	122.60
1	A	327	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	A	396	ILE	CB-CG1-CD1	-7.79	97.43	113.80
1	B	524	HIS	CG-CD2-NE2	-7.76	99.44	107.20
1	B	666	GLN	OE1-CD-NE2	-7.74	114.86	122.60
1	B	374	ILE	N-CA-C	7.74	119.44	110.62
1	A	692	ARG	NE-CZ-NH2	-7.69	112.28	119.20
1	B	690	VAL	N-CA-C	-7.66	96.81	107.99
1	B	540	ASN	CA-CB-CG	-7.61	104.99	112.60
1	A	410	ASN	CA-CB-CG	-7.57	105.03	112.60
1	A	310	GLU	CA-C-N	7.56	127.27	119.56
1	A	310	GLU	C-N-CA	7.56	127.27	119.56
1	A	558	PRO	N-CA-C	7.56	123.85	113.65
1	A	341	MET	CA-CB-CG	-7.46	99.17	114.10
1	B	343	SER	N-CA-C	7.42	121.02	109.52
1	B	482	ILE	N-CA-CB	7.36	121.52	112.10
1	B	262	GLU	O-C-N	7.33	131.51	122.86
1	A	82	GLY	N-CA-C	-7.26	104.47	114.64
1	B	398	ARG	CG-CD-NE	7.23	127.91	112.00
1	B	540	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	A	350	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	B	498	LYS	N-CA-C	-7.17	104.66	113.41
1	A	383	ALA	N-CA-C	7.12	123.04	111.37
1	A	692	ARG	CG-CD-NE	-7.11	96.35	112.00
1	B	362	LEU	N-CA-C	-7.09	100.50	110.50
1	B	644	HIS	CA-C-N	7.08	127.07	119.28
1	B	644	HIS	C-N-CA	7.08	127.07	119.28
1	A	80	GLN	OE1-CD-NE2	7.06	129.66	122.60
1	B	34	LYS	CA-CB-CG	-7.05	100.00	114.10
1	A	524	HIS	CE1-NE2-CD2	7.04	116.04	109.00
1	B	172	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	A	648	ARG	NE-CZ-NH1	7.02	128.52	121.50
1	B	171	ASN	CA-CB-CG	-6.99	105.61	112.60
1	A	526	HIS	ND1-CE1-NE2	-6.96	101.44	108.40
1	B	715	ASP	CA-CB-CG	-6.96	105.64	112.60
1	B	10	MET	N-CA-C	6.95	118.54	110.97
1	B	717	THR	CA-C-N	6.93	126.91	119.28
1	B	717	THR	C-N-CA	6.93	126.91	119.28
1	A	288	MET	N-CA-C	6.92	122.02	113.50
1	B	635	ASP	N-CA-C	6.92	121.89	113.17
1	A	350	ASN	CB-CG-ND2	6.91	126.76	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	LEU	N-CA-C	-6.90	95.75	108.24
1	B	526	HIS	N-CA-C	-6.90	97.17	108.41
1	B	578	GLN	N-CA-C	6.89	119.22	108.96
1	A	421	MET	N-CA-CB	-6.82	99.65	110.77
1	B	381	TYR	CA-C-O	-6.81	113.30	120.58
1	A	39	VAL	N-CA-C	6.79	118.37	108.53
1	A	498	LYS	N-CA-C	-6.75	105.18	113.41
1	A	683	MET	CA-C-N	-6.73	113.71	123.00
1	A	683	MET	C-N-CA	-6.73	113.71	123.00
1	B	472	TRP	N-CA-C	-6.73	96.08	107.99
1	A	690	VAL	N-CA-C	-6.73	98.17	107.99
1	A	61	VAL	CA-C-O	-6.72	114.03	121.23
1	B	428	ALA	CA-C-N	6.71	132.31	122.99
1	B	428	ALA	C-N-CA	6.71	132.31	122.99
1	A	262	GLU	N-CA-C	6.70	119.95	110.23
1	B	39	VAL	N-CA-C	6.67	118.09	108.48
1	A	129	LEU	CA-C-O	6.66	124.96	119.36
1	A	473	ILE	N-CA-C	6.62	117.17	107.37
1	B	262	GLU	N-CA-C	6.62	119.83	110.50
1	B	482	ILE	CA-C-O	-6.62	113.82	120.31
1	A	379	LYS	N-CA-C	6.62	118.68	109.15
1	B	692	ARG	NH1-CZ-NH2	6.61	127.89	119.30
1	A	622	ALA	CA-C-N	6.61	126.30	119.82
1	A	622	ALA	C-N-CA	6.61	126.30	119.82
1	A	588	LEU	N-CA-C	-6.60	94.62	107.62
1	A	53	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	A	721	GLY	CA-C-O	6.53	127.15	122.45
1	B	648	ARG	CD-NE-CZ	6.53	133.54	124.40
1	B	474	PHE	CA-CB-CG	-6.52	107.28	113.80
1	A	153	ASP	N-CA-C	-6.52	98.64	109.46
1	B	61	VAL	N-CA-C	-6.52	101.15	109.30
1	B	307	GLN	OE1-CD-NE2	6.51	129.11	122.60
1	A	534	LEU	CA-C-O	-6.50	113.88	121.16
1	B	274	LYS	N-CA-CB	-6.48	100.84	111.66
1	B	376	TRP	N-CA-C	6.48	122.78	114.56
1	A	362	LEU	N-CA-C	-6.46	100.71	110.28
1	B	129	LEU	CB-CA-C	6.46	118.70	109.08
1	A	566	ASN	N-CA-CB	-6.45	99.73	110.37
1	B	588	LEU	N-CA-C	-6.43	97.20	108.20
1	A	473	ILE	N-CA-CB	-6.42	103.58	111.67
1	B	421	MET	N-CA-CB	-6.41	100.32	110.77
1	A	570	ILE	N-CA-C	-6.41	97.75	106.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ILE	CA-C-O	-6.40	113.41	120.84
1	B	688	THR	N-CA-C	-6.39	96.83	108.02
1	B	450	THR	O-C-N	-6.38	115.44	123.17
1	A	64	LYS	O-C-N	-6.36	115.77	123.27
1	A	343	SER	N-CA-C	6.35	119.06	109.41
1	A	307	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	B	338	VAL	N-CA-C	6.33	119.10	112.83
1	B	420	PRO	N-CA-CB	6.33	108.82	103.25
1	B	482	ILE	O-C-N	6.29	129.13	123.03
1	A	199	ILE	N-CA-C	-6.29	104.62	110.53
1	A	382	LEU	N-CA-C	-6.28	96.87	108.24
1	A	323	ILE	CA-C-O	6.28	127.13	120.48
1	B	6	HIS	CA-CB-CG	-6.27	107.53	113.80
1	B	310	GLU	N-CA-CB	-6.26	103.20	111.40
1	B	7	MET	N-CA-CB	-6.26	101.66	111.05
1	B	540	ASN	N-CA-C	6.25	118.36	108.67
1	B	692	ARG	CG-CD-NE	-6.24	98.28	112.00
1	A	419	VAL	CA-C-O	6.22	123.23	119.19
1	A	526	HIS	N-CA-C	-6.22	98.27	108.41
1	A	292	PRO	CB-CA-C	-6.21	103.28	111.23
1	B	150	ARG	CD-NE-CZ	-6.21	115.71	124.40
1	B	570	ILE	N-CA-C	-6.20	98.05	106.85
1	B	433	TYR	N-CA-C	-6.19	101.11	110.28
1	B	29	LEU	N-CA-C	6.19	119.58	109.24
1	B	595	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	635	ASP	N-CA-C	6.18	120.53	112.92
1	A	621	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	433	TYR	N-CA-C	-6.17	101.15	110.28
1	B	120	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	310	GLU	N-CA-CB	-6.16	103.45	111.09
1	A	547	ASP	CA-C-O	6.16	124.53	119.36
1	A	263	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	B	704	VAL	N-CA-CB	6.12	124.59	111.91
1	B	699	MET	N-CA-C	6.12	117.75	109.24
1	A	469	ILE	O-C-N	6.11	129.60	123.18
1	B	314	LYS	N-CA-C	6.11	119.89	110.42
1	B	261	ILE	N-CA-C	-6.09	96.67	109.34
1	A	519	ILE	N-CA-CB	-6.09	102.63	111.52
1	B	480	ILE	CA-C-N	-6.08	116.70	122.66
1	B	480	ILE	C-N-CA	-6.08	116.70	122.66
1	A	403	PRO	N-CA-CB	6.06	109.09	103.39
1	A	242	LEU	N-CA-C	6.05	119.41	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	LEU	CB-CG-CD1	6.04	128.82	110.70
1	B	262	GLU	CA-C-O	-6.03	114.99	121.56
1	B	78	VAL	N-CA-C	6.02	116.22	110.74
1	A	569	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	B	80	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	A	622	ALA	CB-CA-C	6.00	118.93	109.27
1	A	320	GLY	N-CA-C	-5.99	98.98	113.18
1	A	699	MET	N-CA-C	5.99	117.57	109.24
1	B	84	ASP	N-CA-C	-5.99	98.76	108.41
1	B	524	HIS	CA-C-O	-5.99	114.90	121.31
1	B	208	ALA	CA-C-O	5.98	126.76	120.42
1	B	383	ALA	N-CA-C	5.98	118.31	111.02
1	B	617	LYS	CA-C-O	5.98	125.72	119.14
1	B	272	GLN	CB-CA-C	5.98	121.85	109.95
1	B	581	ASP	CA-C-N	5.98	125.66	119.56
1	B	581	ASP	C-N-CA	5.98	125.66	119.56
1	A	688	THR	N-CA-C	-5.97	97.56	108.02
1	A	321	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	32	LEU	N-CA-CB	-5.96	101.22	110.57
1	B	459	TRP	CA-C-N	-5.96	114.84	123.06
1	B	459	TRP	C-N-CA	-5.96	114.84	123.06
1	B	607	PRO	N-CA-CB	5.96	109.23	103.51
1	B	518	ASN	CA-CB-CG	-5.95	106.66	112.60
1	A	613	HIS	N-CA-C	-5.92	101.34	110.58
1	B	296	ARG	O-C-N	-5.92	115.45	122.20
1	A	46	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	519	ILE	N-CA-C	5.92	116.64	108.12
1	A	588	LEU	N-CA-CB	5.92	120.46	110.46
1	B	497	ALA	CB-CA-C	-5.92	99.53	109.65
1	A	453	ARG	CA-C-O	-5.91	114.32	120.70
1	A	244	LYS	N-CA-C	-5.90	100.68	110.17
1	A	6	HIS	CA-C-N	5.89	131.69	120.97
1	A	6	HIS	C-N-CA	5.89	131.69	120.97
1	B	398	ARG	NH1-CZ-NH2	5.88	126.94	119.30
1	B	237	LYS	CA-CB-CG	5.87	125.84	114.10
1	A	581	ASP	N-CA-C	-5.87	100.12	109.04
1	B	281	GLY	CA-C-O	-5.86	113.13	121.52
1	A	430	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	662	THR	N-CA-C	-5.84	105.46	112.59
1	A	120	ASN	CA-CB-CG	-5.84	106.76	112.60
1	B	415	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	452	ARG	NE-CZ-NH2	5.81	124.43	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ASN	CA-CB-CG	-5.80	106.80	112.60
1	B	453	ARG	CA-C-O	-5.80	114.43	120.70
1	A	23	TRP	O-C-N	-5.80	116.44	123.29
1	B	495	VAL	CA-C-O	-5.80	115.89	121.63
1	A	623	PRO	N-CA-CB	5.79	109.02	103.52
1	B	379	LYS	N-CA-C	5.78	118.58	109.96
1	B	370	GLY	CA-C-O	-5.78	113.78	119.04
1	A	690	VAL	N-CA-CB	5.78	117.97	111.21
1	B	524	HIS	CA-CB-CG	-5.77	108.03	113.80
1	B	621	PHE	CA-C-O	-5.76	113.69	120.60
1	B	503	GLU	N-CA-C	5.76	117.56	111.28
1	A	631	LEU	N-CA-C	5.76	116.66	108.54
1	A	338	VAL	N-CA-C	5.75	118.53	112.83
1	B	656	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	A	570	ILE	CB-CA-C	5.74	119.00	111.53
1	A	689	HIS	CA-CB-CG	5.74	119.54	113.80
1	B	244	LYS	N-CA-C	-5.74	100.93	110.17
1	A	443	MET	CA-CB-CG	5.73	125.56	114.10
1	A	648	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	B	178	GLN	CB-CG-CD	5.71	122.30	112.60
1	A	517	HIS	CA-CB-CG	-5.70	108.10	113.80
1	A	6	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	688	THR	CA-CB-OG1	-5.69	101.06	109.60
1	B	359	GLU	CB-CA-C	5.69	120.10	109.86
1	B	712	ASN	CA-CB-CG	-5.69	106.91	112.60
1	B	633	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	422	GLU	CA-C-N	-5.67	117.12	123.02
1	B	422	GLU	C-N-CA	-5.67	117.12	123.02
1	A	470	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	682	TRP	N-CA-CB	5.66	120.18	110.68
1	B	120	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	236	LEU	N-CA-C	5.65	118.45	109.24
1	A	650	PRO	O-C-N	5.64	129.88	122.27
1	B	669	LYS	N-CA-C	5.64	118.19	111.71
1	B	713	PHE	N-CA-C	-5.63	104.76	111.69
1	A	540	ASN	N-CA-C	5.63	117.39	108.67
1	B	194	SER	CB-CA-C	5.62	120.41	110.85
1	B	309	ILE	O-C-N	5.62	128.93	123.03
1	A	548	PRO	N-CA-CB	5.61	108.32	103.27
1	B	284	VAL	CA-C-N	5.61	125.93	119.93
1	B	284	VAL	C-N-CA	5.61	125.93	119.93
1	A	6	HIS	O-C-N	-5.61	114.03	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	TYR	O-C-N	-5.60	116.13	123.02
1	A	603	TYR	CA-C-N	5.60	129.85	122.30
1	A	603	TYR	C-N-CA	5.60	129.85	122.30
1	A	34	LYS	N-CA-CB	5.59	118.53	110.37
1	A	505	ALA	N-CA-C	5.59	117.81	111.11
1	B	119	PRO	N-CA-C	-5.59	102.68	111.34
1	B	140	ALA	N-CA-C	5.58	117.37	111.28
1	B	530	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	622	ALA	N-CA-C	-5.58	102.38	110.08
1	B	519	ILE	N-CA-CB	-5.58	103.38	111.52
1	A	261	ILE	N-CA-C	-5.57	97.75	109.34
1	A	503	GLU	N-CA-C	5.57	117.79	111.11
1	A	374	ILE	N-CA-C	5.57	116.97	110.62
1	A	491	ALA	N-CA-C	-5.56	100.74	109.25
1	A	605	ILE	CA-C-O	-5.56	114.53	120.59
1	A	259	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	415	ASP	N-CA-CB	5.55	118.04	110.38
1	A	662	THR	N-CA-C	-5.55	105.72	112.88
1	A	526	HIS	CG-CD2-NE2	-5.54	101.66	107.20
1	A	311	PRO	N-CA-CB	5.54	109.02	103.48
1	A	560	THR	N-CA-C	-5.54	106.36	113.23
1	A	197	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	178	GLN	CB-CA-C	-5.53	101.37	110.55
1	B	413	ILE	N-CA-C	-5.53	101.78	108.53
1	B	20	ASP	N-CA-C	-5.53	100.28	109.46
1	B	526	HIS	CE1-NE2-CD2	5.53	114.53	109.00
1	B	223	THR	CA-C-N	5.52	126.37	120.13
1	B	223	THR	C-N-CA	5.52	126.37	120.13
1	B	511	TYR	O-C-N	5.52	128.81	122.25
1	A	292	PRO	N-CA-CB	5.51	108.15	103.35
1	B	421	MET	CA-CB-CG	5.51	125.13	114.10
1	B	715	ASP	CB-CA-C	-5.51	100.86	110.17
1	A	410	ASN	N-CA-C	-5.50	101.32	110.17
1	B	653	LYS	CA-C-O	-5.50	114.59	120.42
1	B	33	ILE	CA-C-N	-5.46	113.52	121.76
1	B	33	ILE	C-N-CA	-5.46	113.52	121.76
1	B	145	PRO	N-CA-CB	5.46	108.10	103.35
1	B	178	GLN	CA-C-N	5.45	125.38	119.76
1	B	178	GLN	C-N-CA	5.45	125.38	119.76
1	A	617	LYS	CA-C-O	5.45	125.64	119.27
1	A	644	HIS	CA-C-N	5.44	125.78	119.47
1	A	644	HIS	C-N-CA	5.44	125.78	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	GLN	CG-CD-NE2	5.43	124.54	116.40
1	A	194	SER	CB-CA-C	-5.41	101.80	110.79
1	A	666	GLN	CG-CD-OE1	5.41	131.62	120.80
1	A	227	VAL	N-CA-C	5.40	119.01	112.80
1	B	149	PRO	CA-C-O	-5.40	115.18	121.34
1	A	610	GLY	CA-C-O	-5.40	118.43	122.37
1	B	665	GLY	N-CA-C	-5.40	105.96	112.49
1	B	470	PHE	CA-CB-CG	-5.39	108.41	113.80
1	B	590	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	469	ILE	CA-C-O	-5.38	114.77	120.48
1	A	472	TRP	N-CA-C	-5.38	98.99	108.20
1	B	407	VAL	N-CA-C	-5.38	100.63	108.17
1	B	539	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	287	PRO	N-CA-C	-5.38	102.24	110.95
1	A	56	ALA	O-C-N	-5.38	116.33	122.89
1	B	148	GLN	CA-C-N	5.37	125.29	119.76
1	B	148	GLN	C-N-CA	5.37	125.29	119.76
1	A	713	PHE	CA-C-N	-5.36	113.35	123.27
1	A	713	PHE	C-N-CA	-5.36	113.35	123.27
1	B	223	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	146	VAL	N-CA-C	-5.36	100.03	108.23
1	A	39	VAL	O-C-N	5.35	128.59	123.14
1	B	131	PRO	CA-C-O	-5.34	115.27	121.95
1	A	300	ALA	CA-C-N	5.34	125.10	119.76
1	A	300	ALA	C-N-CA	5.34	125.10	119.76
1	A	71	SER	CA-CB-OG	-5.33	100.44	111.10
1	B	119	PRO	CA-C-O	-5.33	115.29	121.95
1	A	381	TYR	CA-C-N	5.32	129.90	122.41
1	A	381	TYR	C-N-CA	5.32	129.90	122.41
1	B	273	LYS	CA-CB-CG	-5.31	103.48	114.10
1	A	565	VAL	CA-CB-CG2	-5.31	101.37	110.40
1	B	355	LYS	O-C-N	5.31	129.13	122.86
1	B	385	GLY	N-CA-C	5.31	118.66	112.50
1	B	491	ALA	N-CA-C	-5.30	101.15	109.25
1	A	237	LYS	CA-CB-CG	5.29	124.68	114.10
1	B	410	ASN	CA-CB-CG	-5.29	107.31	112.60
1	B	720	LEU	CA-C-N	-5.28	115.55	122.63
1	B	720	LEU	C-N-CA	-5.28	115.55	122.63
1	B	47	THR	CA-CB-OG1	5.28	117.52	109.60
1	A	308	ILE	N-CA-C	-5.28	98.89	107.28
1	A	326	ARG	NH1-CZ-NH2	5.27	126.15	119.30
1	B	8	VAL	CA-C-N	5.26	126.70	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	VAL	C-N-CA	5.26	126.70	120.23
1	B	680	VAL	CA-C-O	-5.26	114.92	120.39
1	A	713	PHE	CA-CB-CG	5.26	119.06	113.80
1	B	136	VAL	CA-C-O	-5.25	115.49	120.95
1	A	275	ILE	N-CA-C	-5.25	101.96	108.89
1	B	524	HIS	ND1-CE1-NE2	-5.25	103.15	108.40
1	A	546	MET	N-CA-CB	5.25	119.42	110.87
1	A	94	HIS	CA-C-N	5.25	125.33	119.87
1	A	94	HIS	C-N-CA	5.25	125.33	119.87
1	B	657	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	385	GLY	CA-C-O	-5.24	115.34	121.00
1	B	314	LYS	CA-C-N	-5.24	112.32	122.06
1	B	314	LYS	C-N-CA	-5.24	112.32	122.06
1	B	288	MET	N-CA-C	5.24	119.82	113.38
1	B	689	HIS	N-CA-C	5.22	117.13	108.20
1	B	602	SER	N-CA-CB	-5.22	103.31	111.56
1	B	201	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	361	SER	CA-C-N	-5.20	112.77	120.94
1	B	361	SER	C-N-CA	-5.20	112.77	120.94
1	A	130	PRO	N-CA-C	5.20	116.15	110.58
1	B	452	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	A	182	ASP	CA-CB-CG	-5.19	107.41	112.60
1	A	703	TRP	N-CA-CB	-5.19	102.52	111.55
1	A	203	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	315	ASN	N-CA-C	-5.18	106.96	113.28
1	A	680	VAL	N-CA-C	-5.18	100.66	108.12
1	B	648	ARG	N-CA-CB	-5.18	103.73	110.88
1	A	353	LYS	CA-C-O	-5.18	114.57	120.58
1	A	48	ALA	CA-C-N	-5.17	115.75	122.94
1	A	48	ALA	C-N-CA	-5.17	115.75	122.94
1	A	553	ASN	CA-CB-CG	5.17	117.77	112.60
1	B	617	LYS	N-CA-C	-5.17	107.14	113.50
1	B	239	ASP	N-CA-CB	-5.17	102.38	110.44
1	A	83	LEU	CA-C-N	-5.16	115.67	122.85
1	A	83	LEU	C-N-CA	-5.16	115.67	122.85
1	A	340	PRO	N-CA-C	5.16	119.30	111.19
1	A	189	LEU	CA-C-O	-5.16	115.06	120.63
1	B	449	SER	CB-CA-C	-5.16	98.96	109.94
1	A	634	MET	CB-CA-C	-5.14	100.79	110.67
1	B	343	SER	N-CA-CB	-5.14	102.60	111.55
1	A	419	VAL	CA-C-N	5.14	125.14	119.90
1	A	419	VAL	C-N-CA	5.14	125.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	LEU	CA-C-O	-5.14	114.78	120.33
1	A	58	GLN	N-CA-C	-5.13	105.76	111.36
1	B	59	VAL	CA-C-N	5.13	125.11	120.03
1	B	59	VAL	C-N-CA	5.13	125.11	120.03
1	B	642	ARG	O-C-N	-5.13	116.63	122.89
1	B	292	PRO	CA-C-N	-5.13	114.28	122.29
1	B	292	PRO	C-N-CA	-5.13	114.28	122.29
1	A	326	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	B	514	LEU	N-CA-C	-5.13	100.72	108.67
1	A	665	GLY	N-CA-C	-5.12	106.21	112.77
1	B	54	PRO	N-CA-CB	5.12	108.10	103.34
1	B	499	THR	CA-C-O	-5.12	115.78	121.51
1	B	23	TRP	CA-C-O	-5.12	114.81	120.38
1	A	308	ILE	CA-C-N	-5.11	115.02	122.68
1	A	308	ILE	C-N-CA	-5.11	115.02	122.68
1	A	473	ILE	CA-C-N	-5.11	115.98	122.77
1	A	473	ILE	C-N-CA	-5.11	115.98	122.77
1	B	573	GLU	N-CA-C	5.10	117.51	111.33
1	B	707	LEU	N-CA-CB	-5.10	102.03	111.52
1	B	153	ASP	N-CA-C	-5.10	100.99	109.46
1	B	725	LYS	CA-C-O	-5.10	115.35	121.11
1	B	595	ASN	CA-C-N	5.10	127.62	120.28
1	B	595	ASN	C-N-CA	5.10	127.62	120.28
1	A	445	GLN	CG-CD-OE1	-5.09	110.61	120.80
1	A	458	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	53	GLN	CA-C-N	5.08	124.84	119.76
1	A	53	GLN	C-N-CA	5.08	124.84	119.76
1	B	602	SER	CB-CA-C	-5.08	99.57	111.09
1	B	92	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	B	259	HIS	CA-C-N	5.06	124.97	119.76
1	B	259	HIS	C-N-CA	5.06	124.97	119.76
1	A	94	HIS	N-CA-CB	-5.06	102.72	110.11
1	A	287	PRO	N-CA-C	-5.06	102.75	110.95
1	B	544	VAL	CA-C-O	-5.06	114.75	120.67
1	B	473	ILE	N-CA-CB	-5.06	105.30	111.67
1	B	712	ASN	N-CA-C	-5.05	106.69	112.86
1	B	275	ILE	O-C-N	-5.04	117.18	122.83
1	B	132	ASP	OD1-CG-OD2	5.03	134.97	122.90
1	A	79	PHE	CA-CB-CG	-5.02	108.78	113.80
1	B	165	ALA	CA-C-O	5.02	127.32	121.44
1	B	120	ASN	N-CA-CB	5.02	118.97	110.49
1	A	538	GLY	N-CA-C	-5.02	104.99	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	N-CA-C	5.01	117.74	110.42
1	B	498	LYS	N-CA-CB	5.01	117.78	110.47
1	A	566	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	524	HIS	ND1-CE1-NE2	-5.01	103.39	108.40
1	A	689	HIS	N-CA-C	5.01	116.76	108.20
1	B	544	VAL	O-C-N	5.00	128.59	123.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466[B]	TPQ	Mainchain
1	B	466[B]	TPQ	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	5686	0	5553	155	0
1	B	5712	0	5583	172	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	791	0	0	21	0
4	B	700	0	0	24	0
All	All	12895	0	11136	305	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 14.

All (305) 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:B:466[A]:TPQ:H6	4:B:1351:HOH:O	1.25	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466[A]:TPQ:C6	4:B:1351:HOH:O	1.92	1.00
1:B:67:LYS:HG3	1:B:69:TRP:HE1	1.27	0.98
1:A:288:MET:HE2	1:A:288:MET:HA	1.45	0.97
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.30	0.93
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.34	0.92
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.52	0.91
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.01	0.91
1:A:304:LYS:H	1:B:315:ASN:HD21	1.17	0.90
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.18	0.88
1:A:303:VAL:HG22	1:B:326:ARG:HH21	1.37	0.88
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.56	0.88
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.73	0.88
1:A:189:LEU:HG	4:A:843:HOH:O	1.74	0.86
1:A:28:GLN:HG3	4:A:1188:HOH:O	1.74	0.86
1:B:181:LYS:HE2	1:B:181:LYS:H	1.40	0.85
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.09	0.83
1:A:525:GLN:NE2	1:A:620:GLN:H	1.77	0.82
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.62	0.82
1:B:490:GLU:HG2	4:B:1503:HOH:O	1.81	0.81
1:A:303:VAL:HG22	1:B:326:ARG:NH2	1.97	0.79
1:B:251:VAL:HG12	1:B:251:VAL:O	1.82	0.79
1:B:203:GLU:CD	1:B:203:GLU:H	1.92	0.78
1:B:94:HIS:HD2	1:B:96:LEU:H	1.33	0.76
1:B:38:TYR:H	1:B:51:ASN:HD21	1.34	0.76
1:B:642:ARG:HH11	1:B:642:ARG:CB	1.98	0.76
1:B:12:LYS:O	1:B:16:GLU:HG2	1.86	0.76
1:A:38:TYR:H	1:A:51:ASN:HD21	1.34	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:B:580:PHE:H	1:B:637:GLN:HE21	1.34	0.75
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.86	0.75
1:B:189:LEU:HG	4:B:867:HOH:O	1.87	0.75
1:A:580:PHE:H	1:A:637:GLN:HE21	1.33	0.74
1:A:38:TYR:H	1:A:51:ASN:ND2	1.86	0.74
1:A:272:GLN:HE21	1:A:274:LYS:HD3	1.52	0.74
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.53	0.73
1:A:536:VAL:H	1:A:541:ASN:HD21	1.35	0.73
1:A:527:ILE:CD1	1:A:634:MET:HE3	2.18	0.73
1:B:67:LYS:HG3	1:B:69:TRP:NE1	2.03	0.73
1:B:38:TYR:H	1:B:51:ASN:ND2	1.87	0.73
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.71	0.73
1:B:725:LYS:O	1:B:726:ASP:OD1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:CG	1:B:69:TRP:HE1	2.02	0.72
1:A:286:VAL:HG12	1:A:288:MET:CE	2.19	0.72
1:B:525:GLN:NE2	1:B:620:GLN:H	1.88	0.72
1:A:326:ARG:HD2	4:A:1014:HOH:O	1.91	0.71
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.38	0.71
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.04	0.71
1:A:617:LYS:HE3	1:B:581:ASP:OD1	1.91	0.71
1:A:553:ASN:ND2	1:A:555:ALA:H	1.87	0.70
1:A:525:GLN:HE22	1:A:620:GLN:H	1.38	0.70
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.72	0.70
1:B:64:LYS:O	1:B:67:LYS:HG2	1.90	0.70
1:A:315:ASN:HD21	1:B:304:LYS:H	1.38	0.69
1:A:699:MET:HE1	4:A:1574:HOH:O	1.91	0.69
1:A:272:GLN:NE2	1:A:274:LYS:HD3	2.07	0.69
1:B:574:GLN:H	1:B:671:ASN:ND2	1.91	0.68
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.75	0.68
1:B:251:VAL:HG11	4:B:1224:HOH:O	1.92	0.68
1:A:443:MET:HE3	4:B:1119:HOH:O	1.95	0.67
1:A:149:PRO:HB3	1:A:170:GLN:HE21	1.58	0.67
1:B:173:LYS:NZ	1:B:173:LYS:HB3	2.10	0.67
1:B:580:PHE:H	1:B:637:GLN:NE2	1.93	0.67
1:B:119:PRO:O	1:B:120:ASN:OD1	2.12	0.66
1:B:189:LEU:HD11	4:B:1112:HOH:O	1.94	0.66
1:B:10:MET:HG3	1:B:70:VAL:CG1	2.25	0.66
1:B:160:LYS:HD3	1:B:271:GLU:OE1	1.95	0.66
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.78	0.65
1:A:203:GLU:CD	1:A:203:GLU:H	2.05	0.65
1:A:592:ASN:HD21	1:A:676:ASN:ND2	1.93	0.64
1:A:6:HIS:CG	1:A:7:MET:N	2.65	0.64
1:B:79:PHE:C	1:B:80:GLN:OE1	2.40	0.64
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.13	0.64
1:B:7:MET:HE3	1:B:70:VAL:C	2.21	0.64
1:A:629:HIS:HB2	4:A:1241:HOH:O	1.97	0.64
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.80	0.64
1:A:6:HIS:CG	1:A:7:MET:H	2.15	0.64
1:B:22:GLN:HB3	4:B:1478:HOH:O	1.98	0.64
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.26	0.64
1:A:322:MET:HG2	4:A:1312:HOH:O	1.98	0.63
1:B:221:ILE:HD13	1:B:250:ASP:HB2	1.80	0.63
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.64	0.62
1:B:109:GLU:HG2	4:B:1081:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:ASN:HD22	1:B:575:ASP:H	1.46	0.62
1:B:181:LYS:H	1:B:181:LYS:CE	2.11	0.62
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.81	0.62
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.36	0.61
1:A:574:GLN:H	1:A:671:ASN:ND2	1.97	0.60
1:B:178:GLN:HG3	4:B:862:HOH:O	2.00	0.60
1:A:498:LYS:O	1:A:517:HIS:HD2	1.84	0.60
1:B:132:ASP:H	1:B:148:GLN:HE22	1.50	0.59
1:B:196:GLN:HE22	1:B:222:THR:H	1.49	0.59
1:B:613:HIS:HD2	4:B:1267:HOH:O	1.85	0.59
1:A:286:VAL:CG1	1:A:288:MET:HE3	2.30	0.59
1:A:659:THR:OG1	1:A:660:HIS:HD2	1.84	0.59
1:B:477:ASN:HD22	1:B:477:ASN:C	2.08	0.59
1:A:162:ILE:HD11	1:A:185:GLY:N	2.17	0.59
1:B:572:ASN:HD21	1:B:575:ASP:CG	2.11	0.58
1:A:132:ASP:H	1:A:148:GLN:HE22	1.51	0.58
1:A:396:ILE:HD12	1:A:425:ARG:O	2.02	0.58
1:A:477:ASN:C	1:A:477:ASN:HD22	2.11	0.58
1:B:63:MET:HE3	1:B:66:ASN:HA	1.86	0.58
1:B:341:MET:HE2	4:B:922:HOH:O	2.04	0.58
1:B:65:ASP:O	1:B:66:ASN:HB2	2.03	0.58
1:B:525:GLN:HE22	1:B:620:GLN:H	1.51	0.58
1:A:642:ARG:CB	1:A:642:ARG:HH11	2.17	0.57
1:B:307:GLN:HG2	4:B:1178:HOH:O	2.04	0.57
1:A:61:VAL:HG22	1:A:70:VAL:HG12	1.87	0.57
1:B:572:ASN:ND2	1:B:575:ASP:H	2.03	0.57
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.86	0.57
1:B:536:VAL:H	1:B:541:ASN:HD21	1.51	0.56
1:B:527:ILE:CD1	1:B:634:MET:HE3	2.34	0.56
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.23	0.56
1:A:572:ASN:ND2	1:A:575:ASP:H	2.04	0.56
1:B:574:GLN:H	1:B:671:ASN:HD22	1.52	0.56
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.87	0.56
1:B:203:GLU:CD	1:B:203:GLU:N	2.63	0.56
1:A:367:VAL:HG21	1:A:468:TYR:OH	2.06	0.55
1:B:10:MET:HG3	1:B:70:VAL:HG11	1.86	0.55
1:B:359:GLU:HG3	4:B:1446:HOH:O	2.07	0.55
1:A:288:MET:HE2	1:A:288:MET:CA	2.28	0.55
1:B:553:ASN:ND2	1:B:555:ALA:H	2.05	0.55
1:B:196:GLN:NE2	1:B:222:THR:H	2.05	0.54
1:A:131:PRO:HB3	1:A:148:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:ALA:HB2	4:B:1169:HOH:O	2.07	0.54
1:A:10:MET:CG	1:A:14:LEU:HD23	2.37	0.54
1:A:210:LYS:HE2	1:A:210:LYS:HA	1.89	0.54
1:B:221:ILE:HD11	1:B:250:ASP:CB	2.33	0.54
1:A:381:TYR:CD2	1:A:466[A]:TPQ:O5	2.61	0.54
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.16	0.54
1:A:208:ALA:O	1:A:212:ARG:HG3	2.07	0.54
1:B:717:THR:HB	1:B:720:LEU:HG	1.90	0.54
1:A:91:LYS:NZ	4:A:1324:HOH:O	2.37	0.53
1:A:8:VAL:CG2	1:A:9:PRO:HD2	2.37	0.53
1:A:162:ILE:HD11	1:A:184:HIS:C	2.34	0.53
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.73	0.53
1:A:286:VAL:CG1	1:A:288:MET:CE	2.85	0.53
1:A:7:MET:HE1	1:A:59:VAL:HG11	1.91	0.53
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.91	0.52
1:A:237:LYS:HZ2	1:A:239:ASP:CG	2.17	0.52
1:B:726:ASP:CG	1:B:727:LYS:N	2.65	0.52
1:A:203:GLU:CD	1:A:203:GLU:N	2.68	0.52
1:A:22:GLN:HG3	4:A:1418:HOH:O	2.10	0.52
1:A:636:LYS:HE3	4:A:1451:HOH:O	2.10	0.52
1:B:10:MET:HG3	1:B:70:VAL:HG13	1.91	0.52
1:B:381:TYR:CD1	1:B:466[A]:TPQ:O5	2.63	0.51
1:B:498:LYS:O	1:B:517:HIS:HD2	1.93	0.51
1:A:431:GLU:HG2	1:B:306:MET:HE1	1.92	0.51
1:A:62:VAL:HG23	1:A:69:TRP:HB2	1.91	0.51
1:A:237:LYS:HG2	1:A:240:ALA:CB	2.40	0.51
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.23	0.51
1:A:10:MET:HE3	1:A:70:VAL:CG1	2.41	0.51
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.91	0.51
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.91	0.51
1:A:697:PRO:HD2	1:B:720:LEU:HD11	1.93	0.51
1:B:7:MET:HG2	1:B:71:SER:HA	1.92	0.51
1:B:527:ILE:HD12	1:B:634:MET:HE3	1.93	0.50
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.77	0.50
1:B:251:VAL:O	1:B:251:VAL:CG1	2.58	0.50
1:B:572:ASN:HB2	1:B:671:ASN:ND2	2.25	0.50
1:B:7:MET:HE3	1:B:70:VAL:CA	2.42	0.50
1:A:217:ALA:HB2	4:A:1432:HOH:O	2.12	0.50
1:A:551:LYS:NZ	4:A:1453:HOH:O	2.43	0.50
1:B:67:LYS:HD2	1:B:69:TRP:CZ2	2.46	0.50
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.92	0.50
1:A:322:MET:HE1	4:A:1150:HOH:O	2.12	0.50
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.93	0.50
1:B:101:ALA:O	1:B:105:LYS:HG3	2.11	0.50
1:A:29:LEU:HD13	1:A:30:PHE:O	2.11	0.49
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.93	0.49
1:B:619:ALA:HB1	1:B:634:MET:HE2	1.92	0.49
1:A:65:ASP:O	1:A:66:ASN:HB2	2.12	0.49
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.77	0.49
1:A:466[A]:TPQ:HB3	1:A:468:TYR:CE2	2.47	0.49
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.47	0.49
1:B:76:ASN:O	1:B:80:GLN:HB2	2.13	0.49
1:B:239:ASP:OD1	1:B:239:ASP:C	2.55	0.49
1:A:71:SER:OG	1:A:73:THR:HG22	2.13	0.49
1:A:147:ASP:HB2	4:A:1182:HOH:O	2.13	0.49
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.13	0.49
1:A:642:ARG:HG3	1:A:643:TYR:N	2.28	0.49
1:A:670:ASP:OD1	1:A:670:ASP:N	2.46	0.49
1:A:610:GLY:HA3	1:B:610:GLY:HA3	1.95	0.49
1:B:299:VAL:O	1:B:301:PRO:HD3	2.12	0.48
1:B:171:ASN:HB3	1:B:173:LYS:HE2	1.95	0.48
1:B:221:ILE:N	1:B:221:ILE:HD12	2.28	0.48
1:A:29:LEU:HD13	1:A:30:PHE:N	2.28	0.48
1:B:38:TYR:N	1:B:51:ASN:HD21	2.08	0.48
1:A:516:ASP:HB3	1:A:519:ILE:HB	1.96	0.48
1:A:580:PHE:H	1:A:637:GLN:NE2	2.05	0.48
1:B:89:VAL:HG23	4:B:1475:HOH:O	2.14	0.48
1:B:131:PRO:HG3	4:B:1141:HOH:O	2.14	0.48
1:A:288:MET:HA	1:A:288:MET:CE	2.31	0.48
1:B:160:LYS:HB2	1:B:241:ARG:HB2	1.96	0.48
1:A:64:LYS:HB3	1:A:69:TRP:CD1	2.48	0.47
1:A:382:LEU:HD22	4:A:902:HOH:O	2.14	0.47
1:B:367:VAL:HG21	1:B:468:TYR:OH	2.13	0.47
1:B:532:LEU:HD11	1:B:683:MET:HE2	1.96	0.47
1:B:545:ALA:O	1:B:567:GLN:HA	2.14	0.47
1:B:580:PHE:N	1:B:637:GLN:HE21	2.05	0.47
1:B:51:ASN:N	1:B:51:ASN:HD22	2.11	0.47
1:B:578:GLN:HA	1:B:636:LYS:HD2	1.97	0.47
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.50	0.47
1:A:9:PRO:HG3	1:A:12:LYS:NZ	2.29	0.47
1:B:119:PRO:O	1:B:120:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.50	0.46
1:B:118:LYS:HB3	1:B:118:LYS:HE2	1.51	0.46
1:B:322:MET:HB3	1:B:322:MET:HE2	1.67	0.46
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.80	0.46
1:A:40:LYS:CE	4:A:1290:HOH:O	2.64	0.46
4:A:1360:HOH:O	1:B:400:LYS:HE2	2.15	0.46
1:A:558:PRO:HG2	1:B:377:TYR:CE1	2.50	0.46
1:A:572:ASN:HD22	1:A:575:ASP:H	1.62	0.46
1:A:274:LYS:NZ	1:A:275:ILE:O	2.45	0.46
1:A:582:PRO:C	1:B:615:VAL:HG12	2.41	0.46
1:B:10:MET:HE1	1:B:30:PHE:CD1	2.51	0.46
1:A:237:LYS:HG2	1:A:240:ALA:HB2	1.97	0.46
1:B:524:HIS:HE1	4:B:1503:HOH:O	1.99	0.45
1:A:29:LEU:HD13	1:A:29:LEU:C	2.41	0.45
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.99	0.45
1:B:67:LYS:HD2	1:B:69:TRP:HZ2	1.82	0.45
1:B:67:LYS:CD	1:B:69:TRP:HE1	2.29	0.45
1:A:237:LYS:NZ	1:A:239:ASP:CG	2.74	0.45
1:B:121:THR:CG2	1:B:156:MET:HB3	2.47	0.45
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.79	0.45
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.82	0.45
1:A:572:ASN:HD22	1:A:572:ASN:C	2.25	0.45
1:B:208:ALA:O	1:B:212:ARG:HG3	2.17	0.45
1:B:219:LYS:O	1:B:221:ILE:HD12	2.18	0.45
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.64	0.44
1:A:525:GLN:HE22	1:A:620:GLN:N	2.12	0.44
1:A:546:MET:CE	4:A:1025:HOH:O	2.65	0.44
1:A:400:LYS:HE3	1:B:449:SER:HB2	1.99	0.44
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.48	0.44
1:A:359:GLU:CD	1:A:648:ARG:HH22	2.26	0.44
1:A:9:PRO:HG3	1:A:12:LYS:HZ2	1.83	0.43
1:A:90:GLU:CD	1:A:93:PRO:HA	2.43	0.43
1:A:210:LYS:HE2	1:A:214:ILE:O	2.18	0.43
1:A:224:PRO:HB2	1:A:243:LEU:HD13	2.01	0.43
1:A:237:LYS:NZ	1:A:239:ASP:OD1	2.51	0.43
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.54	0.43
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.76	0.43
1:B:725:LYS:NZ	4:B:1489:HOH:O	2.48	0.43
1:A:434:ALA:HB3	1:A:452:ARG:HG2	2.00	0.43
1:A:629:HIS:CE1	4:A:1165:HOH:O	2.71	0.43
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLN:NE2	1:B:274:LYS:HD3	2.14	0.43
1:B:218:LYS:HA	4:B:1466:HOH:O	2.17	0.43
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.34	0.43
1:B:144:LYS:HA	1:B:145:PRO:HD3	1.92	0.42
1:A:203:GLU:OE2	1:A:204:GLU:OE2	2.37	0.42
1:A:595:ASN:C	1:A:595:ASN:HD22	2.26	0.42
1:B:229:TYR:HB3	1:B:630:ARG:HD2	2.01	0.42
1:A:42:LYS:NZ	4:A:1320:HOH:O	2.50	0.42
1:B:447:ASN:CG	1:B:448:VAL:N	2.76	0.42
1:A:642:ARG:HH11	1:A:642:ARG:HG2	1.84	0.42
1:B:642:ARG:CG	1:B:642:ARG:NH1	2.80	0.42
1:B:120:ASN:ND2	4:B:1203:HOH:O	2.32	0.42
1:B:243:LEU:CD1	1:B:270:LEU:HD11	2.50	0.42
1:B:648:ARG:NH2	4:B:1446:HOH:O	2.47	0.42
1:A:117:PHE:CZ	1:A:121:THR:HB	2.54	0.42
1:B:181:LYS:HG2	1:B:181:LYS:O	2.20	0.42
1:A:189:LEU:HG	1:A:189:LEU:H	1.75	0.42
1:A:209:VAL:HG13	1:A:214:ILE:HB	2.02	0.42
1:A:10:MET:HG2	1:A:14:LEU:HD23	2.01	0.42
1:A:29:LEU:HD13	1:A:30:PHE:C	2.45	0.42
1:A:60:PRO:HD2	4:A:1458:HOH:O	2.19	0.42
1:A:237:LYS:HD3	1:A:240:ALA:HB2	2.01	0.42
1:B:162:ILE:HD11	1:B:185:GLY:CA	2.50	0.42
1:A:419:VAL:HA	1:A:420:PRO:HD3	1.95	0.42
1:A:595:ASN:C	1:A:595:ASN:ND2	2.77	0.42
1:B:129:LEU:CD1	1:B:130:PRO:HD2	2.38	0.42
1:A:246:ILE:HD13	1:A:246:ILE:HA	1.81	0.41
1:A:572:ASN:ND2	1:A:671:ASN:HD21	2.18	0.41
1:A:51:ASN:N	1:A:51:ASN:HD22	2.17	0.41
1:A:699:MET:HA	1:A:700:PRO:HD3	1.83	0.41
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.35	0.41
1:A:263:ASN:HB3	1:A:281:GLY:HA3	2.01	0.41
1:B:443:MET:CG	4:B:824:HOH:O	2.68	0.41
1:B:139:PHE:O	1:B:143:ASN:HA	2.19	0.41
1:A:608:TYR:OH	1:A:615:VAL:HG21	2.19	0.41
1:B:118:LYS:HA	1:B:119:PRO:HD3	1.93	0.41
1:A:77:ASP:O	1:A:81:SER:HB3	2.19	0.41
1:B:148:GLN:HA	1:B:149:PRO:HD3	1.76	0.41
1:B:465:ASN:HB2	1:B:489:ILE:O	2.20	0.41
1:A:617:LYS:CE	1:B:581:ASP:OD1	2.65	0.41
1:A:694:GLU:O	1:B:717:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:MET:HE2	1:B:69:TRP:HB3	2.03	0.41
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.51	0.41
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.85	0.41
1:A:29:LEU:HD12	4:A:989:HOH:O	2.20	0.41
1:A:269:ASP:O	1:A:273:LYS:N	2.53	0.41
1:A:578:GLN:HA	1:A:636:LYS:HD2	2.02	0.41
1:A:579:LYS:HA	1:A:637:GLN:NE2	2.36	0.41
1:B:202:SER:CB	1:B:275:ILE:HD12	2.51	0.41
1:B:581:ASP:HA	1:B:582:PRO:HD2	1.94	0.41
1:A:196:GLN:HE22	1:A:222:THR:H	1.68	0.41
1:A:96:LEU:O	1:A:97:ASN:C	2.64	0.40
1:A:615:VAL:HG23	1:B:582:PRO:HB2	2.04	0.40
1:A:284:VAL:O	1:A:285:PRO:C	2.64	0.40
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.34	0.40
1:B:64:LYS:O	1:B:65:ASP:HB2	2.21	0.40
1:B:189:LEU:CD2	4:B:867:HOH:O	2.69	0.40
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.92	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	717/722 (99%)	694 (97%)	23 (3%)	0	100	100
1	B	719/722 (100%)	693 (96%)	25 (4%)	1 (0%)	48	46
All	All	1436/1444 (99%)	1387 (97%)	48 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	726	ASP

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	609/612 (100%)	582 (96%)	27 (4%)	25	24
1	B	612/612 (100%)	577 (94%)	35 (6%)	18	15
All	All	1221/1224 (100%)	1159 (95%)	62 (5%)	21	19

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	32	LEU
1	A	80	GLN
1	A	89	VAL
1	A	129	LEU
1	A	144	LYS
1	A	151	LYS
1	A	162	ILE
1	A	178	GLN
1	A	199	ILE
1	A	203	GLU
1	A	210	LYS
1	A	237	LYS
1	A	239	ASP
1	A	288	MET
1	A	304	LYS
1	A	342	ILE
1	A	374	ILE
1	A	396	ILE
1	A	477	ASN
1	A	520	VAL
1	A	539	GLU
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	642	ARG
1	A	719	THR

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Mol	Chain	Res	Type
1	B	11	ASP
1	B	12	LYS
1	B	15	LYS
1	B	16	GLU
1	B	22	GLN
1	B	34	LYS
1	B	47	THR
1	B	80	GLN
1	B	120	ASN
1	B	129	LEU
1	B	148	GLN
1	B	173	LYS
1	B	178	GLN
1	B	181	LYS
1	B	199	ILE
1	B	203	GLU
1	B	209	VAL
1	B	211	LYS
1	B	218	LYS
1	B	233	LYS
1	B	237	LYS
1	B	239	ASP
1	B	342	ILE
1	B	359	GLU
1	B	477	ASN
1	B	539	GLU
1	B	572	ASN
1	B	595	ASN
1	B	613	HIS
1	B	614	PRO
1	B	617	LYS
1	B	642	ARG
1	B	669	LYS
1	B	726	ASP
1	B	727	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	97	ASN
1	A	120	ASN

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Mol	Chain	Res	Type
1	A	148	GLN
1	A	161	HIS
1	A	170	GLN
1	A	196	GLN
1	A	200	ASN
1	A	272	GLN
1	A	307	GLN
1	A	315	ASN
1	A	324	HIS
1	A	327	ASN
1	A	348	ASN
1	A	350	ASN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	540	ASN
1	A	541	ASN
1	A	553	ASN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	604	GLN
1	A	637	GLN
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	46	GLN
1	B	51	ASN
1	B	53	GLN
1	B	66	ASN
1	B	94	HIS
1	B	97	ASN
1	B	120	ASN
1	B	148	GLN
1	B	196	GLN
1	B	197	ASN
1	B	200	ASN
1	B	238	GLN
1	B	272	GLN
1	B	315	ASN
1	B	327	ASN

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Mol	Chain	Res	Type
1	B	350	ASN
1	B	447	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	518	ASN
1	B	525	GLN
1	B	541	ASN
1	B	553	ASN
1	B	567	GLN
1	B	572	ASN
1	B	574	GLN
1	B	595	ASN
1	B	599	ASN
1	B	604	GLN
1	B	613	HIS
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPQ	A	466[A]	1	13,14,15	2.24	5 (38%)	13,19,21	2.25	4 (30%)
1	TPQ	B	466[B]	1	13,14,15	2.42	5 (38%)	13,19,21	2.36	4 (30%)
1	TPQ	A	466[B]	1	13,14,15	2.44	4 (30%)	13,19,21	2.18	5 (38%)
1	TPQ	B	466[A]	1	13,14,15	2.94	6 (46%)	13,19,21	1.14	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
1	TPQ	A	466[A]	1	-	2/5/22/24	0/1/1/1
1	TPQ	B	466[B]	1	-	2/5/22/24	0/1/1/1
1	TPQ	A	466[B]	1	-	2/5/22/24	0/1/1/1
1	TPQ	B	466[A]	1	-	0/5/22/24	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466[B]	TPQ	C1-C2	-5.99	1.40	1.49
1	A	466[B]	TPQ	C1-C2	-5.81	1.41	1.49
1	B	466[A]	TPQ	C1-C2	-5.55	1.41	1.49
1	A	466[A]	TPQ	C1-C2	-5.42	1.41	1.49
1	B	466[A]	TPQ	O5-C5	-5.06	1.11	1.24
1	B	466[A]	TPQ	O2-C2	-4.98	1.11	1.24
1	A	466[B]	TPQ	C6-C5	-3.46	1.35	1.44
1	B	466[B]	TPQ	C6-C5	-3.33	1.35	1.44
1	A	466[A]	TPQ	C6-C1	3.07	1.42	1.34
1	A	466[B]	TPQ	O5-C5	3.07	1.32	1.24
1	A	466[B]	TPQ	CB-C1	2.84	1.55	1.50
1	B	466[A]	TPQ	C4-C5	-2.83	1.39	1.47
1	A	466[A]	TPQ	CB-C1	2.83	1.55	1.50
1	B	466[B]	TPQ	CB-C1	2.74	1.55	1.50
1	B	466[B]	TPQ	O5-C5	2.52	1.31	1.24
1	A	466[A]	TPQ	C4-C5	-2.31	1.40	1.47
1	A	466[A]	TPQ	C6-C5	-2.10	1.39	1.44
1	B	466[B]	TPQ	CB-CA	2.09	1.58	1.53
1	B	466[A]	TPQ	C6-C5	-2.08	1.39	1.44
1	B	466[A]	TPQ	C6-C1	2.06	1.39	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466[B]	TPQ	CB-C1-C2	6.50	129.93	118.56
1	A	466[A]	TPQ	CB-C1-C2	5.65	128.45	118.56
1	A	466[B]	TPQ	CB-C1-C2	5.07	127.44	118.56
1	A	466[A]	TPQ	O5-C5-C4	3.66	125.21	119.43
1	A	466[A]	TPQ	O5-C5-C6	-3.26	114.40	121.83
1	B	466[B]	TPQ	C4-C3-C2	-2.79	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466[B]	TPQ	C4-C3-C2	-2.77	117.30	120.30
1	A	466[B]	TPQ	C3-C4-C5	-2.50	118.68	121.23
1	A	466[B]	TPQ	C6-C5-C4	2.46	121.09	116.80
1	B	466[B]	TPQ	C6-C5-C4	2.27	120.78	116.80
1	B	466[B]	TPQ	C3-C2-C1	2.10	122.67	118.36
1	A	466[A]	TPQ	C6-C5-C4	2.05	120.38	116.80
1	A	466[B]	TPQ	O2-C2-C3	-2.04	117.19	121.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466[A]	TPQ	N-CA-CB-C1
1	A	466[A]	TPQ	C-CA-CB-C1
1	B	466[B]	TPQ	C-CA-CB-C1
1	A	466[B]	TPQ	N-CA-CB-C1
1	A	466[B]	TPQ	C-CA-CB-C1
1	B	466[B]	TPQ	N-CA-CB-C1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466[A]	TPQ	2	0
1	B	466[A]	TPQ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	719/722 (99%)	-0.37	18 (2%) 58 58	12, 23, 45, 70	0
1	B	721/722 (99%)	-0.32	24 (3%) 49 48	15, 24, 48, 95	0
All	All	1440/1444 (99%)	-0.35	42 (2%) 53 52	12, 24, 47, 95	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	HIS	5.3
1	B	726	ASP	4.2
1	A	189	LEU	4.1
1	B	301	PRO	4.0
1	B	239	ASP	3.6
1	A	149	PRO	3.6
1	A	148	GLN	3.5
1	B	6	HIS	3.5
1	A	239	ASP	3.4
1	A	468	TYR	3.3
1	B	120	ASN	3.3
1	A	130	PRO	3.2
1	B	67	LYS	3.0
1	B	7	MET	3.0
1	A	271	GLU	3.0
1	B	148	GLN	2.9
1	B	727	LYS	2.8
1	A	66	ASN	2.8
1	B	644	HIS	2.8
1	B	8	VAL	2.8
1	B	80	GLN	2.7
1	B	302	ALA	2.6
1	A	147	ASP	2.5
1	A	6	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	170	GLN	2.5
1	B	642	ARG	2.5
1	A	73	THR	2.4
1	A	64	LYS	2.4
1	B	197	ASN	2.4
1	B	670	ASP	2.4
1	A	670	ASP	2.3
1	A	217	ALA	2.3
1	B	539	GLU	2.3
1	B	66	ASN	2.3
1	B	130	PRO	2.3
1	A	443	MET	2.3
1	B	189	LEU	2.2
1	A	215	THR	2.1
1	B	300	ALA	2.1
1	B	76	ASN	2.1
1	B	725	LYS	2.1
1	B	92	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	TPQ	A	466[A]	14/15	0.70	0.27	24,45,47,48	14
1	TPQ	A	466[B]	14/15	0.70	0.27	15,43,53,53	14
1	TPQ	B	466[A]	14/15	0.71	0.29	22,50,57,57	14
1	TPQ	B	466[B]	14/15	0.71	0.29	20,40,50,54	14

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(Å ²)	Q<0.9
3	CA	B	803	1/1	0.94	0.06	49,49,49,49	0
3	CA	A	803	1/1	0.97	0.10	42,42,42,42	0
2	CU	A	801	1/1	0.99	0.02	26,26,26,26	0
3	CA	B	802	1/1	0.99	0.02	22,22,22,22	0
3	CA	A	802	1/1	0.99	0.03	21,21,21,21	0
2	CU	B	801	1/1	1.00	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.