



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 PM UTC

PDB ID : 1DYU / pdb_00001dyu
Title : The active site base controls cofactor reactivity in Escherichia 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.V.; McPherson, M.J.
Deposited on : 2000-02-08
Resolution : 2.04 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

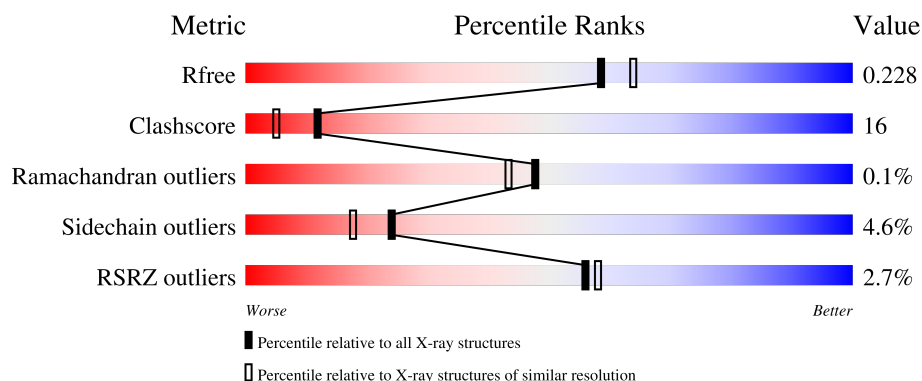
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	727	2% 65% 28% 5% ..
1	B	727	4% 61% 29% 8% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12921 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	718	Total	C	N	O	S	0	0	0
			5664	3602	964	1076	22			
1	B	720	Total	C	N	O	S	0	0	0
			5683	3614	969	1078	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TPQ	TYR	modified residue	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	827	Total	O	0	0
			827	827		

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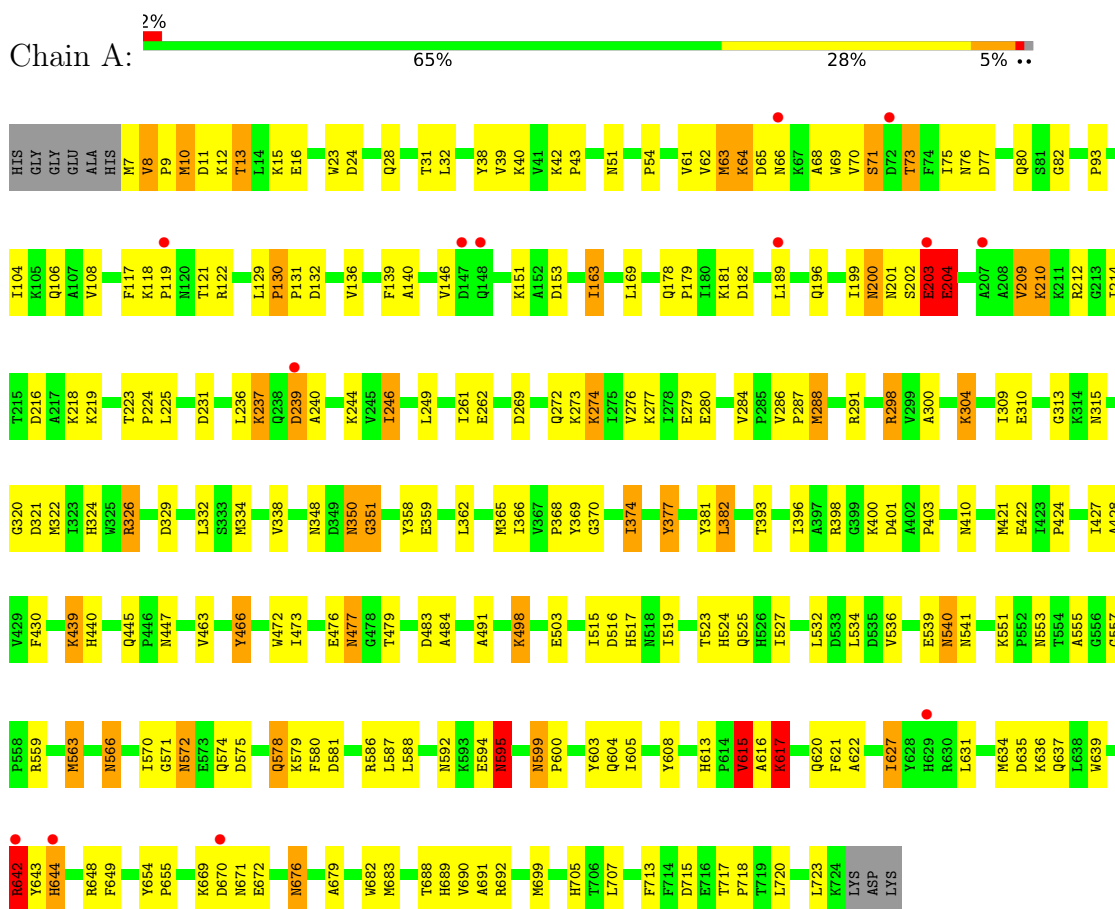
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	741	Total 741	O 741	0	0

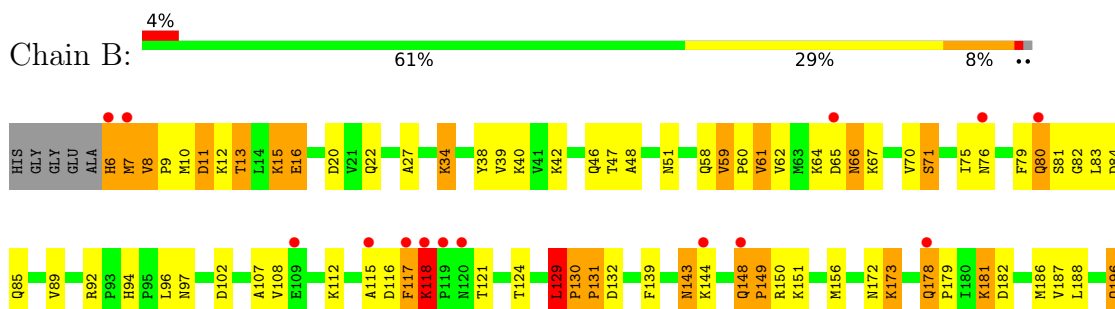
3 Residue-property plots

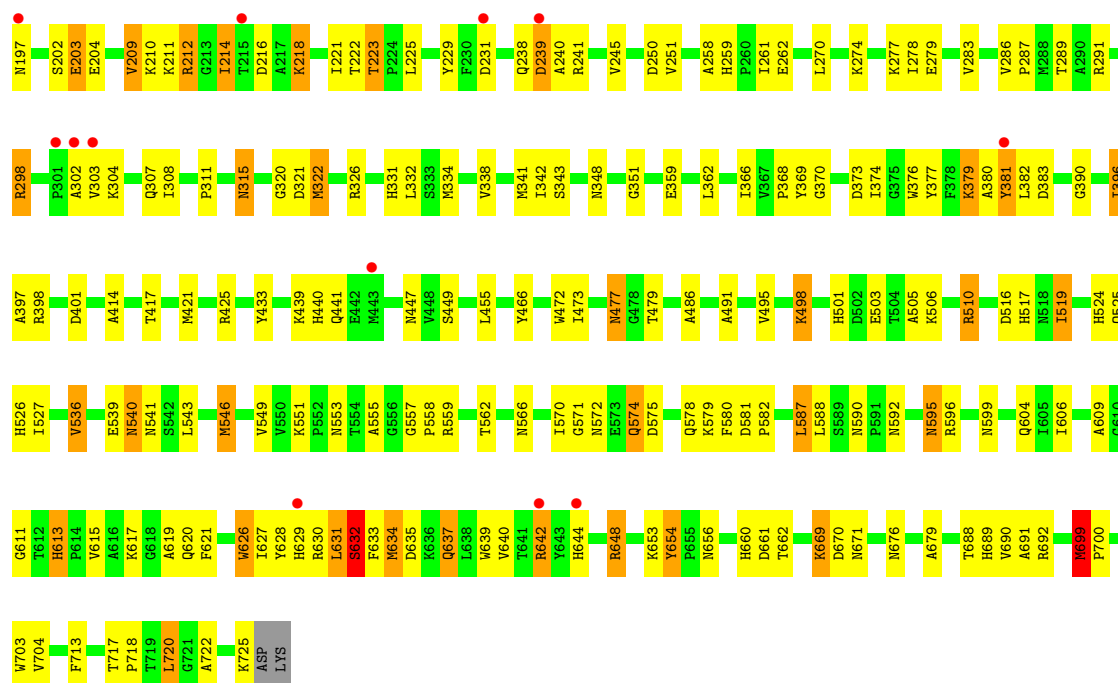
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	135.05Å 167.17Å 79.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.04 20.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.04) 88.5 (20.00-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.237 0.175 , 0.228	Depositor DCC
R_{free} test set	3576 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.884	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12921	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 2.70% 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	0.79	0/5793	1.98	144/7886 (1.8%)
1	B	0.75	0/5813	1.93	168/7912 (2.1%)
All	All	0.77	0/11606	1.95	312/15798 (2.0%)

There are no bond length outliers.

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ASN	OD1-CG-ND2	22.23	144.83	122.60
1	A	130	PRO	O-C-N	17.83	129.53	121.15
1	B	571	GLY	N-CA-C	13.44	130.42	114.16
1	A	571	GLY	N-CA-C	10.80	128.06	114.66
1	A	129	LEU	CA-C-N	10.74	127.39	119.66
1	A	129	LEU	C-N-CA	10.74	127.39	119.66
1	A	642	ARG	CD-NE-CZ	10.45	139.04	124.40
1	A	691	ALA	N-CA-C	10.18	122.94	110.41
1	B	129	LEU	N-CA-C	-9.80	94.14	109.04
1	B	8	VAL	N-CA-CB	-9.75	105.10	111.83
1	A	28	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	B	148	GLN	CB-CA-C	9.48	121.74	108.76
1	A	326	ARG	NE-CZ-NH2	-9.46	110.69	119.20
1	A	288	MET	N-CA-C	9.43	124.92	113.41
1	A	119	PRO	CA-C-N	-9.12	109.59	123.17
1	A	119	PRO	C-N-CA	-9.12	109.59	123.17
1	B	720	LEU	CA-C-N	-9.02	110.54	122.63
1	B	720	LEU	C-N-CA	-9.02	110.54	122.63
1	B	143	ASN	OD1-CG-ND2	8.95	131.55	122.60
1	A	350	ASN	OD1-CG-ND2	8.89	131.49	122.60
1	B	85	GLN	OE1-CD-NE2	8.84	131.44	122.60
1	A	130	PRO	CB-CA-C	-8.76	102.94	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	MET	N-CA-C	8.57	121.15	109.24
1	A	566	ASN	CB-CG-OD1	-8.51	103.78	120.80
1	B	519	ILE	O-C-N	-8.45	114.14	123.26
1	A	692	ARG	NE-CZ-NH2	-8.45	111.60	119.20
1	B	379	LYS	CB-CA-C	8.42	123.46	110.67
1	A	130	PRO	N-CA-CB	8.38	107.58	103.22
1	B	7	MET	N-CA-CB	-8.35	98.37	111.56
1	A	82	GLY	N-CA-C	-8.29	103.92	114.37
1	A	676	ASN	OD1-CG-ND2	-8.29	114.31	122.60
1	B	374	ILE	N-CA-C	8.27	120.05	110.62
1	A	326	ARG	NH1-CZ-NH2	8.25	130.03	119.30
1	A	326	ARG	CB-CA-C	-8.15	106.14	117.23
1	B	495	VAL	CA-C-O	-8.07	113.64	121.63
1	B	590	ASN	OD1-CG-ND2	8.04	130.64	122.60
1	B	691	ALA	N-CA-C	7.99	120.24	110.41
1	A	503	GLU	N-CA-C	7.98	120.69	111.11
1	B	699	MET	N-CA-C	7.91	119.61	109.72
1	A	338	VAL	N-CA-C	7.91	120.66	112.83
1	A	64	LYS	CB-CA-C	-7.90	97.49	110.14
1	A	10	MET	N-CA-C	7.82	119.49	110.97
1	B	348	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	A	146	VAL	N-CA-C	-7.74	98.87	109.55
1	B	118	LYS	CA-C-N	7.73	128.14	119.32
1	B	118	LYS	C-N-CA	7.73	128.14	119.32
1	A	118	LYS	CA-C-N	7.52	129.24	119.84
1	A	118	LYS	C-N-CA	7.52	129.24	119.84
1	B	262	GLU	N-CA-C	7.51	121.40	110.28
1	B	654	TYR	CA-C-N	7.46	127.09	119.56
1	B	654	TYR	C-N-CA	7.46	127.09	119.56
1	A	472	TRP	N-CA-C	-7.40	96.45	108.52
1	A	588	LEU	N-CA-C	-7.40	94.89	107.99
1	A	287	PRO	O-C-N	-7.38	114.94	122.98
1	A	498	LYS	N-CA-C	-7.34	104.30	113.55
1	A	153	ASP	N-CA-C	-7.30	97.69	109.96
1	B	491	ALA	N-CA-C	-7.29	98.09	109.25
1	B	383	ASP	N-CA-C	7.26	119.82	111.11
1	B	510	ARG	NE-CZ-NH2	7.25	125.72	119.20
1	A	310	GLU	CA-C-N	7.19	126.90	119.56
1	A	310	GLU	C-N-CA	7.19	126.90	119.56
1	B	251	VAL	N-CA-CB	-7.18	102.73	112.28
1	A	129	LEU	N-CA-C	-7.12	94.26	109.01
1	A	440	HIS	N-CA-CB	7.11	122.31	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ARG	NH1-CZ-NH2	7.09	128.52	119.30
1	B	8	VAL	N-CA-C	7.09	115.71	107.84
1	A	713	PHE	N-CA-C	-7.07	103.32	112.23
1	B	351	GLY	CA-C-N	-7.06	113.26	123.00
1	B	351	GLY	C-N-CA	-7.06	113.26	123.00
1	A	374	ILE	N-CA-C	7.03	118.63	110.62
1	A	329	ASP	N-CA-CB	7.02	122.60	110.81
1	A	130	PRO	CA-C-O	-6.98	115.22	120.73
1	A	304	LYS	CA-CB-CG	6.95	128.00	114.10
1	B	578	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	B	81	SER	N-CA-C	6.94	118.84	111.28
1	B	609	ALA	CA-C-N	-6.93	113.35	122.63
1	B	609	ALA	C-N-CA	-6.93	113.35	122.63
1	A	484	ALA	CA-C-N	-6.92	117.41	122.18
1	A	484	ALA	C-N-CA	-6.92	117.41	122.18
1	B	588	LEU	N-CA-C	-6.91	96.38	108.20
1	B	498	LYS	N-CA-C	-6.91	104.98	113.41
1	B	648	ARG	N-CA-CB	-6.87	101.76	110.90
1	B	377	TYR	N-CA-C	6.87	120.54	111.75
1	B	578	GLN	N-CA-C	6.85	118.20	108.74
1	A	586	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	A	566	ASN	CA-CB-CG	-6.83	105.77	112.60
1	A	23	TRP	O-C-N	-6.80	115.26	123.29
1	A	28	GLN	CG-CD-NE2	6.77	126.56	116.40
1	A	362	LEU	N-CA-C	-6.76	100.43	110.23
1	B	713	PHE	N-CA-C	-6.73	103.42	111.69
1	B	519	ILE	CA-C-O	6.72	127.45	120.39
1	B	172	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	534	LEU	CA-C-O	-6.66	113.70	121.16
1	B	10	MET	N-CA-C	6.59	119.06	111.02
1	B	343	SER	N-CA-C	6.58	119.88	109.81
1	B	656	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	B	102	ASP	O-C-N	6.55	129.17	122.09
1	B	519	ILE	N-CA-C	6.55	117.28	108.11
1	A	421	MET	N-CA-CB	-6.50	100.57	110.77
1	A	93	PRO	N-CA-CB	6.48	109.10	103.27
1	B	662	THR	N-CA-C	-6.47	103.82	112.94
1	B	326	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	B	557	GLY	CA-C-N	6.44	126.01	119.19
1	B	557	GLY	C-N-CA	6.44	126.01	119.19
1	B	102	ASP	CA-C-O	-6.43	114.08	120.70
1	B	308	ILE	N-CA-C	-6.33	98.62	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	LYS	O-C-N	6.32	126.48	121.55
1	A	196	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	B	85	GLN	CG-CD-NE2	-6.31	106.94	116.40
1	A	615	VAL	N-CA-C	6.30	118.45	108.87
1	A	690	VAL	N-CA-C	-6.30	98.67	107.80
1	A	377	TYR	N-CA-C	6.29	119.80	111.75
1	B	58	GLN	N-CA-CB	6.29	119.19	110.07
1	B	704	VAL	N-CA-CB	6.29	122.33	111.39
1	A	473	ILE	N-CA-C	6.25	116.63	107.37
1	A	61	VAL	N-CA-C	-6.24	101.53	109.58
1	B	505	ALA	N-CA-C	6.23	118.58	111.11
1	A	699	MET	CA-C-O	6.20	123.91	119.32
1	A	578	GLN	N-CA-C	6.19	118.19	108.96
1	B	390	GLY	N-CA-C	-6.18	105.01	112.49
1	B	382	LEU	N-CA-C	-6.17	96.62	107.73
1	B	473	ILE	N-CA-C	6.17	116.70	107.51
1	A	146	VAL	CA-C-N	-6.17	109.76	121.54
1	A	146	VAL	C-N-CA	-6.17	109.76	121.54
1	B	631	LEU	N-CA-C	6.17	119.43	107.71
1	B	433	TYR	N-CA-C	-6.17	101.16	110.28
1	B	117	PHE	CA-C-O	-6.15	114.80	121.44
1	B	414	ALA	CA-C-O	-6.15	113.85	120.92
1	B	148	GLN	N-CA-C	-6.14	101.04	110.32
1	B	212	ARG	O-C-N	6.13	130.04	122.20
1	B	196	GLN	CA-C-O	6.11	127.02	120.55
1	B	197	ASN	OD1-CG-ND2	6.11	128.71	122.60
1	B	398	ARG	CG-CD-NE	6.10	125.42	112.00
1	B	59	VAL	CA-C-N	6.09	126.06	120.03
1	B	59	VAL	C-N-CA	6.09	126.06	120.03
1	A	204	GLU	CA-C-O	6.06	127.18	120.82
1	B	240	ALA	N-CA-C	6.04	119.01	110.50
1	A	539	GLU	N-CA-C	6.04	117.53	111.07
1	B	425	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	A	578	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	B	626	TRP	CA-C-O	5.99	126.88	120.24
1	A	284	VAL	CA-C-O	5.98	123.05	119.94
1	A	139	PHE	N-CA-C	-5.94	104.72	111.14
1	B	261	ILE	N-CA-C	-5.94	96.98	109.34
1	A	648	ARG	N-CA-CB	-5.92	103.13	111.00
1	A	63	MET	CA-C-O	5.91	126.69	120.36
1	B	130	PRO	N-CA-C	5.91	117.91	110.70
1	B	362	LEU	N-CA-C	-5.90	102.18	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	GLU	O-C-N	-5.89	115.44	122.15
1	B	82	GLY	N-CA-C	-5.88	106.41	114.64
1	B	178	GLN	CA-C-N	5.87	125.81	119.76
1	B	178	GLN	C-N-CA	5.87	125.81	119.76
1	B	202	SER	N-CA-C	5.86	117.59	109.15
1	A	476	GLU	O-C-N	5.86	128.33	122.12
1	B	118	LYS	CA-C-O	-5.86	114.84	120.64
1	B	186	MET	CA-C-N	5.85	129.74	121.66
1	B	186	MET	C-N-CA	5.85	129.74	121.66
1	B	223	THR	CB-CA-C	5.84	117.93	110.16
1	B	635	ASP	N-CA-C	5.84	120.40	113.28
1	A	163	ILE	CA-CB-CG1	5.83	120.31	110.40
1	A	350	ASN	CA-CB-CG	-5.82	106.78	112.60
1	B	562	THR	CA-C-O	-5.82	115.00	121.51
1	A	615	VAL	CB-CA-C	-5.81	103.25	111.21
1	B	376	TRP	N-CA-C	5.79	121.22	114.62
1	B	34	LYS	CG-CD-CE	-5.77	98.04	111.30
1	B	570	ILE	N-CA-C	-5.77	98.66	106.85
1	B	440	HIS	N-CA-CB	5.76	120.10	110.59
1	A	540	ASN	N-CA-C	5.76	117.59	108.67
1	B	688	THR	N-CA-C	-5.75	97.96	108.02
1	B	79	PHE	CA-CB-CG	-5.74	108.06	113.80
1	B	689	HIS	N-CA-C	5.73	118.41	107.75
1	A	313	GLY	CA-C-O	-5.73	116.66	122.56
1	B	58	GLN	O-C-N	5.73	128.28	122.09
1	B	48	ALA	N-CA-C	-5.73	100.71	109.41
1	B	84	ASP	N-CA-C	-5.72	99.19	108.41
1	B	338	VAL	N-CA-C	5.72	118.49	112.83
1	B	417	THR	N-CA-CB	5.71	118.94	110.49
1	A	570	ILE	N-CA-C	-5.70	98.76	106.85
1	B	223	THR	CA-C-N	5.68	126.95	119.84
1	B	223	THR	C-N-CA	5.68	126.95	119.84
1	A	309	ILE	CA-C-N	5.68	130.15	123.16
1	A	309	ILE	C-N-CA	5.68	130.15	123.16
1	A	136	VAL	CA-C-O	-5.66	114.85	120.85
1	A	351	GLY	CA-C-N	-5.64	115.03	122.99
1	A	351	GLY	C-N-CA	-5.64	115.03	122.99
1	A	422	GLU	CA-C-N	-5.62	118.78	122.60
1	A	422	GLU	C-N-CA	-5.62	118.78	122.60
1	A	9	PRO	N-CA-CB	5.61	107.79	103.30
1	B	278	ILE	CA-C-O	-5.60	115.23	120.22
1	B	421	MET	N-CA-CB	-5.59	101.41	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	TRP	N-CA-C	5.58	118.65	109.72
1	A	39	VAL	N-CA-C	5.58	116.62	108.53
1	B	156	MET	N-CA-CB	-5.57	102.28	110.85
1	B	503	GLU	N-CA-C	5.57	118.11	111.71
1	A	122	ARG	NH1-CZ-NH2	5.56	126.53	119.30
1	B	258	ALA	CA-C-N	-5.56	116.73	122.85
1	B	258	ALA	C-N-CA	-5.56	116.73	122.85
1	A	581	ASP	N-CA-C	-5.56	100.59	109.04
1	A	140	ALA	N-CA-C	5.54	117.40	111.36
1	A	324	HIS	CA-CB-CG	-5.54	108.26	113.80
1	B	613	HIS	N-CA-C	-5.54	102.08	110.50
1	A	635	ASP	O-C-N	5.53	129.25	122.34
1	B	540	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	401	ASP	N-CA-C	-5.53	106.04	112.89
1	B	287	PRO	N-CA-C	-5.52	102.00	110.95
1	A	599	ASN	CA-C-N	5.52	125.79	119.83
1	A	599	ASN	C-N-CA	5.52	125.79	119.83
1	A	688	THR	N-CA-C	-5.52	99.53	108.52
1	A	669	LYS	CB-CA-C	-5.51	101.59	110.74
1	A	689	HIS	N-CA-C	5.51	117.62	108.20
1	A	635	ASP	N-CA-C	5.50	120.10	113.17
1	B	150	ARG	N-CA-CB	5.50	118.00	109.48
1	B	455	LEU	O-C-N	-5.49	116.79	123.27
1	A	381	TYR	N-CA-C	5.48	118.13	109.96
1	A	269	ASP	N-CA-C	-5.48	99.80	108.73
1	A	692	ARG	CG-CD-NE	-5.47	99.97	112.00
1	A	382	LEU	N-CA-C	-5.46	98.36	108.24
1	B	526	HIS	N-CA-C	-5.45	99.40	108.34
1	A	203	GLU	CA-C-O	5.45	126.20	120.42
1	A	566	ASN	CB-CA-C	-5.44	102.08	110.78
1	B	27	ALA	CA-C-O	-5.44	112.15	119.11
1	B	615	VAL	N-CA-C	5.44	116.61	109.21
1	B	178	GLN	N-CA-C	5.43	120.46	108.73
1	A	649	PHE	O-C-N	5.43	126.22	121.39
1	B	6	HIS	N-CA-CB	5.43	119.72	110.50
1	A	605	ILE	CB-CG1-CD1	-5.42	102.41	113.80
1	A	617	LYS	CA-C-O	5.42	125.63	119.18
1	A	31	THR	N-CA-C	-5.39	99.62	108.41
1	B	690	VAL	N-CA-C	-5.39	100.12	107.99
1	A	200	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	B	381	TYR	N-CA-C	5.38	118.38	110.30
1	B	626	TRP	O-C-N	-5.38	115.23	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	PRO	N-CA-C	-5.37	103.70	111.22
1	A	231	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	131	PRO	N-CA-C	-5.36	103.66	111.33
1	A	261	ILE	N-CA-C	-5.36	98.19	109.34
1	B	632	SER	CB-CA-C	-5.35	100.39	110.67
1	B	472	TRP	N-CA-C	-5.35	98.52	107.99
1	B	149	PRO	N-CA-C	5.34	118.87	110.80
1	B	58	GLN	N-CA-C	-5.34	105.37	111.14
1	B	440	HIS	CB-CA-C	5.32	118.00	110.24
1	A	717	THR	CA-C-N	5.28	124.89	119.56
1	A	717	THR	C-N-CA	5.28	124.89	119.56
1	B	637	GLN	CB-CG-CD	5.27	121.56	112.60
1	A	320	GLY	N-CA-C	-5.27	100.69	113.18
1	A	563	MET	N-CA-CB	5.27	118.82	110.55
1	A	603	TYR	N-CA-CB	5.26	119.90	110.80
1	B	579	LYS	N-CA-C	-5.26	102.70	110.48
1	B	634	MET	N-CA-C	5.25	118.79	112.38
1	B	298	ARG	NH1-CZ-NH2	5.24	126.11	119.30
1	A	13	THR	CA-CB-CG2	5.23	119.39	110.50
1	B	148	GLN	CA-C-N	5.23	125.39	119.90
1	B	148	GLN	C-N-CA	5.23	125.39	119.90
1	A	595	ASN	CA-CB-CG	5.22	117.82	112.60
1	B	150	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	B	89	VAL	N-CA-CB	5.21	116.21	110.53
1	A	473	ILE	N-CA-CB	-5.20	105.12	111.67
1	B	380	ALA	CB-CA-C	-5.20	103.18	111.86
1	A	654	TYR	CA-C-N	5.19	125.26	119.87
1	A	654	TYR	C-N-CA	5.19	125.26	119.87
1	A	287	PRO	CB-CA-C	5.18	118.44	111.71
1	B	89	VAL	CA-C-O	5.17	126.75	120.85
1	B	606	ILE	CA-C-N	5.17	124.78	119.56
1	B	606	ILE	C-N-CA	5.17	124.78	119.56
1	B	578	GLN	CG-CD-NE2	5.17	124.15	116.40
1	B	39	VAL	N-CA-C	5.16	116.73	108.89
1	A	398	ARG	O-C-N	-5.15	116.88	123.06
1	A	491	ALA	N-CA-C	-5.15	101.37	109.25
1	B	15	LYS	O-C-N	5.14	127.37	122.07
1	A	300	ALA	CA-C-O	5.14	125.94	120.64
1	A	644	HIS	CA-C-N	5.14	124.94	119.28
1	A	644	HIS	C-N-CA	5.14	124.94	119.28
1	B	690	VAL	N-CA-CB	5.14	117.22	111.21
1	A	439	LYS	O-C-N	5.14	129.24	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	717	THR	O-C-N	-5.14	117.46	121.47
1	B	373	ASP	N-CA-C	5.14	117.16	110.43
1	B	20	ASP	N-CA-C	-5.13	102.10	110.20
1	B	107	ALA	N-CA-C	-5.13	105.77	111.36
1	B	587	LEU	N-CA-C	5.13	117.76	109.40
1	B	379	LYS	CG-CD-CE	5.12	123.08	111.30
1	A	557	GLY	CA-C-N	5.12	124.91	119.28
1	A	557	GLY	C-N-CA	5.12	124.91	119.28
1	B	546	MET	N-CA-CB	5.12	119.80	110.95
1	A	201	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	B	320	GLY	N-CA-C	-5.11	101.06	113.18
1	A	515	ILE	N-CA-C	5.10	119.50	113.22
1	A	600	PRO	N-CA-CB	5.10	107.86	103.27
1	B	61	VAL	N-CA-C	-5.09	102.93	109.30
1	A	262	GLU	N-CA-C	5.09	117.81	110.28
1	B	311	PRO	N-CA-C	5.09	120.46	113.84
1	B	315	ASN	CA-CB-CG	-5.09	107.51	112.60
1	A	622	ALA	N-CA-C	-5.08	103.07	110.08
1	A	54	PRO	O-C-N	-5.07	117.01	123.10
1	A	600	PRO	CA-C-O	-5.07	115.81	121.23
1	B	214	ILE	N-CA-C	5.07	115.63	107.98
1	A	73	THR	N-CA-CB	-5.05	103.02	110.49
1	B	262	GLU	O-C-N	5.05	129.05	122.89
1	B	648	ARG	N-CA-C	5.04	120.81	114.31
1	B	187	VAL	CB-CA-C	-5.03	104.61	111.15
1	B	83	LEU	N-CA-C	-5.03	106.66	112.89
1	B	397	ALA	N-CA-C	-5.03	100.31	108.41
1	B	692	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	703	TRP	N-CA-CB	-5.03	102.48	111.08
1	A	23	TRP	CA-C-O	5.02	125.86	120.38
1	B	210	LYS	CB-CA-C	-5.02	102.45	110.79
1	A	246	ILE	N-CA-C	-5.02	101.25	108.53
1	A	298	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	B	115	ALA	N-CA-C	5.02	118.89	112.87
1	B	262	GLU	CA-C-O	-5.01	115.54	121.16
1	B	13	THR	CA-CB-OG1	-5.01	102.09	109.60
1	B	148	GLN	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5664	0	5540	171	0
1	B	5683	0	5560	201	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	827	0	0	22	0
4	B	741	0	0	37	0
All	All	12921	0	11100	354	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 16.

All (354) 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:221:ILE:HD11	1:B:250:ASP:HB2	1.36	1.07
1:A:466:TPQ:H6	4:A:2530:HOH:O	1.57	1.01
1:A:463:VAL:HB	4:A:2530:HOH:O	1.60	0.99
1:A:216:ASP:HB3	1:A:219:LYS:HD2	1.44	0.98
1:B:8:VAL:CG2	1:B:9:PRO:HD2	1.93	0.98
1:B:221:ILE:CD1	1:B:250:ASP:HB2	1.98	0.93
1:B:12:LYS:O	1:B:16:GLU:HG2	1.71	0.91
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.55	0.89
1:A:304:LYS:H	1:B:315:ASN:HD21	1.21	0.87
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.57	0.87
1:B:619:ALA:CB	1:B:634:MET:HE2	2.05	0.87
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.42	0.83
1:B:65:ASP:O	1:B:66:ASN:HB2	1.78	0.83
1:B:642:ARG:CB	1:B:642:ARG:HH11	1.92	0.81
1:A:617:LYS:HE2	1:B:581:ASP:OD1	1.81	0.81
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.80	0.81
1:A:527:ILE:HD12	1:A:634:MET:HE2	1.61	0.81
1:B:580:PHE:H	1:B:637:GLN:HE21	1.28	0.80
1:A:71:SER:OG	1:A:73:THR:HG22	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:CD	1:A:203:GLU:H	1.88	0.79
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.12	0.79
1:A:315:ASN:HD21	1:B:304:LYS:H	1.29	0.79
1:A:527:ILE:HD12	1:A:634:MET:CE	2.12	0.78
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.65	0.78
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.27	0.78
1:B:366:ILE:HD13	1:B:634:MET:SD	2.24	0.78
1:B:498:LYS:O	1:B:517:HIS:HD2	1.66	0.78
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.66	0.78
1:B:725:LYS:C	4:B:2741:HOH:O	2.25	0.78
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.48	0.77
1:B:46:GLN:NE2	4:B:2059:HOH:O	1.77	0.77
1:A:553:ASN:ND2	1:A:555:ALA:H	1.83	0.77
1:A:580:PHE:H	1:A:637:GLN:HE21	1.30	0.76
1:A:189:LEU:HG	4:A:2312:HOH:O	1.86	0.75
1:B:525:GLN:HE22	1:B:620:GLN:H	1.34	0.75
1:B:644:HIS:HB3	4:B:2130:HOH:O	1.87	0.75
1:B:322:MET:HG3	4:B:2048:HOH:O	1.87	0.74
1:B:619:ALA:HB1	1:B:634:MET:HE2	1.67	0.73
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.69	0.73
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.70	0.73
1:B:94:HIS:HD2	1:B:96:LEU:H	1.35	0.72
1:B:381:TYR:CD2	4:B:2524:HOH:O	2.40	0.72
1:A:38:TYR:H	1:A:51:ASN:HD21	1.35	0.72
1:B:181:LYS:HE2	1:B:181:LYS:H	1.53	0.72
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.89	0.72
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.55	0.72
1:A:286:VAL:CG1	1:A:288:MET:HE3	2.20	0.71
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.71	0.71
1:B:203:GLU:CD	1:B:203:GLU:H	1.97	0.71
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.56	0.70
1:A:189:LEU:HB3	4:A:2039:HOH:O	1.91	0.70
1:B:7:MET:HG2	1:B:71:SER:HA	1.74	0.70
1:B:525:GLN:NE2	1:B:620:GLN:H	1.90	0.69
1:A:223:THR:HG22	1:A:246:ILE:O	1.93	0.69
1:B:144:LYS:HE3	4:B:2191:HOH:O	1.94	0.68
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.40	0.68
1:B:660:HIS:HA	4:B:2659:HOH:O	1.93	0.68
1:B:619:ALA:HB2	1:B:634:MET:HE2	1.74	0.68
1:A:7:MET:HE2	1:A:7:MET:HA	1.73	0.68
1:A:616:ALA:HA	4:A:2741:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:NZ	1:A:498:LYS:HB3	2.08	0.68
1:B:173:LYS:NZ	1:B:173:LYS:HB3	2.09	0.68
1:A:132:ASP:HB3	4:A:2218:HOH:O	1.94	0.67
1:B:527:ILE:HD12	1:B:634:MET:HE3	1.77	0.67
1:B:8:VAL:HG22	1:B:9:PRO:CD	2.24	0.66
1:A:439:LYS:HZ1	1:A:447:ASN:ND2	1.93	0.66
1:B:574:GLN:H	1:B:671:ASN:ND2	1.94	0.66
1:A:286:VAL:HG12	1:A:288:MET:CE	2.25	0.66
1:B:181:LYS:H	1:B:181:LYS:CE	2.08	0.66
1:B:38:TYR:H	1:B:51:ASN:HD21	1.44	0.66
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.26	0.65
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.32	0.65
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.12	0.65
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.31	0.65
1:B:379:LYS:HG3	1:B:381:TYR:CE1	2.31	0.65
1:B:38:TYR:H	1:B:51:ASN:ND2	1.95	0.64
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.62	0.64
1:A:368:PRO:HG3	1:A:634:MET:CE	2.27	0.64
1:B:322:MET:CG	4:B:2048:HOH:O	2.42	0.64
1:A:130:PRO:HG2	4:A:2214:HOH:O	1.98	0.63
1:A:536:VAL:H	1:A:541:ASN:HD21	1.44	0.63
1:B:216:ASP:OD1	1:B:218:LYS:N	2.32	0.63
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.64	0.62
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.11	0.62
1:B:65:ASP:O	1:B:66:ASN:CB	2.44	0.62
1:B:506:LYS:HE2	1:B:510:ARG:NH2	2.14	0.62
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.15	0.62
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.30	0.62
1:B:341:MET:HB3	4:B:2405:HOH:O	1.99	0.61
1:A:38:TYR:H	1:A:51:ASN:ND2	1.97	0.61
1:A:272:GLN:HB3	1:A:274:LYS:HD3	1.82	0.61
1:B:92:ARG:HD2	4:B:2189:HOH:O	1.99	0.61
1:A:592:ASN:HD21	1:A:676:ASN:ND2	1.97	0.61
1:B:181:LYS:HE2	1:B:181:LYS:N	2.16	0.61
1:A:203:GLU:OE1	1:A:204:GLU:HG3	2.00	0.61
1:B:580:PHE:H	1:B:637:GLN:NE2	1.97	0.60
1:A:286:VAL:CG1	1:A:288:MET:CE	2.79	0.60
1:B:225:LEU:HD22	1:B:381:TYR:CE2	2.37	0.60
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.67	0.60
1:A:274:LYS:HZ2	1:A:276:VAL:HG12	1.67	0.60
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:O	1:A:517:HIS:HD2	1.84	0.59
1:B:203:GLU:CD	1:B:203:GLU:N	2.60	0.59
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.35	0.59
1:A:62:VAL:HG23	1:A:69:TRP:HB2	1.84	0.59
1:A:498:LYS:HB3	1:A:498:LYS:HZ3	1.67	0.59
1:B:277:LYS:NZ	1:B:279:GLU:OE2	2.29	0.59
1:B:341:MET:HE2	4:B:2428:HOH:O	2.01	0.59
1:B:477:ASN:HD22	1:B:479:THR:H	1.51	0.59
1:B:366:ILE:HD12	1:B:631:LEU:HD13	1.84	0.58
1:B:717:THR:HB	1:B:720:LEU:HG	1.85	0.58
1:B:149:PRO:O	1:B:151:LYS:HG3	2.03	0.58
1:B:334:MET:HB3	4:B:2474:HOH:O	2.03	0.58
1:B:216:ASP:HB3	4:B:2271:HOH:O	2.03	0.58
1:B:632:SER:OG	1:B:661:ASP:OD2	2.20	0.58
1:B:94:HIS:CD2	1:B:96:LEU:H	2.21	0.57
1:B:477:ASN:HD22	1:B:477:ASN:C	2.13	0.57
1:A:718:PRO:HD2	4:B:2717:HOH:O	2.04	0.56
1:A:12:LYS:O	1:A:16:GLU:HG3	2.05	0.56
1:B:572:ASN:HD21	1:B:575:ASP:CG	2.13	0.56
1:B:629:HIS:CD2	4:B:2659:HOH:O	2.59	0.56
1:A:326:ARG:NH1	1:B:303:VAL:HG22	2.20	0.56
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.88	0.56
1:B:116:ASP:O	1:B:117:PHE:C	2.45	0.56
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.70	0.56
1:A:439:LYS:NZ	1:A:447:ASN:ND2	2.53	0.55
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.06	0.55
1:A:525:GLN:NE2	1:A:620:GLN:H	2.02	0.55
1:B:274:LYS:NZ	4:B:2339:HOH:O	2.38	0.55
1:B:359:GLU:HG3	4:B:2405:HOH:O	2.06	0.55
1:A:551:LYS:HE3	4:A:2687:HOH:O	2.06	0.55
1:A:203:GLU:CD	1:A:203:GLU:N	2.61	0.55
1:A:525:GLN:HE22	1:A:620:GLN:H	1.55	0.55
1:B:536:VAL:H	1:B:541:ASN:HD21	1.55	0.54
1:A:642:ARG:CB	1:A:642:ARG:HH11	2.19	0.54
1:B:679:ALA:HB2	4:B:2707:HOH:O	2.07	0.54
1:A:477:ASN:C	1:A:477:ASN:HD22	2.14	0.54
4:A:2034:HOH:O	1:B:42:LYS:HE2	2.06	0.54
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.90	0.53
1:B:223:THR:HG21	4:B:2311:HOH:O	2.07	0.53
1:A:76:ASN:O	1:A:80:GLN:HB2	2.08	0.53
1:A:439:LYS:NZ	1:A:447:ASN:HD21	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLN:NE2	4:B:2372:HOH:O	2.39	0.53
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.80	0.53
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.27	0.53
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.21	0.53
1:B:46:GLN:OE1	1:B:60:PRO:HG3	2.08	0.53
1:A:10:MET:HE3	1:A:70:VAL:CG1	2.38	0.53
1:B:196:GLN:HE22	1:B:222:THR:H	1.57	0.53
1:B:572:ASN:ND2	1:B:575:ASP:OD2	2.41	0.53
1:B:108:VAL:CG1	1:B:112:LYS:HE3	2.39	0.52
1:A:274:LYS:NZ	1:A:276:VAL:HG12	2.23	0.52
1:B:551:LYS:NZ	4:B:2579:HOH:O	2.41	0.52
1:A:62:VAL:CG2	1:A:69:TRP:HB2	2.39	0.52
1:A:498:LYS:NZ	1:A:498:LYS:CB	2.73	0.52
1:B:216:ASP:OD1	1:B:216:ASP:C	2.52	0.52
1:B:477:ASN:ND2	1:B:479:THR:H	2.07	0.52
1:A:615:VAL:HG23	1:B:582:PRO:HB2	1.92	0.52
1:A:237:LYS:NZ	1:A:239:ASP:CG	2.68	0.52
1:A:572:ASN:ND2	1:A:575:ASP:H	2.08	0.51
1:A:236:LEU:HD11	1:A:244:LYS:HE3	1.91	0.51
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.35	0.51
1:A:527:ILE:HD12	1:A:634:MET:HE3	1.91	0.51
1:A:210:LYS:HE2	1:A:214:ILE:O	2.10	0.51
1:A:400:LYS:HE3	1:B:449:SER:O	2.10	0.51
1:B:332:LEU:HD13	1:B:342:ILE:CD1	2.40	0.51
1:B:543:LEU:HD22	1:B:640:VAL:HG21	1.92	0.51
1:A:563:MET:HG3	1:B:370:GLY:HA3	1.93	0.51
1:A:7:MET:HE2	1:A:7:MET:CA	2.39	0.51
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.41	0.51
1:B:148:GLN:NE2	4:B:2201:HOH:O	2.41	0.51
1:B:627:ILE:HG23	1:B:628:TYR:N	2.26	0.51
1:A:7:MET:HB3	1:A:69:TRP:HB3	1.93	0.50
1:A:574:GLN:HG3	1:A:671:ASN:CG	2.37	0.50
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.92	0.50
1:A:322:MET:HE1	4:A:2057:HOH:O	2.11	0.50
1:B:574:GLN:H	1:B:671:ASN:HD22	1.57	0.50
1:A:63:MET:SD	1:A:68:ALA:HB2	2.51	0.50
1:A:642:ARG:HH11	1:A:642:ARG:HG2	1.77	0.50
1:B:626:TRP:O	1:B:627:ILE:C	2.53	0.50
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.95	0.50
1:A:181:LYS:HD2	4:A:2305:HOH:O	2.11	0.50
1:A:200:ASN:ND2	4:A:2323:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ASN:HD22	1:A:575:ASP:H	1.58	0.50
1:B:214:ILE:HD12	1:B:214:ILE:N	2.26	0.50
1:B:700:PRO:CG	4:B:2717:HOH:O	2.59	0.50
1:A:42:LYS:HD2	4:A:2058:HOH:O	2.10	0.49
1:A:580:PHE:H	1:A:637:GLN:NE2	2.04	0.49
1:A:288:MET:HE2	1:A:288:MET:HA	1.92	0.49
1:B:553:ASN:ND2	1:B:555:ALA:H	2.11	0.49
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.21	0.49
1:A:237:LYS:HZ2	1:A:239:ASP:CG	2.20	0.49
1:B:642:ARG:CG	1:B:642:ARG:NH1	2.74	0.49
1:A:286:VAL:CB	1:A:288:MET:HE3	2.43	0.49
1:A:608:TYR:HD1	4:A:2813:HOH:O	1.95	0.49
1:A:670:ASP:OD2	1:A:672:GLU:HG3	2.12	0.49
1:B:359:GLU:CD	1:B:648:ARG:NH2	2.71	0.49
1:B:700:PRO:HG3	4:B:2717:HOH:O	2.12	0.49
1:A:366:ILE:HD12	1:A:631:LEU:CD1	2.43	0.48
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.59	0.48
1:A:13:THR:HG22	1:A:75:ILE:HD11	1.96	0.48
1:A:209:VAL:HG13	1:A:214:ILE:HB	1.95	0.48
1:A:15:LYS:HE2	4:A:2022:HOH:O	2.13	0.48
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.48	0.48
1:B:653:LYS:HG2	1:B:654:TYR:CE2	2.48	0.48
1:A:587:LEU:HD23	1:A:604:GLN:HA	1.96	0.48
1:B:572:ASN:ND2	1:B:671:ASN:HD21	2.10	0.48
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.28	0.48
1:B:381:TYR:CE2	4:B:2524:HOH:O	2.64	0.48
1:B:506:LYS:HD3	1:B:506:LYS:C	2.39	0.48
1:A:579:LYS:HA	1:A:637:GLN:NE2	2.29	0.48
1:A:216:ASP:OD1	1:A:218:LYS:HB2	2.14	0.47
1:B:40:LYS:NZ	4:B:2047:HOH:O	2.31	0.47
1:B:7:MET:HE3	1:B:70:VAL:C	2.39	0.47
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.59	0.47
1:A:189:LEU:HD12	4:A:2261:HOH:O	2.15	0.47
1:A:237:LYS:NZ	1:A:239:ASP:OD1	2.47	0.47
1:A:326:ARG:HH12	1:B:303:VAL:CG2	2.22	0.47
1:B:132:ASP:H	1:B:148:GLN:HE22	1.61	0.47
1:A:348:ASN:ND2	1:A:351:GLY:H	2.12	0.47
1:B:642:ARG:HB2	1:B:642:ARG:NH1	2.28	0.47
1:A:51:ASN:N	1:A:51:ASN:HD22	2.12	0.47
1:A:216:ASP:CB	1:A:219:LYS:HD2	2.31	0.47
1:B:116:ASP:O	1:B:118:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASP:HB3	1:B:332:LEU:O	2.15	0.47
1:A:516:ASP:HB3	1:A:519:ILE:HB	1.96	0.47
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.50	0.47
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.80	0.47
1:B:633:PHE:HA	1:B:639:TRP:CZ2	2.49	0.47
1:B:630:ARG:HA	4:B:2659:HOH:O	2.15	0.46
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.30	0.46
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.45	0.46
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.28	0.46
1:B:379:LYS:NZ	4:B:2443:HOH:O	2.48	0.46
1:B:11:ASP:O	1:B:15:LYS:HD3	2.16	0.46
1:B:225:LEU:HD22	1:B:381:TYR:HE2	1.80	0.46
1:A:117:PHE:HE1	4:A:2192:HOH:O	1.99	0.46
1:A:723:LEU:HD23	1:B:298:ARG:HD3	1.98	0.46
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.15	0.46
1:B:239:ASP:OD1	1:B:239:ASP:C	2.57	0.46
1:B:259:HIS:HE1	1:B:289:THR:O	1.99	0.46
1:A:720:LEU:HD23	1:A:720:LEU:HA	1.79	0.46
1:B:67:LYS:HB2	4:B:2085:HOH:O	2.15	0.46
1:B:130:PRO:HB3	4:B:2427:HOH:O	2.16	0.46
1:A:599:ASN:ND2	4:A:2730:HOH:O	2.48	0.46
1:B:203:GLU:OE2	1:B:204:GLU:HG3	2.15	0.45
1:A:332:LEU:HD21	1:A:427:ILE:HG21	1.99	0.45
1:B:7:MET:HE2	1:B:7:MET:HB3	1.81	0.45
1:B:369:TYR:CD1	1:B:379:LYS:HG2	2.51	0.45
1:B:546:MET:HE3	1:B:587:LEU:HD12	1.98	0.45
1:A:24:ASP:OD2	1:B:40:LYS:NZ	2.49	0.45
1:A:214:ILE:N	1:A:214:ILE:HD12	2.31	0.45
1:B:644:HIS:CD2	4:B:2679:HOH:O	2.68	0.45
1:A:151:LYS:NZ	4:A:2249:HOH:O	2.50	0.45
1:A:106:GLN:NE2	1:A:169:LEU:O	2.35	0.45
1:B:549:VAL:HG11	1:B:566:ASN:HD22	1.81	0.45
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.99	0.45
1:A:532:LEU:HD11	1:A:683:MET:HE2	1.99	0.45
1:A:679:ALA:HB2	4:A:2669:HOH:O	2.16	0.45
1:B:76:ASN:O	1:B:80:GLN:HB2	2.17	0.45
1:B:117:PHE:CZ	1:B:121:THR:HB	2.52	0.45
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.32	0.45
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.75	0.44
1:B:546:MET:HE3	1:B:587:LEU:CD1	2.48	0.44
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:VAL:HG12	1:A:616:ALA:N	2.32	0.44
1:B:617:LYS:HA	4:B:2643:HOH:O	2.17	0.44
1:B:359:GLU:CD	1:B:648:ARG:HH22	2.24	0.44
1:A:578:GLN:HA	1:A:636:LYS:HD2	1.99	0.44
1:B:221:ILE:N	1:B:221:ILE:HD12	2.33	0.44
1:A:642:ARG:HG3	1:A:643:TYR:N	2.32	0.44
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.52	0.44
1:B:611:GLY:HA3	4:B:2641:HOH:O	2.18	0.44
1:A:574:GLN:H	1:A:671:ASN:ND2	2.16	0.44
1:A:8:VAL:HG13	1:A:13:THR:OG1	2.18	0.43
1:B:369:TYR:CD2	1:B:524:HIS:HB3	2.53	0.43
1:B:62:VAL:HG12	1:B:64:LYS:HG3	1.99	0.43
1:B:302:ALA:C	1:B:303:VAL:HG23	2.42	0.43
1:B:366:ILE:HD11	1:B:627:ILE:HD11	2.01	0.43
1:B:7:MET:HE3	1:B:70:VAL:CA	2.49	0.43
1:A:572:ASN:HD22	1:A:572:ASN:C	2.27	0.43
1:A:574:GLN:HG3	1:A:671:ASN:HB2	2.00	0.43
1:A:276:VAL:O	1:A:277:LYS:HB2	2.18	0.43
1:A:286:VAL:HB	1:A:288:MET:HE3	2.00	0.43
1:B:525:GLN:HE22	1:B:620:GLN:N	2.09	0.43
1:B:59:VAL:HA	1:B:60:PRO:HD3	1.83	0.43
1:B:439:LYS:HZ1	1:B:447:ASN:ND2	2.16	0.43
1:B:619:ALA:HB2	1:B:634:MET:HB3	2.00	0.43
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.27	0.43
1:A:210:LYS:HE2	1:A:210:LYS:HA	1.99	0.42
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.54	0.42
1:A:477:ASN:HD22	1:A:479:THR:H	1.67	0.42
1:B:209:VAL:HG13	1:B:214:ILE:HB	2.01	0.42
1:A:237:LYS:HD3	1:A:240:ALA:HB2	2.01	0.42
1:A:239:ASP:OD1	1:A:239:ASP:C	2.62	0.42
1:B:439:LYS:NZ	1:B:447:ASN:ND2	2.66	0.42
1:A:348:ASN:HD22	1:A:348:ASN:C	2.28	0.42
1:A:298:ARG:HA	1:B:722:ALA:O	2.20	0.42
1:B:214:ILE:HD11	1:B:286:VAL:HG21	2.01	0.42
1:B:396:ILE:HG23	1:B:401:ASP:HB2	2.00	0.42
1:B:669:LYS:HA	1:B:669:LYS:CE	2.49	0.42
1:B:699:MET:HA	1:B:700:PRO:HD3	1.74	0.42
1:A:321:ASP:HB3	1:A:332:LEU:O	2.20	0.42
1:B:379:LYS:CG	1:B:381:TYR:CE1	3.02	0.42
1:A:365:MET:HE3	1:A:365:MET:HB2	1.98	0.42
1:B:76:ASN:ND2	4:B:2100:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:HG2	1:B:283:VAL:HG22	2.01	0.42
1:B:222:THR:HB	1:B:245:VAL:CG1	2.50	0.42
1:A:410:ASN:OD1	1:A:424:PRO:HA	2.20	0.42
1:A:580:PHE:N	1:A:637:GLN:HE21	2.08	0.42
1:A:224:PRO:C	1:A:225:LEU:HG	2.44	0.42
1:A:181:LYS:O	1:A:182:ASP:HB2	2.20	0.42
1:A:291:ARG:HH11	1:A:291:ARG:HD3	1.71	0.42
1:B:124:THR:HG22	1:B:188:LEU:HD21	2.02	0.41
1:B:129:LEU:HD12	1:B:130:PRO:HD2	2.02	0.41
1:B:587:LEU:HD23	1:B:604:GLN:HA	2.01	0.41
1:B:595:ASN:ND2	1:B:599:ASN:H	2.18	0.41
1:B:642:ARG:NH1	1:B:642:ARG:HG2	2.35	0.41
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.56	0.41
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.21	0.41
1:B:670:ASP:HB2	4:B:2699:HOH:O	2.19	0.41
1:A:334:MET:HE1	1:A:393:THR:OG1	2.19	0.41
1:A:523:THR:HB	4:A:2651:HOH:O	2.20	0.41
1:A:574:GLN:HG3	1:A:671:ASN:CB	2.50	0.41
1:B:229:TYR:CZ	1:B:231:ASP:HA	2.55	0.41
1:A:639:TRP:HB2	1:A:682:TRP:HB2	2.03	0.41
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.36	0.41
1:B:92:ARG:HD3	4:B:2190:HOH:O	2.20	0.41
1:B:64:LYS:HB2	4:B:2085:HOH:O	2.21	0.41
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.51	0.41
1:B:139:PHE:O	1:B:143:ASN:HA	2.21	0.41
1:B:486:ALA:O	1:B:699:MET:HE2	2.20	0.41
1:B:574:GLN:HE22	1:B:669:LYS:NZ	2.19	0.41
1:B:627:ILE:CG2	1:B:628:TYR:N	2.84	0.41
1:B:669:LYS:HA	1:B:669:LYS:HE3	2.03	0.41
1:A:40:LYS:NZ	4:A:2056:HOH:O	2.39	0.41
1:A:178:GLN:HA	1:A:179:PRO:HD3	1.91	0.41
1:A:498:LYS:HB3	1:A:498:LYS:HZ2	1.86	0.41
1:B:241:ARG:HG2	1:B:270:LEU:HB2	2.02	0.41
1:A:65:ASP:O	1:A:66:ASN:HB2	2.20	0.40
1:A:104:ILE:O	1:A:108:VAL:HG23	2.21	0.40
1:B:619:ALA:HB1	1:B:634:MET:CE	2.45	0.40
1:A:117:PHE:CZ	1:A:121:THR:HB	2.57	0.40
1:A:204:GLU:HG3	1:A:204:GLU:H	1.62	0.40
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.70	0.40
1:A:62:VAL:HG23	1:A:62:VAL:O	2.22	0.40
1:A:483:ASP:CG	1:A:705:HIS:HD1	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ILE:CD1	1:B:634:MET:HE3	2.47	0.40
1:B:717:THR:HA	1:B:718:PRO:HD3	1.90	0.40
1:A:181:LYS:HG3	1:A:182:ASP:CG	2.47	0.40
1:B:439:LYS:NZ	1:B:447:ASN:HD21	2.20	0.40
1:A:553:ASN:HD21	1:A:555:ALA:H	1.66	0.40
1:A:643:TYR:O	1:A:644:HIS:CD2	2.74	0.40
1:B:181:LYS:O	1:B:182:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	715/727 (98%)	691 (97%)	24 (3%)	0	100	100
1	B	717/727 (99%)	694 (97%)	21 (3%)	2 (0%)	36	30
All	All	1432/1454 (98%)	1385 (97%)	45 (3%)	2 (0%)	48	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	536	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/615 (99%)	581 (95%)	28 (5%)	24	18
1	B	611/615 (99%)	583 (95%)	28 (5%)	24	18
All	All	1220/1230 (99%)	1164 (95%)	56 (5%)	24	18

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ASP
1	A	32	LEU
1	A	64	LYS
1	A	71	SER
1	A	163	ILE
1	A	199	ILE
1	A	202	SER
1	A	203	GLU
1	A	204	GLU
1	A	209	VAL
1	A	210	LYS
1	A	237	LYS
1	A	239	ASP
1	A	273	LYS
1	A	274	LYS
1	A	350	ASN
1	A	445	GLN
1	A	477	ASN
1	A	566	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	615	VAL
1	A	617	LYS
1	A	627	ILE
1	A	642	ARG
1	A	707	LEU
1	B	6	HIS
1	B	11	ASP
1	B	16	GLU
1	B	22	GLN
1	B	34	LYS
1	B	47	THR
1	B	71	SER

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Mol	Chain	Res	Type
1	B	80	GLN
1	B	118	LYS
1	B	129	LEU
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	209	VAL
1	B	211	LYS
1	B	218	LYS
1	B	239	ASP
1	B	322	MET
1	B	396	ILE
1	B	477	ASN
1	B	539	GLU
1	B	574	GLN
1	B	595	ASN
1	B	613	HIS
1	B	632	SER
1	B	642	ARG
1	B	669	LYS
1	B	699	MET

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	53	GLN
1	A	76	ASN
1	A	97	ASN
1	A	148	GLN
1	A	161	HIS
1	A	170	GLN
1	A	196	GLN
1	A	200	ASN
1	A	201	ASN
1	A	307	GLN
1	A	315	ASN
1	A	324	HIS
1	A	348	ASN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS

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Mol	Chain	Res	Type
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	637	GLN
1	A	644	HIS
1	A	660	HIS
1	A	666	GLN
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	80	GLN
1	B	94	HIS
1	B	97	ASN
1	B	148	GLN
1	B	172	ASN
1	B	196	GLN
1	B	200	ASN
1	B	201	ASN
1	B	238	GLN
1	B	263	ASN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	445	GLN
1	B	447	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	525	GLN
1	B	541	ASN
1	B	553	ASN
1	B	566	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

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Mol	Chain	Res	Type
1	B	613	HIS
1	B	637	GLN
1	B	644	HIS
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 ⓘ

2 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	1	13,14,15	2.91	6 (46%)	13,19,21	1.30	1 (7%)
1	TPQ	B	466	1	13,14,15	2.91	6 (46%)	13,19,21	1.24	2 (15%)

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	1	-	2/5/22/24	0/1/1/1
1	TPQ	B	466	1	-	0/5/22/24	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	C1-C2	-5.24	1.41	1.49
1	B	466	TPQ	C1-C2	-5.22	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	O5-C5	-5.07	1.11	1.24
1	B	466	TPQ	O5-C5	-5.04	1.11	1.24
1	A	466	TPQ	O2-C2	-4.97	1.11	1.24
1	B	466	TPQ	O2-C2	-4.94	1.11	1.24
1	B	466	TPQ	C4-C5	-2.97	1.38	1.47
1	A	466	TPQ	C4-C5	-2.85	1.39	1.47
1	A	466	TPQ	C6-C1	2.11	1.39	1.34
1	B	466	TPQ	C6-C1	2.11	1.39	1.34
1	A	466	TPQ	CB-C1	2.07	1.54	1.50
1	B	466	TPQ	C6-C5	-2.02	1.39	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	TPQ	C6-C1-C2	-2.57	116.83	118.66
1	B	466	TPQ	C6-C1-C2	-2.42	116.93	118.66
1	B	466	TPQ	CB-C1-C2	2.01	122.08	118.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TPQ	O-C-CA-CB
1	A	466	TPQ	N-CA-CB-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466	TPQ	1	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	717/727 (98%)	-0.26	13 (1%) 67 69	15, 27, 46, 62	0
1	B	719/727 (98%)	-0.06	26 (3%) 46 46	17, 29, 51, 65	0
All	All	1436/1454 (98%)	-0.16	39 (2%) 56 58	15, 28, 49, 65	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	ALA	4.6
1	B	119	PRO	4.6
1	A	670	ASP	4.5
1	B	115	ALA	4.2
1	B	301	PRO	4.1
1	A	239	ASP	4.0
1	B	629	HIS	3.9
1	A	189	LEU	3.8
1	B	644	HIS	3.7
1	B	118	LYS	3.7
1	B	239	ASP	3.3
1	A	644	HIS	3.2
1	B	215	THR	3.0
1	B	120	ASN	2.9
1	B	381	TYR	2.8
1	A	203	GLU	2.7
1	A	72	ASP	2.6
1	A	147	ASP	2.6
1	B	6	HIS	2.5
1	B	642	ARG	2.4
1	B	303	VAL	2.4
1	A	207	ALA	2.4
1	B	144	LYS	2.4
1	B	117	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	148	GLN	2.3
1	B	65	ASP	2.3
1	B	7	MET	2.3
1	A	148	GLN	2.3
1	B	178	GLN	2.2
1	B	197	ASN	2.2
1	B	109	GLU	2.2
1	B	76	ASN	2.1
1	B	443	MET	2.1
1	A	66	ASN	2.1
1	B	231	ASP	2.1
1	B	80	GLN	2.0
1	A	642	ARG	2.0
1	A	629	HIS	2.0
1	A	119	PRO	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	14/15	0.92	0.11	21,37,51,52	0
1	TPQ	B	466	14/15	0.94	0.09	23,45,52,53	0

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	A	803	1/1	0.93	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	803	1/1	0.97	0.12	51,51,51,51	0
3	CA	B	802	1/1	0.99	0.03	25,25,25,25	0
2	CU	A	801	1/1	0.99	0.02	30,30,30,30	0
3	CA	A	802	1/1	1.00	0.02	23,23,23,23	0
2	CU	B	801	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.