



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:14 PM UTC

PDB ID : 1QAL / pdb_00001qal
Title : THE ACTIVE SITE BASE CONTROLS COFACTOR REACTIVITY IN ES-
CHERICHIA COLI AMINE OXIDASE : X-RAY CRYSTALLOGRAPHIC
STUDIES WITH MUTATIONAL VARIANTS
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S.E.; McPherson, M.J.
Deposited on : 1999-03-19
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<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

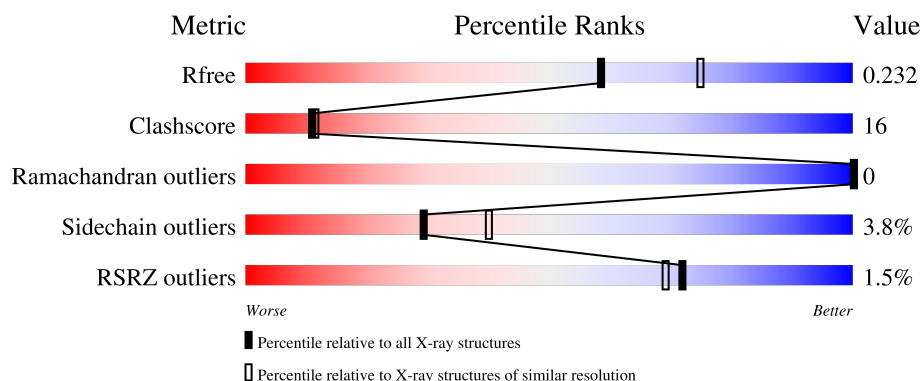
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	721	59% 33% 7%
1	B	721	2% 61% 31% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12909 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	719	Total	C	N	O	S	0	0	1
			5665	3602	966	1075	22			
1	B	721	Total	C	N	O	S	0	0	0
			5692	3618	971	1081	22			

There are 4 discrepancies between the modelled and reference sequences:

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

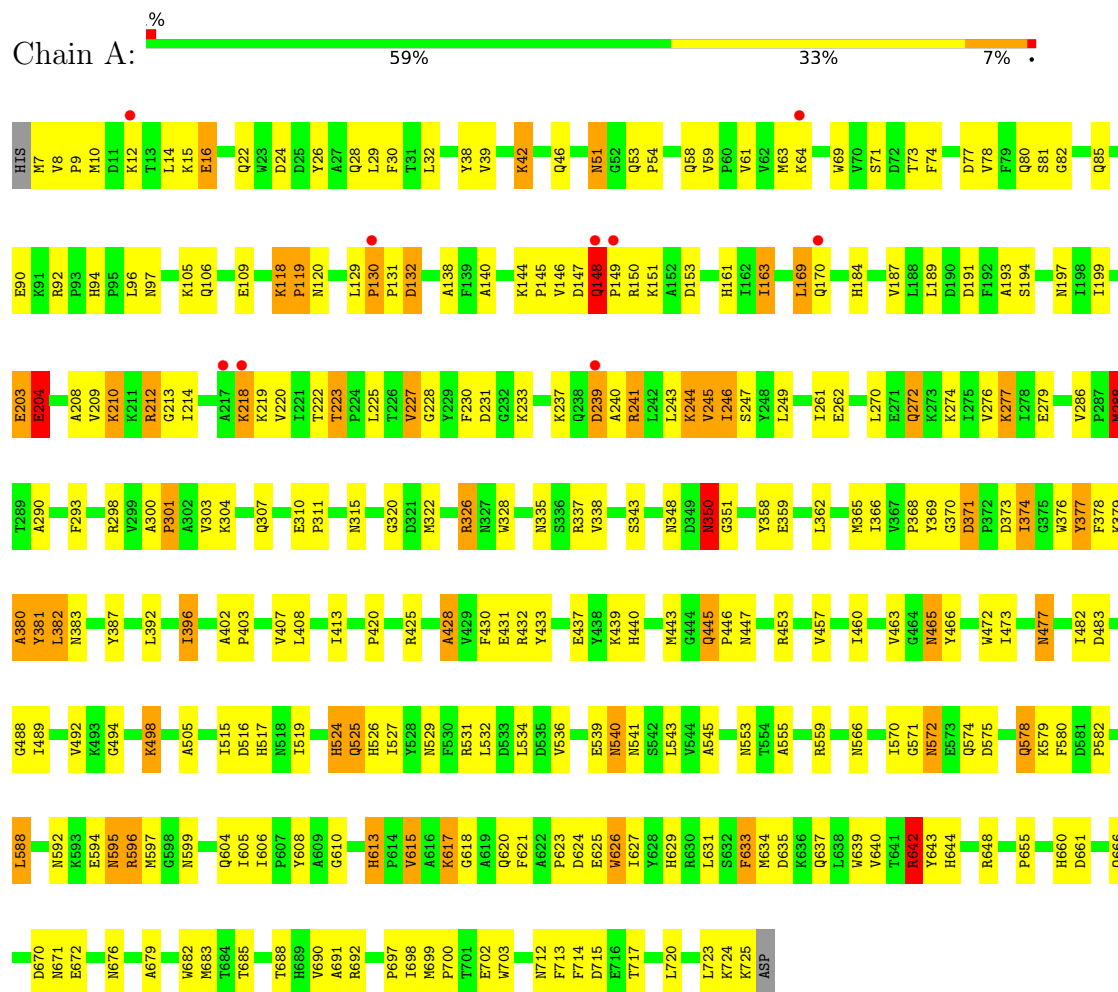
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	801	Total 801	O 801	0	0
4	B	745	Total 745	O 745	0	0

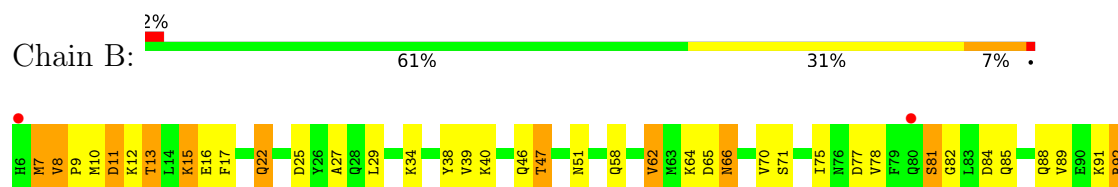
3 Residue-property plots

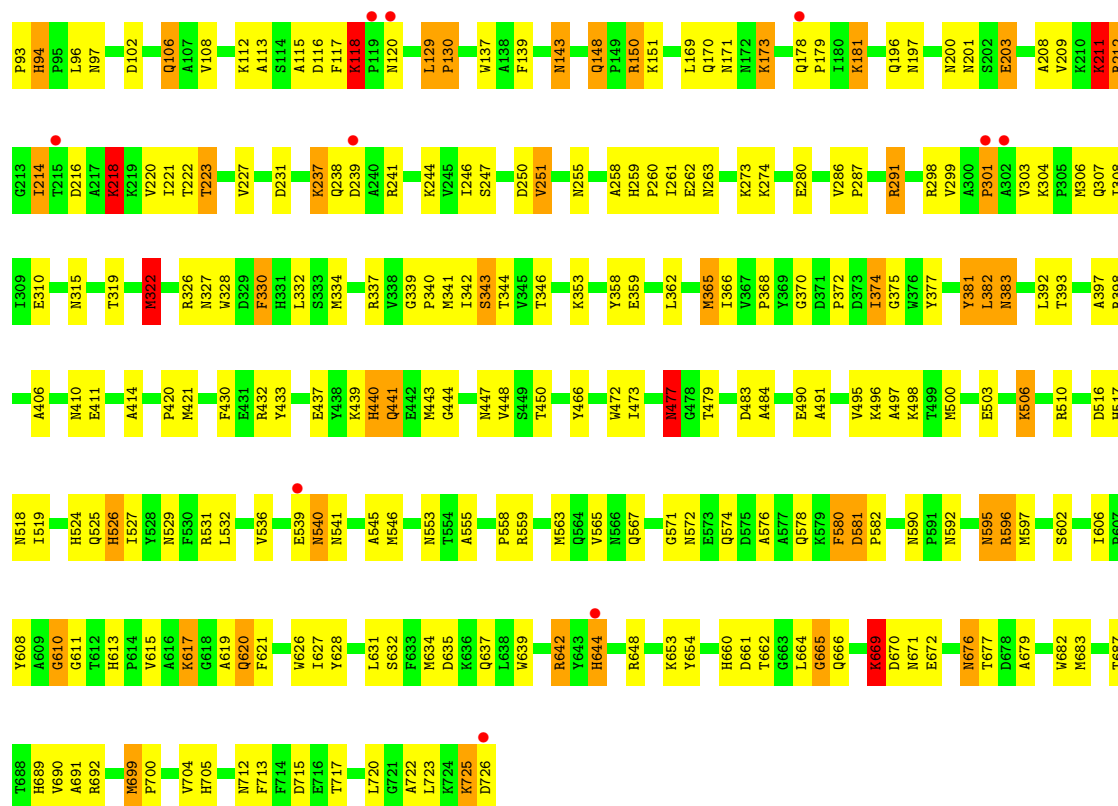
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 166.52Å 79.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.20) 93.4 (20.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.241 0.177 , 0.232	Depositor DCC
R_{free} test set	2923 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.9	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	12909	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, CA, CU

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	1/5794 (0.0%)	2.06	198/7888 (2.5%)
1	B	0.76	0/5822	2.01	194/7923 (2.4%)
All	All	0.77	1/11616 (0.0%)	2.03	392/15811 (2.5%)

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 (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	ARG	NE-CZ-NH2	-16.32	104.51	119.20
1	A	596	ARG	NE-CZ-NH2	-15.31	105.42	119.20
1	A	307	GLN	OE1-CD-NE2	-13.70	108.90	122.60
1	A	642	ARG	NH1-CZ-NH2	13.40	136.72	119.30
1	A	666	GLN	OE1-CD-NE2	-12.64	109.96	122.60
1	A	129	LEU	CA-C-N	12.63	128.88	119.66
1	A	129	LEU	C-N-CA	12.63	128.88	119.66
1	B	725	LYS	CA-C-O	-12.49	107.00	121.11
1	A	197	ASN	OD1-CG-ND2	-12.38	110.22	122.60
1	A	596	ARG	NH1-CZ-NH2	11.80	134.65	119.30
1	A	130	PRO	O-C-N	11.79	126.73	121.31
1	B	610	GLY	CA-C-O	-10.79	114.68	122.45
1	B	15	LYS	CA-C-O	-10.74	109.54	120.82
1	A	350	ASN	OD1-CG-ND2	10.53	133.13	122.60
1	A	130	PRO	CB-CA-C	-10.22	101.78	111.39
1	B	15	LYS	O-C-N	10.13	132.51	122.07
1	A	524	HIS	CE1-NE2-CD2	10.00	119.00	109.00
1	B	118	LYS	CA-C-N	9.72	129.35	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	LYS	C-N-CA	9.72	129.35	119.24
1	A	692	ARG	NE-CZ-NH2	-9.64	110.52	119.20
1	B	692	ARG	NE-CZ-NH2	-9.60	110.56	119.20
1	B	291	ARG	NE-CZ-NH2	9.57	127.81	119.20
1	B	170	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	B	129	LEU	N-CA-C	-9.06	96.64	109.24
1	B	571	GLY	N-CA-C	9.01	124.58	114.67
1	B	578	GLN	OE1-CD-NE2	-8.95	113.65	122.60
1	B	22	GLN	OE1-CD-NE2	-8.93	113.67	122.60
1	A	46	GLN	OE1-CD-NE2	-8.78	113.82	122.60
1	A	571	GLY	N-CA-C	8.72	124.71	114.16
1	B	291	ARG	NE-CZ-NH1	-8.63	112.87	121.50
1	B	526	HIS	CE1-NE2-CD2	8.61	117.61	109.00
1	B	725	LYS	O-C-N	8.48	134.22	123.19
1	A	138	ALA	CA-C-O	8.26	129.31	120.55
1	B	699	MET	N-CA-C	8.24	120.02	109.72
1	B	620	GLN	OE1-CD-NE2	-8.19	114.41	122.60
1	B	7	MET	N-CA-CB	-8.17	98.44	111.43
1	A	53	GLN	OE1-CD-NE2	-8.10	114.50	122.60
1	B	85	GLN	OE1-CD-NE2	8.04	130.64	122.60
1	B	524	HIS	CE1-NE2-CD2	7.94	116.94	109.00
1	A	130	PRO	N-CA-CB	7.92	107.62	103.19
1	B	118	LYS	O-C-N	7.92	129.10	121.66
1	A	298	ARG	NE-CZ-NH2	-7.89	112.09	119.20
1	B	691	ALA	N-CA-C	7.73	119.92	110.41
1	A	626	TRP	O-C-N	7.72	130.30	122.12
1	A	119	PRO	CA-C-N	-7.68	110.28	123.25
1	A	119	PRO	C-N-CA	-7.68	110.28	123.25
1	A	566	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	B	699	MET	CA-C-O	7.64	125.93	119.66
1	B	713	PHE	N-CA-C	-7.56	103.12	111.36
1	B	310	GLU	CA-C-N	7.55	127.26	119.56
1	B	310	GLU	C-N-CA	7.55	127.26	119.56
1	A	524	HIS	ND1-CE1-NE2	-7.53	100.87	108.40
1	A	515	ILE	CA-C-O	7.53	127.18	119.20
1	A	588	LEU	N-CA-C	-7.47	94.76	107.99
1	B	326	ARG	CD-NE-CZ	7.46	134.85	124.40
1	B	689	HIS	N-CA-C	7.46	121.13	107.99
1	A	540	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	A	604	GLN	OE1-CD-NE2	7.43	130.03	122.60
1	A	106	GLN	OE1-CD-NE2	-7.42	115.18	122.60
1	A	713	PHE	N-CA-C	-7.39	102.60	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	578	GLN	CG-CD-NE2	7.37	127.45	116.40
1	B	58	GLN	N-CA-CB	7.29	120.65	110.07
1	B	92	ARG	NE-CZ-NH1	-7.27	114.23	121.50
1	A	371	ASP	CA-C-O	7.25	126.93	120.19
1	A	615	VAL	CA-C-O	7.25	128.90	120.71
1	A	118	LYS	CA-C-N	7.24	128.89	119.84
1	A	118	LYS	C-N-CA	7.24	128.89	119.84
1	A	307	GLN	CG-CD-OE1	7.22	135.23	120.80
1	B	13	THR	CA-C-O	7.20	128.38	120.82
1	A	288	MET	N-CA-C	7.19	122.18	113.41
1	A	525	GLN	OE1-CD-NE2	7.18	129.78	122.60
1	A	120	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	A	594	GLU	CA-C-O	-7.15	113.07	121.44
1	A	724	LYS	O-C-N	7.12	134.39	123.00
1	A	524	HIS	CG-CD2-NE2	-7.12	100.08	107.20
1	B	397	ALA	CA-C-O	7.11	128.32	120.92
1	A	402	ALA	O-C-N	7.07	126.90	121.88
1	B	13	THR	O-C-N	-7.06	114.79	122.07
1	B	653	LYS	CA-C-O	-7.03	113.10	120.55
1	A	465	ASN	OD1-CG-ND2	7.00	129.60	122.60
1	A	132	ASP	O-C-N	7.00	131.12	122.86
1	A	534	LEU	CA-C-O	-7.00	113.32	121.16
1	A	220	VAL	CA-C-O	-6.99	112.48	120.65
1	B	89	VAL	N-CA-CB	6.97	118.88	110.31
1	B	327	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	B	262	GLU	N-CA-C	6.91	119.75	110.35
1	A	326	ARG	CA-CB-CG	-6.89	100.32	114.10
1	B	617	LYS	CA-C-O	6.84	127.79	119.38
1	A	310	GLU	CA-C-N	6.83	126.53	119.56
1	A	310	GLU	C-N-CA	6.83	126.53	119.56
1	B	602	SER	N-CA-CB	-6.83	100.78	111.56
1	A	194	SER	N-CA-CB	6.82	120.10	109.94
1	A	626	TRP	CA-C-O	-6.82	113.33	120.55
1	A	53	GLN	CA-C-N	6.81	126.78	119.76
1	A	53	GLN	C-N-CA	6.81	126.78	119.76
1	A	362	LEU	N-CA-C	-6.80	100.22	110.28
1	A	439	LYS	O-C-N	6.78	130.75	123.56
1	B	143	ASN	OD1-CG-ND2	6.77	129.37	122.60
1	A	241	ARG	CA-C-O	-6.77	113.67	120.98
1	B	359	GLU	CB-CA-C	6.76	122.03	109.86
1	B	337	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	B	263	ASN	OD1-CG-ND2	-6.72	115.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	MET	N-CA-C	6.71	118.57	109.24
1	B	129	LEU	CB-CA-C	6.71	119.04	109.38
1	B	116	ASP	OD1-CG-OD2	-6.68	106.86	122.90
1	B	590	ASN	OD1-CG-ND2	6.68	129.28	122.60
1	A	130	PRO	CA-C-O	-6.67	116.10	120.90
1	B	526	HIS	ND1-CE1-NE2	-6.67	101.73	108.40
1	B	200	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	A	594	GLU	O-C-N	6.65	131.80	123.15
1	A	380	ALA	O-C-N	-6.65	117.38	123.50
1	B	66	ASN	OD1-CG-ND2	6.64	129.25	122.60
1	B	211	LYS	CA-C-O	6.63	127.68	119.05
1	A	374	ILE	N-CA-C	6.63	117.33	110.36
1	B	106	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	B	47	THR	CA-CB-OG1	6.62	119.53	109.60
1	A	447	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	138	ALA	O-C-N	-6.58	115.15	122.12
1	B	381	TYR	N-CA-C	6.58	119.42	108.96
1	A	660	HIS	O-C-N	6.57	130.16	123.26
1	B	322	MET	CA-C-O	6.56	127.95	120.54
1	A	153	ASP	N-CA-C	-6.55	99.02	109.76
1	A	526	HIS	CE1-NE2-CD2	6.52	115.52	109.00
1	A	488	GLY	O-C-N	-6.52	116.66	122.85
1	A	144	LYS	CA-C-O	6.52	125.56	119.76
1	A	61	VAL	N-CA-C	-6.51	101.18	109.58
1	A	692	ARG	NH1-CZ-NH2	6.50	127.75	119.30
1	B	39	VAL	N-CA-C	6.50	117.83	108.48
1	B	10	MET	N-CA-C	6.48	118.88	111.11
1	A	566	ASN	CB-CG-OD1	6.47	133.74	120.80
1	B	92	ARG	CA-C-O	6.47	125.54	119.59
1	B	106	GLN	CG-CD-NE2	6.47	126.10	116.40
1	A	28	GLN	OE1-CD-NE2	6.46	129.06	122.60
1	B	437	GLU	N-CA-C	-6.46	104.24	111.28
1	A	148	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	B	148	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	B	81	SER	N-CA-C	6.42	117.94	111.07
1	A	328	TRP	CA-C-O	6.42	129.06	121.36
1	B	22	GLN	CG-CD-OE1	6.39	133.59	120.80
1	B	258	ALA	CA-C-N	-6.38	115.83	122.85
1	B	258	ALA	C-N-CA	-6.38	115.83	122.85
1	B	648	ARG	NH1-CZ-NH2	-6.36	111.04	119.30
1	A	290	ALA	O-C-N	6.35	130.74	122.93
1	B	420	PRO	N-CA-CB	6.33	108.82	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	THR	CA-C-N	-6.33	114.61	122.84
1	A	688	THR	C-N-CA	-6.33	114.61	122.84
1	B	672	GLU	CA-C-O	6.31	128.81	121.87
1	B	712	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	398	ARG	O-C-N	-6.27	116.09	123.11
1	A	408	LEU	CA-C-O	6.26	127.26	120.43
1	A	223	THR	CA-C-N	6.25	127.19	120.13
1	A	223	THR	C-N-CA	6.25	127.19	120.13
1	B	255	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	B	362	LEU	N-CA-C	-6.24	101.05	110.28
1	A	463	VAL	CA-C-O	6.23	127.05	120.51
1	B	662	THR	N-CA-C	-6.22	105.00	112.59
1	B	635	ASP	N-CA-C	6.22	120.87	113.16
1	B	328	TRP	O-C-N	6.21	130.02	123.06
1	B	540	ASN	N-CA-C	6.21	118.30	108.67
1	B	358	TYR	CA-C-O	6.20	127.00	120.42
1	B	218	LYS	CA-C-O	6.20	127.01	119.38
1	B	440	HIS	CA-CB-CG	-6.20	107.60	113.80
1	B	117	PHE	CA-C-O	-6.19	114.75	121.44
1	B	441	GLN	O-C-N	-6.18	115.42	122.84
1	A	28	GLN	CB-CG-CD	-6.15	102.14	112.60
1	B	473	ILE	N-CA-C	6.14	116.67	107.51
1	B	472	TRP	N-CA-C	-6.14	97.12	107.99
1	A	539	GLU	N-CA-C	6.12	117.74	111.14
1	A	261	ILE	N-CA-C	-6.11	97.91	106.53
1	B	704	VAL	N-CA-CB	6.09	121.99	111.39
1	B	524	HIS	CG-CD2-NE2	-6.08	101.12	107.20
1	A	301	PRO	N-CD-CG	-6.07	94.10	103.20
1	A	145	PRO	CA-C-O	6.05	128.24	121.34
1	A	39	VAL	N-CA-C	6.05	117.30	108.53
1	B	78	VAL	N-CA-C	6.04	116.24	110.74
1	B	237	LYS	CB-CA-C	6.04	118.86	110.16
1	B	220	VAL	CA-C-O	6.03	127.53	120.71
1	A	193	ALA	N-CA-CB	6.03	119.08	110.16
1	A	617	LYS	CA-C-O	6.03	126.82	119.11
1	A	660	HIS	CA-C-O	-6.02	115.00	121.38
1	B	398	ARG	CA-C-O	6.02	126.97	120.95
1	A	408	LEU	O-C-N	-6.01	116.48	123.27
1	B	11	ASP	O-C-N	6.00	128.27	122.03
1	B	531	ARG	CD-NE-CZ	-5.98	116.03	124.40
1	B	611	GLY	CA-C-O	-5.98	115.76	121.62
1	B	130	PRO	O-C-N	5.96	128.50	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ILE	N-CA-C	-5.95	96.95	109.34
1	B	374	ILE	N-CA-C	5.95	117.40	110.62
1	B	8	VAL	CA-C-N	5.94	126.87	119.98
1	B	8	VAL	C-N-CA	5.94	126.87	119.98
1	A	335	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	B	273	LYS	CA-CB-CG	-5.93	102.23	114.10
1	A	428	ALA	CA-C-O	-5.93	114.43	120.71
1	A	691	ALA	N-CA-C	5.92	117.97	110.33
1	B	94	HIS	CA-C-N	5.91	125.59	119.56
1	B	94	HIS	C-N-CA	5.91	125.59	119.56
1	B	7	MET	N-CA-C	5.91	118.40	109.41
1	B	666	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	B	218	LYS	CA-CB-CG	5.90	125.90	114.10
1	A	58	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	B	212	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	343	SER	N-CA-C	5.89	119.16	109.85
1	A	407	VAL	CA-C-N	-5.88	114.61	122.72
1	A	407	VAL	C-N-CA	-5.88	114.61	122.72
1	B	526	HIS	CG-CD2-NE2	-5.87	101.33	107.20
1	B	576	ALA	CA-C-O	-5.85	112.06	119.31
1	A	432	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	A	387	TYR	CA-C-O	-5.84	112.28	118.77
1	B	578	GLN	N-CA-C	5.84	116.80	108.74
1	A	377	TYR	N-CA-C	5.84	119.22	111.75
1	A	26	TYR	CA-C-O	5.83	126.73	120.55
1	A	69	TRP	CA-C-O	-5.83	114.29	121.11
1	B	377	TYR	N-CA-C	5.82	119.20	111.75
1	A	378	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	446	PRO	N-CA-CB	5.80	108.49	103.27
1	B	151	LYS	CA-C-O	5.79	128.51	121.68
1	A	191	ASP	O-C-N	5.78	128.99	122.22
1	A	246	ILE	N-CA-C	-5.78	100.15	108.53
1	B	503	GLU	CA-C-O	-5.78	114.39	120.63
1	A	425	ARG	CD-NE-CZ	-5.77	116.32	124.40
1	B	580	PHE	CA-C-O	5.77	126.67	120.32
1	A	472	TRP	N-CA-C	-5.76	98.35	108.20
1	A	373	ASP	CA-C-N	5.75	128.02	120.60
1	A	373	ASP	C-N-CA	5.75	128.02	120.60
1	B	690	VAL	N-CA-C	-5.75	99.60	107.99
1	A	698	ILE	O-C-N	-5.75	116.87	123.07
1	A	212	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	54	PRO	O-C-N	-5.74	116.09	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	A	515	ILE	O-C-N	-5.72	116.48	122.20
1	A	498	LYS	N-CA-C	-5.71	106.86	113.88
1	B	644	HIS	CA-C-N	5.71	125.39	119.56
1	B	644	HIS	C-N-CA	5.71	125.39	119.56
1	A	290	ALA	CA-C-O	-5.71	114.25	120.81
1	B	247	SER	N-CA-C	5.69	119.00	109.95
1	A	380	ALA	CA-C-O	5.68	126.60	120.63
1	A	473	ILE	N-CA-C	5.68	116.04	107.80
1	A	648	ARG	N-CA-CB	-5.68	102.34	110.80
1	A	633	PHE	O-C-N	5.66	129.75	122.39
1	A	433	TYR	N-CA-C	-5.66	101.91	110.28
1	B	495	VAL	CA-C-O	-5.66	116.03	121.63
1	A	714	PHE	CA-C-O	-5.64	114.11	121.73
1	B	251	VAL	CA-CB-CG1	5.64	119.98	110.40
1	B	421	MET	N-CA-CB	-5.63	101.34	110.81
1	B	359	GLU	CA-C-O	5.63	127.07	120.43
1	A	262	GLU	N-CA-C	5.62	118.61	110.28
1	B	491	ALA	N-CA-C	-5.62	99.95	108.67
1	B	654	TYR	CA-C-N	5.62	125.72	119.87
1	B	654	TYR	C-N-CA	5.62	125.72	119.87
1	A	473	ILE	N-CA-CB	-5.62	104.38	111.46
1	A	392	LEU	CA-C-N	-5.61	112.74	120.71
1	A	392	LEU	C-N-CA	-5.61	112.74	120.71
1	A	666	GLN	CG-CD-OE1	5.61	132.02	120.80
1	B	322	MET	O-C-N	-5.59	116.84	123.22
1	A	132	ASP	CA-C-O	-5.59	115.47	121.56
1	A	231	ASP	O-C-N	-5.58	115.16	122.59
1	A	247	SER	N-CA-C	5.58	118.65	109.72
1	B	437	GLU	CA-C-O	5.58	126.46	120.55
1	A	145	PRO	O-C-N	-5.58	116.28	123.03
1	B	365	MET	CA-C-O	-5.58	115.48	121.45
1	A	688	THR	N-CA-C	-5.57	99.44	108.52
1	B	433	TYR	N-CA-C	-5.57	102.04	110.28
1	B	116	ASP	O-C-N	5.56	130.07	122.46
1	A	204	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	184	HIS	CB-CG-CD2	5.55	138.41	131.20
1	A	482	ILE	O-C-N	5.54	127.96	122.97
1	B	260	PRO	CB-CA-C	-5.54	103.72	110.98
1	A	148	GLN	CG-CD-NE2	5.54	124.71	116.40
1	B	13	THR	CA-CB-OG1	-5.53	101.30	109.60
1	B	565	VAL	N-CA-C	5.51	115.83	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	VAL	O-C-N	5.50	129.65	122.94
1	B	301	PRO	N-CA-CB	5.47	108.42	103.33
1	B	383	ASN	N-CA-C	5.47	117.67	111.11
1	B	503	GLU	N-CA-C	5.46	117.94	111.33
1	A	140	ALA	O-C-N	5.45	128.60	122.22
1	A	272	GLN	N-CA-C	-5.45	106.13	112.89
1	B	343	SER	N-CA-C	5.45	118.45	109.85
1	B	596	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	B	150	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	690	VAL	N-CA-C	-5.44	99.32	107.37
1	B	129	LEU	CA-C-N	5.44	125.98	120.38
1	B	129	LEU	C-N-CA	5.44	125.98	120.38
1	B	441	GLN	CA-C-O	5.44	127.80	121.11
1	A	245	VAL	CA-CB-CG1	5.43	119.64	110.40
1	A	129	LEU	N-CA-C	-5.43	97.76	109.01
1	A	685	THR	OG1-CB-CG2	-5.42	98.46	109.30
1	B	669	LYS	N-CA-C	5.42	117.18	111.28
1	A	233	LYS	O-C-N	5.41	129.43	122.39
1	A	635	ASP	O-C-N	5.41	129.11	122.34
1	A	635	ASP	N-CA-C	5.41	119.99	113.17
1	A	338	VAL	N-CA-C	5.41	118.09	112.90
1	B	631	LEU	N-CA-C	5.41	117.99	107.71
1	B	524	HIS	CA-CB-CG	-5.41	108.39	113.80
1	B	477	ASN	N-CA-C	5.40	119.58	113.15
1	A	163	ILE	CA-CB-CG1	5.40	119.58	110.40
1	B	581	ASP	CA-C-N	5.39	125.11	119.82
1	B	581	ASP	C-N-CA	5.39	125.11	119.82
1	A	488	GLY	CA-C-O	5.39	127.59	122.25
1	B	259	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	618	GLY	CA-C-O	-5.38	116.79	121.04
1	B	218	LYS	O-C-N	-5.38	115.22	122.43
1	B	414	ALA	CA-C-O	-5.38	114.83	120.80
1	B	546	MET	N-CA-CB	5.37	119.63	110.87
1	B	223	THR	CB-CA-C	5.35	116.61	109.65
1	B	410	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	B	692	ARG	NH1-CZ-NH2	5.34	126.24	119.30
1	A	277	LYS	O-C-N	5.33	129.68	122.59
1	A	446	PRO	O-C-N	-5.33	116.88	123.01
1	B	699	MET	CA-C-N	5.30	125.22	119.76
1	B	699	MET	C-N-CA	5.30	125.22	119.76
1	A	191	ASP	CA-C-O	-5.29	114.12	120.10
1	A	413	ILE	O-C-N	5.28	128.34	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	VAL	CA-CB-CG1	5.27	119.36	110.40
1	B	84	ASP	N-CA-C	-5.27	99.92	108.41
1	A	631	LEU	N-CA-CB	-5.26	101.12	110.60
1	B	201	ASN	OD1-CG-ND2	-5.26	117.33	122.60
1	B	25	ASP	OD1-CG-OD2	5.26	135.53	122.90
1	B	46	GLN	CA-C-O	5.26	125.65	119.28
1	A	337	ARG	CA-C-O	-5.25	114.93	120.55
1	A	381	TYR	N-CA-C	5.25	116.81	108.67
1	B	648	ARG	N-CA-CB	-5.25	103.39	110.95
1	B	497	ALA	CB-CA-C	-5.23	100.71	109.65
1	B	62	VAL	CA-C-O	5.23	126.02	120.48
1	A	16	GLU	OE1-CD-OE2	-5.22	110.36	122.90
1	A	230	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	337	ARG	NH1-CZ-NH2	-5.22	112.52	119.30
1	B	197	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	382	LEU	N-CA-C	-5.21	99.49	108.56
1	A	505	ALA	N-CA-C	5.20	117.35	111.11
1	A	661	ASP	N-CA-C	5.20	116.63	109.15
1	B	648	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	665	GLY	N-CA-C	-5.20	106.12	112.77
1	B	432	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	465	ASN	CA-C-O	-5.19	111.98	120.80
1	B	628	TYR	O-C-N	5.18	127.61	122.12
1	B	330	PHE	CA-C-O	-5.17	115.91	121.45
1	B	382	LEU	N-CA-C	-5.17	98.88	108.24
1	A	712	ASN	N-CA-C	-5.17	105.62	112.24
1	A	578	GLN	N-CA-CB	-5.17	103.40	111.56
1	B	150	ARG	N-CA-C	-5.17	102.00	109.59
1	B	669	LYS	CA-CB-CG	-5.17	103.77	114.10
1	B	58	GLN	N-CA-C	-5.16	105.56	111.14
1	B	212	ARG	O-C-N	5.16	128.70	122.35
1	A	85	GLN	CG-CD-NE2	5.16	124.14	116.40
1	B	82	GLY	N-CA-C	-5.16	107.89	114.85
1	A	605	ILE	CB-CG1-CD1	-5.15	102.98	113.80
1	A	703	TRP	N-CA-C	5.15	117.99	109.85
1	A	90	GLU	CA-C-O	-5.14	115.29	120.84
1	A	606	ILE	CA-C-N	5.14	124.80	119.56
1	A	606	ILE	C-N-CA	5.14	124.80	119.56
1	A	189	LEU	O-C-N	-5.13	116.68	122.12
1	A	92	ARG	CA-C-N	5.13	125.37	119.83
1	A	92	ARG	C-N-CA	5.13	125.37	119.83
1	B	116	ASP	CA-C-O	-5.13	113.27	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	THR	O-C-N	-5.12	116.24	123.11
1	B	518	ASN	CA-C-O	-5.12	114.27	120.32
1	B	676	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	92	ARG	CA-C-O	5.11	125.91	120.08
1	B	346	THR	CA-C-O	5.11	127.44	121.46
1	A	457	VAL	N-CA-C	-5.11	99.16	107.28
1	B	689	HIS	ND1-CE1-NE2	-5.10	103.30	108.40
1	A	130	PRO	N-CA-C	5.10	115.37	110.47
1	A	445	GLN	O-C-N	-5.10	117.57	121.55
1	A	213	GLY	O-C-N	5.10	128.87	122.39
1	A	227	VAL	N-CA-C	5.10	120.05	113.07
1	A	244	LYS	N-CA-C	-5.09	102.53	110.42
1	A	531	ARG	CA-C-O	-5.09	115.25	120.54
1	A	82	GLY	N-CA-C	-5.09	107.52	114.64
1	A	39	VAL	CB-CA-C	-5.08	103.08	110.81
1	A	440	HIS	N-CA-CB	5.08	118.98	110.59
1	A	420	PRO	N-CA-CB	5.08	107.72	103.25
1	A	42	LYS	CB-CG-CD	5.08	122.97	111.30
1	B	484	ALA	CA-C-O	-5.07	114.88	120.36
1	B	606	ILE	CA-C-N	5.07	124.68	119.56
1	B	606	ILE	C-N-CA	5.07	124.68	119.56
1	A	320	GLY	N-CA-C	-5.06	101.18	113.18
1	B	113	ALA	CB-CA-C	-5.06	100.00	109.72
1	A	51	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	169	LEU	CA-C-O	5.05	125.77	120.42
1	B	308	ILE	N-CA-C	-5.03	100.64	107.99
1	B	241	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	A	119	PRO	N-CA-C	5.03	122.82	112.47
1	A	413	ILE	CA-C-O	-5.03	116.16	121.44
1	B	450	THR	N-CA-C	-5.02	101.45	109.23
1	B	102	ASP	O-C-N	5.01	127.86	122.15
1	B	115	ALA	O-C-N	5.01	129.15	122.43
1	B	479	THR	CA-C-O	-5.01	116.10	121.56
1	A	494	GLY	O-C-N	5.01	127.30	122.99
1	B	85	GLN	O-C-N	5.01	128.85	122.39
1	A	483	ASP	O-C-N	-5.01	116.68	123.19
1	B	722	ALA	CA-C-N	5.01	127.96	120.95
1	B	722	ALA	C-N-CA	5.01	127.96	120.95

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	5665	0	5542	203	0
1	B	5692	0	5566	199	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	801	0	0	28	3
4	B	745	0	0	27	2
All	All	12909	0	11108	370	4

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 (370) 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:A:642:ARG:HD2	4:A:1498:HOH:O	1.34	1.27
1:A:625:GLU:O	1:A:629:HIS:CD2	2.11	1.02
1:A:130:PRO:HG2	4:A:1115:HOH:O	1.61	0.99
1:B:725:LYS:O	1:B:726:ASP:OD1	1.83	0.95
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.31	0.95
1:A:625:GLU:O	1:A:629:HIS:HD2	1.48	0.94
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.49	0.92
1:B:181:LYS:HE2	1:B:181:LYS:H	1.33	0.91
1:A:304:LYS:H	1:B:315:ASN:HD21	1.17	0.90
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.52	0.89
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.21	0.86
1:A:368:PRO:HG3	1:A:634:MET:CE	2.04	0.86
1:A:130:PRO:O	4:A:1115:HOH:O	1.92	0.85
1:A:596:ARG:NH2	1:B:516:ASP:OD1	2.10	0.84
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.07	0.84
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.60	0.84
1:A:131:PRO:HB3	1:A:148:GLN:NE2	1.94	0.83
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.27	0.83
1:B:642:ARG:HH11	1:B:642:ARG:CB	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.80	0.81
1:B:525:GLN:HE22	1:B:620:GLN:H	1.27	0.81
1:B:181:LYS:H	1:B:181:LYS:CE	1.95	0.80
1:A:431:GLU:HB3	1:B:306:MET:HE1	1.64	0.79
1:A:326:ARG:NH2	1:B:303:VAL:HG13	1.98	0.79
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.13	0.79
1:B:540:ASN:HB3	1:B:676:ASN:ND2	1.97	0.78
1:B:617:LYS:HA	4:B:1051:HOH:O	1.84	0.77
1:B:580:PHE:H	1:B:637:GLN:HE21	1.33	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:A:624:ASP:C	1:A:629:HIS:NE2	2.44	0.76
1:A:624:ASP:HA	1:A:629:HIS:CE1	2.20	0.76
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.68	0.75
1:B:525:GLN:NE2	1:B:620:GLN:H	1.84	0.75
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.68	0.75
1:A:225:LEU:HD22	4:A:1575:HOH:O	1.86	0.75
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.00	0.75
1:A:580:PHE:H	1:A:637:GLN:HE21	1.33	0.75
1:B:94:HIS:HD2	1:B:96:LEU:H	1.34	0.75
1:B:94:HIS:HB3	1:B:97:ASN:HD21	1.51	0.74
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.21	0.74
1:A:38:TYR:H	1:A:51:ASN:ND2	1.86	0.74
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.21	0.74
1:A:24:ASP:OD2	1:B:40:LYS:NZ	2.20	0.73
1:A:532:LEU:HD11	1:A:683:MET:HE2	1.70	0.73
1:A:38:TYR:H	1:A:51:ASN:HD21	1.34	0.73
1:A:203:GLU:CD	1:A:203:GLU:H	1.97	0.72
1:A:315:ASN:HD21	1:B:304:LYS:H	1.37	0.72
1:A:350:ASN:OD1	4:A:1074:HOH:O	2.08	0.71
1:B:203:GLU:CD	1:B:203:GLU:H	2.00	0.70
1:B:27:ALA:HA	4:B:827:HOH:O	1.92	0.70
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.74	0.70
1:A:288:MET:HE2	1:A:288:MET:HA	1.72	0.69
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.73	0.69
1:A:241:ARG:HG2	1:A:270:LEU:HD12	1.74	0.69
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.74	0.69
1:B:679:ALA:HB2	4:B:1177:HOH:O	1.93	0.69
1:B:574:GLN:H	1:B:671:ASN:ND2	1.90	0.69
1:B:700:PRO:HD2	4:B:1012:HOH:O	1.93	0.68
1:A:525:GLN:HE22	1:A:620:GLN:H	1.41	0.68
1:B:38:TYR:H	1:B:51:ASN:HD21	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:THR:HB	1:B:720:LEU:HG	1.75	0.68
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.94	0.67
1:A:527:ILE:HD12	1:A:634:MET:HE2	1.77	0.67
1:B:580:PHE:H	1:B:637:GLN:NE2	1.93	0.66
1:B:12:LYS:O	1:B:16:GLU:HG2	1.94	0.66
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.77	0.66
1:A:210:LYS:HE2	1:A:214:ILE:O	1.96	0.66
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.60	0.66
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.31	0.66
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.26	0.65
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.78	0.65
1:B:670:ASP:HB2	4:B:1055:HOH:O	1.95	0.65
1:A:223:THR:HG22	1:A:246:ILE:O	1.97	0.65
1:A:553:ASN:ND2	1:A:555:ALA:H	1.94	0.65
1:A:617:LYS:HE2	1:B:581:ASP:OD1	1.97	0.65
1:B:173:LYS:NZ	1:B:173:LYS:HB3	2.12	0.64
1:A:498:LYS:O	1:A:517:HIS:HD2	1.81	0.64
1:A:286:VAL:CG1	1:A:288:MET:HE3	2.28	0.64
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.06	0.63
1:B:38:TYR:H	1:B:51:ASN:ND2	1.97	0.63
1:A:572:ASN:ND2	1:A:575:ASP:H	1.96	0.63
1:A:527:ILE:HD12	1:A:634:MET:CE	2.28	0.63
1:B:441:GLN:OE1	1:B:447:ASN:HB2	1.98	0.63
1:A:570:ILE:HD13	1:A:578:GLN:HE22	1.62	0.63
1:B:120:ASN:CG	4:B:851:HOH:O	2.42	0.63
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.64	0.62
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.63	0.62
1:A:149:PRO:HB3	1:A:170:GLN:HE21	1.65	0.62
1:B:506:LYS:CE	1:B:510:ARG:HH22	2.12	0.62
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.82	0.62
1:A:536:VAL:H	1:A:541:ASN:HD21	1.46	0.62
1:B:221:ILE:N	1:B:221:ILE:HD12	2.15	0.61
1:A:379:LYS:HG3	4:A:1575:HOH:O	1.99	0.61
1:B:148:GLN:NE2	4:B:1287:HOH:O	2.34	0.61
1:A:381:TYR:CE2	4:A:1575:HOH:O	2.51	0.61
1:A:71:SER:OG	1:A:73:THR:HG22	2.00	0.61
1:A:365:MET:CE	1:A:383:ASN:HD22	2.14	0.60
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.83	0.60
1:B:443:MET:HE3	1:B:444:GLY:H	1.67	0.60
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.50	0.59
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.17	0.59
1:A:237:LYS:HD3	1:A:240:ALA:HB2	1.83	0.59
1:A:326:ARG:HH22	1:B:303:VAL:HG13	1.64	0.59
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.18	0.59
1:A:326:ARG:NH1	1:B:303:VAL:HG22	2.17	0.59
1:A:12:LYS:O	1:A:16:GLU:HG3	2.03	0.59
1:A:525:GLN:NE2	1:A:620:GLN:H	2.01	0.58
1:A:7:MET:HE2	1:A:7:MET:HA	1.85	0.58
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.68	0.58
1:B:527:ILE:HD12	1:B:634:MET:HE3	1.85	0.58
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.03	0.58
1:B:334:MET:HB3	4:B:1464:HOH:O	2.02	0.58
1:B:572:ASN:ND2	1:B:671:ASN:HD21	1.95	0.58
1:A:222:THR:HB	1:A:245:VAL:HG13	1.85	0.57
1:B:334:MET:HE2	1:B:411:GLU:HG3	1.86	0.57
1:A:322:MET:HG2	4:A:1375:HOH:O	2.03	0.57
1:B:65:ASP:O	1:B:66:ASN:HB2	2.02	0.57
1:B:477:ASN:HD22	1:B:477:ASN:C	2.10	0.57
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.85	0.57
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.68	0.57
1:A:365:MET:HE2	1:A:383:ASN:ND2	2.19	0.56
1:B:130:PRO:HG3	4:B:1172:HOH:O	2.05	0.56
1:A:723:LEU:HD23	1:B:298:ARG:HD3	1.88	0.56
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.71	0.55
1:B:307:GLN:OE1	4:B:1189:HOH:O	2.18	0.55
1:A:29:LEU:HD13	1:A:30:PHE:N	2.21	0.55
1:A:203:GLU:CD	1:A:203:GLU:N	2.64	0.55
1:A:670:ASP:OD2	1:A:672:GLU:HG3	2.06	0.55
1:B:723:LEU:HD23	1:B:726:ASP:OD1	2.07	0.55
1:A:620:GLN:HB2	1:B:563:MET:HE2	1.87	0.55
1:A:77:ASP:O	1:A:81:SER:HB3	2.07	0.55
1:A:477:ASN:C	1:A:477:ASN:HD22	2.14	0.54
1:A:326:ARG:NH2	1:B:303:VAL:HG22	2.22	0.54
1:A:572:ASN:HD21	1:A:575:ASP:CG	2.16	0.54
1:A:624:ASP:HA	1:A:629:HIS:NE2	2.23	0.53
1:B:596:ARG:NH1	1:B:596:ARG:HG2	2.24	0.53
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.21	0.53
1:A:225:LEU:HD21	1:A:381:TYR:OH	2.09	0.53
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.44	0.53
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.43	0.53
1:B:216:ASP:OD1	1:B:218:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ARG:HG2	1:B:596:ARG:HH11	1.74	0.53
1:B:239:ASP:OD1	1:B:239:ASP:C	2.51	0.53
1:B:291:ARG:CG	1:B:291:ARG:HH11	2.22	0.53
1:A:582:PRO:C	1:B:615:VAL:HG12	2.34	0.53
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.09	0.53
1:A:150:ARG:O	1:A:169:LEU:HB2	2.09	0.53
1:B:498:LYS:O	1:B:517:HIS:HD2	1.92	0.52
1:A:642:ARG:HB2	1:A:642:ARG:HH11	1.73	0.52
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.38	0.52
1:A:326:ARG:HH22	1:B:303:VAL:HG22	1.74	0.52
1:A:10:MET:O	1:A:14:LEU:HD23	2.10	0.52
1:A:274:LYS:NZ	1:A:276:VAL:HG12	2.24	0.52
1:B:94:HIS:CD2	1:B:96:LEU:H	2.22	0.52
1:B:553:ASN:ND2	1:B:555:ALA:H	2.06	0.52
1:A:203:GLU:OE2	1:A:204:GLU:HG3	2.09	0.52
1:B:540:ASN:HB3	1:B:676:ASN:HD22	1.73	0.52
1:B:322:MET:CG	4:B:1160:HOH:O	2.57	0.52
1:B:322:MET:HE3	1:B:330:PHE:C	2.35	0.52
1:A:498:LYS:NZ	1:A:498:LYS:HB3	2.24	0.52
1:A:29:LEU:HD13	1:A:30:PHE:O	2.09	0.52
1:B:27:ALA:C	4:B:827:HOH:O	2.53	0.52
1:B:572:ASN:HB2	1:B:671:ASN:ND2	2.24	0.52
1:A:10:MET:CG	1:A:14:LEU:HD23	2.40	0.52
1:A:130:PRO:HD2	4:A:1536:HOH:O	2.09	0.52
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.92	0.51
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.28	0.51
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.35	0.51
1:A:679:ALA:HB2	4:A:1524:HOH:O	2.10	0.51
1:B:322:MET:HG3	4:B:1160:HOH:O	2.10	0.51
1:A:272:GLN:HE22	1:A:274:LYS:HZ1	1.57	0.51
1:A:210:LYS:HE2	1:A:210:LYS:HA	1.92	0.51
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.91	0.51
1:B:669:LYS:HZ1	1:B:669:LYS:HA	1.76	0.51
1:A:326:ARG:CZ	1:B:303:VAL:HG22	2.41	0.51
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.46	0.51
1:B:725:LYS:O	1:B:726:ASP:CG	2.53	0.51
1:A:700:PRO:HD2	4:A:975:HOH:O	2.11	0.51
1:A:365:MET:HE2	1:A:383:ASN:HD22	1.76	0.51
1:A:579:LYS:HA	1:A:637:GLN:NE2	2.26	0.51
1:B:527:ILE:CD1	1:B:634:MET:HE3	2.40	0.50
1:A:94:HIS:HB3	1:A:97:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:TYR:O	1:A:644:HIS:CD2	2.64	0.50
1:B:223:THR:HG22	1:B:246:ILE:O	2.11	0.50
1:A:625:GLU:C	1:A:629:HIS:CD2	2.89	0.50
1:B:291:ARG:HH11	1:B:291:ARG:HG3	1.77	0.50
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.94	0.50
1:A:8:VAL:HG22	1:A:9:PRO:CD	2.41	0.50
1:B:669:LYS:HA	1:B:669:LYS:NZ	2.27	0.49
1:A:10:MET:HG3	1:A:14:LEU:CD2	2.43	0.49
1:A:371:ASP:HB3	1:A:376:TRP:HB3	1.94	0.49
1:A:580:PHE:H	1:A:637:GLN:NE2	2.05	0.49
1:A:276:VAL:O	1:A:277:LYS:HB2	2.11	0.49
1:B:203:GLU:CD	1:B:203:GLU:N	2.70	0.49
1:B:353:LYS:HE2	4:B:1031:HOH:O	2.12	0.49
1:A:223:THR:HG21	4:A:1302:HOH:O	2.11	0.49
1:B:7:MET:HE3	1:B:70:VAL:C	2.38	0.49
1:B:299:VAL:O	1:B:301:PRO:HD3	2.13	0.49
1:A:237:LYS:NZ	1:A:239:ASP:OD1	2.45	0.49
1:A:595:ASN:HD22	1:A:595:ASN:C	2.21	0.48
1:A:15:LYS:HE2	4:A:1264:HOH:O	2.12	0.48
1:A:725:LYS:N	4:A:1525:HOH:O	2.46	0.48
1:B:62:VAL:HG12	1:B:64:LYS:HG3	1.95	0.48
1:A:38:TYR:N	1:A:51:ASN:HD21	2.08	0.48
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.49	0.48
1:A:365:MET:CE	1:A:383:ASN:ND2	2.76	0.48
1:A:460:ILE:HG21	1:B:439:LYS:HE2	1.95	0.48
1:B:17:PHE:O	1:B:34:LYS:HE2	2.13	0.48
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.95	0.48
1:B:7:MET:HE3	1:B:70:VAL:CA	2.43	0.48
1:B:196:GLN:HE22	1:B:222:THR:H	1.62	0.48
1:A:437:GLU:OE2	1:B:700:PRO:HB3	2.14	0.48
1:A:572:ASN:HD22	1:A:575:ASP:H	1.61	0.48
1:A:592:ASN:HD21	1:A:676:ASN:ND2	2.04	0.47
1:B:529:ASN:HA	1:B:683:MET:O	2.14	0.47
1:B:92:ARG:HD2	4:B:1400:HOH:O	2.14	0.47
1:A:63:MET:HG3	4:A:1350:HOH:O	2.14	0.47
1:A:161:HIS:HB3	4:A:1256:HOH:O	2.15	0.47
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.44	0.47
1:B:532:LEU:HD11	1:B:683:MET:HE2	1.97	0.47
1:B:536:VAL:H	1:B:541:ASN:HD21	1.62	0.47
1:A:219:LYS:HD2	4:A:1185:HOH:O	2.14	0.47
1:A:572:ASN:HD22	1:A:572:ASN:C	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HB3	1:A:170:GLN:HB3	1.96	0.47
1:B:644:HIS:CD2	4:B:1003:HOH:O	2.68	0.47
1:B:644:HIS:HD2	4:B:1003:HOH:O	1.97	0.47
1:A:272:GLN:NE2	1:A:274:LYS:NZ	2.63	0.47
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.45	0.47
1:A:642:ARG:HH12	1:A:672:GLU:HB3	1.80	0.46
1:B:22:GLN:HG3	4:B:838:HOH:O	2.14	0.46
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.30	0.46
1:A:595:ASN:C	1:A:595:ASN:ND2	2.73	0.46
1:B:642:ARG:NE	1:B:677:THR:OG1	2.48	0.46
1:B:108:VAL:CG1	1:B:112:LYS:HE3	2.46	0.46
1:A:218:LYS:HE2	4:A:1571:HOH:O	2.15	0.46
1:B:118:LYS:HB3	1:B:118:LYS:HE2	1.41	0.46
1:B:660:HIS:HA	4:B:1242:HOH:O	2.16	0.46
1:A:105:LYS:O	1:A:109:GLU:HG3	2.15	0.46
1:A:29:LEU:HD13	1:A:30:PHE:C	2.41	0.46
1:A:642:ARG:NH2	4:A:1398:HOH:O	2.48	0.46
1:B:642:ARG:CG	1:B:642:ARG:NH1	2.77	0.46
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.46	0.46
1:B:595:ASN:HB2	1:B:715:ASP:OD1	2.16	0.46
1:A:626:TRP:HA	1:A:629:HIS:HD2	1.81	0.46
1:A:209:VAL:HG12	1:A:214:ILE:HB	1.96	0.45
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.30	0.45
1:A:74:PHE:CE1	1:A:78:VAL:HG21	2.52	0.45
1:B:8:VAL:HG22	1:B:9:PRO:CD	2.47	0.45
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.87	0.45
1:B:365:MET:HE2	1:B:383:ASN:HD22	1.81	0.45
1:B:699:MET:HA	1:B:700:PRO:HD3	1.74	0.45
1:A:613:HIS:CE1	1:A:702:GLU:HG3	2.51	0.45
1:B:108:VAL:HG13	1:B:112:LYS:HE3	1.99	0.45
1:A:541:ASN:HD22	1:A:588:LEU:HD21	1.81	0.45
1:A:574:GLN:H	1:A:671:ASN:ND2	2.14	0.45
1:B:29:LEU:HD11	1:B:40:LYS:HB3	1.99	0.45
1:A:697:PRO:HD2	1:B:720:LEU:HD11	1.98	0.45
1:A:218:LYS:HZ3	1:A:218:LYS:HB2	1.82	0.45
1:B:173:LYS:NZ	1:B:173:LYS:CB	2.78	0.45
1:B:580:PHE:N	1:B:637:GLN:HE21	2.07	0.45
1:A:187:VAL:HG22	1:A:243:LEU:HD21	1.97	0.45
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.52	0.45
1:B:51:ASN:N	1:B:51:ASN:HD22	2.14	0.45
1:B:595:ASN:C	1:B:595:ASN:ND2	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ASN:ND2	1:B:500:MET:HG3	2.33	0.44
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.46	0.44
1:A:150:ARG:N	4:A:1242:HOH:O	2.49	0.44
1:A:131:PRO:CB	1:A:148:GLN:NE2	2.73	0.44
1:A:225:LEU:HD21	1:A:381:TYR:CZ	2.52	0.44
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.89	0.44
1:A:599:ASN:ND2	4:A:950:HOH:O	2.49	0.44
1:B:595:ASN:ND2	1:B:597:MET:H	2.15	0.44
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.66	0.43
1:A:597:MET:SD	1:B:516:ASP:HA	2.58	0.43
1:A:228:GLY:HA3	4:A:1599:HOH:O	2.18	0.43
1:A:366:ILE:HD11	1:A:380:ALA:HB1	2.00	0.43
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.44	0.43
1:A:209:VAL:CG1	1:A:214:ILE:HB	2.48	0.43
1:B:209:VAL:HG13	1:B:214:ILE:HB	2.01	0.43
1:B:339:GLY:HA3	1:B:340:PRO:HD2	1.82	0.43
1:B:620:GLN:HG3	4:B:995:HOH:O	2.17	0.43
1:B:483:ASP:CG	1:B:705:HIS:HD1	2.25	0.43
1:A:131:PRO:HG2	1:A:146:VAL:HG11	2.00	0.43
1:A:624:ASP:CA	1:A:629:HIS:NE2	2.81	0.43
1:A:720:LEU:HD23	1:A:720:LEU:HA	1.87	0.43
1:B:332:LEU:CD1	1:B:342:ILE:HD13	2.49	0.43
1:A:208:ALA:O	1:A:212:ARG:HG3	2.18	0.43
1:A:293:PHE:CZ	1:B:440:HIS:HD2	2.37	0.43
1:A:453:ARG:NH2	4:A:1573:HOH:O	2.38	0.43
1:B:106:GLN:OE1	4:B:1166:HOH:O	2.21	0.43
1:B:343:SER:O	1:B:344:THR:C	2.61	0.43
1:A:623:PRO:O	1:A:629:HIS:CE1	2.72	0.43
1:B:77:ASP:O	1:B:81:SER:HB3	2.19	0.43
1:B:150:ARG:O	1:B:169:LEU:HB2	2.18	0.43
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.86	0.42
1:A:7:MET:HE1	1:A:59:VAL:HG11	2.00	0.42
1:B:88:GLN:O	1:B:319:THR:HA	2.19	0.42
1:B:129:LEU:HD12	1:B:130:PRO:HD2	2.01	0.42
1:B:545:ALA:O	1:B:567:GLN:HA	2.19	0.42
1:A:80:GLN:N	1:A:80:GLN:OE1	2.53	0.42
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.53	0.42
1:A:465:ASN:HB2	1:A:489:ILE:O	2.19	0.42
1:B:322:MET:HE3	1:B:330:PHE:O	2.19	0.42
1:B:332:LEU:HD13	1:B:342:ILE:HD13	2.02	0.42
1:B:341:MET:HE2	4:B:937:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ASP:HB3	1:A:519:ILE:HB	2.01	0.42
1:B:129:LEU:HA	1:B:130:PRO:HD2	1.81	0.42
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.81	0.42
1:B:632:SER:OG	1:B:661:ASP:OD2	2.35	0.42
1:A:633:PHE:HA	1:A:639:TRP:CZ2	2.55	0.42
1:B:171:ASN:HB3	1:B:173:LYS:HE2	2.01	0.42
1:A:516:ASP:HA	1:B:597:MET:SD	2.60	0.42
1:B:120:ASN:ND2	4:B:851:HOH:O	2.53	0.42
1:A:38:TYR:CG	1:A:311:PRO:HA	2.55	0.42
1:A:492:VAL:HB	1:A:519:ILE:HG23	2.00	0.42
1:B:148:GLN:HB3	4:B:1144:HOH:O	2.19	0.42
1:B:526:HIS:HB2	1:B:687:THR:OG1	2.19	0.42
1:B:665:GLY:O	1:B:669:LYS:NZ	2.49	0.42
1:A:580:PHE:CE2	1:A:582:PRO:HA	2.54	0.42
1:A:272:GLN:NE2	1:A:274:LYS:HZ1	2.17	0.42
1:A:443:MET:CE	1:B:392:LEU:HD22	2.50	0.42
1:A:717:THR:HB	1:A:720:LEU:HG	2.02	0.42
1:B:366:ILE:HA	1:B:381:TYR:O	2.19	0.42
1:B:496:LYS:HE3	4:B:1255:HOH:O	2.19	0.42
1:B:723:LEU:HD12	1:B:723:LEU:HA	1.90	0.42
1:A:96:LEU:O	1:A:97:ASN:C	2.61	0.41
1:A:608:TYR:HE2	1:B:608:TYR:CE2	2.39	0.41
1:B:7:MET:HG2	1:B:71:SER:HA	2.01	0.41
1:B:139:PHE:CD1	1:B:139:PHE:C	2.97	0.41
1:B:353:LYS:CE	4:B:1031:HOH:O	2.67	0.41
1:B:572:ASN:HD22	1:B:671:ASN:ND2	2.02	0.41
1:B:619:ALA:HB1	1:B:634:MET:HE2	2.02	0.41
1:A:237:LYS:HZ2	1:A:239:ASP:CG	2.28	0.41
1:A:580:PHE:HA	4:A:1287:HOH:O	2.20	0.41
1:B:92:ARG:HA	1:B:93:PRO:HD2	1.85	0.41
1:A:22:GLN:HG3	4:A:1278:HOH:O	2.20	0.41
1:B:196:GLN:NE2	1:B:222:THR:H	2.18	0.41
1:B:374:ILE:HG13	1:B:375:GLY:N	2.35	0.41
1:A:203:GLU:OE2	1:A:204:GLU:OE2	2.39	0.41
1:A:572:ASN:CB	1:A:671:ASN:HD21	2.32	0.41
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.88	0.41
1:A:118:LYS:HA	1:A:119:PRO:HD3	1.87	0.41
1:A:543:LEU:HD22	1:A:640:VAL:HG21	2.03	0.41
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.45	0.41
1:B:27:ALA:CA	4:B:827:HOH:O	2.60	0.41
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:HIS:CD2	1:A:629:HIS:H	2.39	0.41
4:A:959:HOH:O	1:B:563:MET:HB3	2.21	0.41
1:B:208:ALA:O	1:B:211:LYS:HG2	2.21	0.41
1:B:368:PRO:HB2	1:B:621:PHE:CE2	2.56	0.41
1:B:406:ALA:HA	1:B:430:PHE:HB3	2.03	0.41
1:A:149:PRO:HA	4:A:1242:HOH:O	2.21	0.41
1:A:529:ASN:HA	1:A:683:MET:O	2.20	0.41
1:A:529:ASN:HD21	1:A:682:TRP:HE3	1.68	0.41
1:A:626:TRP:HA	1:A:629:HIS:CD2	2.55	0.41
1:B:139:PHE:O	1:B:143:ASN:HA	2.21	0.41
1:B:639:TRP:CG	1:B:664:LEU:HD13	2.56	0.41
1:A:132:ASP:HB3	4:A:1567:HOH:O	2.21	0.41
1:A:223:THR:CG2	1:A:246:ILE:HB	2.51	0.41
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.56	0.41
1:A:545:ALA:HB2	1:A:570:ILE:HD11	2.03	0.40
1:B:212:ARG:HH21	1:B:280:GLU:HB3	1.85	0.40
1:B:447:ASN:CG	1:B:448:VAL:N	2.78	0.40
1:A:536:VAL:H	1:A:541:ASN:ND2	2.17	0.40
1:B:382:LEU:N	1:B:382:LEU:HD12	2.36	0.40
1:B:619:ALA:CB	1:B:634:MET:HE2	2.51	0.40
1:A:610:GLY:HA3	1:B:610:GLY:HA3	2.04	0.40
1:B:392:LEU:O	1:B:393:THR:C	2.63	0.40
1:A:374:ILE:HD12	1:A:374:ILE:HA	1.83	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1283:HOH:O	4:B:1261:HOH:O[2_565]	1.53	0.67
4:B:827:HOH:O	4:B:1460:HOH:O[2_565]	1.88	0.32
4:A:1175:HOH:O	4:A:1434:HOH:O[2_565]	2.05	0.15
4:A:1153:HOH:O	4:A:1552:HOH:O[2_565]	2.14	0.06

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	716/721 (99%)	689 (96%)	27 (4%)	0	100	100
1	B	718/721 (100%)	695 (97%)	23 (3%)	0	100	100
All	All	1434/1442 (99%)	1384 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	587 (96%)	22 (4%)	31	42
1	B	612/612 (100%)	587 (96%)	25 (4%)	27	37
All	All	1221/1224 (100%)	1174 (96%)	47 (4%)	29	40

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	42	LYS
1	A	64	LYS
1	A	147	ASP
1	A	148	GLN
1	A	151	LYS
1	A	163	ILE
1	A	199	ILE
1	A	203	GLU
1	A	204	GLU
1	A	210	LYS
1	A	218	LYS
1	A	239	ASP
1	A	288	MET
1	A	350	ASN

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Mol	Chain	Res	Type
1	A	396	ILE
1	A	445	GLN
1	A	477	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	642	ARG
1	B	11	ASP
1	B	15	LYS
1	B	47	THR
1	B	91	LYS
1	B	118	LYS
1	B	137	TRP
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	211	LYS
1	B	214	ILE
1	B	218	LYS
1	B	237	LYS
1	B	251	VAL
1	B	274	LYS
1	B	322	MET
1	B	372	PRO
1	B	477	ASN
1	B	490	GLU
1	B	506	LYS
1	B	539	GLU
1	B	595	ASN
1	B	613	HIS
1	B	642	ARG
1	B	669	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	51	ASN
1	A	53	GLN
1	A	97	ASN
1	A	148	GLN
1	A	161	HIS

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	178	GLN
1	A	196	GLN
1	A	197	ASN
1	A	200	ASN
1	A	201	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	445	GLN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	540	ASN
1	A	541	ASN
1	A	553	ASN
1	A	566	ASN
1	A	567	GLN
1	A	572	ASN
1	A	592	ASN
1	A	595	ASN
1	A	599	ASN
1	A	629	HIS
1	A	637	GLN
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	148	GLN
1	B	196	GLN
1	B	200	ASN
1	B	201	ASN
1	B	238	GLN
1	B	272	GLN

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Mol	Chain	Res	Type
1	B	315	ASN
1	B	327	ASN
1	B	348	ASN
1	B	350	ASN
1	B	383	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	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	572	ASN
1	B	595	ASN
1	B	599	ASN
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 ⓘ

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	2.71	6 (46%)	13,19,21	1.31	1 (7%)
1	TPQ	B	466	1	13,14,15	2.04	3 (23%)	13,19,21	1.63	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	-	2/5/22/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	C1-C2	-5.46	1.41	1.49
1	B	466	TPQ	C1-C2	-5.10	1.42	1.49
1	A	466	TPQ	O5-C5	-4.12	1.13	1.24
1	A	466	TPQ	O2-C2	-4.00	1.14	1.24
1	B	466	TPQ	CB-C1	3.20	1.56	1.50
1	A	466	TPQ	C4-C5	-2.98	1.38	1.47
1	B	466	TPQ	C4-C5	-2.79	1.39	1.47
1	A	466	TPQ	C6-C1	2.71	1.41	1.34
1	A	466	TPQ	CB-C1	2.53	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TPQ	C4-C3-C2	-3.14	116.90	120.30
1	B	466	TPQ	CB-C1-C2	3.12	124.02	118.56
1	A	466	TPQ	C6-C1-C2	-2.41	116.94	118.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	718/721 (99%)	-0.45	9 (1%) 75 73	14, 25, 44, 65	0
1	B	720/721 (99%)	-0.41	12 (1%) 69 66	16, 26, 46, 66	0
All	All	1438/1442 (99%)	-0.43	21 (1%) 72 69	14, 26, 45, 66	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	PRO	4.7
1	A	217	ALA	3.6
1	B	120	ASN	3.6
1	A	148	GLN	3.5
1	B	302	ALA	3.2
1	B	726	ASP	3.1
1	A	149	PRO	2.9
1	A	239	ASP	2.6
1	B	239	ASP	2.6
1	B	6	HIS	2.6
1	A	130	PRO	2.6
1	A	170	GLN	2.4
1	B	215	THR	2.4
1	B	539	GLU	2.4
1	B	80	GLN	2.3
1	A	64	LYS	2.3
1	B	178	GLN	2.3
1	B	119	PRO	2.1
1	A	12	LYS	2.1
1	B	644	HIS	2.1
1	A	218	LYS	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	B	466	14/15	0.84	0.14	24,45,55,57	0
1	TPQ	A	466	14/15	0.87	0.15	24,50,58,59	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	B	803	1/1	0.96	0.05	45,45,45,45	0
3	CA	A	803	1/1	0.97	0.04	47,47,47,47	0
3	CA	A	802	1/1	0.99	0.06	25,25,25,25	0
2	CU	A	801	1/1	0.99	0.03	30,30,30,30	0
3	CA	B	802	1/1	0.99	0.03	25,25,25,25	0
2	CU	B	801	1/1	0.99	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.