



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:19 PM UTC

PDB ID : 1JRQ / pdb_00001jrq
Title : X-ray Structure Analysis of the Role of the Conserved Tyrosine-369 in Active Site of E. coli Amine Oxidase
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Deposited on : 2001-08-14
Resolution : 2.15 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

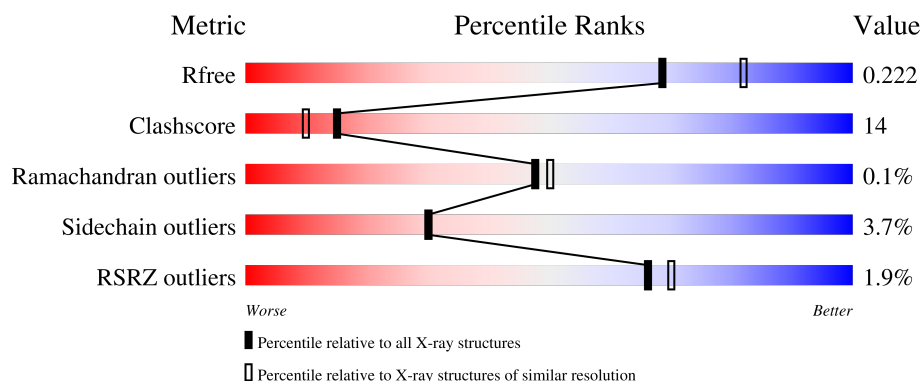
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	% 67% 27% 5%
1	B	727	2% 70% 25% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12750 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
			5663	3602	964	1075	22			
1	B	721	Total	C	N	O	S	0	0	0
			5687	3617	970	1078	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	PHE	TYR	engineered mutation	UNP P46883
A	466	TPQ	TYR	modified residue	UNP P46883
B	369	PHE	TYR	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		

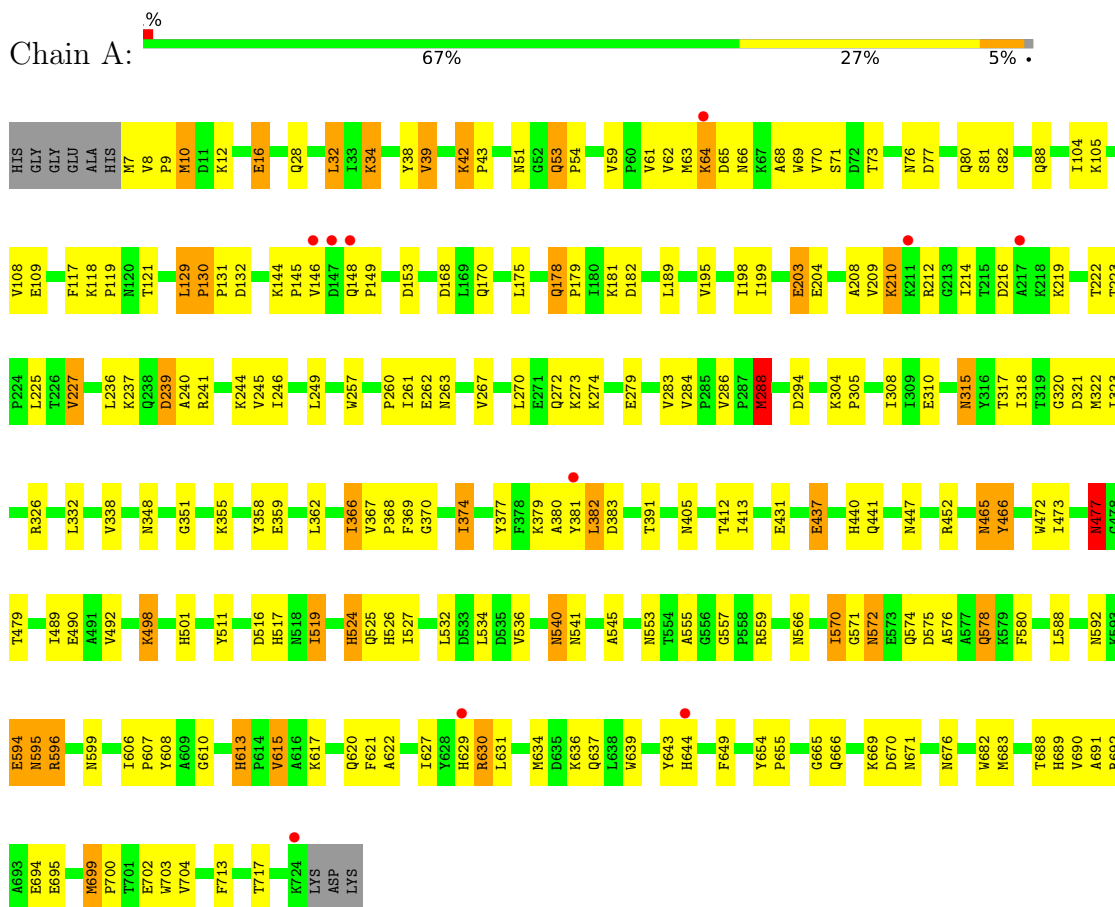
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	749	Total 749	O 749	0	0
4	B	645	Total 645	O 645	0	0

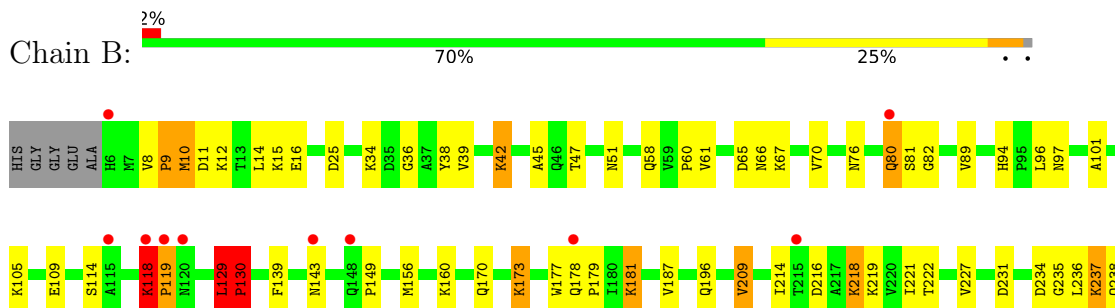
3 Residue-property plots

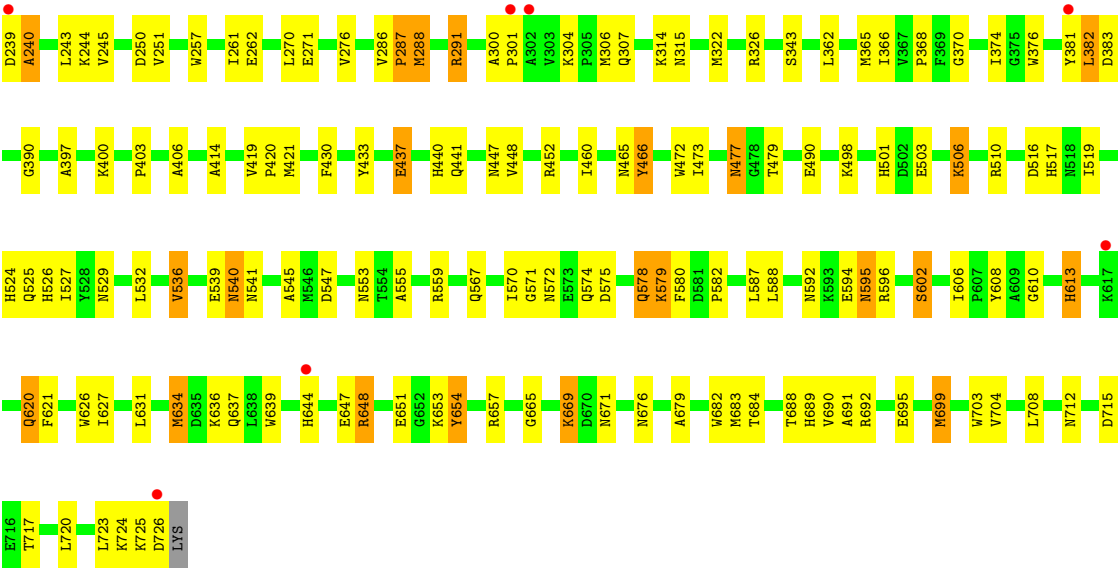
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Copper amine oxidase



• Molecule 1: Copper amine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.54Å 166.45Å 79.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 20.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.15) 92.4 (20.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.235 0.184 , 0.222	Depositor DCC
R_{free} test set	3092 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	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	0.96	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.43	0/5792	1.59	87/7884 (1.1%)
1	B	0.41	0/5817	1.55	72/7917 (0.9%)
All	All	0.42	0/11609	1.57	159/15801 (1.0%)

There are no bond length outliers.

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ASN	OD1-CG-ND2	11.13	133.73	122.60
1	B	691	ALA	N-CA-C	9.02	121.50	110.41
1	A	129	LEU	CA-C-N	8.93	126.09	119.66
1	A	129	LEU	C-N-CA	8.93	126.09	119.66
1	A	596	ARG	CD-NE-CZ	8.78	136.69	124.40
1	A	524	HIS	CE1-NE2-CD2	8.67	117.67	109.00
1	A	571	GLY	N-CA-C	8.54	126.51	115.32
1	A	713	PHE	N-CA-C	-8.23	101.86	112.23
1	B	81	SER	N-CA-C	7.98	119.97	111.28
1	A	699	MET	N-CA-C	7.76	120.03	109.24
1	B	699	MET	N-CA-C	7.73	119.99	109.24
1	A	588	LEU	N-CA-C	-7.67	94.42	107.99
1	A	118	LYS	CA-C-N	7.49	129.20	119.84
1	A	118	LYS	C-N-CA	7.49	129.20	119.84
1	A	362	LEU	N-CA-C	-7.47	99.23	110.28
1	B	118	LYS	CA-C-N	7.44	127.80	119.32
1	B	118	LYS	C-N-CA	7.44	127.80	119.32
1	B	654	TYR	CA-C-N	7.36	126.99	119.56
1	B	654	TYR	C-N-CA	7.36	126.99	119.56
1	A	524	HIS	CG-CD2-NE2	-7.33	99.87	107.20
1	B	10	MET	N-CA-C	7.29	118.92	110.97
1	B	362	LEU	N-CA-C	-7.23	99.58	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ARG	NE-CZ-NH2	-7.22	112.70	119.20
1	A	262	GLU	N-CA-C	7.19	120.65	110.23
1	B	262	GLU	N-CA-C	7.16	120.88	110.28
1	A	146	VAL	N-CA-C	-7.14	97.97	108.54
1	A	288	MET	N-CA-C	7.13	122.27	113.50
1	A	130	PRO	O-C-N	7.08	124.48	121.15
1	B	39	VAL	N-CA-C	7.07	118.66	108.48
1	B	588	LEU	N-CA-C	-7.05	95.52	107.99
1	A	691	ALA	N-CA-C	7.03	119.40	110.33
1	A	129	LEU	N-CA-C	-6.75	95.04	109.01
1	B	524	HIS	CE1-NE2-CD2	6.74	115.74	109.00
1	A	472	TRP	N-CA-C	-6.73	96.69	108.20
1	B	382	LEU	N-CA-C	-6.70	96.11	108.24
1	B	58	GLN	N-CA-C	-6.64	103.97	111.14
1	B	129	LEU	CA-C-N	6.61	127.19	120.38
1	B	129	LEU	C-N-CA	6.61	127.19	120.38
1	A	578	GLN	N-CA-C	6.59	118.78	108.96
1	A	440	HIS	N-CA-CB	6.53	120.70	110.71
1	B	540	ASN	N-CA-C	6.53	119.08	108.63
1	B	34	LYS	CA-CB-CG	-6.50	101.09	114.10
1	A	39	VAL	N-CA-C	6.48	117.92	108.53
1	B	82	GLY	N-CA-C	-6.47	106.78	114.48
1	A	53	GLN	CA-C-N	6.43	126.38	119.76
1	A	53	GLN	C-N-CA	6.43	126.38	119.76
1	B	689	HIS	N-CA-C	6.42	119.18	108.20
1	B	602	SER	N-CA-C	6.40	117.88	108.86
1	B	437	GLU	N-CA-C	-6.33	104.39	111.28
1	A	326	ARG	NE-CZ-NH2	-6.32	113.51	119.20
1	A	310	GLU	CA-C-N	6.32	126.00	119.56
1	A	310	GLU	C-N-CA	6.32	126.00	119.56
1	A	689	HIS	N-CA-C	6.31	119.02	108.73
1	A	130	PRO	N-CA-C	6.30	117.32	110.58
1	B	578	GLN	N-CA-C	6.28	117.41	108.74
1	B	571	GLY	N-CA-C	6.26	123.53	115.32
1	B	381	TYR	CA-C-O	-6.22	113.46	120.43
1	A	130	PRO	CB-CA-C	-6.18	105.36	111.17
1	A	377	TYR	N-CA-C	6.16	119.64	111.75
1	B	473	ILE	N-CA-C	6.16	116.49	107.37
1	A	473	ILE	N-CA-C	6.13	116.69	107.80
1	A	338	VAL	N-CA-C	6.07	118.84	112.83
1	A	526	HIS	CE1-NE2-CD2	6.06	115.06	109.00
1	B	261	ILE	N-CA-C	-6.06	96.74	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	704	VAL	N-CA-CB	6.04	121.34	111.44
1	A	294	ASP	N-CA-C	6.03	120.26	113.02
1	A	34	LYS	N-CA-CB	6.03	119.17	110.37
1	B	374	ILE	N-CA-C	6.03	117.49	110.62
1	A	717	THR	CA-C-N	6.02	125.70	119.56
1	A	717	THR	C-N-CA	6.02	125.70	119.56
1	B	688	THR	N-CA-C	-6.01	97.50	108.02
1	B	524	HIS	CG-CD2-NE2	-5.95	101.25	107.20
1	B	440	HIS	CA-CB-CG	-5.92	107.88	113.80
1	B	526	HIS	CE1-NE2-CD2	5.91	114.91	109.00
1	B	89	VAL	N-CA-CB	5.87	116.93	110.53
1	B	570	ILE	N-CA-C	-5.87	98.52	106.85
1	B	606	ILE	CA-C-N	5.87	125.48	119.56
1	B	606	ILE	C-N-CA	5.87	125.48	119.56
1	B	291	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	B	376	TRP	N-CA-C	5.83	121.27	114.62
1	B	620	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	689	HIS	ND1-CE1-NE2	-5.80	102.60	108.40
1	A	119	PRO	CA-C-N	-5.79	114.54	123.17
1	A	119	PRO	C-N-CA	-5.79	114.54	123.17
1	B	690	VAL	N-CA-C	-5.79	98.80	107.37
1	A	374	ILE	N-CA-C	5.71	116.35	110.36
1	A	477	ASN	OD1-CG-ND2	-5.67	116.94	122.60
1	A	688	THR	N-CA-C	-5.66	99.30	108.52
1	A	606	ILE	CA-C-N	5.65	125.27	119.56
1	A	606	ILE	C-N-CA	5.65	125.27	119.56
1	A	10	MET	N-CA-C	5.64	117.29	111.03
1	A	382	LEU	N-CA-C	-5.63	97.59	107.73
1	B	440	HIS	N-CA-CB	5.63	118.59	110.37
1	A	578	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	82	GLY	N-CA-C	-5.62	106.78	114.64
1	B	130	PRO	N-CA-C	5.62	117.55	110.70
1	A	437	GLU	N-CA-C	-5.60	105.18	111.28
1	A	261	ILE	N-CA-C	-5.59	97.72	109.34
1	A	524	HIS	ND1-CE1-NE2	-5.57	102.83	108.40
1	A	383	ASP	N-CA-C	5.53	120.43	111.37
1	A	690	VAL	N-CA-C	-5.53	99.19	107.37
1	B	524	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	320	GLY	N-CA-C	-5.46	100.23	113.18
1	A	315	ASN	N-CA-C	-5.46	106.61	113.28
1	B	472	TRP	N-CA-C	-5.46	98.33	107.99
1	A	227	VAL	N-CA-C	5.44	120.52	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	ARG	N-CA-CB	-5.42	103.15	110.95
1	A	534	LEU	CA-C-O	-5.41	115.10	121.16
1	A	540	ASN	N-CA-C	5.41	117.06	108.67
1	A	16	GLU	N-CA-C	-5.41	105.47	111.36
1	A	629	HIS	CA-CB-CG	-5.40	108.40	113.80
1	B	665	GLY	N-CA-C	-5.40	105.86	112.77
1	B	503	GLU	N-CA-C	5.39	117.16	111.28
1	B	703	TRP	N-CA-C	5.35	118.29	109.72
1	B	343	SER	N-CA-C	5.35	118.30	109.85
1	A	704	VAL	N-CA-CB	5.34	120.20	111.44
1	B	326	ARG	CD-NE-CZ	5.33	131.87	124.40
1	B	588	LEU	N-CA-CB	5.33	119.31	110.47
1	B	240	ALA	N-CA-C	5.32	118.35	110.48
1	A	622	ALA	N-CA-C	-5.32	102.74	110.08
1	A	153	ASP	N-CA-C	-5.31	100.59	109.24
1	A	617	LYS	CA-C-O	5.30	125.49	119.18
1	A	654	TYR	CA-C-N	5.29	125.37	119.87
1	A	654	TYR	C-N-CA	5.29	125.37	119.87
1	B	287	PRO	N-CA-C	-5.29	102.39	110.95
1	B	397	ALA	N-CA-C	-5.28	99.91	108.41
1	B	587	LEU	N-CA-C	5.27	118.16	109.72
1	B	129	LEU	CB-CA-C	5.27	116.97	109.38
1	B	119	PRO	N-CA-C	5.26	121.58	113.75
1	B	613	HIS	N-CA-C	-5.25	101.00	109.82
1	A	145	PRO	N-CA-CB	5.24	107.97	103.31
1	A	498	LYS	N-CA-C	-5.21	106.60	113.12
1	A	665	GLY	N-CA-C	-5.19	106.50	112.73
1	A	692	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	570	ILE	N-CA-C	-5.18	99.49	106.85
1	B	288	MET	N-CA-C	5.17	119.72	113.41
1	B	579	LYS	N-CA-C	-5.17	102.83	110.48
1	A	557	GLY	CA-C-N	5.15	124.94	119.28
1	A	557	GLY	C-N-CA	5.15	124.94	119.28
1	A	703	TRP	N-CA-C	5.13	117.96	109.85
1	A	260	PRO	CB-CA-C	-5.13	104.26	110.98
1	A	284	VAL	CA-C-O	5.13	122.69	119.51
1	A	630	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	B	421	MET	N-CA-CB	-5.11	102.44	110.77
1	A	473	ILE	N-CA-CB	-5.10	105.03	111.46
1	B	25	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	649	PHE	O-C-N	5.10	125.93	121.39
1	B	390	GLY	N-CA-C	-5.10	106.59	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	N-CA-C	-5.08	102.18	109.24
1	A	689	HIS	ND1-CG-CD2	-5.07	101.03	106.10
1	B	414	ALA	CA-C-O	-5.07	115.17	120.80
1	A	412	THR	N-CA-C	5.05	117.20	109.07
1	B	9	PRO	N-CA-CB	5.05	107.66	103.17
1	A	267	VAL	O-C-N	5.04	129.00	123.10
1	B	234	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	657	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	440	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	519	ILE	N-CA-C	5.02	115.20	107.77
1	B	433	TYR	N-CA-C	-5.02	102.27	110.20

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	5663	0	5540	171	0
1	B	5687	0	5562	154	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	749	0	0	17	0
4	B	645	0	0	19	0
All	All	12750	0	11102	308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (308) 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:572:ASN:HD22	1:B:671:ASN:HD21	1.07	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ILE:HD12	1:A:634:MET:HE2	1.46	0.98
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.45	0.96
1:A:225:LEU:HD22	1:A:381:TYR:HE2	1.28	0.96
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.48	0.95
1:A:304:LYS:H	1:B:315:ASN:HD21	1.13	0.91
1:B:322:MET:HG3	4:B:1156:HOH:O	1.73	0.89
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.57	0.87
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.04	0.86
1:B:466:TPQ:O5	4:B:1201:HOH:O	1.93	0.85
1:A:465:ASN:HD22	1:A:465:ASN:H	1.24	0.82
1:B:94:HIS:HD2	1:B:96:LEU:H	1.27	0.82
1:A:580:PHE:H	1:A:637:GLN:HE21	1.26	0.82
1:B:572:ASN:ND2	1:B:671:ASN:HD21	1.77	0.82
1:B:12:LYS:O	1:B:16:GLU:HG2	1.82	0.80
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.62	0.79
1:A:62:VAL:HG23	1:A:69:TRP:HB2	1.61	0.79
1:A:288:MET:HE2	1:A:288:MET:HA	1.65	0.79
1:B:181:LYS:HE2	1:B:181:LYS:H	1.50	0.77
1:A:368:PRO:HG3	1:A:634:MET:CE	2.15	0.77
1:A:553:ASN:ND2	1:A:555:ALA:H	1.82	0.76
1:B:271:GLU:HG2	4:B:811:HOH:O	1.87	0.74
1:A:203:GLU:CD	1:A:203:GLU:H	1.95	0.74
1:B:490:GLU:HG2	4:B:818:HOH:O	1.87	0.74
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.88	0.73
1:B:580:PHE:H	1:B:637:GLN:HE21	1.34	0.73
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.70	0.73
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.37	0.73
1:B:699:MET:HE1	4:B:1017:HOH:O	1.88	0.73
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.18	0.72
1:B:38:TYR:H	1:B:51:ASN:HD21	1.38	0.72
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.36	0.72
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.54	0.71
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.05	0.71
1:A:525:GLN:HE22	1:A:620:GLN:H	1.38	0.71
1:B:466:TPQ:C5	4:B:1201:HOH:O	2.39	0.70
1:A:596:ARG:NH1	4:A:1517:HOH:O	2.17	0.70
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.74	0.69
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.75	0.69
1:A:225:LEU:HD22	1:A:381:TYR:CE2	2.20	0.69
1:B:38:TYR:H	1:B:51:ASN:ND2	1.91	0.69
1:A:237:LYS:NZ	1:A:239:ASP:HB3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:H	1:A:51:ASN:HD21	1.40	0.68
1:B:572:ASN:HD22	1:B:671:ASN:ND2	1.85	0.68
1:A:322:MET:HE1	4:A:1140:HOH:O	1.94	0.67
1:A:315:ASN:HD21	1:B:304:LYS:H	1.41	0.67
1:B:648:ARG:NH1	4:B:1044:HOH:O	2.26	0.67
1:A:38:TYR:H	1:A:51:ASN:ND2	1.91	0.67
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.11	0.66
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.04	0.66
1:B:572:ASN:HB2	1:B:671:ASN:ND2	2.11	0.66
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.78	0.66
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.32	0.65
1:A:572:ASN:ND2	1:A:575:ASP:H	1.94	0.65
1:A:525:GLN:NE2	1:A:620:GLN:H	1.95	0.65
1:B:553:ASN:ND2	1:B:555:ALA:H	1.94	0.65
1:B:580:PHE:H	1:B:637:GLN:NE2	1.94	0.65
1:B:237:LYS:HE2	1:B:239:ASP:HB3	1.77	0.65
1:A:225:LEU:CD2	1:A:381:TYR:HE2	2.08	0.64
1:A:272:GLN:HE21	1:A:274:LYS:HD3	1.62	0.64
1:A:131:PRO:HB3	1:A:148:GLN:NE2	2.12	0.64
1:B:216:ASP:OD1	1:B:218:LYS:HB2	1.98	0.64
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.80	0.64
1:A:465:ASN:H	1:A:465:ASN:ND2	1.95	0.64
1:B:525:GLN:HE22	1:B:620:GLN:H	1.44	0.63
1:B:525:GLN:NE2	1:B:620:GLN:H	1.95	0.63
1:B:65:ASP:O	1:B:66:ASN:HB2	1.98	0.63
1:A:527:ILE:HD12	1:A:634:MET:CE	2.24	0.63
1:A:216:ASP:HB3	1:A:219:LYS:HD2	1.81	0.63
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.17	0.62
1:B:181:LYS:H	1:B:181:LYS:CE	2.12	0.62
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.81	0.62
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.81	0.62
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.81	0.62
1:B:498:LYS:O	1:B:517:HIS:HD2	1.83	0.62
1:A:28:GLN:HG3	4:A:1170:HOH:O	2.00	0.61
1:B:196:GLN:HE22	1:B:222:THR:H	1.48	0.61
1:A:286:VAL:CG1	1:A:288:MET:HE3	2.31	0.61
1:A:580:PHE:H	1:A:637:GLN:NE2	1.99	0.60
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.34	0.60
1:A:149:PRO:HB3	1:A:170:GLN:NE2	2.16	0.60
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.84	0.59
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:HD11	1:B:683:MET:HE2	1.85	0.59
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.33	0.59
1:B:466:TPQ:O2	4:B:832:HOH:O	2.17	0.58
1:B:574:GLN:H	1:B:671:ASN:ND2	2.02	0.58
1:B:105:LYS:O	1:B:109:GLU:HG3	2.03	0.58
1:B:251:VAL:HG12	4:B:1373:HOH:O	2.04	0.58
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.86	0.58
1:A:574:GLN:H	1:A:671:ASN:ND2	2.02	0.57
1:B:10:MET:HG2	1:B:14:LEU:HD12	1.87	0.57
1:A:644:HIS:HB3	4:A:1265:HOH:O	2.05	0.57
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.87	0.56
1:A:636:LYS:HE3	4:A:1465:HOH:O	2.05	0.56
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.35	0.56
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.35	0.56
1:A:366:ILE:HG13	1:A:367:VAL:N	2.21	0.56
1:B:67:LYS:HD3	4:B:1429:HOH:O	2.06	0.56
1:B:366:ILE:HG21	1:B:634:MET:HE3	1.88	0.55
1:A:203:GLU:CD	1:A:203:GLU:N	2.62	0.55
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.88	0.55
1:B:506:LYS:HE2	1:B:510:ARG:HH12	1.71	0.55
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.71	0.55
1:B:181:LYS:HE2	1:B:181:LYS:N	2.19	0.55
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.53	0.55
1:B:679:ALA:HB2	4:B:1167:HOH:O	2.07	0.55
1:A:477:ASN:C	1:A:477:ASN:HD22	2.15	0.54
1:A:572:ASN:C	1:A:572:ASN:HD22	2.16	0.54
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.33	0.54
1:A:198:ILE:HD11	1:A:273:LYS:HA	1.90	0.54
1:A:366:ILE:CG2	1:A:634:MET:HE3	2.37	0.54
1:A:73:THR:HG23	1:A:77:ASP:OD2	2.07	0.54
1:A:62:VAL:CG2	1:A:69:TRP:HB2	2.34	0.54
1:A:149:PRO:HB3	1:A:170:GLN:HE21	1.72	0.53
1:B:45:ALA:O	1:B:60:PRO:HB3	2.07	0.53
1:B:717:THR:HB	1:B:720:LEU:HG	1.91	0.53
1:A:237:LYS:HD3	1:A:240:ALA:HB2	1.90	0.53
1:B:243:LEU:CD1	1:B:270:LEU:HD11	2.38	0.53
1:B:307:GLN:HB3	4:B:1093:HOH:O	2.09	0.53
1:A:288:MET:HA	1:A:288:MET:CE	2.37	0.53
1:A:219:LYS:HD3	4:A:1177:HOH:O	2.08	0.53
1:B:437:GLU:HA	1:B:452:ARG:HB2	1.89	0.52
1:A:366:ILE:HD13	1:A:631:LEU:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:TPQ:O5	1:A:490:GLU:HA	2.10	0.52
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.91	0.52
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.44	0.52
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.45	0.52
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.39	0.52
1:A:615:VAL:HG23	1:B:582:PRO:HB2	1.92	0.52
1:A:214:ILE:N	1:A:214:ILE:HD12	2.25	0.52
1:A:12:LYS:O	1:A:16:GLU:HG3	2.08	0.51
1:B:580:PHE:N	1:B:637:GLN:HE21	2.05	0.51
1:A:7:MET:HE1	1:A:59:VAL:HG11	1.93	0.51
1:B:527:ILE:HD12	1:B:634:MET:HE2	1.93	0.51
1:A:498:LYS:O	1:A:517:HIS:HD2	1.93	0.51
1:B:139:PHE:O	1:B:143:ASN:HA	2.10	0.51
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.92	0.51
1:A:318:ILE:HG12	1:A:323:ILE:HG12	1.92	0.51
1:A:536:VAL:H	1:A:541:ASN:HD21	1.59	0.51
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.26	0.51
1:A:131:PRO:HA	1:A:148:GLN:HE22	1.75	0.50
1:B:94:HIS:CD2	1:B:96:LEU:H	2.16	0.50
1:A:366:ILE:HG23	1:A:634:MET:HE3	1.93	0.50
1:A:88:GLN:HG2	1:A:317:THR:CG2	2.42	0.50
1:A:203:GLU:HA	4:A:1374:HOH:O	2.12	0.50
1:A:492:VAL:HB	1:A:519:ILE:HG23	1.94	0.50
1:B:36:GLY:HA2	1:B:314:LYS:HE2	1.94	0.50
1:B:214:ILE:HD12	1:B:214:ILE:H	1.76	0.50
1:A:545:ALA:HB2	1:A:570:ILE:HD11	1.94	0.50
1:B:572:ASN:HB2	1:B:671:ASN:HD21	1.74	0.50
1:A:210:LYS:HE2	1:A:214:ILE:O	2.12	0.50
1:A:61:VAL:HG22	1:A:70:VAL:HG12	1.94	0.49
1:A:214:ILE:HD12	1:A:214:ILE:H	1.77	0.49
1:A:366:ILE:HD11	1:A:380:ALA:HB1	1.94	0.49
1:A:477:ASN:HD22	1:A:479:THR:H	1.61	0.49
1:A:501:HIS:NE2	1:B:594:GLU:OE1	2.41	0.49
4:A:1238:HOH:O	1:B:400:LYS:HE2	2.12	0.49
1:A:498:LYS:NZ	1:A:498:LYS:HB3	2.27	0.49
1:B:477:ASN:HD22	1:B:477:ASN:C	2.21	0.49
1:A:379:LYS:HD3	1:A:381:TYR:OH	2.12	0.49
1:A:237:LYS:HZ3	1:A:239:ASP:HB3	1.77	0.49
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.26	0.49
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.13	0.49
1:A:670:ASP:HB2	4:A:1523:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:HG2	1:A:270:LEU:HD12	1.94	0.48
1:A:532:LEU:HD11	1:A:683:MET:HE2	1.95	0.48
1:A:553:ASN:HD21	1:A:555:ALA:H	1.55	0.48
1:A:580:PHE:N	1:A:637:GLN:HE21	2.03	0.48
1:B:76:ASN:O	1:B:80:GLN:HB2	2.13	0.48
1:A:257:TRP:HB2	1:A:489:ILE:HG21	1.96	0.48
1:A:369:PHE:CD2	1:A:524:HIS:HB3	2.49	0.48
1:A:10:MET:HE3	1:A:70:VAL:CG1	2.43	0.48
1:A:286:VAL:O	1:A:288:MET:HG2	2.14	0.48
1:A:437:GLU:HA	1:A:452:ARG:HB2	1.96	0.48
1:B:595:ASN:HB2	1:B:715:ASP:OD1	2.14	0.48
1:A:272:GLN:NE2	1:A:274:LYS:HD3	2.27	0.48
1:B:406:ALA:HA	1:B:430:PHE:HB3	1.95	0.48
1:B:101:ALA:O	1:B:105:LYS:HG3	2.14	0.47
1:A:64:LYS:HD3	1:A:65:ASP:N	2.29	0.47
1:B:726:ASP:O	4:B:1239:HOH:O	2.20	0.47
1:A:348:ASN:HD22	1:A:348:ASN:C	2.23	0.47
1:B:365:MET:HE2	1:B:383:ASP:OD2	2.14	0.47
1:B:631:LEU:O	1:B:634:MET:HG3	2.14	0.47
1:A:516:ASP:HB3	1:A:519:ILE:HB	1.96	0.47
1:A:595:ASN:ND2	1:A:599:ASN:H	2.13	0.47
1:B:51:ASN:N	1:B:51:ASN:HD22	2.13	0.47
1:B:237:LYS:HD3	1:B:240:ALA:HB2	1.96	0.47
1:B:506:LYS:HD3	1:B:506:LYS:C	2.39	0.47
1:A:32:LEU:HB2	1:A:39:VAL:HB	1.96	0.46
1:A:263:ASN:HD22	1:A:374:ILE:HG22	1.81	0.46
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.81	0.46
1:B:65:ASP:O	1:B:66:ASN:CB	2.64	0.46
1:B:129:LEU:HD12	1:B:129:LEU:C	2.40	0.46
1:A:431:GLU:HB3	1:B:306:MET:HE1	1.98	0.46
1:B:695:GLU:HB3	1:B:699:MET:HG3	1.97	0.46
1:A:203:GLU:OE2	1:A:204:GLU:HG3	2.16	0.46
1:A:144:LYS:HE3	4:A:1495:HOH:O	2.15	0.46
1:B:129:LEU:HA	1:B:130:PRO:HD2	1.79	0.46
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.72	0.46
1:A:38:TYR:N	1:A:51:ASN:HD21	2.10	0.45
1:B:366:ILE:CG2	1:B:634:MET:HE3	2.47	0.45
1:B:644:HIS:HB2	1:B:647:GLU:HG3	1.97	0.45
1:B:725:LYS:O	1:B:726:ASP:CB	2.64	0.45
1:A:208:ALA:O	1:A:212:ARG:HG3	2.16	0.45
1:A:553:ASN:HD21	1:A:555:ALA:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:OE1	1:B:501:HIS:CE1	2.68	0.45
1:B:276:VAL:HG11	4:B:1275:HOH:O	2.17	0.45
1:A:576:ALA:O	1:A:578:GLN:HG2	2.17	0.45
1:B:466:TPQ:O4	4:B:818:HOH:O	1.99	0.45
1:A:168:ASP:HB2	1:A:175:LEU:HD21	1.99	0.45
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.82	0.45
1:B:536:VAL:H	1:B:541:ASN:HD21	1.64	0.45
1:A:104:ILE:O	1:A:108:VAL:HG23	2.17	0.45
1:A:608:TYR:HE2	1:B:608:TYR:CE2	2.32	0.45
1:B:579:LYS:HA	1:B:637:GLN:NE2	2.30	0.45
1:B:118:LYS:HA	1:B:119:PRO:HD3	1.70	0.45
1:A:572:ASN:HD22	1:A:575:ASP:H	1.65	0.44
1:A:694:GLU:O	1:B:717:THR:HA	2.17	0.44
1:B:61:VAL:HG22	1:B:70:VAL:CG1	2.46	0.44
1:A:222:THR:HB	1:A:245:VAL:HG13	1.98	0.44
1:B:160:LYS:HD3	1:B:271:GLU:OE1	2.18	0.44
1:A:308:ILE:O	1:A:405:ASN:HB3	2.18	0.44
1:A:441:GLN:OE1	1:A:447:ASN:HB2	2.18	0.44
1:A:613:HIS:CE1	1:A:702:GLU:HG3	2.52	0.44
1:A:643:TYR:O	1:A:644:HIS:CD2	2.70	0.44
1:B:235:GLY:O	1:B:236:LEU:HD23	2.16	0.44
1:B:723:LEU:HD12	1:B:723:LEU:HA	1.86	0.44
1:B:669:LYS:HA	1:B:669:LYS:CE	2.47	0.44
1:A:210:LYS:HE2	1:A:210:LYS:HA	1.99	0.43
1:A:236:LEU:HD11	1:A:244:LYS:HE3	2.00	0.43
1:B:238:GLN:HB2	4:B:1089:HOH:O	2.17	0.43
1:A:77:ASP:O	1:A:81:SER:HB3	2.17	0.43
1:B:149:PRO:HB3	1:B:170:GLN:HB3	1.99	0.43
1:B:196:GLN:NE2	1:B:222:THR:H	2.15	0.43
1:A:391:THR:HA	1:A:413:ILE:HD11	2.00	0.43
1:A:610:GLY:HA3	1:B:610:GLY:HA3	2.01	0.43
1:A:699:MET:HA	1:A:700:PRO:HD3	1.88	0.43
1:B:300:ALA:HA	1:B:301:PRO:HD2	1.90	0.43
1:A:595:ASN:HD22	1:A:595:ASN:C	2.27	0.43
1:B:251:VAL:HG12	1:B:251:VAL:O	2.19	0.43
1:B:257:TRP:CE2	1:B:465:ASN:HB3	2.53	0.43
1:B:572:ASN:OD1	1:B:575:ASP:OD2	2.37	0.43
1:A:88:GLN:HG2	1:A:317:THR:HG23	2.01	0.43
1:A:572:ASN:HD21	1:A:575:ASP:CG	2.26	0.43
1:B:720:LEU:HD23	1:B:720:LEU:HA	1.87	0.43
1:A:148:GLN:NE2	4:A:1166:HOH:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HA	1:A:179:PRO:HD3	1.88	0.42
1:B:447:ASN:CG	1:B:448:VAL:N	2.76	0.42
1:B:129:LEU:HD12	1:B:130:PRO:N	2.35	0.42
1:B:139:PHE:CD1	1:B:139:PHE:C	2.97	0.42
1:A:595:ASN:ND2	1:A:595:ASN:C	2.76	0.42
1:B:173:LYS:NZ	1:B:173:LYS:HB3	2.34	0.42
1:B:547:ASP:HB3	4:B:1127:HOH:O	2.19	0.42
1:A:63:MET:SD	1:A:68:ALA:HB2	2.59	0.42
1:A:71:SER:OG	1:A:73:THR:HG22	2.20	0.42
1:A:348:ASN:HD21	1:A:351:GLY:C	2.28	0.42
1:A:42:LYS:HE2	4:B:822:HOH:O	2.19	0.42
1:A:304:LYS:H	1:B:315:ASN:ND2	1.96	0.42
1:B:286:VAL:O	1:B:288:MET:HG2	2.19	0.42
1:A:131:PRO:HA	1:A:148:GLN:NE2	2.34	0.42
1:A:105:LYS:O	1:A:109:GLU:HG3	2.20	0.42
1:A:580:PHE:CE2	1:A:607:PRO:HD2	2.55	0.42
1:B:553:ASN:HD21	1:B:555:ALA:H	1.68	0.42
1:B:653:LYS:HG2	1:B:654:TYR:CE2	2.55	0.42
1:A:63:MET:HG3	4:A:1492:HOH:O	2.20	0.42
1:B:477:ASN:HD22	1:B:479:THR:H	1.68	0.42
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.90	0.41
1:A:355:LYS:NZ	4:A:1472:HOH:O	2.52	0.41
1:A:511:TYR:HB3	4:A:906:HOH:O	2.20	0.41
1:B:221:ILE:N	1:B:221:ILE:HD12	2.35	0.41
1:A:34:LYS:NZ	4:A:1371:HOH:O	2.52	0.41
1:A:246:ILE:HD13	1:A:246:ILE:HA	1.95	0.41
1:B:403:PRO:HG3	1:B:430:PHE:CD2	2.55	0.41
1:A:181:LYS:O	1:A:182:ASP:HB2	2.19	0.41
1:A:209:VAL:HG13	1:A:214:ILE:HB	2.01	0.41
1:B:237:LYS:HG2	1:B:240:ALA:H	1.84	0.41
1:A:130:PRO:HA	1:A:131:PRO:HD3	1.87	0.41
1:B:382:LEU:HD23	1:B:651:GLU:HG3	2.01	0.41
1:A:553:ASN:ND2	1:A:553:ASN:C	2.77	0.41
1:A:666:GLN:O	1:A:669:LYS:HB2	2.19	0.41
1:B:578:GLN:HG3	1:B:579:LYS:O	2.21	0.41
1:A:559:ARG:NH2	1:B:370:GLY:HA2	2.28	0.41
1:B:545:ALA:O	1:B:567:GLN:HA	2.21	0.41
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.35	0.41
1:A:670:ASP:O	1:A:671:ASN:C	2.64	0.41
1:B:532:LEU:HD13	1:B:708:LEU:HD11	2.03	0.41
1:A:132:ASP:HB3	4:A:1511:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:VAL:HA	1:B:420:PRO:HD3	1.96	0.41
1:B:529:ASN:HD21	1:B:682:TRP:HE3	1.69	0.41
1:B:595:ASN:HB3	1:B:712:ASN:O	2.20	0.41
1:B:637:GLN:HA	1:B:684:THR:HB	2.03	0.41
1:B:156:MET:HE1	1:B:177:TRP:CZ3	2.56	0.41
1:A:117:PHE:CZ	1:A:121:THR:HB	2.56	0.40
1:B:222:THR:HB	1:B:245:VAL:CG1	2.51	0.40
1:A:76:ASN:O	1:A:80:GLN:HB2	2.20	0.40
1:A:321:ASP:HB3	1:A:332:LEU:O	2.22	0.40
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.79	0.40
1:A:305:PRO:HB2	4:A:1391:HOH:O	2.20	0.40
1:A:490:GLU:OE2	1:A:695:GLU:HB2	2.22	0.40
1:B:42:LYS:HB3	4:B:1419:HOH:O	2.21	0.40
1:B:536:VAL:HG11	1:B:602:SER:HA	2.03	0.40
1:B:366:ILE:HD12	1:B:631:LEU:HD13	2.03	0.40
1:A:212:ARG:NH1	1:A:283:VAL:HA	2.37	0.40
1:A:366:ILE:HG21	1:A:634:MET:HE3	2.03	0.40
1:A:630:ARG:HH11	1:A:630:ARG:HD3	1.70	0.40
1:B:187:VAL:HG22	1:B:243:LEU:HD21	2.03	0.40
1:B:578:GLN:HA	1:B:636:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	715/727 (98%)	688 (96%)	27 (4%)	0	100	100
1	B	718/727 (99%)	693 (96%)	23 (3%)	2 (0%)	36	34
All	All	1433/1454 (99%)	1381 (96%)	50 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	536	VAL
1	B	130	PRO

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%)	586 (96%)	23 (4%)	29	29
1	B	611/615 (99%)	589 (96%)	22 (4%)	31	31
All	All	1220/1230 (99%)	1175 (96%)	45 (4%)	30	30

All (45) 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	66	ASN
1	A	129	LEU
1	A	178	GLN
1	A	189	LEU
1	A	195	VAL
1	A	199	ILE
1	A	203	GLU
1	A	210	LYS
1	A	223	THR
1	A	239	ASP
1	A	288	MET
1	A	366	ILE
1	A	465	ASN
1	A	477	ASN
1	A	572	ASN
1	A	594	GLU
1	A	595	ASN
1	A	613	HIS
1	A	615	VAL

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Mol	Chain	Res	Type
1	A	627	ILE
1	B	11	ASP
1	B	15	LYS
1	B	42	LYS
1	B	47	THR
1	B	80	GLN
1	B	114	SER
1	B	118	LYS
1	B	129	LEU
1	B	173	LYS
1	B	181	LYS
1	B	209	VAL
1	B	218	LYS
1	B	237	LYS
1	B	460	ILE
1	B	477	ASN
1	B	506	LYS
1	B	539	GLU
1	B	595	ASN
1	B	613	HIS
1	B	634	MET
1	B	669	LYS
1	B	724	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	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	263	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

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Mol	Chain	Res	Type
1	A	447	ASN
1	A	465	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	567	GLN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	604	GLN
1	A	637	GLN
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	161	HIS
1	B	184	HIS
1	B	196	GLN
1	B	197	ASN
1	B	200	ASN
1	B	238	GLN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	447	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	518	ASN
1	B	525	GLN
1	B	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	564	GLN
1	B	567	GLN

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Mol	Chain	Res	Type
1	B	572	ASN
1	B	595	ASN
1	B	599	ASN
1	B	637	GLN
1	B	644	HIS
1	B	656	ASN
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	B	466	1	13,14,15	2.52	4 (30%)	13,19,21	1.82	4 (30%)
1	TPQ	A	466	1	13,14,15	2.35	3 (23%)	13,19,21	1.48	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	B	466	1	-	1/5/22/24	0/1/1/1
1	TPQ	A	466	1	-	2/5/22/24	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	TPQ	C1-C2	-5.50	1.41	1.49
1	A	466	TPQ	C1-C2	-5.40	1.41	1.49
1	B	466	TPQ	C6-C5	-4.37	1.33	1.44
1	A	466	TPQ	CB-C1	4.00	1.57	1.50
1	B	466	TPQ	CB-C1	3.64	1.57	1.50
1	A	466	TPQ	C6-C5	-3.08	1.36	1.44
1	B	466	TPQ	O5-C5	2.48	1.31	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TPQ	C6-C5-C4	3.27	122.51	116.80
1	B	466	TPQ	C3-C4-C5	-3.00	118.17	121.23
1	B	466	TPQ	CB-C1-C2	2.56	123.04	118.56
1	A	466	TPQ	C6-C5-C4	2.20	120.65	116.80
1	A	466	TPQ	O2-C2-C3	-2.01	117.26	121.83
1	B	466	TPQ	O4-C4-C5	2.00	122.39	117.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TPQ	C2-C1-CB-CA
1	B	466	TPQ	C2-C1-CB-CA
1	A	466	TPQ	C6-C1-CB-CA

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	TPQ	4	0
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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	717/727 (98%)	-0.30	10 (1%) 73 77	15, 26, 46, 62	0
1	B	720/727 (99%)	-0.20	17 (2%) 59 63	17, 29, 50, 65	0
All	All	1437/1454 (98%)	-0.25	27 (1%) 66 70	15, 28, 48, 65	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	ASP	4.9
1	B	6	HIS	4.8
1	A	381	TYR	4.0
1	A	148	GLN	3.1
1	A	644	HIS	3.0
1	B	301	PRO	3.0
1	B	644	HIS	2.9
1	A	629	HIS	2.8
1	B	115	ALA	2.6
1	B	215	THR	2.6
1	A	64	LYS	2.5
1	B	120	ASN	2.5
1	A	147	ASP	2.4
1	B	80	GLN	2.4
1	B	239	ASP	2.4
1	A	211	LYS	2.4
1	A	146	VAL	2.4
1	B	302	ALA	2.3
1	B	119	PRO	2.3
1	A	217	ALA	2.3
1	B	118	LYS	2.3
1	B	381	TYR	2.2
1	B	148	GLN	2.1
1	B	178	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	617	LYS	2.1
1	B	143	ASN	2.0
1	A	724	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	A	466	14/15	0.85	0.18	20,43,47,48	0
1	TPQ	B	466	14/15	0.88	0.14	22,45,49,50	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	0.94	0.12	54,54,54,54	0
3	CA	B	803	1/1	0.96	0.07	54,54,54,54	0
3	CA	B	802	1/1	0.98	0.04	29,29,29,29	0
3	CA	A	802	1/1	0.99	0.05	26,26,26,26	0
2	CU	A	801	1/1	0.99	0.05	28,28,28,28	0
2	CU	B	801	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.