



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:23 PM GMT

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

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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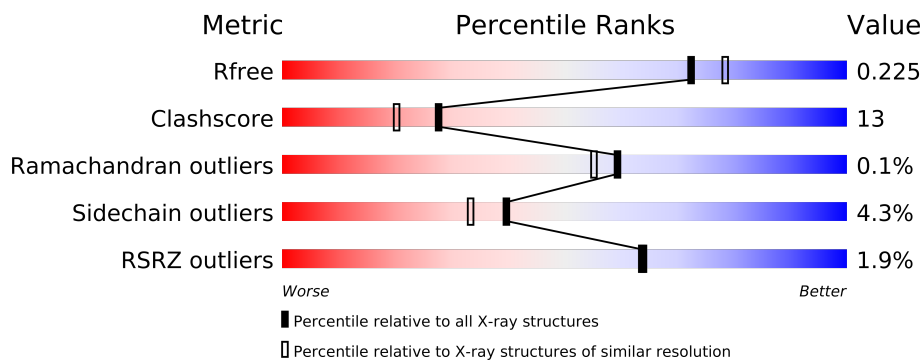
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	722	
1	B	722	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12895 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called COPPER AMINE OXIDASE.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	ASP	ENGINEERED	UNP P46883
A	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883
B	383	ALA	ASP	ENGINEERED	UNP P46883
B	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

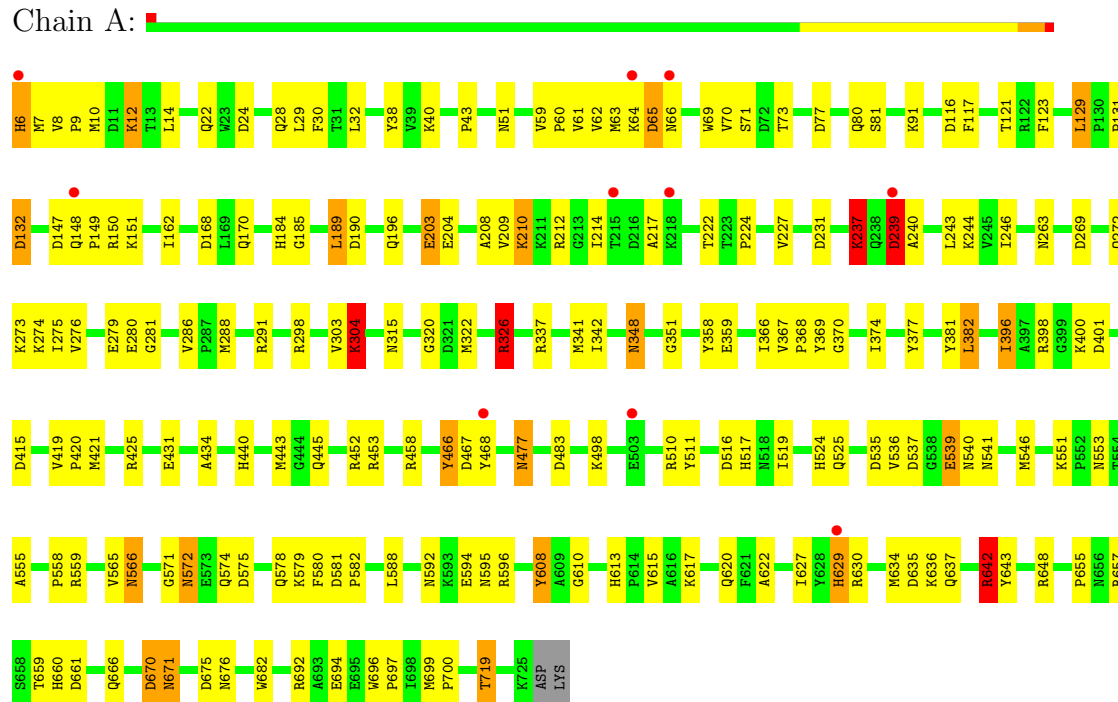
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	791	Total 791	O 791	0	0
4	B	700	Total 700	O 700	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

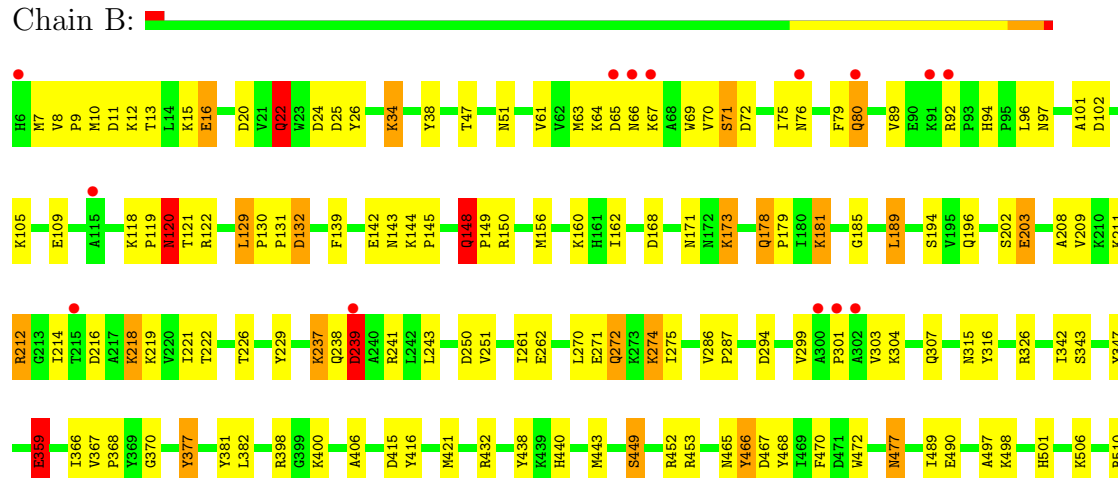
#### • Molecule 1: COPPER AMINE OXIDASE

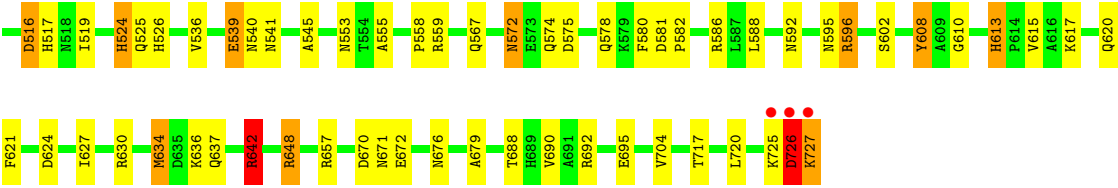
Chain A:



#### • Molecule 1: COPPER AMINE OXIDASE

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.66Å 166.17Å 79.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.00) 90.0 (19.94-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.36 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.176 , 0.244 0.175 , 0.225	Depositor DCC
$R_{free}$ test set	3766 reflections (3.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 109646 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, TPQ, 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	0.53	0/5802	1.71	80/7899 (1.0%)
1	B	0.51	0/5828	1.65	89/7930 (1.1%)
All	All	0.52	0/11630	1.68	169/15829 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ARG	NE-CZ-NH2	-20.10	110.25	120.30
1	A	596	ARG	CD-NE-CZ	19.41	150.78	123.60
1	A	648	ARG	NE-CZ-NH1	16.45	128.52	120.30
1	A	692	ARG	NE-CZ-NH2	-16.04	112.28	120.30
1	A	648	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	291	ARG	CD-NE-CZ	11.36	139.50	123.60
1	B	72	ASP	CB-CG-OD1	10.97	128.17	118.30
1	A	566	ASN	OD1-CG-ND2	10.86	146.89	121.90
1	A	642	ARG	CD-NE-CZ	10.77	138.68	123.60
1	A	189	LEU	CB-CG-CD1	10.48	128.82	111.00
1	A	692	ARG	CD-NE-CZ	10.27	137.98	123.60
1	B	20	ASP	CB-CG-OD2	10.13	127.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	A	692	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	401	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	A	24	ASP	CB-CG-OD1	9.77	127.09	118.30
1	A	566	ASN	CB-CG-OD1	-9.68	102.24	121.60
1	B	415	ASP	CB-CG-OD1	9.52	126.87	118.30
1	B	359	GLU	CA-CB-CG	9.41	134.11	113.40
1	B	586	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	635	ASP	CB-CG-OD2	-9.34	109.89	118.30
1	B	516	ASP	CB-CG-OD1	9.26	126.63	118.30
1	B	648	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	B	648	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	122	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	B	189	LEU	CB-CG-CD2	8.59	125.60	111.00
1	A	415	ASP	CB-CG-OD1	8.58	126.02	118.30
1	B	132	ASP	CB-CG-OD1	-8.46	110.68	118.30
1	A	341	MET	CA-CB-CG	-8.31	99.17	113.30
1	B	452	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	B	608	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	A	453	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	440	HIS	N-CA-CB	8.11	125.19	110.60
1	A	304	LYS	CA-CB-CG	8.10	131.21	113.40
1	A	642	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	452	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	326	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	B	92	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	608	TYR	CB-CG-CD1	7.72	125.63	121.00
1	B	692	ARG	NH1-CZ-NH2	7.72	127.89	119.40
1	A	398	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	398	ARG	CG-CD-NE	7.67	127.91	111.80
1	A	511	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	B	416	TYR	CB-CG-CD2	-7.57	116.46	121.00
1	A	189	LEU	CB-CA-C	7.53	124.50	110.20
1	A	596	ARG	NE-CZ-NH1	-7.53	116.54	120.30
1	B	72	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	337	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	692	ARG	CG-CD-NE	-7.36	96.35	111.80
1	B	657	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	608	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	A	443	MET	CA-CB-CG	7.21	125.56	113.30
1	A	483	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	629	HIS	CA-CB-CG	-7.13	101.47	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	ARG	CD-NE-CZ	7.10	133.54	123.60
1	B	624	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	116	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	A	190	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	129	LEU	N-CA-C	-7.08	91.87	111.00
1	A	719	THR	CA-CB-CG2	-7.07	102.50	112.40
1	B	497	ALA	CB-CA-C	-7.04	99.53	110.10
1	B	102	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	231	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	458	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	421	MET	CA-CB-CG	6.96	125.13	113.30
1	B	440	HIS	N-CA-CB	6.87	122.96	110.60
1	B	726	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	398	ARG	NH1-CZ-NH2	6.85	126.94	119.40
1	B	239	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	22	GLN	CB-CG-CD	6.82	129.32	111.60
1	A	431	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	A	630	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	511	TYR	CB-CG-CD2	6.78	125.07	121.00
1	A	537	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	25	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	581	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	672	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	A	298	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	571	GLY	N-CA-C	6.45	129.22	113.10
1	B	692	ARG	CG-CD-NE	-6.44	98.28	111.80
1	A	635	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	565	VAL	CA-CB-CG2	-6.35	101.37	110.90
1	A	132	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	B	189	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	A	168	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	132	ASP	OD1-CG-OD2	6.14	134.97	123.30
1	A	326	ARG	NH1-CZ-NH2	6.13	126.15	119.40
1	B	34	LYS	CA-CB-CG	-6.09	100.00	113.40
1	A	421	MET	N-CA-CB	-6.08	99.65	110.60
1	A	588	LEU	N-CA-C	-6.07	94.62	111.00
1	A	566	ASN	N-CA-CB	-6.04	99.73	110.60
1	B	316	TYR	CG-CD2-CE2	6.04	126.13	121.30
1	B	657	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	A	539	GLU	CB-CG-CD	6.02	130.45	114.20
1	B	608	TYR	CB-CG-CD1	5.95	124.57	121.00
1	B	704	VAL	N-CA-CB	5.95	124.59	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	622	ALA	CB-CA-C	5.89	118.93	110.10
1	A	396	ILE	CB-CG1-CD1	-5.88	97.43	113.90
1	B	449	SER	CB-CA-C	-5.87	98.96	110.10
1	B	415	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	453	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	150	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	142	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	B	272	GLN	CB-CA-C	5.72	121.85	110.40
1	B	421	MET	N-CA-CB	-5.71	100.32	110.60
1	B	237	LYS	CA-CB-CG	5.65	125.84	113.40
1	A	320	GLY	N-CA-C	-5.65	98.98	113.10
1	B	382	LEU	N-CA-C	-5.65	95.75	111.00
1	A	326	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	150	ARG	CD-NE-CZ	-5.63	115.71	123.60
1	A	231	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	670	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	123	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	A	596	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	B	602	SER	CB-CA-C	-5.54	99.57	110.10
1	B	472	TRP	N-CA-C	-5.53	96.08	111.00
1	B	262	GLU	O-C-N	5.50	131.51	122.70
1	B	438	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	445	GLN	CG-CD-OE1	-5.49	110.61	121.60
1	B	526	HIS	CA-CB-CG	-5.49	104.27	113.60
1	A	675	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	120	ASN	CA-CB-CG	5.45	125.38	113.40
1	B	470	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	B	194	SER	CB-CA-C	5.42	120.41	110.10
1	A	6	HIS	O-C-N	-5.42	114.03	122.70
1	B	274	LYS	N-CA-CB	-5.42	100.84	110.60
1	B	406	ALA	CB-CA-C	-5.39	102.01	110.10
1	B	642	ARG	CD-NE-CZ	5.38	131.14	123.60
1	A	65	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	377	TYR	CG-CD2-CE2	5.37	125.59	121.30
1	B	212	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	682	TRP	N-CA-CB	5.32	120.18	110.60
1	B	634	MET	CG-SD-CE	5.32	108.70	100.20
1	A	661	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	261	ILE	N-CA-C	-5.31	96.67	111.00
1	B	148	GLN	CB-CA-C	5.30	121.00	110.40
1	B	24	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	B	432	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	343	SER	N-CA-CB	-5.27	102.60	110.50
1	B	294	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	690	VAL	N-CA-C	-5.26	96.81	111.00
1	A	535	ASP	N-CA-C	-5.25	96.82	111.00
1	B	688	THR	N-CA-C	-5.25	96.83	111.00
1	B	26	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	382	LEU	N-CA-C	-5.23	96.87	111.00
1	A	239	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	239	ASP	OD1-CG-OD2	5.21	133.19	123.30
1	B	695	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	B	670	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	398	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	696	TRP	N-CA-CB	-5.17	101.30	110.60
1	A	657	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	524	HIS	CG-CD2-NE2	-5.14	99.44	109.20
1	B	438	TYR	CB-CG-CD1	5.14	124.08	121.00
1	A	237	LYS	CA-CB-CG	5.13	124.68	113.40
1	B	226	THR	CA-CB-CG2	-5.13	105.22	112.40
1	B	526	HIS	N-CA-C	-5.12	97.17	111.00
1	B	122	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	596	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	588	LEU	N-CA-C	-5.11	97.20	111.00
1	B	539	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	A	467	ASP	O-C-N	5.03	130.75	122.70
1	B	347	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	588	LEU	N-CA-CB	5.03	120.46	110.40
1	B	168	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	421	MET	CG-SD-CE	-5.01	92.17	100.20
1	A	666	GLN	CG-CD-OE1	5.01	131.62	121.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466[B]	TPQ	Mainchain
1	B	466[B]	TPQ	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5686	0	5553	148	0
1	B	5712	0	5583	161	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	791	0	0	23	0
4	B	700	0	0	21	0
All	All	12895	0	11136	288	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (288) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:466[A]:TPQ:H6	4:B:1351:HOH:O	1.25	1.29
1:B:466[A]:TPQ:C6	4:B:1351:HOH:O	1.92	1.00
1:B:67:LYS:HG3	1:B:69:TRP:HE1	1.27	0.98
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.30	0.93
1:A:466[A]:TPQ:O5	4:A:1575:HOH:O	1.86	0.93
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.34	0.92
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.52	0.91
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.01	0.91
1:A:304:LYS:H	1:B:315:ASN:HD21	1.17	0.90
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.18	0.88
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.56	0.88
1:A:303:VAL:HG22	1:B:326:ARG:HH21	1.37	0.88
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.73	0.88
1:A:189:LEU:HG	4:A:843:HOH:O	1.74	0.86
1:A:28:GLN:HG3	4:A:1188:HOH:O	1.74	0.86
1:B:181:LYS:HE2	1:B:181:LYS:H	1.40	0.85
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.09	0.83
1:A:525:GLN:NE2	1:A:620:GLN:H	1.77	0.82
1:B:490:GLU:HG2	4:B:1503:HOH:O	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:VAL:HG22	1:B:326:ARG:NH2	1.97	0.79
1:B:251:VAL:O	1:B:251:VAL:HG12	1.82	0.79
1:B:94:HIS:HD2	1:B:96:LEU:H	1.33	0.76
1:B:38:TYR:H	1:B:51:ASN:HD21	1.34	0.76
1:B:642:ARG:HH11	1:B:642:ARG:CB	1.98	0.76
1:B:12:LYS:O	1:B:16:GLU:HG2	1.86	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:A:38:TYR:H	1:A:51:ASN:HD21	1.34	0.76
1:B:580:PHE:H	1:B:637:GLN:HE21	1.34	0.75
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.86	0.75
1:B:189:LEU:HG	4:B:867:HOH:O	1.87	0.75
1:A:580:PHE:H	1:A:637:GLN:HE21	1.33	0.74
1:A:38:TYR:H	1:A:51:ASN:ND2	1.86	0.74
1:A:272:GLN:HE21	1:A:274:LYS:HD3	1.52	0.74
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.53	0.73
1:A:536:VAL:H	1:A:541:ASN:HD21	1.35	0.73
1:B:67:LYS:HG3	1:B:69:TRP:NE1	2.03	0.73
1:B:38:TYR:H	1:B:51:ASN:ND2	1.87	0.73
1:B:203:GLU:H	1:B:203:GLU:CD	1.92	0.73
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.71	0.73
1:B:725:LYS:O	1:B:726:ASP:OD1	2.06	0.73
1:B:67:LYS:CG	1:B:69:TRP:HE1	2.02	0.72
1:A:286:VAL:HG12	1:A:288:MET:CE	2.19	0.72
1:B:525:GLN:NE2	1:B:620:GLN:H	1.88	0.72
1:A:326:ARG:HD2	4:A:1014:HOH:O	1.91	0.71
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.38	0.71
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.04	0.71
1:A:617:LYS:HE3	1:B:581:ASP:OD1	1.91	0.71
1:A:553:ASN:ND2	1:A:555:ALA:H	1.87	0.70
1:A:525:GLN:HE22	1:A:620:GLN:H	1.38	0.70
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.72	0.70
1:B:64:LYS:O	1:B:67:LYS:HG2	1.90	0.70
1:A:286:VAL:CG1	1:A:288:MET:HE1	2.21	0.70
1:A:315:ASN:HD21	1:B:304:LYS:H	1.38	0.69
1:A:699:MET:HE1	4:A:1574:HOH:O	1.91	0.69
1:A:272:GLN:NE2	1:A:274:LYS:HD3	2.07	0.69
1:B:574:GLN:H	1:B:671:ASN:ND2	1.91	0.68
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.75	0.68
1:B:251:VAL:HG11	4:B:1224:HOH:O	1.92	0.68
1:B:580:PHE:H	1:B:637:GLN:NE2	1.93	0.67
1:A:149:PRO:HB3	1:A:170:GLN:HE21	1.58	0.67
1:B:173:LYS:HB3	1:B:173:LYS:NZ	2.10	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:119:PRO:O	1:B:120:ASN:OD1	2.12	0.66
1:B:189:LEU:HD11	4:B:1112:HOH:O	1.94	0.66
1:B:10:MET:HG3	1:B:70:VAL:CG1	2.25	0.66
1:A:288:MET:HA	1:A:288:MET:HE2	1.78	0.66
1:B:160:LYS:HD3	1:B:271:GLU:OE1	1.95	0.66
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.78	0.65
1:A:592:ASN:HD21	1:A:676:ASN:ND2	1.93	0.64
1:A:6:HIS:CG	1:A:7:MET:N	2.65	0.64
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.13	0.64
1:A:629:HIS:HB2	4:A:1241:HOH:O	1.97	0.64
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.80	0.64
1:A:6:HIS:CG	1:A:7:MET:H	2.15	0.64
1:B:22:GLN:HB3	4:B:1478:HOH:O	1.98	0.64
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.26	0.64
1:A:322:MET:HG2	4:A:1312:HOH:O	1.98	0.63
1:B:221:ILE:HD13	1:B:250:ASP:HB2	1.80	0.63
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.64	0.62
1:B:109:GLU:HG2	4:B:1081:HOH:O	1.98	0.62
1:A:286:VAL:HG12	1:A:288:MET:HE1	1.81	0.62
1:B:572:ASN:HD22	1:B:575:ASP:H	1.46	0.62
1:B:181:LYS:CE	1:B:181:LYS:H	2.11	0.62
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.81	0.62
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.36	0.61
1:A:574:GLN:H	1:A:671:ASN:ND2	1.97	0.60
1:B:178:GLN:HG3	4:B:862:HOH:O	2.00	0.60
1:A:203:GLU:CD	1:A:203:GLU:H	2.05	0.60
1:A:498:LYS:O	1:A:517:HIS:HD2	1.84	0.60
1:B:79:PHE:C	1:B:80:GLN:OE1	2.40	0.60
1:B:196:GLN:HE22	1:B:222:THR:H	1.49	0.59
1:B:132:ASP:H	1:B:148:GLN:HE22	1.50	0.59
1:B:613:HIS:HD2	4:B:1267:HOH:O	1.85	0.59
1:A:288:MET:CE	1:A:288:MET:HA	2.31	0.59
1:A:659:THR:OG1	1:A:660:HIS:HD2	1.84	0.59
1:A:162:ILE:HD11	1:A:185:GLY:N	2.17	0.59
1:A:132:ASP:H	1:A:148:GLN:HE22	1.51	0.58
1:A:396:ILE:HD12	1:A:425:ARG:O	2.02	0.58
1:B:65:ASP:O	1:B:66:ASN:HB2	2.03	0.58
1:B:525:GLN:HE22	1:B:620:GLN:H	1.51	0.58
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.17	0.57
1:B:307:GLN:HG2	4:B:1178:HOH:O	2.04	0.57
1:A:61:VAL:HG22	1:A:70:VAL:HG12	1.87	0.57
1:B:572:ASN:ND2	1:B:575:ASP:H	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.86	0.57
1:B:536:VAL:H	1:B:541:ASN:HD21	1.51	0.56
1:A:572:ASN:ND2	1:A:575:ASP:H	2.04	0.56
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.23	0.56
1:B:574:GLN:H	1:B:671:ASN:HD22	1.52	0.56
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.87	0.56
1:A:367:VAL:HG21	1:A:468:TYR:OH	2.06	0.55
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.88	0.55
1:B:10:MET:HG3	1:B:70:VAL:HG11	1.86	0.55
1:B:359:GLU:HG3	4:B:1446:HOH:O	2.07	0.55
1:B:553:ASN:ND2	1:B:555:ALA:H	2.05	0.55
1:B:196:GLN:NE2	1:B:222:THR:H	2.05	0.54
1:B:477:ASN:HD22	1:B:477:ASN:C	2.08	0.54
1:A:131:PRO:HB3	1:A:148:GLN:NE2	2.23	0.54
1:B:679:ALA:HB2	4:B:1169:HOH:O	2.07	0.54
1:B:221:ILE:HD11	1:B:250:ASP:CB	2.33	0.54
1:A:10:MET:CG	1:A:14:LEU:HD23	2.37	0.54
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.89	0.54
1:A:381:TYR:CD2	1:A:466[A]:TPQ:O5	2.61	0.54
1:B:572:ASN:HD21	1:B:575:ASP:CG	2.11	0.54
1:A:208:ALA:O	1:A:212:ARG:HG3	2.07	0.54
1:B:717:THR:HB	1:B:720:LEU:HG	1.90	0.54
1:A:477:ASN:HD22	1:A:477:ASN:C	2.11	0.53
1:A:91:LYS:NZ	4:A:1324:HOH:O	2.37	0.53
1:A:8:VAL:CG2	1:A:9:PRO:HD2	2.37	0.53
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.73	0.53
1:A:237:LYS:HZ2	1:A:239:ASP:CG	2.12	0.53
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.91	0.52
1:B:10:MET:HG3	1:B:70:VAL:HG13	1.91	0.52
1:A:636:LYS:HE3	4:A:1451:HOH:O	2.10	0.52
1:A:22:GLN:HG3	4:A:1418:HOH:O	2.10	0.52
1:B:381:TYR:CD1	1:B:466[A]:TPQ:O5	2.63	0.51
1:B:498:LYS:O	1:B:517:HIS:HD2	1.93	0.51
1:B:203:GLU:N	1:B:203:GLU:CD	2.63	0.51
1:A:400:LYS:NZ	4:A:1225:HOH:O	2.44	0.51
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.23	0.51
1:A:237:LYS:HG2	1:A:240:ALA:CB	2.40	0.51
1:A:62:VAL:HG23	1:A:69:TRP:HB2	1.91	0.51
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.91	0.51
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.91	0.51
1:A:286:VAL:CG1	1:A:288:MET:CE	2.85	0.51
1:A:697:PRO:HD2	1:B:720:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:7:MET:HG2	1:B:71:SER:HA	1.92	0.51
1:B:251:VAL:O	1:B:251:VAL:CG1	2.58	0.50
1:B:572:ASN:HB2	1:B:671:ASN:ND2	2.25	0.50
1:B:238:GLN:HA	1:B:238:GLN:HE21	1.77	0.50
1:A:217:ALA:HB2	4:A:1432:HOH:O	2.12	0.50
1:B:67:LYS:HD2	1:B:69:TRP:CZ2	2.46	0.50
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.24	0.50
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.92	0.50
1:A:7:MET:HE1	1:A:59:VAL:HG11	1.94	0.50
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.93	0.50
1:B:101:ALA:O	1:B:105:LYS:HG3	2.11	0.50
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.93	0.49
1:A:29:LEU:HD13	1:A:30:PHE:O	2.11	0.49
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.77	0.49
1:A:65:ASP:O	1:A:66:ASN:HB2	2.12	0.49
1:A:466[A]:TPQ:HB3	1:A:468:TYR:CE2	2.47	0.49
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.16	0.49
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.47	0.49
1:B:76:ASN:O	1:B:80:GLN:HB2	2.13	0.49
1:A:551:LYS:NZ	4:A:1453:HOH:O	2.43	0.49
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.13	0.49
1:A:71:SER:OG	1:A:73:THR:HG22	2.13	0.49
1:A:147:ASP:HB2	4:A:1182:HOH:O	2.13	0.49
1:A:642:ARG:HG3	1:A:643:TYR:N	2.28	0.49
1:A:670:ASP:N	1:A:670:ASP:OD1	2.46	0.49
1:A:610:GLY:HA3	1:B:610:GLY:HA3	1.95	0.49
1:B:299:VAL:O	1:B:301:PRO:HD3	2.12	0.48
1:B:221:ILE:N	1:B:221:ILE:HD12	2.28	0.48
1:B:171:ASN:HB3	1:B:173:LYS:HE2	1.95	0.48
1:B:38:TYR:N	1:B:51:ASN:HD21	2.08	0.48
1:A:29:LEU:HD13	1:A:30:PHE:N	2.28	0.48
1:A:580:PHE:H	1:A:637:GLN:NE2	2.05	0.48
1:A:516:ASP:HB3	1:A:519:ILE:HB	1.96	0.48
1:B:131:PRO:HG3	4:B:1141:HOH:O	2.14	0.48
1:B:89:VAL:HG23	4:B:1475:HOH:O	2.14	0.48
1:A:162:ILE:HD11	1:A:184:HIS:C	2.34	0.48
1:B:160:LYS:HB2	1:B:241:ARG:HB2	1.96	0.48
1:A:64:LYS:HB3	1:A:69:TRP:CD1	2.48	0.47
1:A:382:LEU:HD22	4:A:902:HOH:O	2.14	0.47
1:B:367:VAL:HG21	1:B:468:TYR:OH	2.13	0.47
1:B:726:ASP:CG	1:B:727:LYS:N	2.65	0.47
1:B:580:PHE:N	1:B:637:GLN:HE21	2.05	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:GLU:N	1:A:203:GLU:CD	2.68	0.47
1:B:545:ALA:O	1:B:567:GLN:HA	2.14	0.47
1:B:51:ASN:N	1:B:51:ASN:HD22	2.11	0.47
1:B:578:GLN:HA	1:B:636:LYS:HD2	1.97	0.47
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.50	0.47
1:A:9:PRO:HG3	1:A:12:LYS:NZ	2.29	0.47
1:B:119:PRO:O	1:B:120:ASN:CB	2.63	0.47
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.50	0.46
1:B:118:LYS:HE2	1:B:118:LYS:HB3	1.51	0.46
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.80	0.46
1:A:40:LYS:CE	4:A:1290:HOH:O	2.64	0.46
4:A:1360:HOH:O	1:B:400:LYS:HE2	2.15	0.46
1:B:634:MET:HE2	1:B:634:MET:HB3	1.87	0.46
1:A:558:PRO:HG2	1:B:377:TYR:CE1	2.50	0.46
1:A:572:ASN:HD22	1:A:575:ASP:H	1.62	0.46
1:A:274:LYS:NZ	1:A:275:ILE:O	2.45	0.46
1:A:237:LYS:HG2	1:A:240:ALA:HB2	1.97	0.46
1:B:524:HIS:HE1	4:B:1503:HOH:O	1.99	0.45
1:A:286:VAL:HG11	1:A:288:MET:HE1	1.97	0.45
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.99	0.45
1:B:67:LYS:HD2	1:B:69:TRP:HZ2	1.82	0.45
1:B:67:LYS:CD	1:B:69:TRP:HE1	2.29	0.45
1:B:121:THR:CG2	1:B:156:MET:HB3	2.47	0.45
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.79	0.45
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.82	0.45
1:B:219:LYS:O	1:B:221:ILE:HD12	2.18	0.45
1:B:208:ALA:O	1:B:212:ARG:HG3	2.17	0.45
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.64	0.44
1:A:10:MET:HE2	1:A:70:VAL:HG11	2.00	0.44
1:B:239:ASP:OD1	1:B:239:ASP:C	2.55	0.44
1:A:525:GLN:HE22	1:A:620:GLN:N	2.12	0.44
1:B:7:MET:HB3	1:B:7:MET:HE2	1.71	0.44
1:A:546:MET:CE	4:A:1025:HOH:O	2.65	0.44
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.48	0.44
1:A:400:LYS:HE3	1:B:449:SER:HB2	1.99	0.44
1:A:368:PRO:HG3	1:A:634:MET:HE3	1.99	0.44
1:A:210:LYS:HE2	1:A:214:ILE:O	2.18	0.43
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.76	0.43
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.54	0.43
1:A:237:LYS:NZ	1:A:239:ASP:OD1	2.51	0.43
1:A:224:PRO:HB2	1:A:243:LEU:HD13	2.01	0.43
1:B:272:GLN:NE2	1:B:274:LYS:HD3	2.14	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.34	0.43
1:A:629:HIS:CE1	4:A:1165:HOH:O	2.71	0.43
1:A:322:MET:HE1	4:A:1150:HOH:O	2.17	0.43
1:A:434:ALA:HB3	1:A:452:ARG:HG2	2.00	0.43
1:B:218:LYS:HA	4:B:1466:HOH:O	2.17	0.43
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.34	0.43
1:B:144:LYS:HA	1:B:145:PRO:HD3	1.92	0.42
1:A:203:GLU:OE2	1:A:204:GLU:OE2	2.37	0.42
1:B:229:TYR:HB3	1:B:630:ARG:HD2	2.01	0.42
1:B:642:ARG:CG	1:B:642:ARG:NH1	2.80	0.42
1:A:642:ARG:HH11	1:A:642:ARG:HG2	1.84	0.42
1:B:120:ASN:ND2	4:B:1203:HOH:O	2.32	0.42
1:B:648:ARG:NH2	4:B:1446:HOH:O	2.47	0.42
1:B:243:LEU:CD1	1:B:270:LEU:HD11	2.50	0.42
1:B:181:LYS:HG2	1:B:181:LYS:O	2.20	0.42
1:A:117:PHE:CZ	1:A:121:THR:HB	2.54	0.42
1:A:189:LEU:HG	1:A:189:LEU:H	1.75	0.42
1:A:209:VAL:HG13	1:A:214:ILE:HB	2.02	0.42
1:A:10:MET:HG2	1:A:14:LEU:HD23	2.01	0.42
1:A:237:LYS:HD3	1:A:240:ALA:HB2	2.01	0.42
1:B:162:ILE:HD11	1:B:185:GLY:CA	2.50	0.42
1:A:60:PRO:HD2	4:A:1458:HOH:O	2.19	0.42
1:B:129:LEU:CD1	1:B:130:PRO:HD2	2.38	0.42
1:A:419:VAL:HA	1:A:420:PRO:HD3	1.95	0.42
1:A:572:ASN:ND2	1:A:671:ASN:HD21	2.18	0.41
1:A:246:ILE:HD13	1:A:246:ILE:HA	1.81	0.41
1:A:51:ASN:N	1:A:51:ASN:HD22	2.17	0.41
1:A:699:MET:HA	1:A:700:PRO:HD3	1.83	0.41
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.35	0.41
1:B:443:MET:CG	4:B:824:HOH:O	2.68	0.41
1:A:263:ASN:HB3	1:A:281:GLY:HA3	2.01	0.41
1:B:139:PHE:O	1:B:143:ASN:HA	2.19	0.41
1:A:608:TYR:OH	1:A:615:VAL:HG21	2.19	0.41
1:B:118:LYS:HA	1:B:119:PRO:HD3	1.93	0.41
1:A:77:ASP:O	1:A:81:SER:HB3	2.19	0.41
1:A:274:LYS:HZ2	1:A:276:VAL:HG12	1.85	0.41
1:B:148:GLN:HA	1:B:149:PRO:HD3	1.76	0.41
1:B:465:ASN:HB2	1:B:489:ILE:O	2.20	0.41
1:A:582:PRO:C	1:B:615:VAL:HG12	2.41	0.41
1:A:617:LYS:CE	1:B:581:ASP:OD1	2.65	0.41
1:A:694:GLU:O	1:B:717:THR:HA	2.20	0.41
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.85	0.41
1:B:63:MET:HE3	1:B:66:ASN:HA	2.03	0.41
1:A:579:LYS:HA	1:A:637:GLN:NE2	2.36	0.41
1:B:581:ASP:HA	1:B:582:PRO:HD2	1.94	0.41
1:A:578:GLN:HA	1:A:636:LYS:HD2	2.02	0.41
1:A:29:LEU:HD12	4:A:989:HOH:O	2.20	0.41
1:B:202:SER:CB	1:B:275:ILE:HD12	2.51	0.41
1:A:269:ASP:O	1:A:273:LYS:N	2.53	0.41
1:A:288:MET:CE	1:A:288:MET:CA	2.98	0.41
1:A:29:LEU:HD13	1:A:29:LEU:C	2.41	0.41
1:A:196:GLN:HE22	1:A:222:THR:H	1.68	0.41
1:A:466[A]:TPQ:H6	4:A:1575:HOH:O	2.06	0.40
1:A:615:VAL:HG23	1:B:582:PRO:HB2	2.04	0.40
1:B:64:LYS:O	1:B:65:ASP:HB2	2.21	0.40
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.34	0.40
1:B:189:LEU:CD2	4:B:867:HOH:O	2.69	0.40
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	717/722 (99%)	694 (97%)	23 (3%)	0	100	100
1	B	719/722 (100%)	693 (96%)	25 (4%)	1 (0%)	59	55
All	All	1436/1444 (99%)	1387 (97%)	48 (3%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	726	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/612 (100%)	587 (96%)	22 (4%)	47	42
1	B	612/612 (100%)	581 (95%)	31 (5%)	33	26
All	All	1221/1224 (100%)	1168 (96%)	53 (4%)	40	33

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	32	LEU
1	A	80	GLN
1	A	129	LEU
1	A	151	LYS
1	A	203	GLU
1	A	210	LYS
1	A	237	LYS
1	A	239	ASP
1	A	304	LYS
1	A	326	ARG
1	A	342	ILE
1	A	348	ASN
1	A	477	ASN
1	A	539	GLU
1	A	566	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	642	ARG
1	A	671	ASN
1	A	719	THR
1	B	11	ASP
1	B	15	LYS
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	120	ASN
1	B	129	LEU
1	B	148	GLN
1	B	173	LYS
1	B	178	GLN
1	B	181	LYS
1	B	203	GLU
1	B	211	LYS
1	B	218	LYS
1	B	237	LYS
1	B	239	ASP
1	B	342	ILE
1	B	359	GLU
1	B	467	ASP
1	B	477	ASN
1	B	539	GLU
1	B	572	ASN
1	B	595	ASN
1	B	613	HIS
1	B	617	LYS
1	B	642	ARG
1	B	726	ASP
1	B	727	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	97	ASN
1	A	120	ASN
1	A	148	GLN
1	A	161	HIS
1	A	170	GLN
1	A	196	GLN
1	A	200	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

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Mol	Chain	Res	Type
1	A	348	ASN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	541	ASN
1	A	553	ASN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	604	GLN
1	A	637	GLN
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	66	ASN
1	B	94	HIS
1	B	97	ASN
1	B	120	ASN
1	B	148	GLN
1	B	196	GLN
1	B	197	ASN
1	B	200	ASN
1	B	238	GLN
1	B	263	ASN
1	B	272	GLN
1	B	307	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	525	GLN
1	B	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	567	GLN
1	B	572	ASN

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Mol	Chain	Res	Type
1	B	595	ASN
1	B	599	ASN
1	B	604	GLN
1	B	613	HIS
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPQ	A	466[A]	1	14,14,15	5.39	6 (42%)	17,19,21	3.00	7 (41%)
1	TPQ	A	466[B]	1	14,14,15	6.07	6 (42%)	17,19,21	3.63	8 (47%)
1	TPQ	B	466[A]	1	14,14,15	5.79	6 (42%)	17,19,21	1.92	2 (11%)
1	TPQ	B	466[B]	1	14,14,15	6.28	6 (42%)	17,19,21	3.76	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	A	466[A]	1	-	0/4/22/24	0/1/1/1
1	TPQ	A	466[B]	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	466[A]	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	466[B]	1	-	0/4/22/24	0/1/1/1



All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466[B]	TPQ	O-C	22.18	1.26	1.11
1	A	466[B]	TPQ	O-C	21.31	1.26	1.11
1	B	466[A]	TPQ	O-C	19.37	1.24	1.11
1	A	466[A]	TPQ	O-C	18.82	1.24	1.11
1	B	466[B]	TPQ	C1-C2	-5.35	1.40	1.48
1	A	466[B]	TPQ	C1-C2	-5.18	1.41	1.48
1	B	466[A]	TPQ	C1-C2	-4.94	1.41	1.48
1	A	466[A]	TPQ	C1-C2	-4.83	1.41	1.48
1	B	466[A]	TPQ	O5-C5	-4.77	1.11	1.24
1	B	466[A]	TPQ	O2-C2	-4.69	1.11	1.24
1	A	466[B]	TPQ	C6-C5	-2.99	1.35	1.44
1	B	466[B]	TPQ	C6-C5	-2.88	1.35	1.44
1	A	466[B]	TPQ	O5-C5	2.78	1.32	1.24
1	A	466[A]	TPQ	C6-C1	2.69	1.42	1.34
1	B	466[A]	TPQ	C4-C5	-2.62	1.39	1.48
1	A	466[A]	TPQ	C3-C4	2.43	1.39	1.35
1	B	466[B]	TPQ	O5-C5	2.28	1.31	1.24
1	B	466[A]	TPQ	C3-C4	2.26	1.39	1.35
1	A	466[B]	TPQ	CB-C1	2.23	1.55	1.50
1	A	466[A]	TPQ	CB-C1	2.22	1.55	1.50
1	A	466[A]	TPQ	C4-C5	-2.18	1.40	1.48
1	B	466[B]	TPQ	CB-C1	2.15	1.55	1.50
1	A	466[B]	TPQ	C3-C4	2.14	1.39	1.35
1	B	466[B]	TPQ	C3-C4	2.11	1.39	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466[B]	TPQ	C-CA-N	12.22	126.04	113.83
1	A	466[B]	TPQ	C-CA-N	11.38	125.20	113.83
1	A	466[A]	TPQ	C-CA-N	7.55	121.37	113.83
1	B	466[A]	TPQ	C-CA-N	5.96	119.78	113.83
1	B	466[B]	TPQ	CB-C1-C2	5.50	129.93	118.76
1	B	466[B]	TPQ	CB-C1-C6	-5.26	112.78	122.61
1	A	466[A]	TPQ	CB-C1-C6	-5.25	112.80	122.61
1	A	466[A]	TPQ	CB-C1-C2	4.77	128.45	118.76
1	A	466[B]	TPQ	CA-CB-C1	-4.64	105.00	114.41
1	A	466[B]	TPQ	CB-C1-C2	4.27	127.44	118.76
1	A	466[B]	TPQ	CB-C1-C6	-4.25	114.67	122.61
1	A	466[A]	TPQ	O5-C5-C4	3.88	125.21	119.05
1	B	466[A]	TPQ	CA-CB-C1	-3.49	107.33	114.41
1	B	466[B]	TPQ	CA-CB-C1	-3.20	107.92	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466[A]	TPQ	O5-C5-C6	-3.03	114.40	121.73
1	B	466[B]	TPQ	C4-C3-C2	-2.91	117.28	120.40
1	A	466[B]	TPQ	C4-C3-C2	-2.88	117.30	120.40
1	A	466[A]	TPQ	CB-CA-N	2.86	125.35	112.03
1	A	466[A]	TPQ	CA-CB-C1	-2.71	108.91	114.41
1	A	466[B]	TPQ	CB-CA-N	2.70	124.60	112.03
1	A	466[B]	TPQ	C3-C4-C5	-2.35	118.68	121.27
1	A	466[B]	TPQ	C6-C5-C4	2.21	121.09	117.44
1	B	466[B]	TPQ	C6-C5-C4	2.02	120.78	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	720/722 (99%)	-0.38	10 (1%) 72 72	12, 23, 45, 70	0
1	B	722/722 (100%)	-0.30	17 (2%) 56 56	15, 24, 48, 95	0
All	All	1442/1444 (99%)	-0.34	27 (1%) 64 64	12, 24, 47, 95	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	727	LYS	7.2
1	B	301	PRO	4.7
1	B	302	ALA	4.6
1	A	629	HIS	3.9
1	B	6	HIS	3.7
1	A	6	HIS	3.6
1	B	92	ARG	3.5
1	B	726	ASP	3.4
1	B	215	THR	3.4
1	A	66	ASN	3.0
1	B	65	ASP	2.9
1	A	148	GLN	2.9
1	B	66	ASN	2.8
1	B	91	LYS	2.8
1	B	300	ALA	2.8
1	A	64	LYS	2.8
1	B	115	ALA	2.5
1	A	468	TYR	2.3
1	B	239	ASP	2.3
1	B	725	LYS	2.3
1	A	215	THR	2.2
1	A	218	LYS	2.2
1	A	239	ASP	2.2
1	A	503	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	67	LYS	2.1
1	B	76	ASN	2.0
1	B	80	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	B	466[A]	14/15	0.18	4.52	22,50,57,57	14
1	TPQ	B	466[B]	14/15	0.18	3.76	20,40,50,54	14
1	TPQ	A	466[B]	14/15	0.20	2.99	15,43,53,53	14
1	TPQ	A	466[A]	14/15	0.20	2.79	24,45,47,48	14

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	A	802	1/1	0.08	-0.70	21,21,21,21	0
3	CA	A	803	1/1	0.09	-0.82	42,42,42,42	0
3	CA	B	802	1/1	0.07	-0.99	22,22,22,22	0
3	CA	B	803	1/1	0.06	-1.29	49,49,49,49	0
2	CU	B	801	1/1	0.04	-4.53	23,23,23,23	0
2	CU	A	801	1/1	0.04	-8.33	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.