



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:43 PM GMT

PDB ID : 1QAF  
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 : 1999-03-11  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

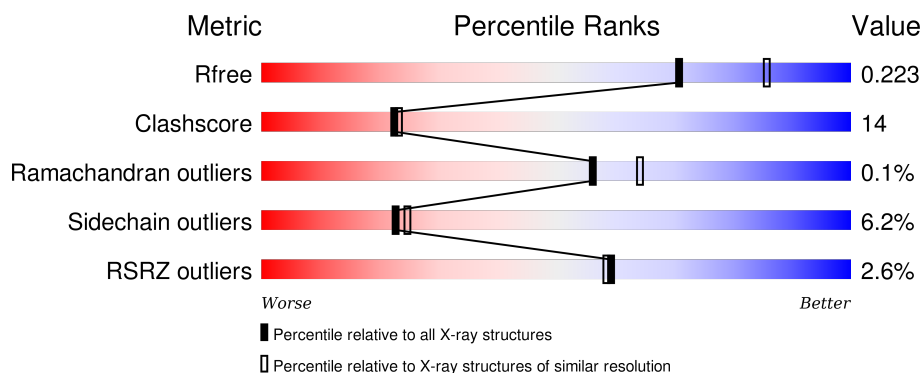
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	721	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	1450	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12775 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 PROTEIN (COPPER AMINE OXIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	1
			5666	3603	965	1076	22			
1	B	721	Total	C	N	O	S	0	0	0
			5690	3618	970	1080	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	GLU	ASP	ENGINEERED	UNP P46883
A	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883
B	383	GLU	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 GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

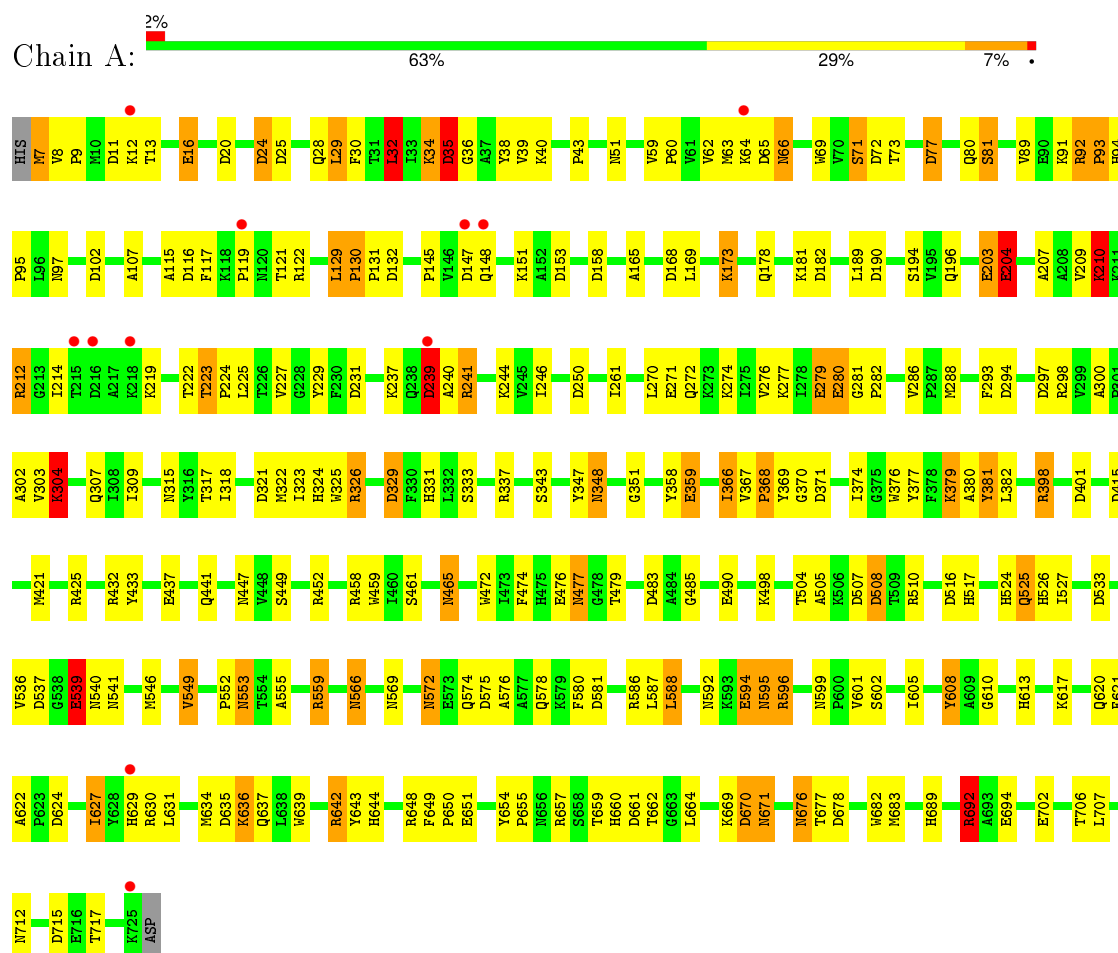
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	767	Total	O	0	0
			767	767		
5	B	640	Total	O	0	0
			640	640		

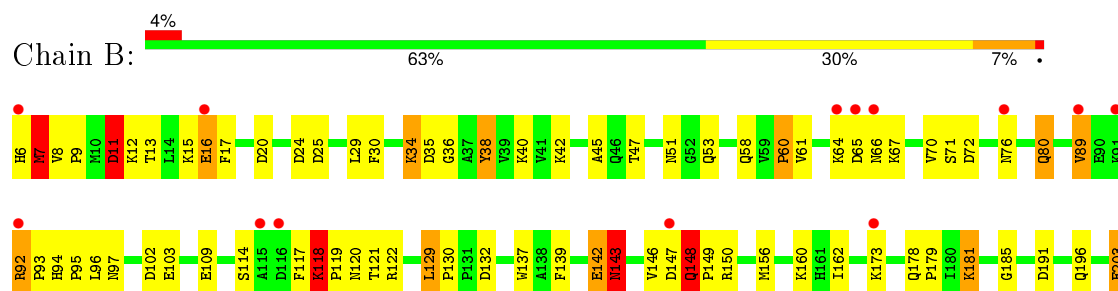
### 3 Residue-property plots [i](#)

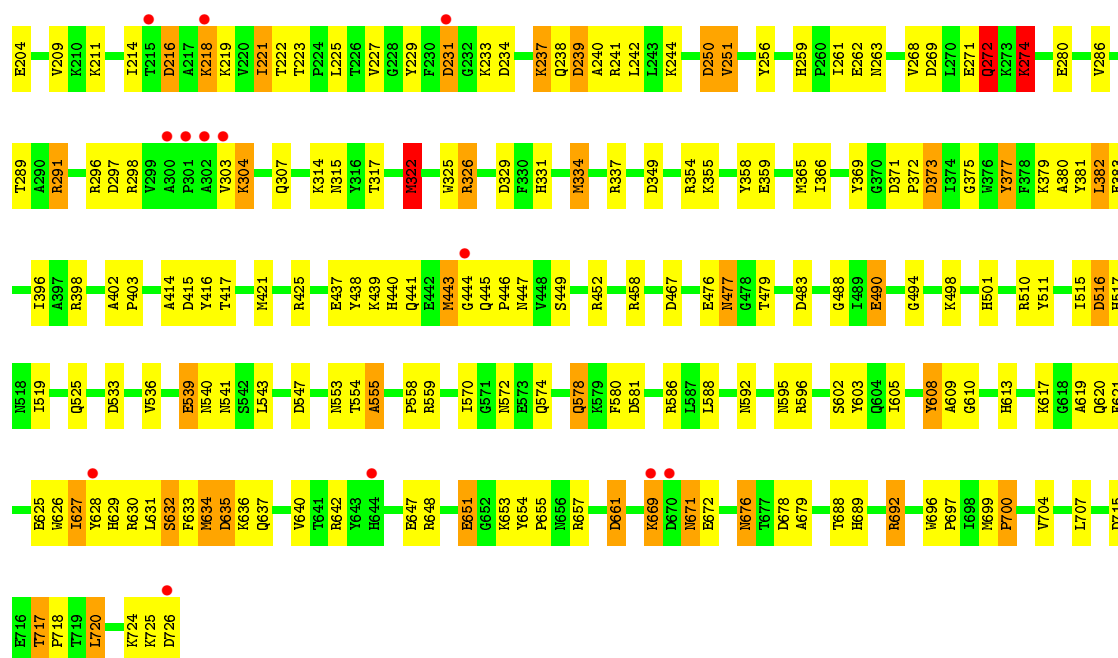
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PROTEIN (COPPER AMINE OXIDASE)



#### • Molecule 1: PROTEIN (COPPER AMINE OXIDASE)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.20 Å   167.00 Å   79.93 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-2.20) 88.9 (19.98-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.19 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.176   ,   0.244 0.164   ,   0.223	Depositor DCC
$R_{free}$ test set	2854 reflections (3.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 84274 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.62	2/5795 (0.0%)	2.02	171/7889 (2.2%)
1	B	0.62	2/5820 (0.0%)	2.04	173/7920 (2.2%)
All	All	0.62	4/11615 (0.0%)	2.03	344/15809 (2.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	LYS	C-N	10.15	1.57	1.34
1	B	326	ARG	C-N	-9.90	1.11	1.34
1	B	325	TRP	C-N	-6.26	1.19	1.34
1	A	35	ASP	C-N	-5.94	1.22	1.33

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ARG	NE-CZ-NH2	-24.01	108.30	120.30
1	B	642	ARG	NE-CZ-NH1	-22.84	108.88	120.30
1	A	596	ARG	NE-CZ-NH2	22.58	131.59	120.30
1	B	648	ARG	CD-NE-CZ	19.27	150.57	123.60
1	B	586	ARG	NE-CZ-NH1	17.76	129.18	120.30
1	A	642	ARG	NE-CZ-NH2	-16.89	111.86	120.30
1	B	661	ASP	CB-CG-OD2	16.68	133.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ARG	NE-CZ-NH2	-16.52	112.04	120.30
1	A	539	GLU	OE1-CD-OE2	-16.44	103.57	123.30
1	B	102	ASP	CB-CG-OD1	15.87	132.58	118.30
1	A	398	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	B	72	ASP	CB-CG-OD1	14.69	131.52	118.30
1	B	241	ARG	NE-CZ-NH1	14.46	127.53	120.30
1	A	657	ARG	NE-CZ-NH2	-14.07	113.26	120.30
1	A	25	ASP	CB-CG-OD1	14.05	130.94	118.30
1	A	212	ARG	NE-CZ-NH2	-13.98	113.31	120.30
1	B	642	ARG	NH1-CZ-NH2	13.87	134.65	119.40
1	B	657	ARG	NE-CZ-NH1	-13.70	113.45	120.30
1	B	586	ARG	NE-CZ-NH2	-13.55	113.52	120.30
1	A	586	ARG	NE-CZ-NH2	13.35	126.97	120.30
1	A	642	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	A	72	ASP	CB-CG-OD1	12.79	129.81	118.30
1	A	630	ARG	NE-CZ-NH1	-12.04	114.28	120.30
1	A	304	LYS	CA-CB-CG	11.95	139.68	113.40
1	B	239	ASP	CB-CG-OD2	-11.90	107.59	118.30
1	A	539	GLU	CG-CD-OE2	11.89	142.09	118.30
1	A	566	ASN	OD1-CG-ND2	11.79	149.02	121.90
1	B	326	ARG	O-C-N	-11.71	103.97	122.70
1	B	322	MET	CG-SD-CE	11.43	118.49	100.20
1	B	373	ASP	CB-CG-OD1	-11.31	108.12	118.30
1	B	291	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	B	490	GLU	OE1-CD-OE2	11.04	136.55	123.30
1	A	415	ASP	CB-CG-OD1	10.84	128.05	118.30
1	B	608	TYR	CB-CG-CD2	-10.72	114.57	121.00
1	B	415	ASP	CB-CG-OD1	10.60	127.84	118.30
1	B	280	GLU	OE1-CD-OE2	10.55	135.96	123.30
1	A	279	GLU	OE1-CD-OE2	-10.53	110.67	123.30
1	B	516	ASP	CB-CG-OD1	10.52	127.77	118.30
1	B	458	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	483	ASP	CB-CG-OD1	9.97	127.27	118.30
1	B	20	ASP	CB-CG-OD2	9.84	127.15	118.30
1	A	566	ASN	CB-CG-OD1	-9.82	101.96	121.60
1	A	122	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	415	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	A	92	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	A	516	ASP	CB-CG-OD2	-9.66	109.61	118.30
1	A	635	ASP	CB-CG-OD1	9.64	126.97	118.30
1	B	354	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	A	241	ARG	NE-CZ-NH1	9.52	125.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	CA-C-N	9.51	135.21	116.20
1	B	239	ASP	CB-CG-OD1	9.48	126.83	118.30
1	A	516	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	635	ASP	CB-CG-OD2	-9.33	109.90	118.30
1	A	92	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	B	11	ASP	CB-CG-OD2	-9.23	109.99	118.30
1	A	241	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	234	ASP	CB-CG-OD1	9.09	126.48	118.30
1	B	17	PHE	CB-CG-CD1	-9.07	114.45	120.80
1	B	326	ARG	CA-C-N	9.00	137.01	117.20
1	A	35	ASP	O-C-N	-8.94	108.00	123.20
1	A	596	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	B	547	ASP	CB-CG-OD2	8.80	126.22	118.30
1	B	398	ARG	NH1-CZ-NH2	8.68	128.95	119.40
1	B	511	TYR	CB-CG-CD2	8.67	126.20	121.00
1	B	608	TYR	CB-CG-CD1	8.58	126.15	121.00
1	A	231	ASP	CB-CG-OD1	8.57	126.01	118.30
1	A	537	ASP	CB-CG-OD1	8.46	125.92	118.30
1	B	148	GLN	CB-CA-C	8.46	127.31	110.40
1	B	425	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	317	THR	OG1-CB-CG2	-8.42	90.63	110.00
1	A	13	THR	CA-CB-CG2	8.35	124.08	112.40
1	A	507	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	377	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	B	216	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	692	ARG	CA-CB-CG	8.26	131.58	113.40
1	B	452	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	191	ASP	CB-CG-OD2	8.18	125.66	118.30
1	B	377	TYR	CB-CG-CD1	8.12	125.88	121.00
1	B	692	ARG	NH1-CZ-NH2	8.00	128.20	119.40
1	B	510	ARG	NE-CZ-NH1	-8.00	116.30	120.30
1	A	433	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	B	150	ARG	CD-NE-CZ	-7.92	112.51	123.60
1	B	296	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	132	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	A	458	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	B	147	ASP	CB-CG-OD1	-7.79	111.29	118.30
1	A	194	SER	N-CA-CB	7.78	122.17	110.50
1	A	608	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	B	414	ALA	CB-CA-C	-7.73	98.50	110.10
1	B	642	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	B	6	HIS	N-CA-CB	7.63	124.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	678	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	16	GLU	OE1-CD-OE2	-7.60	114.18	123.30
1	B	555	ALA	N-CA-CB	-7.59	99.47	110.10
1	A	72	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	B	102	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	657	ARG	NH1-CZ-NH2	7.54	127.70	119.40
1	B	439	LYS	CD-CE-NZ	7.53	129.02	111.70
1	B	65	ASP	CB-CG-OD2	7.53	125.08	118.30
1	A	608	TYR	CB-CG-CD1	7.52	125.51	121.00
1	A	692	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	661	ASP	CB-CG-OD1	7.35	124.92	118.30
1	A	116	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	A	437	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	B	458	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	415	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	B	17	PHE	CB-CG-CD2	7.24	125.87	120.80
1	B	628	TYR	CB-CG-CD1	-7.24	116.66	121.00
1	A	302	ALA	CB-CA-C	7.14	120.81	110.10
1	B	233	LYS	N-CA-CB	7.14	123.45	110.60
1	A	490	GLU	OE1-CD-OE2	7.13	131.86	123.30
1	B	251	VAL	CG1-CB-CG2	7.08	122.23	110.90
1	A	271	GLU	CG-CD-OE1	7.05	132.39	118.30
1	A	586	ARG	NH1-CZ-NH2	-7.02	111.67	119.40
1	A	483	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	516	ASP	OD1-CG-OD2	-6.99	110.02	123.30
1	A	525	GLN	CG-CD-OE1	-6.96	107.68	121.60
1	A	624	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	165	ALA	CB-CA-C	-6.89	99.77	110.10
1	A	271	GLU	CG-CD-OE2	-6.88	104.54	118.30
1	A	715	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	72	ASP	OD1-CG-OD2	-6.85	110.28	123.30
1	A	474	PHE	CB-CG-CD2	6.84	125.58	120.80
1	B	337	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	425	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	505	ALA	N-CA-CB	6.82	119.64	110.10
1	A	212	ARG	NH1-CZ-NH2	6.81	126.89	119.40
1	A	559	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	654	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	B	371	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	A	321	ASP	CB-CG-OD1	6.73	124.35	118.30
1	B	421	MET	N-CA-CB	-6.72	98.50	110.60
1	A	210	LYS	CD-CE-NZ	6.71	127.13	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	VAL	CA-CB-CG2	6.70	120.95	110.90
1	A	239	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	24	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	24	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	438	TYR	CZ-CE2-CD2	-6.67	113.80	119.80
1	A	401	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	661	ASP	OD1-CG-OD2	-6.65	110.67	123.30
1	A	300	ALA	N-CA-CB	-6.64	100.81	110.10
1	A	643	TYR	CB-CG-CD1	6.64	124.98	121.00
1	B	7	MET	N-CA-CB	-6.62	98.69	110.60
1	B	438	TYR	CG-CD2-CE2	6.61	126.59	121.30
1	B	65	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	A	293	PHE	CB-CG-CD2	6.60	125.42	120.80
1	A	636	LYS	N-CA-CB	6.60	122.47	110.60
1	B	256	TYR	CB-CG-CD1	6.60	124.96	121.00
1	A	119	PRO	C-N-CA	-6.54	105.36	121.70
1	B	25	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	483	ASP	OD1-CG-OD2	-6.53	110.89	123.30
1	B	678	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	569	ASN	CB-CG-OD1	-6.45	108.69	121.60
1	A	7	MET	N-CA-CB	6.43	122.18	110.60
1	B	58	GLN	N-CA-CB	6.42	122.16	110.60
1	B	117	PHE	CB-CG-CD1	-6.42	116.31	120.80
1	A	168	ASP	CB-CG-OD2	6.39	124.06	118.30
1	A	36	GLY	O-C-N	-6.38	112.49	122.70
1	B	122	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	432	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	715	ASP	CB-CG-OD1	6.31	123.97	118.30
1	B	103	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	B	672	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	A	596	ARG	NH1-CZ-NH2	-6.21	112.57	119.40
1	A	596	ARG	CD-NE-CZ	6.21	132.29	123.60
1	A	677	THR	N-CA-CB	-6.21	98.51	110.30
1	A	190	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	369	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	B	296	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	633	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	B	334	MET	N-CA-CB	-6.17	99.50	110.60
1	A	581	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	539	GLU	CB-CG-CD	6.16	130.82	114.20
1	A	648	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	241	ARG	NE-CZ-NH2	-6.12	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	707	LEU	N-CA-CB	-6.11	98.18	110.40
1	A	34	LYS	C-N-CA	-6.09	106.47	121.70
1	B	109	GLU	OE1-CD-OE2	-6.09	116.00	123.30
1	A	654	TYR	CB-CG-CD1	6.08	124.65	121.00
1	B	704	VAL	N-CA-CB	6.07	124.86	111.50
1	A	129	LEU	CA-C-O	6.07	132.84	120.10
1	A	715	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	588	LEU	CB-CA-C	6.04	121.67	110.20
1	B	692	ARG	CB-CA-C	6.03	122.47	110.40
1	B	359	GLU	CA-CB-CG	6.03	126.66	113.40
1	A	129	LEU	N-CA-C	-6.01	94.77	111.00
1	A	371	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	A	240	ALA	N-CA-CB	-6.00	101.70	110.10
1	B	692	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	239	ASP	CB-CA-C	-5.99	98.42	110.40
1	A	569	ASN	CB-CG-ND2	5.99	131.07	116.70
1	B	494	GLY	CA-C-O	-5.99	109.82	120.60
1	A	204	GLU	OE1-CD-OE2	-5.99	116.12	123.30
1	A	662	THR	CA-CB-CG2	-5.98	104.03	112.40
1	A	707	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	194	SER	CB-CA-C	-5.95	98.79	110.10
1	B	34	LYS	CA-CB-CG	-5.92	100.37	113.40
1	B	398	ARG	CG-CD-NE	5.91	124.22	111.80
1	A	297	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	298	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	B	142	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	594	GLU	O-C-N	5.88	132.10	122.70
1	B	38	TYR	CD1-CE1-CZ	5.86	125.07	119.80
1	A	20	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	692	ARG	CG-CD-NE	-5.83	99.55	111.80
1	B	117	PHE	CB-CG-CD2	5.83	124.88	120.80
1	B	717	THR	CA-CB-CG2	-5.83	104.24	112.40
1	A	115	ALA	CB-CA-C	-5.82	101.38	110.10
1	B	369	TYR	CG-CD2-CE2	-5.82	116.65	121.30
1	A	379	LYS	CG-CD-CE	-5.80	94.51	111.90
1	B	437	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	B	554	THR	CA-CB-CG2	5.78	120.50	112.40
1	A	92	ARG	CD-NE-CZ	-5.78	115.51	123.60
1	B	38	TYR	CG-CD1-CE1	-5.78	116.68	121.30
1	A	77	ASP	CB-CG-OD1	5.77	123.50	118.30
1	B	143	ASN	OD1-CG-ND2	5.76	135.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ALA	N-CA-CB	-5.75	102.05	110.10
1	A	588	LEU	N-CA-C	-5.74	95.50	111.00
1	A	129	LEU	CB-CA-C	5.73	121.08	110.20
1	B	720	LEU	C-N-CA	-5.73	110.28	122.30
1	B	329	ASP	N-CA-CB	5.71	120.88	110.60
1	A	329	ASP	N-CA-CB	5.68	120.83	110.60
1	B	66	ASN	OD1-CG-ND2	5.68	134.96	121.90
1	B	250	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	32	LEU	CB-CG-CD1	5.67	120.64	111.00
1	A	130	PRO	O-C-N	5.67	131.87	121.10
1	A	95	PRO	N-CA-CB	5.66	110.10	103.30
1	A	343	SER	O-C-N	5.66	131.76	122.70
1	A	93	PRO	N-CA-CB	5.66	110.09	103.30
1	B	651	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	165	ALA	O-C-N	5.65	131.74	122.70
1	A	294	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	11	ASP	OD1-CG-OD2	5.63	134.00	123.30
1	A	347	TYR	CB-CG-CD1	5.62	124.37	121.00
1	A	337	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	630	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	566	ASN	N-CA-CB	-5.60	100.52	110.60
1	A	689	HIS	CG-ND1-CE1	5.59	116.02	108.20
1	B	602	SER	N-CA-CB	-5.59	102.12	110.50
1	B	25	ASP	OD1-CG-OD2	5.58	133.91	123.30
1	B	440	HIS	N-CA-CB	5.57	120.63	110.60
1	B	30	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	B	416	TYR	CB-CG-CD1	5.54	124.33	121.00
1	B	274	LYS	CA-CB-CG	5.54	125.60	113.40
1	A	472	TRP	N-CA-C	-5.54	96.05	111.00
1	A	566	ASN	CA-CB-CG	-5.53	101.23	113.40
1	B	298	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	11	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	173	LYS	CB-CA-C	-5.50	99.41	110.40
1	B	438	TYR	CB-CG-CD1	5.48	124.29	121.00
1	A	280	GLU	OE1-CD-OE2	5.47	129.86	123.30
1	A	483	ASP	OD1-CG-OD2	-5.47	112.91	123.30
1	A	307	GLN	N-CA-CB	5.46	120.44	110.60
1	B	358	TYR	O-C-N	-5.46	113.97	122.70
1	B	635	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	B	700	PRO	N-CD-CG	-5.45	95.03	103.20
1	B	35	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	648	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	688	THR	CA-CB-CG2	-5.41	104.83	112.40
1	B	118	LYS	CD-CE-NZ	5.41	124.13	111.70
1	A	229	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	B	359	GLU	CB-CA-C	5.40	121.20	110.40
1	B	204	GLU	OE1-CD-OE2	5.39	129.76	123.30
1	B	715	ASP	OD1-CG-OD2	-5.38	113.08	123.30
1	B	268	VAL	CA-CB-CG2	5.38	118.97	110.90
1	B	657	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	508	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	231	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	119	PRO	N-CA-C	5.36	126.04	112.10
1	B	603	TYR	N-CA-CB	5.36	120.25	110.60
1	A	421	MET	N-CA-CB	5.36	120.25	110.60
1	A	207	ALA	CB-CA-C	5.35	118.13	110.10
1	A	452	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	190	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	81	SER	CB-CA-C	-5.34	99.95	110.10
1	B	223	THR	OG1-CB-CG2	-5.33	97.73	110.00
1	A	359	GLU	CB-CA-C	-5.32	99.76	110.40
1	B	297	ASP	N-CA-CB	-5.32	101.03	110.60
1	A	717	THR	CA-CB-CG2	-5.31	104.97	112.40
1	A	303	VAL	CA-CB-CG1	5.30	118.84	110.90
1	A	476	GLU	CB-CA-C	-5.29	99.81	110.40
1	A	559	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	A	158	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	272	GLN	CG-CD-OE1	-5.29	111.02	121.60
1	A	576	ALA	CB-CA-C	5.28	118.02	110.10
1	A	510	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	533	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	417	THR	N-CA-CB	5.26	120.30	110.30
1	A	587	LEU	O-C-N	5.26	131.12	122.70
1	A	602	SER	N-CA-CB	-5.26	102.61	110.50
1	B	89	VAL	N-CA-CB	5.26	123.06	111.50
1	B	449	SER	CB-CA-C	-5.24	100.15	110.10
1	A	712	ASN	N-CA-CB	5.23	120.01	110.60
1	B	609	ALA	C-N-CA	-5.23	111.32	122.30
1	B	317	THR	CA-CB-CG2	-5.22	105.09	112.40
1	B	467	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	533	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	670	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	689	HIS	CG-ND1-CE1	5.21	115.49	108.20
1	B	25	ASP	CB-CG-OD1	-5.20	113.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ILE	N-CA-C	-5.20	96.96	111.00
1	B	291	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	304	LYS	N-CA-CB	-5.19	101.25	110.60
1	B	92	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	359	GLU	N-CA-CB	-5.18	101.28	110.60
1	B	443	MET	CA-CB-CG	-5.17	104.51	113.30
1	B	280	GLU	O-C-N	5.16	131.98	123.20
1	B	647	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	A	650	PRO	O-C-N	5.15	130.94	122.70
1	B	570	ILE	N-CA-C	-5.15	97.09	111.00
1	A	449	SER	CB-CA-C	-5.15	100.32	110.10
1	B	697	PRO	N-CA-C	5.15	125.49	112.10
1	A	566	ASN	CB-CA-C	-5.15	100.11	110.40
1	B	416	TYR	CG-CD1-CE1	5.15	125.42	121.30
1	A	250	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	398	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	349	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	B	715	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	649	PHE	CB-CG-CD2	5.13	124.39	120.80
1	A	153	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	322	MET	CA-CB-CG	-5.13	104.58	113.30
1	A	549	VAL	CB-CA-C	-5.13	101.66	111.40
1	A	145	PRO	N-CA-CB	5.11	109.44	103.30
1	B	510	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	A	261	ILE	N-CA-C	-5.11	97.21	111.00
1	A	381	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	B	581	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	16	GLU	CA-CB-CG	5.08	124.58	113.40
1	B	377	TYR	N-CA-CB	-5.08	101.45	110.60
1	B	13	THR	CA-CB-OG1	-5.08	98.34	109.00
1	A	303	VAL	CA-CB-CG2	-5.07	103.29	110.90
1	B	382	LEU	CB-CA-C	5.07	119.84	110.20
1	B	718	PRO	N-CD-CG	-5.07	95.59	103.20
1	A	526	HIS	N-CA-CB	5.07	119.72	110.60
1	B	578	GLN	CG-CD-NE2	5.07	128.85	116.70
1	B	234	ASP	OD1-CG-OD2	-5.05	113.70	123.30
1	A	622	ALA	CB-CA-C	5.05	117.67	110.10
1	B	396	ILE	O-C-N	-5.04	114.64	122.70
1	B	692	ARG	CG-CD-NE	-5.03	101.24	111.80
1	A	25	ASP	OD1-CG-OD2	-5.01	113.77	123.30
1	A	537	ASP	OD1-CG-OD2	-5.01	113.77	123.30
1	A	601	VAL	CA-CB-CG2	5.01	118.42	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	PRO	N-CA-CB	5.01	109.31	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ASP	Mainchain

## 5.2 Too-close contacts [i](#)

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	5666	0	5541	161	0
1	B	5690	0	5562	157	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	B	6	0	7	6	0
5	A	767	0	0	21	0
5	B	640	0	0	13	0
All	All	12775	0	11110	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:322:MET:HG3	5:B:1792:HOH:O	1.60	1.00
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.14	0.93
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.50	0.93
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.50	0.93
1:B:326:ARG:HH11	1:B:476:GLU:CD	1.74	0.91
1:A:304:LYS:H	1:B:315:ASN:HD21	1.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:H	1:B:203:GLU:CD	1.74	0.90
1:A:35:ASP:OD1	1:A:398:ARG:NH1	2.06	0.88
1:B:120:ASN:HA	5:B:1818:HOH:O	1.73	0.87
1:A:223:THR:HG23	1:A:225:LEU:HD21	1.56	0.86
1:B:580:PHE:H	1:B:637:GLN:HE21	1.21	0.84
1:A:465:ASN:H	1:A:465:ASN:HD22	1.25	0.84
1:B:382:LEU:HD23	1:B:651:GLU:HG3	1.58	0.84
1:B:572:ASN:ND2	1:B:671:ASN:HD21	1.77	0.83
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.62	0.81
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.62	0.81
1:B:237:LYS:HD3	1:B:240:ALA:HB2	1.63	0.81
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.63	0.80
1:B:94:HIS:HD2	1:B:96:LEU:H	1.25	0.80
4:B:1450:GOL:O1	5:B:1465:HOH:O	1.99	0.79
1:A:572:ASN:ND2	1:A:575:ASP:H	1.80	0.78
1:A:227:VAL:CG1	1:A:244:LYS:HG3	2.13	0.77
1:A:574:GLN:H	1:A:671:ASN:ND2	1.82	0.77
1:A:71:SER:OG	1:A:73:THR:HG22	1.85	0.77
1:A:28:GLN:HG3	5:A:1176:HOH:O	1.84	0.76
1:A:527:ILE:HD12	1:A:634:MET:HE2	1.65	0.76
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.66	0.76
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.69	0.74
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.69	0.74
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.19	0.73
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.68	0.73
1:B:574:GLN:H	1:B:671:ASN:ND2	1.84	0.73
1:B:38:TYR:H	1:B:51:ASN:ND2	1.86	0.73
1:A:272:GLN:HE21	1:A:274:LYS:HD3	1.53	0.73
1:B:578:GLN:HA	1:B:636:LYS:HD2	1.71	0.72
1:A:580:PHE:H	1:A:637:GLN:HE21	1.37	0.72
1:A:132:ASP:HB3	5:A:1534:HOH:O	1.88	0.72
1:B:38:TYR:H	1:B:51:ASN:HD21	1.37	0.71
1:A:498:LYS:O	1:A:517:HIS:HD2	1.73	0.71
1:A:465:ASN:H	1:A:465:ASN:ND2	1.88	0.71
1:A:527:ILE:HD12	1:A:634:MET:CE	2.20	0.71
1:A:315:ASN:HD21	1:B:304:LYS:H	1.37	0.71
1:B:218:LYS:HD2	1:B:218:LYS:H	1.56	0.71
1:A:553:ASN:ND2	1:A:555:ALA:H	1.89	0.71
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.72	0.71
1:A:539:GLU:CD	5:A:1201:HOH:O	2.29	0.70
1:A:203:GLU:CD	1:A:203:GLU:H	1.93	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:OD2	5:A:1084:HOH:O	2.09	0.70
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.92	0.69
1:B:382:LEU:HD22	1:B:655:PRO:HB2	1.75	0.69
1:B:326:ARG:NH1	1:B:476:GLU:CD	2.46	0.68
1:B:536:VAL:H	1:B:541:ASN:HD21	1.40	0.68
1:A:670:ASP:HB2	5:A:1547:HOH:O	1.94	0.67
1:A:219:LYS:HD3	5:A:1183:HOH:O	1.93	0.67
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.12	0.67
1:A:536:VAL:H	1:A:541:ASN:HD21	1.42	0.67
4:B:1450:GOL:C1	5:B:1465:HOH:O	2.42	0.67
1:B:580:PHE:H	1:B:637:GLN:NE2	1.90	0.67
1:B:632:SER:OG	1:B:661:ASP:OD2	2.13	0.66
1:B:225:LEU:HD23	4:B:1450:GOL:H31	1.76	0.66
1:B:203:GLU:N	1:B:203:GLU:CD	2.49	0.66
1:B:553:ASN:HD21	1:B:555:ALA:HB3	1.59	0.66
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.26	0.66
1:A:286:VAL:CG1	1:A:288:MET:HE1	2.25	0.65
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.32	0.65
1:B:525:GLN:HE22	1:B:620:GLN:H	1.42	0.65
1:B:381:TYR:CE1	4:B:1450:GOL:H11	2.32	0.65
1:A:203:GLU:OE2	1:A:204:GLU:HG3	1.96	0.65
1:A:38:TYR:H	1:A:51:ASN:ND2	1.94	0.65
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.32	0.64
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.28	0.64
1:B:525:GLN:NE2	1:B:620:GLN:H	1.95	0.64
1:B:366:ILE:CD1	1:B:627:ILE:HD11	2.26	0.64
1:A:692:ARG:HG3	1:A:694:GLU:OE1	1.97	0.64
1:A:379:LYS:HG2	1:A:381:TYR:CZ	2.33	0.64
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.79	0.63
1:A:644:HIS:HB3	5:A:1278:HOH:O	1.98	0.63
1:A:322:MET:HE1	5:A:1147:HOH:O	1.99	0.63
1:B:498:LYS:O	1:B:517:HIS:HD2	1.82	0.63
1:A:241:ARG:HG2	1:A:270:LEU:HD12	1.80	0.63
1:B:12:LYS:O	1:B:16:GLU:HG2	1.98	0.62
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.15	0.62
1:A:574:GLN:HG2	1:A:671:ASN:ND2	2.15	0.62
1:A:572:ASN:HD22	1:A:575:ASP:H	1.45	0.62
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.82	0.62
1:A:38:TYR:H	1:A:51:ASN:HD21	1.48	0.61
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.83	0.61
1:A:210:LYS:CA	1:A:210:LYS:HE2	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:OE1	1:A:374:ILE:HD11	2.01	0.61
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.15	0.61
1:B:381:TYR:CD1	4:B:1450:GOL:H11	2.37	0.60
1:B:326:ARG:NH1	1:B:476:GLU:OE1	2.33	0.60
1:A:574:GLN:H	1:A:671:ASN:HD22	1.50	0.60
1:B:620:GLN:HG3	5:B:1637:HOH:O	2.02	0.59
1:B:214:ILE:HD11	1:B:286:VAL:HG21	1.83	0.59
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.66	0.59
1:A:286:VAL:HG12	1:A:288:MET:CE	2.33	0.59
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.51	0.59
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.32	0.59
1:A:629:HIS:HB2	5:A:1184:HOH:O	2.01	0.59
1:A:223:THR:HG21	5:A:858:HOH:O	2.03	0.58
1:B:218:LYS:N	1:B:218:LYS:HD2	2.19	0.57
1:A:525:GLN:HE22	1:A:620:GLN:H	1.50	0.57
1:B:490:GLU:HG3	1:B:699:MET:SD	2.44	0.57
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.87	0.57
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.04	0.57
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.51	0.57
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.38	0.57
1:A:29:LEU:HD13	1:A:30:PHE:N	2.20	0.57
1:B:380:ALA:CB	1:B:627:ILE:HD12	2.36	0.56
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.88	0.56
1:A:286:VAL:CG1	1:A:288:MET:CE	2.83	0.56
1:B:366:ILE:HD12	1:B:631:LEU:HD13	1.88	0.56
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.21	0.56
1:B:445:GLN:HB3	1:B:446:PRO:HD2	1.88	0.56
1:A:525:GLN:NE2	1:A:620:GLN:H	2.04	0.56
1:A:366:ILE:HG13	1:A:367:VAL:N	2.20	0.55
1:B:29:LEU:HD21	1:B:40:LYS:HD2	1.88	0.55
1:A:578:GLN:HA	1:A:636:LYS:HD2	1.88	0.55
1:B:45:ALA:O	1:B:60:PRO:HB3	2.07	0.55
1:B:160:LYS:HD3	1:B:271:GLU:OE1	2.07	0.55
1:B:717:THR:HB	1:B:720:LEU:HG	1.89	0.55
1:A:224:PRO:O	1:A:224:PRO:HG2	2.06	0.54
1:A:286:VAL:HG11	1:A:288:MET:HE1	1.89	0.54
1:A:196:GLN:HE22	1:A:222:THR:H	1.56	0.54
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.43	0.53
1:B:53:GLN:OE1	5:B:2011:HOH:O	2.19	0.53
1:B:262:GLU:O	1:B:263:ASN:HB2	2.08	0.53
1:A:29:LEU:HD13	1:A:30:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASN:CA	5:B:1818:HOH:O	2.40	0.53
1:B:366:ILE:HG21	1:B:634:MET:HE3	1.91	0.53
1:A:552:PRO:HD2	5:A:1352:HOH:O	2.08	0.52
1:A:325:TRP:O	1:A:326:ARG:HB2	2.09	0.52
1:A:34:LYS:O	1:A:35:ASP:C	2.48	0.52
1:A:580:PHE:H	1:A:637:GLN:NE2	2.06	0.52
1:A:379:LYS:HG2	1:A:381:TYR:OH	2.10	0.51
1:B:95:PRO:HB3	1:B:146:VAL:HG21	1.93	0.51
1:B:216:ASP:OD1	1:B:216:ASP:C	2.49	0.51
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.76	0.51
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.93	0.51
1:A:366:ILE:HD13	1:A:631:LEU:CD1	2.41	0.50
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.40	0.50
1:A:596:ARG:NH1	5:A:1541:HOH:O	2.30	0.50
1:A:559:ARG:HD2	1:B:625:GLU:OE1	2.12	0.49
1:A:117:PHE:CZ	1:A:121:THR:HB	2.47	0.49
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.32	0.49
1:A:477:ASN:HD22	1:A:477:ASN:C	2.15	0.49
1:A:7:MET:HE1	1:A:59:VAL:HG11	1.94	0.49
1:B:580:PHE:N	1:B:637:GLN:HE21	1.99	0.49
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.60	0.49
1:B:619:ALA:HB2	1:B:634:MET:HB2	1.94	0.49
1:B:488:GLY:O	1:B:699:MET:HG3	2.13	0.49
1:B:129:LEU:CD1	1:B:130:PRO:HD2	2.42	0.49
1:B:621:PHE:CZ	1:B:627:ILE:HG21	2.48	0.49
1:A:223:THR:HG22	1:A:246:ILE:HB	1.95	0.49
1:A:77:ASP:O	1:A:81:SER:HB3	2.12	0.49
1:B:40:LYS:HE2	5:B:1864:HOH:O	2.13	0.49
1:B:307:GLN:HB3	5:B:1730:HOH:O	2.12	0.49
1:B:380:ALA:HB1	1:B:627:ILE:HD12	1.94	0.49
1:A:237:LYS:HG2	1:A:239:ASP:H	1.78	0.48
1:B:578:GLN:CA	1:B:636:LYS:HD2	2.42	0.48
1:A:441:GLN:OE1	1:A:447:ASN:HB2	2.13	0.48
1:A:65:ASP:O	1:A:66:ASN:HB2	2.14	0.48
1:A:549:VAL:HA	5:A:1306:HOH:O	2.13	0.48
1:A:227:VAL:HG11	1:A:244:LYS:HG3	1.91	0.48
1:B:380:ALA:HB1	1:B:627:ILE:CD1	2.43	0.48
1:A:664:LEU:HD21	1:A:682:TRP:CD2	2.48	0.48
1:B:148:GLN:HA	1:B:149:PRO:HD3	1.75	0.48
1:A:131:PRO:HB3	1:A:148:GLN:NE2	2.29	0.48
1:A:588:LEU:HB2	1:A:605:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:GLN:H	1:B:671:ASN:HD22	1.59	0.47
1:B:619:ALA:HB2	1:B:634:MET:HE2	1.96	0.47
1:A:32:LEU:HB2	1:A:39:VAL:HB	1.96	0.47
1:B:272:GLN:HE21	1:B:274:LYS:CD	2.27	0.47
1:B:61:VAL:HG22	1:B:70:VAL:CG1	2.42	0.47
1:A:272:GLN:NE2	1:A:274:LYS:HD3	2.26	0.47
1:B:214:ILE:HD12	1:B:214:ILE:N	2.30	0.47
1:A:147:ASP:HB2	5:A:1171:HOH:O	2.14	0.47
1:A:12:LYS:O	1:A:16:GLU:HG3	2.14	0.47
1:A:181:LYS:HG2	1:A:182:ASP:OD2	2.15	0.47
1:A:527:ILE:CD1	1:A:634:MET:CE	2.88	0.47
1:B:553:ASN:ND2	1:B:555:ALA:H	2.13	0.47
1:A:574:GLN:HB3	5:A:1562:HOH:O	2.15	0.47
1:B:725:LYS:O	1:B:726:ASP:CB	2.63	0.47
1:A:324:HIS:HD2	1:A:329:ASP:OD1	1.97	0.47
1:B:93:PRO:HG2	5:B:1921:HOH:O	2.15	0.47
1:B:619:ALA:CB	1:B:634:MET:HE2	2.45	0.47
1:A:465:ASN:N	1:A:465:ASN:ND2	2.60	0.47
1:A:43:PRO:HD2	5:A:1236:HOH:O	2.13	0.47
1:A:209:VAL:HG13	1:A:214:ILE:HB	1.96	0.47
1:A:214:ILE:HD12	1:A:214:ILE:H	1.80	0.47
1:A:331:HIS:HE1	1:A:333:SER:HB3	1.79	0.47
1:B:669:LYS:CE	1:B:669:LYS:HA	2.45	0.46
1:B:382:LEU:CD2	1:B:655:PRO:HB2	2.45	0.46
1:A:498:LYS:HB3	1:A:498:LYS:NZ	2.31	0.46
1:A:223:THR:HG23	1:A:225:LEU:CD2	2.39	0.46
1:B:445:GLN:HB3	1:B:446:PRO:CD	2.44	0.46
1:A:8:VAL:CG2	1:A:9:PRO:HD2	2.41	0.46
1:A:381:TYR:HE1	5:A:1546:HOH:O	1.98	0.46
1:B:525:GLN:HE22	1:B:619:ALA:HA	1.80	0.46
1:B:51:ASN:N	1:B:51:ASN:HD22	2.14	0.46
1:B:181:LYS:HE2	5:B:1989:HOH:O	2.16	0.46
1:A:366:ILE:HD11	1:A:380:ALA:HB1	1.98	0.46
1:A:331:HIS:CE1	1:A:333:SER:HB3	2.50	0.46
1:A:227:VAL:HG12	1:A:244:LYS:CG	2.41	0.46
1:A:203:GLU:N	1:A:203:GLU:CD	2.66	0.46
1:A:214:ILE:HD12	1:A:214:ILE:N	2.30	0.46
1:A:595:ASN:ND2	1:A:599:ASN:H	2.14	0.46
1:A:28:GLN:CG	5:A:1176:HOH:O	2.54	0.45
1:B:699:MET:HA	1:B:700:PRO:HD3	1.70	0.45
1:B:118:LYS:HE2	1:B:118:LYS:HB3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:HIS:CE1	1:B:596:ARG:NH1	2.83	0.45
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.36	0.45
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.97	0.45
1:B:196:GLN:HE22	1:B:222:THR:H	1.63	0.45
1:B:38:TYR:N	1:B:51:ASN:HD21	2.11	0.45
1:A:38:TYR:N	1:A:51:ASN:HD21	2.11	0.45
1:A:366:ILE:HD13	1:A:631:LEU:HD12	1.98	0.45
1:A:224:PRO:O	1:A:224:PRO:CG	2.65	0.45
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.64	0.45
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.20	0.45
1:A:477:ASN:HD22	1:A:479:THR:H	1.65	0.45
1:B:272:GLN:HE21	1:B:274:LYS:HG2	1.81	0.45
1:A:485:GLY:HA2	1:A:702:GLU:O	2.16	0.45
1:A:7:MET:CE	1:A:59:VAL:HG11	2.47	0.45
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.30	0.45
1:B:626:TRP:O	1:B:629:HIS:N	2.48	0.45
1:A:574:GLN:CG	1:A:671:ASN:ND2	2.80	0.45
1:A:382:LEU:HD22	1:A:651:GLU:HG3	1.98	0.45
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.44	0.45
1:B:181:LYS:H	1:B:181:LYS:CD	2.29	0.44
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.52	0.44
1:B:402:ALA:HB1	1:B:403:PRO:HD2	2.00	0.44
1:B:259:HIS:HE1	1:B:289:THR:O	2.01	0.44
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.98	0.44
1:A:64:LYS:O	1:A:66:ASN:N	2.44	0.44
1:B:7:MET:HB3	1:B:7:MET:HE3	1.75	0.44
1:B:626:TRP:O	1:B:627:ILE:C	2.56	0.44
1:B:229:TYR:HB3	1:B:630:ARG:HD2	1.98	0.44
1:B:477:ASN:HD22	1:B:477:ASN:C	2.20	0.44
1:B:653:LYS:HE2	1:B:654:TYR:OH	2.18	0.44
1:B:11:ASP:O	1:B:15:LYS:HD3	2.18	0.44
1:A:465:ASN:N	1:A:465:ASN:HD22	2.04	0.43
1:B:588:LEU:HD12	1:B:588:LEU:HA	1.92	0.43
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.83	0.43
1:B:242:LEU:HD23	1:B:269:ASP:HA	1.99	0.43
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.83	0.43
1:B:121:THR:CG2	1:B:156:MET:HB3	2.49	0.43
1:A:683:MET:HE1	1:A:706:THR:HB	2.01	0.43
1:A:574:GLN:CG	1:A:671:ASN:CG	2.87	0.43
1:B:76:ASN:O	1:B:80:GLN:HB2	2.18	0.43
1:A:28:GLN:CD	5:A:1176:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HD13	1:B:250:ASP:HB2	1.99	0.43
1:A:24:ASP:OD2	1:B:40:LYS:HE3	2.17	0.43
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.34	0.43
1:B:375:GLY:O	1:B:379:LYS:HE3	2.19	0.43
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.48	0.43
1:B:272:GLN:NE2	1:B:274:LYS:HG2	2.33	0.43
1:B:139:PHE:O	1:B:143:ASN:HA	2.19	0.43
1:B:239:ASP:HB2	5:B:1806:HOH:O	2.18	0.43
1:A:130:PRO:O	1:A:130:PRO:HG2	2.18	0.42
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.54	0.42
1:B:679:ALA:HB2	5:B:1803:HOH:O	2.19	0.42
1:B:543:LEU:HD22	1:B:640:VAL:HG21	2.01	0.42
1:B:379:LYS:HD3	1:B:381:TYR:OH	2.19	0.42
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.76	0.42
1:A:281:GLY:O	1:A:282:PRO:C	2.58	0.42
1:B:214:ILE:HD11	1:B:286:VAL:CG2	2.47	0.42
1:B:653:LYS:HG2	1:B:654:TYR:CE2	2.55	0.42
1:B:373:ASP:N	1:B:373:ASP:OD1	2.53	0.42
1:B:381:TYR:CD1	4:B:1450:GOL:C1	3.02	0.42
1:B:142:GLU:O	1:B:143:ASN:CB	2.66	0.42
1:B:443:MET:HG3	1:B:444:GLY:N	2.35	0.42
1:B:477:ASN:HD22	1:B:479:THR:H	1.67	0.41
1:A:91:LYS:NZ	5:A:1298:HOH:O	2.52	0.41
1:B:515:ILE:HD12	1:B:696:TRP:HB2	2.02	0.41
1:B:669:LYS:HA	1:B:669:LYS:HE3	2.02	0.41
1:A:659:THR:OG1	1:A:660:HIS:HD2	2.02	0.41
1:A:610:GLY:HA3	1:B:610:GLY:HA3	2.03	0.41
1:A:276:VAL:O	1:A:277:LYS:HB2	2.20	0.41
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.50	0.41
1:A:376:TRP:O	1:A:379:LYS:HB2	2.20	0.41
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.84	0.41
1:B:36:GLY:HA2	1:B:314:LYS:HE2	2.03	0.41
1:A:29:LEU:HD21	1:A:40:LYS:HB3	2.02	0.41
1:A:92:ARG:HH11	1:A:92:ARG:HD2	1.73	0.41
1:A:379:LYS:CG	1:A:381:TYR:OH	2.68	0.41
1:A:318:ILE:HG12	1:A:323:ILE:HG12	2.02	0.41
1:B:229:TYR:CZ	1:B:231:ASP:HA	2.56	0.41
1:A:107:ALA:HB2	1:A:169:LEU:HD21	2.03	0.41
1:A:309:ILE:HD13	1:A:309:ILE:HG21	1.91	0.41
1:A:546:MET:CE	5:A:1030:HOH:O	2.69	0.41
1:A:348:ASN:HD22	1:A:348:ASN:C	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:THR:O	1:A:508:ASP:HB2	2.21	0.41
1:B:216:ASP:OD1	1:B:218:LYS:N	2.52	0.41
1:A:59:VAL:HA	1:A:60:PRO:HD3	1.89	0.41
1:B:540:ASN:HB3	1:B:676:ASN:HD22	1.84	0.40
1:B:365:MET:HE2	1:B:383:GLU:HG3	2.03	0.40
1:B:162:ILE:HD11	1:B:185:GLY:CA	2.51	0.40
1:A:94:HIS:HB3	1:A:97:ASN:ND2	2.36	0.40
1:A:80:GLN:OE1	1:A:80:GLN:N	2.54	0.40
1:B:605:ILE:HG21	1:B:605:ILE:HD13	1.88	0.40
1:B:238:GLN:HE21	1:B:238:GLN:CA	2.33	0.40
1:A:129:LEU:HA	1:A:130:PRO:HD2	1.77	0.40
1:A:459:TRP:CZ2	1:A:461:SER:HB2	2.56	0.40
1:B:137:TRP:CD2	1:B:355:LYS:HE2	2.55	0.40
1:A:92:ARG:HA	1:A:93:PRO:HD2	1.87	0.40
1:A:62:VAL:HG23	1:A:69:TRP:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/721 (99%)	691 (96%)	24 (3%)	1 (0%)	56	64
1	B	718/721 (100%)	687 (96%)	31 (4%)	0	100	100
All	All	1434/1442 (99%)	1378 (96%)	55 (4%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	ARG

### 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%)	577 (95%)	32 (5%)	28	32
1	B	611/612 (100%)	567 (93%)	44 (7%)	18	18
All	All	1220/1224 (100%)	1144 (94%)	76 (6%)	23	25

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	LEU
1	A	66	ASN
1	A	71	SER
1	A	151	LYS
1	A	173	LYS
1	A	178	GLN
1	A	189	LEU
1	A	203	GLU
1	A	204	GLU
1	A	210	LYS
1	A	223	THR
1	A	239	ASP
1	A	304	LYS
1	A	348	ASN
1	A	366	ILE
1	A	368	PRO
1	A	465	ASN
1	A	477	ASN
1	A	539	GLU
1	A	553	ASN
1	A	566	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	617	LYS
1	A	627	ILE

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Mol	Chain	Res	Type
1	A	642	ARG
1	A	669	LYS
1	A	671	ASN
1	A	676	ASN
1	A	692	ARG
1	B	7	MET
1	B	11	ASP
1	B	34	LYS
1	B	42	LYS
1	B	47	THR
1	B	64	LYS
1	B	67	LYS
1	B	71	SER
1	B	80	GLN
1	B	89	VAL
1	B	92	ARG
1	B	114	SER
1	B	118	LYS
1	B	129	LEU
1	B	143	ASN
1	B	148	GLN
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	211	LYS
1	B	218	LYS
1	B	221	ILE
1	B	237	LYS
1	B	251	VAL
1	B	272	GLN
1	B	274	LYS
1	B	322	MET
1	B	334	MET
1	B	372	PRO
1	B	377	TYR
1	B	477	ASN
1	B	539	GLU
1	B	595	ASN
1	B	613	HIS
1	B	617	LYS
1	B	627	ILE
1	B	632	SER

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Mol	Chain	Res	Type
1	B	634	MET
1	B	635	ASP
1	B	669	LYS
1	B	671	ASN
1	B	676	ASN
1	B	692	ARG
1	B	724	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	97	ASN
1	A	148	GLN
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
1	A	445	GLN
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	541	ASN
1	A	553	ASN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	637	GLN
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN

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Mol	Chain	Res	Type
1	B	76	ASN
1	B	80	GLN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	161	HIS
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	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
1	B	595	ASN
1	B	599	ASN
1	B	604	GLN
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	2.06	4 (30%)	15,19,21	2.49	7 (46%)
1	TPQ	B	466	1	13,14,15	1.91	3 (23%)	15,19,21	2.21	7 (46%)

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	-	0/4/22/24	0/1/1/1
1	TPQ	B	466	1	-	0/4/22/24	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	C1-C2	-5.15	1.42	1.49
1	B	466	TPQ	C1-C2	-4.84	1.42	1.49
1	A	466	TPQ	C4-C5	-2.88	1.38	1.47
1	B	466	TPQ	C3-C4	2.09	1.39	1.35
1	B	466	TPQ	CB-C1	2.53	1.56	1.50
1	A	466	TPQ	C3-C4	2.56	1.39	1.35
1	A	466	TPQ	CB-C1	2.76	1.56	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	TPQ	CA-CB-C1	-3.90	105.81	113.63
1	A	466	TPQ	C4-C3-C2	-3.70	116.06	120.77
1	A	466	TPQ	O5-C5-C4	-3.09	114.23	119.16
1	B	466	TPQ	CA-CB-C1	-3.04	107.53	113.63
1	B	466	TPQ	O5-C5-C4	-3.02	114.34	119.16
1	B	466	TPQ	O-C-CA	-2.59	118.75	125.49
1	A	466	TPQ	O2-C2-C3	-2.51	116.23	121.89
1	B	466	TPQ	O2-C2-C1	-2.15	118.97	120.85
1	A	466	TPQ	CB-C1-C2	2.03	121.50	118.33
1	B	466	TPQ	CB-C1-C2	2.03	121.50	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	TPQ	O5-C5-C6	2.17	126.76	121.89
1	B	466	TPQ	O5-C5-C6	2.75	128.07	121.89
1	B	466	TPQ	C3-C2-C1	4.69	121.81	118.30
1	A	466	TPQ	C3-C2-C1	5.44	122.37	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	B	1450	-	5,5,5	0.50	0	5,5,5	1.47	2 (40%)

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
4	GOL	B	1450	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.



All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1450	GOL	O2-C2-C1	2.03	117.94	108.65
4	B	1450	GOL	C3-C2-C1	2.40	120.53	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1450	GOL	6	0

## 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	718/721 (99%)	-0.46	11 (1%) 76 75	16, 28, 51, 71	0
1	B	720/721 (99%)	-0.36	26 (3%) 46 45	17, 29, 55, 84	0
All	All	1438/1442 (99%)	-0.41	37 (2%) 59 58	16, 28, 53, 84	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	HIS	7.5
1	B	301	PRO	5.6
1	B	726	ASP	4.3
1	A	725	LYS	4.1
1	B	65	ASP	3.7
1	B	115	ALA	3.6
1	A	64	LYS	3.2
1	B	92	ARG	3.1
1	B	215	THR	2.9
1	B	302	ALA	2.9
1	B	218	LYS	2.9
1	A	216	ASP	2.8
1	A	215	THR	2.7
1	A	119	PRO	2.7
1	B	147	ASP	2.7
1	B	76	ASN	2.6
1	B	303	VAL	2.6
1	B	669	LYS	2.5
1	B	670	ASP	2.5
1	A	239	ASP	2.5
1	B	300	ALA	2.5
1	B	628	TYR	2.5
1	B	116	ASP	2.4
1	A	629	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	64	LYS	2.4
1	B	231	ASP	2.4
1	B	91	LYS	2.4
1	A	218	LYS	2.2
1	B	644	HIS	2.2
1	B	16	GLU	2.2
1	B	66	ASN	2.2
1	A	147	ASP	2.2
1	A	12	LYS	2.1
1	B	89	VAL	2.1
1	B	444	GLY	2.0
1	A	148	GLN	2.0
1	B	173	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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	A	466	14/15	0.98	0.09	-	22,28,32,33	0
1	TPQ	B	466	14/15	0.95	0.09	-	22,29,36,38	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	1450	6/6	0.86	0.17	6.75	63,67,68,68	0
3	CA	A	802	1/1	0.99	0.12	0.17	25,25,25,25	0
3	CA	B	802	1/1	0.99	0.11	-0.60	28,28,28,28	0
3	CA	B	803	1/1	0.94	0.10	-0.82	53,53,53,53	0
3	CA	A	803	1/1	0.94	0.08	-0.85	53,53,53,53	0
2	CU	A	801	1/1	1.00	0.04	-	33,33,33,33	0
2	CU	B	801	1/1	0.99	0.04	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.