



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:04 PM GMT

PDB ID : 1DYU  
Title : THE ACTIVE SITE BASE CONTROLS COFACTOR REACTIVITY IN  
ESCHERICHIA COLI AMINE OXIDASE: X-RAY CRYSTALLOGRAPHIC  
STUDIES WITH MUTATIONAL VARIANTS.  
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Deposited on : 2000-02-08  
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

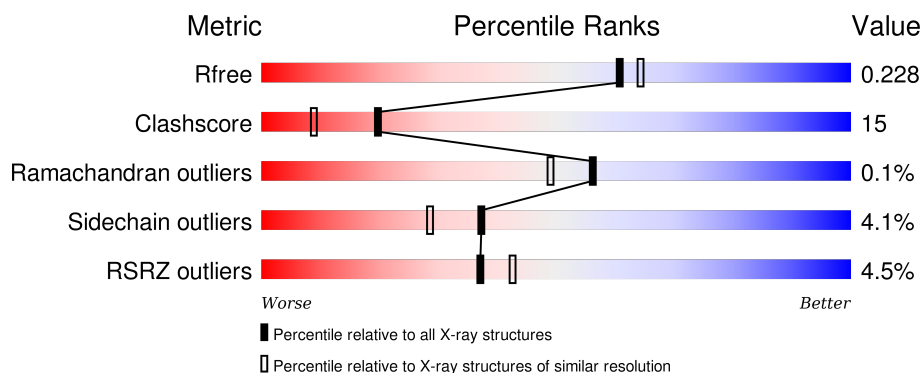
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	727	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	727	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>5% ••</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5664	3602	964	1076	22			
1	B	720	Total	C	N	O	S	0	0	0
			5683	3614	969	1078	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883
B	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883

- Molecule 2 is COPPER (II) ION (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.

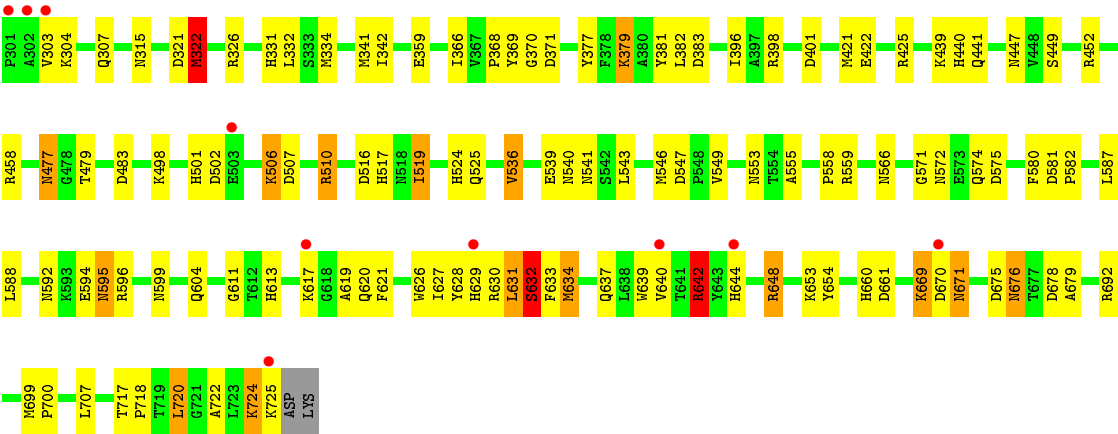
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	827	Total	O	0	0
			827	827		

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.05Å 167.17Å 79.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.04 19.43 – 2.04	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.04) 88.5 (19.43-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.11 (at 2.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.185 , 0.237 0.175 , 0.228	Depositor DCC
$R_{free}$ test set	3576 reflections (3.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.884	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 78.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 104326 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: 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	0.60	0/5793	1.62	76/7886 (1.0%)
1	B	0.57	0/5813	1.55	72/7912 (0.9%)
All	All	0.59	0/11606	1.59	148/15798 (0.9%)

There are no bond length outliers.

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	NE-CZ-NH2	-19.22	110.69	120.30
1	A	692	ARG	NE-CZ-NH2	-17.40	111.60	120.30
1	A	147	ASP	CB-CG-OD1	12.75	129.78	118.30
1	A	298	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	A	642	ARG	CD-NE-CZ	11.03	139.04	123.60
1	B	510	ARG	NE-CZ-NH2	10.85	125.72	120.30
1	B	326	ARG	NE-CZ-NH1	-10.51	115.05	120.30
1	B	398	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	B	298	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	453	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	B	642	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	231	ASP	CB-CG-OD1	10.12	127.41	118.30
1	A	586	ARG	NE-CZ-NH2	10.11	125.36	120.30
1	A	566	ASN	OD1-CG-ND2	9.97	144.83	121.90
1	A	326	ARG	NH1-CZ-NH2	9.66	130.03	119.40
1	B	692	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	122	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	559	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	B	216	ASP	CB-CG-OD2	9.40	126.76	118.30
1	A	241	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	25	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	566	ASN	CB-CG-OD1	-8.91	103.78	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	425	ARG	NE-CZ-NH2	8.65	124.63	120.30
1	B	72	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	648	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	B	398	ARG	NH1-CZ-NH2	8.29	128.52	119.40
1	B	92	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	72	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	92	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	147	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	A	16	GLU	OE1-CD-OE2	-7.97	113.73	123.30
1	B	398	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	20	ASP	CB-CG-OD2	7.84	125.36	118.30
1	B	122	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	24	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	547	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	692	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	132	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	A	239	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	102	ASP	CB-CG-OD1	7.19	124.78	118.30
1	A	231	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	507	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	322	MET	CG-SD-CE	7.10	111.55	100.20
1	A	483	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	425	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	35	ASP	CB-CG-OD2	6.98	124.58	118.30
1	A	596	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	B	571	GLY	N-CA-C	6.93	130.42	113.10
1	B	7	MET	N-CA-CB	-6.80	98.37	110.60
1	B	296	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	453	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	329	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	415	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	432	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	329	ASP	N-CA-CB	6.67	122.60	110.60
1	B	291	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	304	LYS	CA-CB-CG	6.64	128.00	113.40
1	B	452	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	11	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	483	ASP	CB-CG-OD2	6.59	124.24	118.30
1	B	379	LYS	CB-CA-C	6.53	123.46	110.40
1	A	440	HIS	N-CA-CB	6.51	122.31	110.60
1	A	122	ARG	NH1-CZ-NH2	6.49	126.53	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ARG	CG-CD-NE	6.48	125.42	111.80
1	A	291	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	458	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	64	LYS	CB-CA-C	-6.45	97.49	110.40
1	A	483	ASP	OD1-CG-OD2	-6.42	111.10	123.30
1	A	150	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	271	GLU	OE1-CD-OE2	-6.39	115.64	123.30
1	A	581	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	695	GLU	OE1-CD-OE2	-6.37	115.65	123.30
1	A	707	LEU	CB-CG-CD1	6.30	121.71	111.00
1	B	371	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	670	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	129	LEU	N-CA-C	-6.25	94.14	111.00
1	A	129	LEU	N-CA-C	-6.20	94.26	111.00
1	B	678	ASP	CB-CG-OD2	6.19	123.88	118.30
1	B	158	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	661	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	298	ARG	NH1-CZ-NH2	6.10	126.11	119.40
1	B	153	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	428	ALA	CB-CA-C	-6.01	101.09	110.10
1	A	571	GLY	N-CA-C	5.98	128.06	113.10
1	A	588	LEU	N-CA-C	-5.96	94.89	111.00
1	A	383	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	657	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	77	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	B	250	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	692	ARG	NH1-CZ-NH2	5.72	125.70	119.40
1	A	116	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	559	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	148	GLN	CB-CA-C	5.67	121.74	110.40
1	A	511	TYR	CB-CG-CD2	5.66	124.40	121.00
1	A	596	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	B	269	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	692	ARG	CG-CD-NE	-5.64	99.97	111.80
1	B	231	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	72	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	692	ARG	CD-NE-CZ	5.60	131.44	123.60
1	B	720	LEU	C-N-CA	-5.60	110.54	122.30
1	A	421	MET	N-CA-CB	-5.57	100.57	110.60
1	B	383	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	675	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	377	TYR	CZ-CE2-CD2	-5.47	114.88	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	226	THR	CA-CB-CG2	-5.45	104.77	112.40
1	B	168	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	502	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	347	TYR	CB-CG-CD1	5.43	124.26	121.00
1	B	72	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	588	LEU	N-CA-C	-5.41	96.38	111.00
1	A	472	TRP	N-CA-C	-5.39	96.45	111.00
1	A	401	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	B	547	ASP	OD1-CG-OD2	-5.36	113.12	123.30
1	B	519	ILE	O-C-N	-5.35	114.14	122.70
1	B	594	GLU	OE1-CD-OE2	5.34	129.71	123.30
1	A	398	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	382	LEU	N-CA-C	-5.33	96.62	111.00
1	B	631	LEU	N-CA-CB	-5.30	99.80	110.40
1	B	510	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	B	483	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	440	HIS	N-CA-CB	5.28	120.10	110.60
1	A	596	ARG	CD-NE-CZ	5.25	130.95	123.60
1	A	293	PHE	CB-CG-CD2	5.23	124.46	120.80
1	A	502	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	516	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	261	ILE	N-CA-C	-5.19	96.98	111.00
1	A	692	ARG	CD-NE-CZ	5.18	130.85	123.60
1	A	603	TYR	N-CA-CB	5.17	119.90	110.60
1	A	288	MET	N-CA-C	5.15	124.92	111.00
1	B	707	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	539	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	326	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	635	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	432	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	A	634	MET	CG-SD-CE	5.12	108.40	100.20
1	B	546	MET	N-CA-CB	5.11	119.80	110.60
1	B	632	SER	CB-CA-C	-5.11	100.39	110.10
1	B	421	MET	N-CA-CB	-5.10	101.41	110.60
1	B	20	ASP	OD1-CG-OD2	-5.10	113.61	123.30
1	B	458	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	280	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	A	670	ASP	OD1-CG-OD2	-5.07	113.67	123.30
1	B	6	HIS	N-CA-CB	5.07	119.72	110.60
1	B	422	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	B	634	MET	CB-CA-C	-5.05	100.31	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5664	0	5540	161	0
1	B	5683	0	5560	192	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	827	0	0	22	0
4	B	741	0	0	35	0
All	All	12921	0	11100	335	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 15.

All (335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.36	1.07
1:A:466:TPQ:H6	4:A:2530:HOH:O	1.57	1.01
1:A:463:VAL:HB	4:A:2530:HOH:O	1.60	0.99
1:A:216:ASP:HB3	1:A:219:LYS:HD2	1.44	0.98
1:B:8:VAL:CG2	1:B:9:PRO:HD2	1.93	0.98
1:A:527:ILE:HD12	1:A:634:MET:HE3	1.46	0.96
1:B:221:ILE:CD1	1:B:250:ASP:HB2	1.98	0.93
1:B:12:LYS:O	1:B:16:GLU:HG2	1.71	0.91
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.55	0.89
1:A:304:LYS:H	1:B:315:ASN:HD21	1.21	0.87
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.57	0.87
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.42	0.83
1:B:65:ASP:O	1:B:66:ASN:HB2	1.78	0.83
1:B:642:ARG:HH11	1:B:642:ARG:CB	1.92	0.81
1:A:617:LYS:HE2	1:B:581:ASP:OD1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.80	0.81
1:B:580:PHE:H	1:B:637:GLN:HE21	1.28	0.80
1:A:71:SER:OG	1:A:73:THR:HG22	1.82	0.80
1:A:315:ASN:HD21	1:B:304:LYS:H	1.29	0.79
1:A:527:ILE:HD12	1:A:634:MET:CE	2.12	0.78
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.27	0.78
1:B:366:ILE:HD13	1:B:634:MET:SD	2.24	0.78
1:B:498:LYS:O	1:B:517:HIS:HD2	1.66	0.78
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.66	0.78
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.48	0.77
1:B:46:GLN:NE2	4:B:2059:HOH:O	1.77	0.77
1:A:553:ASN:ND2	1:A:555:ALA:H	1.83	0.77
1:A:580:PHE:H	1:A:637:GLN:HE21	1.30	0.76
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.67	0.76
1:A:189:LEU:HG	4:A:2312:HOH:O	1.86	0.75
1:A:203:GLU:CD	1:A:203:GLU:H	1.88	0.75
1:B:525:GLN:HE22	1:B:620:GLN:H	1.34	0.75
1:B:644:HIS:HB3	4:B:2130:HOH:O	1.87	0.75
1:B:725:LYS:C	4:B:2741:HOH:O	2.25	0.74
1:B:322:MET:HG3	4:B:2048:HOH:O	1.87	0.74
1:B:94:HIS:HD2	1:B:96:LEU:H	1.35	0.72
1:B:381:TYR:CD2	4:B:2524:HOH:O	2.40	0.72
1:A:38:TYR:H	1:A:51:ASN:HD21	1.35	0.72
1:B:181:LYS:HE2	1:B:181:LYS:H	1.53	0.72
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.55	0.72
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.89	0.72
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.71	0.71
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.56	0.70
1:A:189:LEU:HB3	4:A:2039:HOH:O	1.91	0.70
1:B:7:MET:HG2	1:B:71:SER:HA	1.74	0.70
1:B:525:GLN:NE2	1:B:620:GLN:H	1.90	0.69
1:A:223:THR:HG22	1:A:246:ILE:O	1.93	0.69
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.40	0.68
1:B:660:HIS:HA	4:B:2659:HOH:O	1.93	0.68
1:B:144:LYS:HE3	4:B:2191:HOH:O	1.94	0.68
1:A:616:ALA:HA	4:A:2741:HOH:O	1.92	0.68
1:A:498:LYS:HB3	1:A:498:LYS:NZ	2.08	0.68
1:B:173:LYS:HB3	1:B:173:LYS:NZ	2.09	0.68
1:A:286:VAL:HG12	1:A:288:MET:CE	2.25	0.67
1:A:132:ASP:HB3	4:A:2218:HOH:O	1.94	0.67
1:B:203:GLU:H	1:B:203:GLU:CD	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:HG22	1:B:9:PRO:CD	2.24	0.66
1:B:574:GLN:H	1:B:671:ASN:ND2	1.94	0.66
1:B:181:LYS:CE	1:B:181:LYS:H	2.08	0.66
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.76	0.66
1:A:439:LYS:HZ2	1:A:447:ASN:HD21	1.43	0.66
1:B:38:TYR:H	1:B:51:ASN:HD21	1.44	0.66
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.26	0.65
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.12	0.65
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.32	0.65
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.31	0.65
1:B:379:LYS:HG3	1:B:381:TYR:CE1	2.31	0.65
1:B:38:TYR:H	1:B:51:ASN:ND2	1.95	0.64
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.62	0.64
1:A:368:PRO:HG3	1:A:634:MET:CE	2.27	0.64
1:B:322:MET:CG	4:B:2048:HOH:O	2.42	0.64
1:B:341:MET:HE2	4:B:2428:HOH:O	1.97	0.63
1:A:130:PRO:HG2	4:A:2214:HOH:O	1.98	0.63
1:A:536:VAL:H	1:A:541:ASN:HD21	1.44	0.63
1:B:216:ASP:OD1	1:B:218:LYS:N	2.32	0.63
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.64	0.62
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.11	0.62
1:B:506:LYS:HE2	1:B:510:ARG:NH2	2.14	0.62
1:B:65:ASP:O	1:B:66:ASN:CB	2.44	0.62
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.15	0.62
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.30	0.62
1:B:341:MET:HB3	4:B:2405:HOH:O	1.99	0.61
1:A:38:TYR:H	1:A:51:ASN:ND2	1.97	0.61
1:B:92:ARG:HD2	4:B:2189:HOH:O	1.99	0.61
1:A:272:GLN:HB3	1:A:274:LYS:HD3	1.82	0.61
1:A:592:ASN:HD21	1:A:676:ASN:ND2	1.97	0.61
1:B:181:LYS:HE2	1:B:181:LYS:N	2.16	0.61
1:A:203:GLU:OE1	1:A:204:GLU:HG3	2.00	0.61
1:A:7:MET:HE2	1:A:7:MET:HA	1.83	0.60
1:B:368:PRO:HG3	1:B:634:MET:HE3	1.82	0.60
1:B:580:PHE:H	1:B:637:GLN:NE2	1.97	0.60
1:B:225:LEU:HD22	1:B:381:TYR:CE2	2.37	0.60
1:A:286:VAL:CG1	1:A:288:MET:CE	2.79	0.60
1:A:274:LYS:HZ2	1:A:276:VAL:HG12	1.67	0.60
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.83	0.60
1:A:498:LYS:O	1:A:517:HIS:HD2	1.84	0.59
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG23	1:A:69:TRP:HB2	1.84	0.59
1:B:277:LYS:NZ	1:B:279:GLU:OE2	2.29	0.59
1:B:477:ASN:HD22	1:B:479:THR:H	1.51	0.59
1:B:366:ILE:HD12	1:B:631:LEU:HD13	1.84	0.58
1:B:717:THR:HB	1:B:720:LEU:HG	1.85	0.58
1:B:149:PRO:O	1:B:151:LYS:HG3	2.03	0.58
1:B:334:MET:HB3	4:B:2474:HOH:O	2.03	0.58
1:A:498:LYS:HB3	1:A:498:LYS:HZ3	1.69	0.58
1:B:216:ASP:HB3	4:B:2271:HOH:O	2.03	0.58
1:B:632:SER:OG	1:B:661:ASP:OD2	2.20	0.58
1:B:94:HIS:CD2	1:B:96:LEU:H	2.21	0.57
1:A:718:PRO:HD2	4:B:2717:HOH:O	2.04	0.56
1:A:439:LYS:NZ	1:A:447:ASN:ND2	2.53	0.56
1:A:12:LYS:O	1:A:16:GLU:HG3	2.05	0.56
1:B:629:HIS:CD2	4:B:2659:HOH:O	2.59	0.56
1:A:326:ARG:NH1	1:B:303:VAL:HG22	2.20	0.56
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.88	0.56
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.70	0.56
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.06	0.55
1:A:525:GLN:NE2	1:A:620:GLN:H	2.02	0.55
1:B:274:LYS:NZ	4:B:2339:HOH:O	2.38	0.55
1:B:203:GLU:N	1:B:203:GLU:CD	2.60	0.55
1:B:359:GLU:HG3	4:B:2405:HOH:O	2.06	0.55
1:A:551:LYS:HE3	4:A:2687:HOH:O	2.06	0.55
1:A:525:GLN:HE22	1:A:620:GLN:H	1.55	0.55
1:B:536:VAL:H	1:B:541:ASN:HD21	1.55	0.54
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.19	0.54
1:B:679:ALA:HB2	4:B:2707:HOH:O	2.07	0.54
4:A:2034:HOH:O	1:B:42:LYS:HE2	2.06	0.54
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.90	0.53
1:B:223:THR:HG21	4:B:2311:HOH:O	2.07	0.53
1:A:76:ASN:O	1:A:80:GLN:HB2	2.08	0.53
1:B:307:GLN:NE2	4:B:2372:HOH:O	2.39	0.53
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.80	0.53
1:A:40:LYS:NZ	4:A:2056:HOH:O	2.39	0.53
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.27	0.53
1:B:46:GLN:OE1	1:B:60:PRO:HG3	2.08	0.53
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.21	0.53
1:A:527:ILE:CD1	1:A:634:MET:HE3	2.31	0.53
1:B:196:GLN:HE22	1:B:222:THR:H	1.57	0.53
1:A:286:VAL:CG1	1:A:288:MET:HE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:ASN:ND2	1:B:575:ASP:OD2	2.41	0.53
1:A:439:LYS:NZ	1:A:447:ASN:HD21	2.06	0.53
1:B:108:VAL:CG1	1:B:112:LYS:HE3	2.39	0.52
1:B:619:ALA:HB1	1:B:634:MET:HE1	1.90	0.52
1:A:274:LYS:NZ	1:A:276:VAL:HG12	2.23	0.52
1:A:7:MET:HE2	1:A:71:SER:HA	1.92	0.52
1:B:477:ASN:HD22	1:B:477:ASN:C	2.13	0.52
1:A:62:VAL:CG2	1:A:69:TRP:HB2	2.39	0.52
1:A:498:LYS:CB	1:A:498:LYS:NZ	2.73	0.52
1:B:477:ASN:ND2	1:B:479:THR:H	2.07	0.52
1:A:615:VAL:HG23	1:B:582:PRO:HB2	1.92	0.52
1:B:572:ASN:HD21	1:B:575:ASP:CG	2.13	0.52
1:A:572:ASN:ND2	1:A:575:ASP:H	2.08	0.51
1:A:236:LEU:HD11	1:A:244:LYS:HE3	1.91	0.51
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.35	0.51
1:B:116:ASP:O	1:B:117:PHE:C	2.45	0.51
1:A:210:LYS:HE2	1:A:214:ILE:O	2.10	0.51
1:B:332:LEU:HD13	1:B:342:ILE:CD1	2.40	0.51
1:A:400:LYS:HE3	1:B:449:SER:O	2.10	0.51
1:B:543:LEU:HD22	1:B:640:VAL:HG21	1.92	0.51
1:A:563:MET:HG3	1:B:370:GLY:HA3	1.93	0.51
1:B:627:ILE:HG23	1:B:628:TYR:N	2.26	0.51
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.41	0.51
1:B:148:GLN:NE2	4:B:2201:HOH:O	2.41	0.51
1:A:7:MET:HB3	1:A:69:TRP:HB3	1.93	0.50
1:B:439:LYS:HZ2	1:B:447:ASN:HD21	1.58	0.50
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.92	0.50
1:B:574:GLN:H	1:B:671:ASN:HD22	1.57	0.50
1:A:322:MET:HE1	4:A:2057:HOH:O	2.11	0.50
1:A:203:GLU:N	1:A:203:GLU:CD	2.61	0.50
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.93	0.50
1:A:63:MET:SD	1:A:68:ALA:HB2	2.51	0.50
1:A:642:ARG:HG2	1:A:642:ARG:HH11	1.77	0.50
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.95	0.50
1:A:200:ASN:ND2	4:A:2323:HOH:O	2.43	0.50
1:A:181:LYS:HD2	4:A:2305:HOH:O	2.11	0.50
1:A:572:ASN:HD22	1:A:575:ASP:H	1.58	0.50
1:B:214:ILE:HD12	1:B:214:ILE:N	2.26	0.50
1:B:700:PRO:CG	4:B:2717:HOH:O	2.59	0.50
1:A:439:LYS:HZ2	1:A:447:ASN:ND2	2.09	0.49
1:A:580:PHE:H	1:A:637:GLN:NE2	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HD2	4:A:2058:HOH:O	2.10	0.49
1:B:553:ASN:ND2	1:B:555:ALA:H	2.11	0.49
1:A:477:ASN:HD22	1:A:477:ASN:C	2.14	0.49
1:B:642:ARG:CG	1:B:642:ARG:NH1	2.74	0.49
1:B:700:PRO:HG3	4:B:2717:HOH:O	2.12	0.49
1:A:670:ASP:OD2	1:A:672:GLU:HG3	2.12	0.49
1:A:608:TYR:HD1	4:A:2813:HOH:O	1.95	0.49
1:A:366:ILE:HD12	1:A:631:LEU:CD1	2.43	0.48
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.59	0.48
1:A:209:VAL:HG13	1:A:214:ILE:HB	1.95	0.48
1:A:13:THR:HG22	1:A:75:ILE:HD11	1.96	0.48
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.48	0.48
1:A:15:LYS:HE2	4:A:2022:HOH:O	2.13	0.48
1:B:653:LYS:HG2	1:B:654:TYR:CE2	2.48	0.48
1:B:572:ASN:ND2	1:B:671:ASN:HD21	2.10	0.48
1:A:587:LEU:HD23	1:A:604:GLN:HA	1.96	0.48
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.28	0.48
1:B:381:TYR:CE2	4:B:2524:HOH:O	2.64	0.48
1:A:579:LYS:HA	1:A:637:GLN:NE2	2.29	0.48
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.78	0.48
1:A:216:ASP:OD1	1:A:218:LYS:HB2	2.14	0.47
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.59	0.47
1:A:326:ARG:HH12	1:B:303:VAL:CG2	2.22	0.47
1:A:189:LEU:HD12	4:A:2261:HOH:O	2.15	0.47
1:B:132:ASP:H	1:B:148:GLN:HE22	1.61	0.47
1:A:237:LYS:NZ	1:A:239:ASP:OD1	2.47	0.47
1:B:216:ASP:OD1	1:B:216:ASP:C	2.52	0.47
1:A:348:ASN:ND2	1:A:351:GLY:H	2.12	0.47
1:B:642:ARG:HB2	1:B:642:ARG:NH1	2.28	0.47
1:A:216:ASP:CB	1:A:219:LYS:HD2	2.31	0.47
1:A:51:ASN:N	1:A:51:ASN:HD22	2.12	0.47
1:B:116:ASP:O	1:B:118:LYS:HG2	2.15	0.47
1:B:321:ASP:HB3	1:B:332:LEU:O	2.15	0.47
1:A:237:LYS:NZ	1:A:239:ASP:CG	2.68	0.47
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.50	0.47
1:B:633:PHE:HA	1:B:639:TRP:CZ2	2.49	0.47
1:B:238:GLN:HA	1:B:238:GLN:HE21	1.80	0.47
1:A:516:ASP:HB3	1:A:519:ILE:HB	1.96	0.47
1:B:630:ARG:HA	4:B:2659:HOH:O	2.15	0.46
1:B:619:ALA:CB	1:B:634:MET:HE2	2.46	0.46
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.45	0.46
1:A:527:ILE:CD1	1:A:634:MET:CE	2.87	0.46
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.28	0.46
1:B:225:LEU:HD22	1:B:381:TYR:HE2	1.80	0.46
1:B:11:ASP:O	1:B:15:LYS:HD3	2.16	0.46
1:A:117:PHE:HE1	4:A:2192:HOH:O	1.99	0.46
1:A:723:LEU:HD23	1:B:298:ARG:HD3	1.98	0.46
1:B:619:ALA:HB1	1:B:634:MET:CE	2.45	0.46
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.15	0.46
1:B:259:HIS:HE1	1:B:289:THR:O	1.99	0.46
1:A:574:GLN:HG3	1:A:671:ASN:CG	2.37	0.46
1:B:67:LYS:HB2	4:B:2085:HOH:O	2.15	0.46
1:A:720:LEU:HA	1:A:720:LEU:HD23	1.79	0.46
1:B:130:PRO:HB3	4:B:2427:HOH:O	2.16	0.46
1:A:599:ASN:ND2	4:A:2730:HOH:O	2.48	0.46
1:B:626:TRP:O	1:B:627:ILE:C	2.53	0.45
1:B:203:GLU:OE2	1:B:204:GLU:HG3	2.15	0.45
1:B:369:TYR:CD1	1:B:379:LYS:HG2	2.51	0.45
1:A:332:LEU:HD21	1:A:427:ILE:HG21	1.99	0.45
1:A:214:ILE:HD12	1:A:214:ILE:N	2.31	0.45
1:B:644:HIS:CD2	4:B:2679:HOH:O	2.68	0.45
1:A:151:LYS:NZ	4:A:2249:HOH:O	2.50	0.45
1:B:549:VAL:HG11	1:B:566:ASN:HD22	1.81	0.45
1:A:106:GLN:NE2	1:A:169:LEU:O	2.35	0.45
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.99	0.45
1:A:237:LYS:HZ2	1:A:239:ASP:CG	2.20	0.45
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.21	0.45
1:B:117:PHE:CZ	1:B:121:THR:HB	2.52	0.45
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.32	0.45
1:A:679:ALA:HB2	4:A:2669:HOH:O	2.16	0.45
1:B:76:ASN:O	1:B:80:GLN:HB2	2.17	0.45
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.75	0.44
1:A:615:VAL:HG12	1:A:616:ALA:N	2.32	0.44
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.51	0.44
1:B:617:LYS:HA	4:B:2643:HOH:O	2.17	0.44
1:B:173:LYS:HB3	1:B:173:LYS:HZ2	1.80	0.44
1:B:221:ILE:N	1:B:221:ILE:HD12	2.33	0.44
1:A:578:GLN:HA	1:A:636:LYS:HD2	1.99	0.44
1:A:642:ARG:HG3	1:A:643:TYR:N	2.32	0.44
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.52	0.44
1:B:359:GLU:CD	1:B:648:ARG:NH2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:GLY:HA3	4:B:2641:HOH:O	2.18	0.44
1:A:574:GLN:H	1:A:671:ASN:ND2	2.16	0.44
1:B:369:TYR:CD2	1:B:524:HIS:HB3	2.53	0.43
1:A:8:VAL:HG13	1:A:13:THR:OG1	2.18	0.43
1:B:62:VAL:HG12	1:B:64:LYS:HG3	1.99	0.43
1:B:366:ILE:HD11	1:B:627:ILE:HD11	2.01	0.43
1:A:574:GLN:HG3	1:A:671:ASN:HB2	2.00	0.43
1:B:506:LYS:HD3	1:B:506:LYS:C	2.39	0.43
1:B:525:GLN:HE22	1:B:620:GLN:N	2.09	0.43
1:A:276:VAL:O	1:A:277:LYS:HB2	2.18	0.43
1:B:59:VAL:HA	1:B:60:PRO:HD3	1.83	0.43
1:B:724:LYS:NZ	4:B:2738:HOH:O	2.49	0.43
1:B:619:ALA:HB2	1:B:634:MET:HB3	2.00	0.43
1:A:10:MET:HE2	1:A:70:VAL:HG11	2.01	0.43
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.27	0.43
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.99	0.42
1:B:209:VAL:HG13	1:B:214:ILE:HB	2.01	0.42
1:A:477:ASN:HD22	1:A:479:THR:H	1.67	0.42
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.54	0.42
1:B:439:LYS:NZ	1:B:447:ASN:ND2	2.66	0.42
1:A:237:LYS:HD3	1:A:240:ALA:HB2	2.01	0.42
1:B:619:ALA:HB2	1:B:634:MET:HE2	2.00	0.42
1:B:669:LYS:CE	1:B:669:LYS:HA	2.49	0.42
1:B:214:ILE:HD11	1:B:286:VAL:HG21	2.01	0.42
1:A:298:ARG:HA	1:B:722:ALA:O	2.20	0.42
1:B:396:ILE:HG23	1:B:401:ASP:HB2	2.00	0.42
1:B:699:MET:HA	1:B:700:PRO:HD3	1.74	0.42
1:B:379:LYS:CG	1:B:381:TYR:CE1	3.02	0.42
1:A:321:ASP:HB3	1:A:332:LEU:O	2.20	0.42
1:A:498:LYS:HB3	1:A:498:LYS:HZ2	1.84	0.42
1:B:222:THR:HB	1:B:245:VAL:CG1	2.50	0.42
1:B:76:ASN:ND2	4:B:2100:HOH:O	2.52	0.42
1:B:212:ARG:HG2	1:B:283:VAL:HG22	2.01	0.42
1:A:580:PHE:N	1:A:637:GLN:HE21	2.08	0.42
1:A:410:ASN:OD1	1:A:424:PRO:HA	2.20	0.42
1:A:181:LYS:O	1:A:182:ASP:HB2	2.20	0.42
1:A:291:ARG:HH11	1:A:291:ARG:HD3	1.71	0.42
1:A:24:ASP:OD2	1:B:40:LYS:NZ	2.49	0.42
1:B:642:ARG:NH1	1:B:642:ARG:HG2	2.35	0.41
1:A:286:VAL:HG11	1:A:288:MET:HE1	2.01	0.41
1:B:129:LEU:HD12	1:B:130:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HG22	1:B:188:LEU:HD21	2.02	0.41
1:B:595:ASN:ND2	1:B:599:ASN:H	2.18	0.41
1:B:587:LEU:HD23	1:B:604:GLN:HA	2.01	0.41
1:B:670:ASP:HB2	4:B:2699:HOH:O	2.19	0.41
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.56	0.41
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.21	0.41
1:A:574:GLN:HG3	1:A:671:ASN:CB	2.50	0.41
1:A:523:THR:HB	4:A:2651:HOH:O	2.20	0.41
1:B:229:TYR:CZ	1:B:231:ASP:HA	2.55	0.41
1:B:239:ASP:OD1	1:B:239:ASP:C	2.57	0.41
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.36	0.41
1:A:639:TRP:HB2	1:A:682:TRP:HB2	2.03	0.41
1:B:619:ALA:CB	1:B:634:MET:CE	2.98	0.41
1:B:92:ARG:HD3	4:B:2190:HOH:O	2.20	0.41
1:B:627:ILE:CG2	1:B:628:TYR:N	2.84	0.41
1:B:574:GLN:HE22	1:B:669:LYS:NZ	2.19	0.41
1:B:669:LYS:HA	1:B:669:LYS:HE3	2.03	0.41
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.51	0.41
1:B:64:LYS:HB2	4:B:2085:HOH:O	2.21	0.41
1:B:139:PHE:O	1:B:143:ASN:HA	2.21	0.41
1:B:241:ARG:HG2	1:B:270:LEU:HB2	2.02	0.41
1:A:178:GLN:HA	1:A:179:PRO:HD3	1.91	0.41
1:A:104:ILE:O	1:A:108:VAL:HG23	2.21	0.40
1:A:65:ASP:O	1:A:66:ASN:HB2	2.20	0.40
1:A:204:GLU:H	1:A:204:GLU:HG3	1.62	0.40
1:A:117:PHE:CZ	1:A:121:THR:HB	2.57	0.40
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.70	0.40
1:A:62:VAL:HG23	1:A:62:VAL:O	2.22	0.40
1:B:717:THR:HA	1:B:718:PRO:HD3	1.90	0.40
1:B:439:LYS:NZ	1:B:447:ASN:HD21	2.20	0.40
1:A:553:ASN:HD21	1:A:555:ALA:H	1.66	0.40
1:B:181:LYS:O	1:B:182:ASP:HB2	2.21	0.40
1:A:643:TYR:O	1:A:644:HIS:CD2	2.74	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%)	691 (97%)	24 (3%)	0	100	100
1	B	717/727 (99%)	694 (97%)	21 (3%)	2 (0%)	46	36
All	All	1432/1454 (98%)	1385 (97%)	45 (3%)	2 (0%)	56	49

All (2) Ramachandran outliers are listed below:

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

### 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	609/615 (99%)	586 (96%)	23 (4%)	40	31
1	B	611/615 (99%)	584 (96%)	27 (4%)	35	26
All	All	1220/1230 (99%)	1170 (96%)	50 (4%)	37	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ASP
1	A	32	LEU
1	A	71	SER

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Mol	Chain	Res	Type
1	A	163	ILE
1	A	202	SER
1	A	203	GLU
1	A	204	GLU
1	A	210	LYS
1	A	239	ASP
1	A	273	LYS
1	A	274	LYS
1	A	348	ASN
1	A	350	ASN
1	A	477	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
1	A	642	ARG
1	A	671	ASN
1	B	11	ASP
1	B	22	GLN
1	B	34	LYS
1	B	47	THR
1	B	71	SER
1	B	80	GLN
1	B	129	LEU
1	B	144	LYS
1	B	160	LYS
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	211	LYS
1	B	218	LYS
1	B	239	ASP
1	B	322	MET
1	B	477	ASN
1	B	506	LYS
1	B	539	GLU
1	B	595	ASN
1	B	613	HIS
1	B	632	SER
1	B	642	ARG

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Mol	Chain	Res	Type
1	B	669	LYS
1	B	671	ASN
1	B	676	ASN
1	B	724	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	148	GLN
1	A	170	GLN
1	A	196	GLN
1	A	200	ASN
1	A	272	GLN
1	A	307	GLN
1	A	315	ASN
1	A	327	ASN
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	637	GLN
1	A	660	HIS
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	76	ASN
1	B	80	GLN
1	B	94	HIS
1	B	97	ASN
1	B	148	GLN
1	B	196	GLN
1	B	200	ASN
1	B	238	GLN
1	B	263	ASN

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Mol	Chain	Res	Type
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	566	ASN
1	B	567	GLN
1	B	572	ASN
1	B	574	GLN
1	B	595	ASN
1	B	599	ASN
1	B	604	GLN
1	B	613	HIS
1	B	637	GLN
1	B	644	HIS
1	B	671	ASN
1	B	676	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPQ	A	466	1	13,14,15	2.86	6 (46%)	15,19,21	1.82	4 (26%)
1	TPQ	B	466	1	13,14,15	2.86	6 (46%)	15,19,21	1.98	5 (33%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	C1-C2	-5.49	1.41	1.49
1	B	466	TPQ	C1-C2	-5.46	1.41	1.49
1	A	466	TPQ	O5-C5	-4.96	1.11	1.24
1	B	466	TPQ	O5-C5	-4.93	1.11	1.24
1	A	466	TPQ	O2-C2	-4.86	1.11	1.24
1	B	466	TPQ	O2-C2	-4.83	1.11	1.24
1	B	466	TPQ	C4-C5	-2.75	1.38	1.47
1	A	466	TPQ	C4-C5	-2.64	1.39	1.47
1	A	466	TPQ	C6-C1	2.01	1.39	1.34
1	B	466	TPQ	C6-C1	2.01	1.39	1.34
1	A	466	TPQ	C3-C4	2.13	1.39	1.35
1	B	466	TPQ	C3-C4	2.14	1.39	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TPQ	O-C-CA	-3.91	115.30	125.49
1	A	466	TPQ	O-C-CA	-2.72	118.41	125.49
1	B	466	TPQ	CA-CB-C1	-2.45	108.72	113.63
1	A	466	TPQ	C6-C1-C2	-2.29	116.83	118.44
1	B	466	TPQ	C6-C1-C2	-2.13	116.93	118.44
1	A	466	TPQ	CB-C1-C2	2.34	121.99	118.33
1	B	466	TPQ	CB-C1-C2	2.40	122.08	118.33
1	B	466	TPQ	C3-C2-C1	4.11	121.37	118.30
1	A	466	TPQ	C3-C2-C1	4.19	121.44	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466	TPQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	717/727 (98%)	-0.11	22 (3%) 52 60	15, 27, 46, 62	0
1	B	719/727 (98%)	0.06	43 (5%) 25 28	17, 29, 51, 65	0
All	All	1436/1454 (98%)	-0.02	65 (4%) 37 42	15, 28, 49, 65	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	HIS	5.9
1	B	301	PRO	5.7
1	B	115	ALA	5.6
1	B	65	ASP	5.3
1	B	91	LYS	4.8
1	B	302	ALA	4.8
1	A	119	PRO	4.1
1	B	178	GLN	4.0
1	B	215	THR	3.9
1	A	215	THR	3.7
1	B	239	ASP	3.6
1	B	173	LYS	3.5
1	B	119	PRO	3.5
1	B	76	ASN	3.4
1	B	92	ARG	3.3
1	B	629	HIS	3.2
1	B	303	VAL	3.1
1	A	503	GLU	3.1
1	B	16	GLU	3.1
1	B	147	ASP	3.1
1	A	218	LYS	3.1
1	A	147	ASP	3.1
1	B	218	LYS	3.0
1	B	66	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	239	ASP	2.9
1	A	210	LYS	2.9
1	A	670	ASP	2.9
1	B	143	ASN	2.8
1	B	64	LYS	2.8
1	B	725	LYS	2.7
1	B	203	GLU	2.7
1	B	12	LYS	2.7
1	B	144	LYS	2.7
1	A	303	VAL	2.7
1	A	211	LYS	2.7
1	A	203	GLU	2.6
1	A	723	LEU	2.6
1	B	216	ASP	2.6
1	B	231	ASP	2.5
1	B	644	HIS	2.5
1	B	617	LYS	2.5
1	B	300	ALA	2.4
1	A	64	LYS	2.4
1	B	80	GLN	2.4
1	A	16	GLU	2.4
1	B	113	ALA	2.3
1	A	72	ASP	2.3
1	A	640	VAL	2.3
1	B	670	ASP	2.3
1	B	197	ASN	2.3
1	A	76	ASN	2.3
1	B	118	LYS	2.3
1	B	640	VAL	2.2
1	B	503	GLU	2.2
1	A	12	LYS	2.2
1	A	644	HIS	2.2
1	B	58	GLN	2.2
1	B	116	ASP	2.1
1	A	148	GLN	2.1
1	A	181	LYS	2.1
1	B	72	ASP	2.1
1	B	109	GLU	2.1
1	B	210	LYS	2.0
1	B	120	ASN	2.0
1	A	41	VAL	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	0.94	0.14	-	21,37,51,52	0
1	TPQ	B	466	14/15	0.92	0.13	-	23,45,52,53	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(Å <sup>2</sup> )	Q<0.9
3	CA	A	803	1/1	0.97	0.17	0.06	54,54,54,54	0
3	CA	B	803	1/1	0.98	0.15	-0.01	51,51,51,51	0
3	CA	A	802	1/1	1.00	0.08	-1.12	23,23,23,23	0
3	CA	B	802	1/1	0.99	0.08	-1.20	25,25,25,25	0
2	CU	B	801	1/1	1.00	0.04	-	28,28,28,28	0
2	CU	A	801	1/1	0.99	0.04	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.