



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:15 AM UTC

PDB ID : 1SPU / pdb_00001spu
Title : STRUCTURE OF OXIDOREDUCTASE
Authors : Wilmot, C.M.; Phillips, S.E.V.
Deposited on : 1996-11-13
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

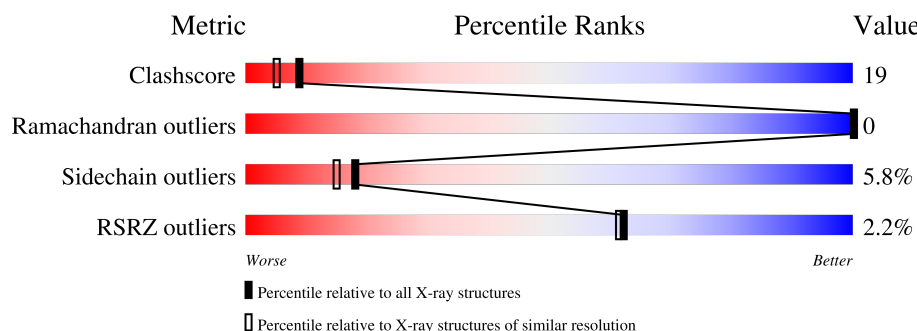
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	% 57% 34% 8% .
1	B	727	3% 54% 35% 10% ..

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
1	PAQ	A	466	X	-	-	-
1	PAQ	B	466	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12431 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
			5671	3607	967	1075	22			
1	B	720	Total	C	N	O	S	0	0	0
			5690	3619	972	1077	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	PAQ	TYR	modified residue	UNP P46883
B	466	PAQ	TYR	modified residue	UNP P46883

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	539	Total	O	0	0
			539	539		

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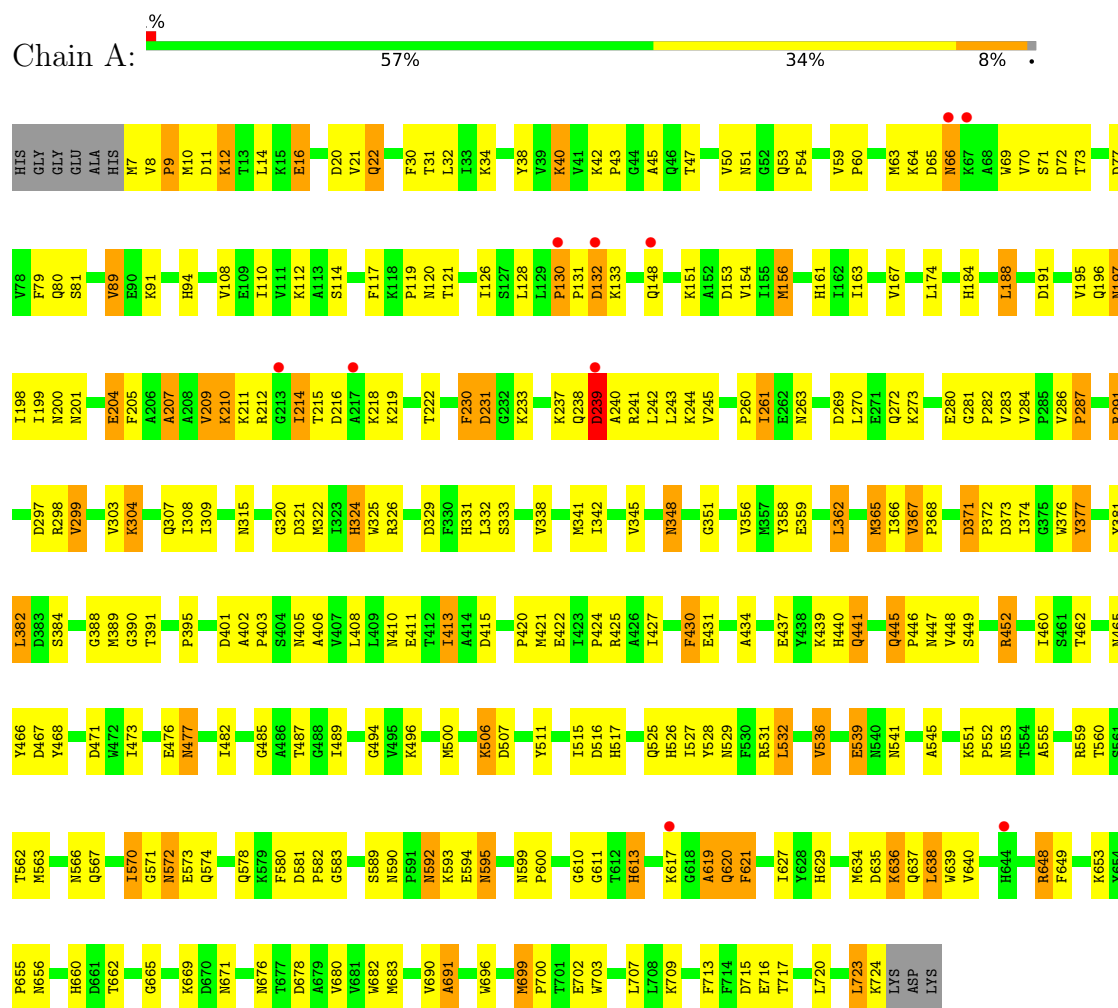
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	525	Total	O	0	0
			525	525		

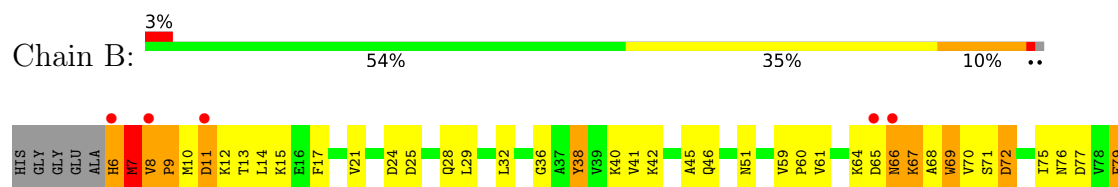
3 Residue-property plots

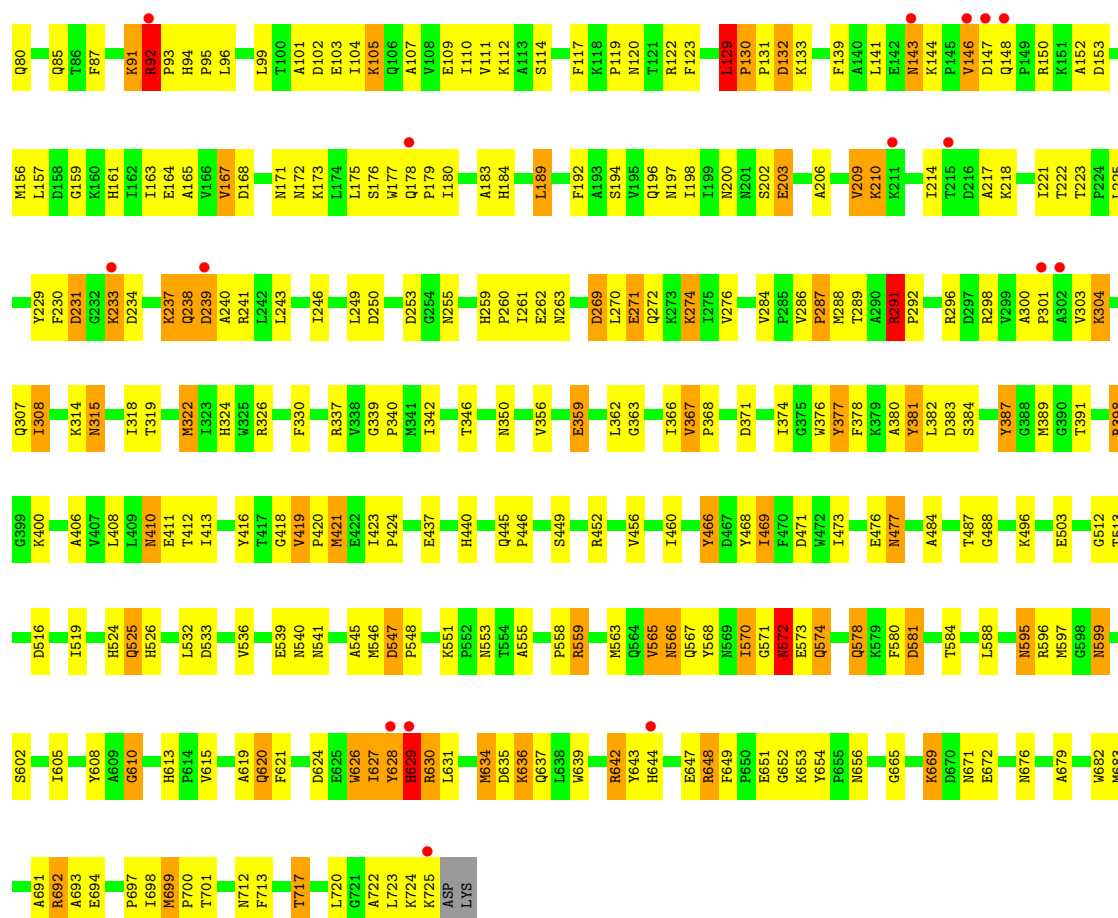
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: COPPER AMINE OXIDASE



• Molecule 1: COPPER AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.46Å 166.07Å 79.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.7 (20.00-2.00) 80.6 (20.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 1.99Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.206 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 115.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12431	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CU, PAQ

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	1.01	3/5793 (0.1%)	1.94	148/7886 (1.9%)
1	B	0.98	1/5813 (0.0%)	2.00	158/7912 (2.0%)
All	All	0.99	4/11606 (0.0%)	1.97	306/15798 (1.9%)

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	1	1
1	B	1	0
All	All	2	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ASP	CA-C	7.09	1.62	1.52
1	A	133	LYS	N-CA	7.04	1.55	1.46
1	A	130	PRO	CA-C	-6.28	1.46	1.52
1	B	513	THR	CA-CB	5.03	1.60	1.53

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ARG	CD-NE-CZ	14.42	144.59	124.40
1	A	238	GLN	CA-C-N	11.72	135.68	120.44
1	A	238	GLN	C-N-CA	11.72	135.68	120.44
1	B	239	ASP	CA-CB-CG	11.62	124.22	112.60
1	B	581	ASP	O-C-N	10.85	131.39	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	A	371	ASP	CB-CA-C	9.29	120.74	109.31
1	B	566	ASN	CA-C-O	9.29	130.40	120.46
1	B	202	SER	CA-C-N	9.12	133.25	120.29
1	B	202	SER	C-N-CA	9.12	133.25	120.29
1	A	20	ASP	CA-CB-CG	9.07	121.67	112.60
1	B	146	VAL	CB-CA-C	8.86	123.31	111.97
1	B	376	TRP	N-CA-C	8.75	124.45	113.43
1	A	161	HIS	CA-CB-CG	-8.65	105.15	113.80
1	B	203	GLU	CB-CG-CD	8.63	127.28	112.60
1	A	374	ILE	O-C-N	8.60	130.54	121.94
1	A	374	ILE	CA-C-O	-8.58	112.35	121.27
1	B	234	ASP	CA-CB-CG	8.54	121.14	112.60
1	B	547	ASP	O-C-N	8.37	130.65	121.36
1	B	25	ASP	CA-CB-CG	-8.27	104.33	112.60
1	A	31	THR	O-C-N	8.19	132.77	123.27
1	B	406	ALA	CA-C-N	8.17	133.74	123.12
1	B	406	ALA	C-N-CA	8.17	133.74	123.12
1	A	649	PHE	O-C-N	8.08	128.58	121.39
1	A	448	VAL	N-CA-CB	8.04	122.38	112.10
1	A	50	VAL	O-C-N	7.96	130.75	123.03
1	B	566	ASN	CB-CA-C	7.91	123.68	110.79
1	B	183	ALA	O-C-N	7.86	132.29	123.01
1	B	384	SER	CA-C-N	7.74	128.53	119.94
1	B	384	SER	C-N-CA	7.74	128.53	119.94
1	B	238	GLN	CA-C-N	7.72	130.93	120.44
1	B	238	GLN	C-N-CA	7.72	130.93	120.44
1	B	6	HIS	CA-CB-CG	7.69	121.49	113.80
1	B	566	ASN	CA-CB-CG	7.55	120.15	112.60
1	A	440	HIS	N-CA-CB	7.49	122.17	110.71
1	B	699	MET	CA-C-O	7.41	125.74	119.66
1	A	362	LEU	N-CA-C	-7.41	98.49	110.20
1	B	359	GLU	CA-CB-CG	7.38	128.85	114.10
1	B	571	GLY	N-CA-C	7.35	123.22	113.37
1	A	205	PHE	CA-CB-CG	-7.32	106.48	113.80
1	B	526	HIS	N-CA-CB	7.22	121.91	110.65
1	A	66	ASN	CA-C-N	7.18	133.81	122.74
1	A	66	ASN	C-N-CA	7.18	133.81	122.74
1	A	578	GLN	N-CA-C	7.18	119.66	108.96
1	B	132	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	713	PHE	N-CA-C	-7.13	103.59	111.36
1	A	31	THR	CA-C-O	-7.12	112.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	PHE	CA-CB-CG	-7.10	106.70	113.80
1	A	65	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	350	ASN	CA-CB-CG	-7.09	105.51	112.60
1	A	307	GLN	O-C-N	7.04	131.44	123.27
1	B	7	MET	N-CA-C	7.01	120.58	109.50
1	A	211	LYS	O-C-N	6.97	129.25	122.07
1	A	699	MET	N-CA-C	6.93	119.68	109.42
1	A	410	ASN	O-C-N	6.92	131.06	123.10
1	B	573	GLU	N-CA-C	6.91	119.69	111.33
1	A	656	ASN	CA-CB-CG	6.88	119.48	112.60
1	B	146	VAL	CA-C-N	6.88	132.40	122.35
1	B	146	VAL	C-N-CA	6.88	132.40	122.35
1	A	473	ILE	N-CA-C	6.86	117.74	107.51
1	A	635	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	231	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	30	PHE	O-C-N	6.79	130.94	123.27
1	A	9	PRO	N-CA-C	-6.78	100.57	110.80
1	B	12	LYS	CA-C-N	6.74	129.61	120.38
1	B	12	LYS	C-N-CA	6.74	129.61	120.38
1	A	167	VAL	O-C-N	6.71	130.07	123.03
1	B	72	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	130	PRO	N-CA-C	6.65	118.81	110.70
1	B	129	LEU	CB-CA-C	6.65	117.43	109.85
1	B	418	GLY	CA-C-O	6.65	126.70	119.06
1	B	8	VAL	N-CA-CB	-6.62	101.94	111.21
1	B	578	GLN	N-CA-C	6.62	117.88	108.74
1	B	387	TYR	CA-C-O	-6.61	111.90	118.97
1	A	430	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	230	PHE	CA-CB-CG	-6.58	107.22	113.80
1	B	565	VAL	CA-C-N	-6.58	113.76	123.11
1	B	565	VAL	C-N-CA	-6.58	113.76	123.11
1	A	415	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	315	ASN	OD1-CG-ND2	6.58	129.18	122.60
1	B	581	ASP	CA-C-O	-6.58	113.84	119.36
1	A	581	ASP	CB-CA-C	6.56	117.32	109.85
1	B	630	ARG	CD-NE-CZ	6.54	133.56	124.40
1	A	713	PHE	N-CA-C	-6.53	103.66	111.69
1	B	350	ASN	O-C-N	6.51	130.71	122.57
1	B	102	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	627	ILE	CA-C-O	6.49	127.80	121.05
1	A	79	PHE	O-C-N	6.46	130.21	122.27
1	B	691	ALA	N-CA-C	6.45	119.26	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	630	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	B	423	ILE	O-C-N	6.42	127.16	121.57
1	B	627	ILE	CA-C-N	6.39	128.84	120.28
1	B	627	ILE	C-N-CA	6.39	128.84	120.28
1	B	440	HIS	N-CA-CB	6.38	120.47	110.71
1	A	441	GLN	O-C-N	6.37	129.40	122.64
1	A	291	ARG	CD-NE-CZ	6.37	133.32	124.40
1	A	197	ASN	O-C-N	6.36	128.64	122.03
1	A	148	GLN	O-C-N	6.34	125.77	121.71
1	A	507	ASP	CA-C-N	6.31	128.73	120.28
1	A	507	ASP	C-N-CA	6.31	128.73	120.28
1	A	471	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	66	ASN	CB-CA-C	6.29	120.29	111.86
1	B	129	LEU	O-C-N	6.26	128.31	121.36
1	B	378	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	299	VAL	N-CA-CB	6.24	121.22	111.99
1	A	284	VAL	O-C-N	6.21	126.67	120.59
1	A	34	LYS	N-CA-CB	6.20	119.43	110.37
1	A	184	HIS	N-CA-CB	6.19	120.73	110.52
1	A	566	ASN	CA-CB-CG	6.18	118.78	112.60
1	B	524	HIS	CA-CB-CG	-6.17	107.63	113.80
1	B	377	TYR	N-CA-C	6.16	119.64	111.75
1	B	147	ASP	N-CA-C	6.16	120.17	111.92
1	B	291	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	B	274	LYS	O-C-N	6.14	130.25	123.25
1	B	419	VAL	CB-CA-C	6.13	117.02	110.53
1	B	572	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	B	699	MET	N-CA-C	6.11	117.36	109.72
1	A	309	ILE	CA-C-N	6.11	130.67	123.16
1	A	309	ILE	C-N-CA	6.11	130.67	123.16
1	B	629	HIS	CA-C-N	6.10	129.29	120.38
1	B	629	HIS	C-N-CA	6.10	129.29	120.38
1	A	570	ILE	CB-CA-C	6.09	119.44	111.53
1	A	411	GLU	CB-CG-CD	6.06	122.90	112.60
1	A	571	GLY	N-CA-C	6.06	122.95	113.86
1	B	296	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	A	324	HIS	CA-CB-CG	-6.05	107.75	113.80
1	B	284	VAL	O-C-N	6.05	127.98	120.66
1	A	506	LYS	N-CA-C	6.02	117.51	111.07
1	A	299	VAL	CA-C-O	6.01	126.20	120.25
1	A	421	MET	N-CA-CB	-6.00	100.98	110.77
1	B	652	GLY	CA-C-N	5.98	128.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	652	GLY	C-N-CA	5.98	128.29	120.28
1	A	648	ARG	NE-CZ-NH2	-5.97	113.82	119.20
1	A	382	LEU	N-CA-C	-5.96	101.31	109.71
1	B	223	THR	O-C-N	5.95	127.55	121.72
1	B	717	THR	O-C-N	5.94	128.15	121.32
1	A	709	LYS	O-C-N	5.91	127.21	121.66
1	B	356	VAL	N-CA-C	-5.91	106.95	111.62
1	A	619	ALA	CA-C-O	-5.90	113.88	120.54
1	B	574	GLN	CB-CG-CD	5.89	122.61	112.60
1	B	223	THR	CA-C-O	-5.88	113.11	120.23
1	B	68	ALA	O-C-N	5.88	129.98	123.16
1	B	362	LEU	N-CA-C	-5.86	102.38	110.35
1	A	589	SER	O-C-N	5.84	130.63	123.10
1	A	662	THR	O-C-N	5.83	129.08	122.20
1	B	105	LYS	CA-C-N	5.82	128.08	120.28
1	B	105	LYS	C-N-CA	5.82	128.08	120.28
1	A	239	ASP	CA-C-N	5.82	129.13	120.87
1	A	239	ASP	C-N-CA	5.82	129.13	120.87
1	B	77	ASP	O-C-N	5.81	128.78	122.15
1	B	643	TYR	O-C-N	5.80	130.15	122.95
1	A	592	ASN	O-C-N	5.80	130.01	122.42
1	A	420	PRO	CB-CA-C	5.79	118.92	111.56
1	A	690	VAL	N-CA-C	-5.78	99.42	107.80
1	B	526	HIS	O-C-N	5.77	129.96	123.27
1	B	526	HIS	CA-C-O	-5.76	114.14	120.30
1	B	382	LEU	N-CA-C	-5.75	100.94	109.11
1	B	161	HIS	O-C-N	5.74	129.91	123.19
1	A	188	LEU	CB-CA-C	5.74	119.27	109.80
1	A	12	LYS	O-C-N	5.74	128.00	122.03
1	A	261	ILE	N-CA-CB	5.74	118.88	111.83
1	B	255	ASN	CA-CB-CG	5.73	118.33	112.60
1	B	324	HIS	CA-CB-CG	-5.71	108.09	113.80
1	B	525	GLN	OE1-CD-NE2	5.69	128.29	122.60
1	A	287	PRO	CB-CA-C	5.69	117.76	111.56
1	B	471	ASP	O-C-N	5.67	130.05	123.30
1	A	620	GLN	CA-C-N	5.65	131.89	122.73
1	A	620	GLN	C-N-CA	5.65	131.89	122.73
1	B	488	GLY	N-CA-C	-5.65	105.85	111.56
1	A	110	ILE	CA-C-O	-5.63	115.42	121.27
1	A	406	ALA	CA-C-N	5.62	130.75	123.11
1	A	406	ALA	C-N-CA	5.62	130.75	123.11
1	A	283	VAL	O-C-N	5.61	128.79	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	356	VAL	N-CA-C	-5.56	107.23	111.62
1	A	594	GLU	O-C-N	5.56	129.89	123.17
1	A	338	VAL	N-CA-C	5.55	120.05	113.22
1	B	9	PRO	N-CA-CB	5.52	107.71	103.30
1	A	214	ILE	CA-C-N	5.51	128.13	120.63
1	A	214	ILE	C-N-CA	5.51	128.13	120.63
1	B	626	TRP	CA-C-N	5.51	128.30	120.53
1	B	626	TRP	C-N-CA	5.51	128.30	120.53
1	A	507	ASP	O-C-N	5.50	128.42	122.15
1	B	7	MET	CA-C-O	5.50	127.54	121.11
1	A	422	GLU	CA-C-N	-5.49	118.64	122.59
1	A	422	GLU	C-N-CA	-5.49	118.64	122.59
1	B	371	ASP	CB-CA-C	5.49	117.26	109.08
1	A	482	ILE	O-C-N	5.49	127.91	122.97
1	A	431	GLU	CG-CD-OE1	5.48	131.01	118.40
1	B	654	TYR	O-C-N	5.46	126.28	121.37
1	B	389	MET	CA-C-N	5.46	126.04	119.98
1	B	389	MET	C-N-CA	5.46	126.04	119.98
1	B	148	GLN	CB-CA-C	5.45	117.38	109.20
1	B	410	ASN	CB-CA-C	5.45	118.71	109.50
1	B	411	GLU	CB-CG-CD	5.45	121.86	112.60
1	A	373	ASP	CA-C-N	5.45	127.62	120.60
1	A	373	ASP	C-N-CA	5.45	127.62	120.60
1	A	204	GLU	O-C-N	5.43	127.66	122.07
1	A	445	GLN	O-C-N	5.43	125.96	121.35
1	B	570	ILE	CA-C-N	5.42	127.11	120.22
1	B	570	ILE	C-N-CA	5.42	127.11	120.22
1	A	209	VAL	O-C-N	5.41	127.21	121.91
1	B	161	HIS	CA-C-N	5.40	129.12	122.37
1	B	161	HIS	C-N-CA	5.40	129.12	122.37
1	B	701	THR	CA-CB-OG1	-5.40	101.51	109.60
1	A	239	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	536	VAL	O-C-N	5.39	129.31	122.57
1	B	11	ASP	CA-CB-CG	-5.39	107.21	112.60
1	B	398	ARG	CA-C-O	5.39	125.94	120.88
1	B	610	GLY	CA-C-O	5.38	126.33	122.45
1	A	163	ILE	O-C-N	5.37	129.00	123.20
1	A	282	PRO	CA-C-O	5.37	127.46	121.34
1	A	448	VAL	CA-C-O	-5.36	115.06	120.31
1	B	642	ARG	CA-C-O	5.35	127.15	121.16
1	B	304	LYS	O-C-N	5.34	128.91	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	VAL	CA-C-O	5.34	126.36	120.64
1	B	122	ARG	CD-NE-CZ	5.34	131.87	124.40
1	B	69	TRP	O-C-N	5.33	129.77	123.27
1	A	413	ILE	CA-C-O	-5.32	116.42	121.64
1	B	202	SER	CA-C-O	5.32	126.66	120.49
1	A	691	ALA	N-CA-C	5.32	117.55	110.53
1	B	570	ILE	CB-CA-C	5.32	118.44	111.53
1	A	494	GLY	N-CA-C	-5.31	103.30	111.64
1	A	22	GLN	N-CA-CB	5.30	120.06	110.83
1	B	526	HIS	CA-C-N	-5.30	116.05	123.10
1	B	526	HIS	C-N-CA	-5.30	116.05	123.10
1	A	218	LYS	CA-C-N	5.30	131.97	122.38
1	A	218	LYS	C-N-CA	5.30	131.97	122.38
1	A	517	HIS	CA-CB-CG	-5.29	108.51	113.80
1	B	602	SER	N-CA-C	5.28	117.00	109.14
1	A	207	ALA	CA-C-N	5.28	127.35	120.28
1	A	207	ALA	C-N-CA	5.28	127.35	120.28
1	A	420	PRO	CA-C-O	5.28	127.32	121.36
1	A	566	ASN	N-CA-CB	5.26	119.07	110.39
1	A	211	LYS	N-CA-CB	5.25	117.62	110.01
1	A	381	TYR	N-CA-C	5.25	117.28	109.25
1	B	308	ILE	O-C-N	5.24	129.23	123.10
1	B	319	THR	CA-C-O	-5.24	114.73	120.70
1	A	467	ASP	CA-C-N	5.23	130.22	123.00
1	A	467	ASP	C-N-CA	5.23	130.22	123.00
1	A	471	ASP	O-C-N	5.23	129.34	123.27
1	A	482	ILE	N-CA-CB	5.23	119.14	112.34
1	B	512	GLY	CA-C-O	-5.23	116.49	121.62
1	A	372	PRO	CA-C-N	5.23	129.70	120.87
1	A	372	PRO	C-N-CA	5.23	129.70	120.87
1	A	367	VAL	O-C-N	5.22	127.05	121.10
1	A	303	VAL	CA-C-O	5.21	127.33	121.28
1	A	320	GLY	N-CA-C	-5.21	100.84	113.18
1	B	153	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	452	ARG	O-C-N	5.20	129.27	123.19
1	A	665	GLY	N-CA-C	-5.20	106.49	112.73
1	B	287	PRO	N-CA-C	-5.20	102.34	110.50
1	A	462	THR	CA-C-O	-5.20	114.75	120.36
1	A	592	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	B	79	PHE	CB-CA-C	5.19	119.02	110.88
1	A	660	HIS	CA-CB-CG	-5.18	108.62	113.80
1	B	526	HIS	CA-CB-CG	-5.18	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	PRO	N-CA-CB	5.18	107.93	103.27
1	A	552	PRO	CB-CA-C	5.18	118.10	111.21
1	A	638	LEU	O-C-N	5.17	129.58	123.27
1	B	129	LEU	N-CA-C	-5.17	101.19	109.04
1	A	47	THR	CA-CB-OG1	-5.16	101.85	109.60
1	A	153	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	269	ASP	N-CA-C	-5.16	99.37	108.20
1	A	304	LYS	N-CA-C	-5.16	103.17	110.29
1	B	421	MET	N-CA-CB	-5.16	102.37	110.77
1	A	374	ILE	N-CA-C	5.15	115.77	110.36
1	B	381	TYR	N-CA-C	5.15	117.68	109.96
1	B	132	ASP	CB-CA-C	5.15	117.93	109.90
1	B	64	LYS	CA-C-O	5.14	125.89	120.33
1	B	92	ARG	O-C-N	5.14	126.03	121.19
1	A	572	ASN	O-C-N	5.14	129.62	122.78
1	A	244	LYS	N-CA-C	-5.14	102.45	110.42
1	B	473	ILE	N-CA-C	5.14	115.16	107.51
1	B	691	ALA	CA-C-O	5.13	127.86	121.81
1	A	487	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	456	VAL	O-C-N	5.12	128.36	122.93
1	A	573	GLU	O-C-N	5.12	127.54	122.12
1	A	390	GLY	N-CA-C	-5.11	106.60	112.73
1	B	79	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	590	ASN	O-C-N	5.11	126.01	120.85
1	A	16	GLU	CA-CB-CG	5.11	124.32	114.10
1	A	211	LYS	CB-CA-C	-5.11	102.86	110.88
1	B	608	TYR	CA-CB-CG	-5.11	104.71	113.90
1	B	209	VAL	CA-C-O	-5.10	115.44	120.85
1	B	628	TYR	CA-CB-CG	-5.09	104.75	113.90
1	B	38	TYR	CB-CA-C	5.08	118.92	110.74
1	B	634	MET	N-CA-C	5.08	118.58	112.38
1	B	261	ILE	O-C-N	5.07	128.91	122.57
1	B	287	PRO	CB-CA-C	5.07	117.09	111.56
1	A	287	PRO	N-CA-C	-5.07	102.54	110.50
1	B	150	ARG	N-CA-CB	5.07	117.40	109.85
1	A	526	HIS	N-CA-CB	5.07	118.54	110.84
1	B	107	ALA	CA-C-O	-5.05	115.07	120.42
1	B	363	GLY	N-CA-C	-5.05	101.21	113.18
1	A	707	LEU	N-CA-CB	-5.05	102.13	111.52
1	A	72	ASP	CA-C-N	5.04	130.98	122.26
1	A	72	ASP	C-N-CA	5.04	130.98	122.26
1	B	269	ASP	CB-CA-C	5.04	118.84	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	651	GLU	CB-CG-CD	5.04	121.16	112.60
1	A	648	ARG	CD-NE-CZ	5.04	131.45	124.40
1	B	85	GLN	O-C-N	5.04	128.38	122.34
1	A	539	GLU	CA-CB-CG	5.03	124.15	114.10
1	A	231	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	192	PHE	O-C-N	5.01	127.24	122.07
1	B	367	VAL	O-C-N	5.01	126.82	121.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	466	PAQ	CG
1	B	466	PAQ	CG

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	648	ARG	Sidechain

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	5671	0	5545	200	0
1	B	5690	0	5563	252	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	539	0	0	18	0
4	B	525	0	0	20	0
All	All	12431	0	11108	418	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 19.

All (418) 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:210:LYS:HE3	1:B:217:ALA:HB2	1.24	1.14
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.09	1.12
1:B:92:ARG:HB2	1:B:92:ARG:HH11	1.24	1.00
1:B:368:PRO:HB2	1:B:621:PHE:CZ	1.97	0.98
1:A:297:ASP:HB2	1:B:725:LYS:HE3	1.46	0.98
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.03	0.97
1:B:644:HIS:HB3	4:B:1413:HOH:O	1.67	0.91
1:A:304:LYS:H	1:B:315:ASN:HD21	1.20	0.90
1:B:7:MET:HE2	1:B:70:VAL:C	1.97	0.90
1:A:38:TYR:H	1:A:51:ASN:ND2	1.70	0.89
1:A:38:TYR:H	1:A:51:ASN:HD21	1.21	0.85
1:A:699:MET:SD	4:A:1422:HOH:O	2.34	0.85
1:B:322:MET:HE3	1:B:330:PHE:O	1.77	0.85
1:B:92:ARG:HB2	1:B:92:ARG:NH1	1.91	0.85
1:B:621:PHE:HE2	1:B:634:MET:HE1	1.39	0.85
1:A:315:ASN:HD21	1:B:304:LYS:H	1.26	0.84
1:A:216:ASP:HB3	1:A:219:LYS:HD2	1.60	0.82
1:B:269:ASP:HB2	1:B:276:VAL:HG11	1.62	0.81
1:A:94:HIS:HD2	1:A:322:MET:HE3	1.45	0.81
1:B:7:MET:HE2	1:B:71:SER:N	1.96	0.80
1:A:439:LYS:HZ1	1:A:447:ASN:ND2	1.82	0.78
1:A:592:ASN:HD21	1:A:676:ASN:ND2	1.80	0.78
1:A:545:ALA:HB2	1:A:570:ILE:HD11	1.66	0.78
1:B:38:TYR:H	1:B:51:ASN:HD21	1.31	0.78
1:B:6:HIS:HB3	1:B:72:ASP:OD1	1.84	0.77
1:B:322:MET:HE3	1:B:330:PHE:C	2.09	0.77
1:B:139:PHE:O	1:B:143:ASN:HA	1.83	0.77
1:A:297:ASP:CB	1:B:725:LYS:HE3	2.15	0.77
1:B:38:TYR:H	1:B:51:ASN:ND2	1.84	0.76
1:B:38:TYR:HE1	1:B:40:LYS:HE3	1.49	0.76
1:A:326:ARG:HH22	1:B:303:VAL:CG1	2.00	0.74
1:B:445:GLN:HB3	1:B:446:PRO:CD	2.16	0.74
1:B:200:ASN:ND2	4:B:1597:HOH:O	2.16	0.74
1:B:445:GLN:HB3	1:B:446:PRO:HD2	1.70	0.73
1:B:7:MET:HE3	1:B:59:VAL:CG1	2.19	0.72
1:A:198:ILE:HD11	1:A:273:LYS:HD3	1.70	0.72
1:A:536:VAL:H	1:A:541:ASN:HD21	1.37	0.71
1:A:525:GLN:NE2	1:A:620:GLN:H	1.87	0.71
1:A:94:HIS:CD2	1:A:322:MET:HE3	2.26	0.71
1:A:237:LYS:HE2	1:A:239:ASP:HB2	1.71	0.70
1:A:525:GLN:HE22	1:A:620:GLN:H	1.39	0.70
1:A:326:ARG:HH22	1:B:303:VAL:HG11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:O	1:A:16:GLU:HB2	1.92	0.70
1:B:65:ASP:O	1:B:66:ASN:HB2	1.91	0.70
1:A:214:ILE:HD11	1:A:261:ILE:HG12	1.74	0.69
1:A:7:MET:HE2	1:A:59:VAL:CG1	2.23	0.69
1:B:239:ASP:HB2	4:B:1388:HOH:O	1.91	0.69
1:A:325:TRP:CE2	1:A:326:ARG:HD2	2.28	0.69
1:B:237:LYS:HE2	1:B:240:ALA:HB2	1.75	0.68
1:A:21:VAL:HG13	1:A:32:LEU:CD2	2.23	0.68
1:A:260:PRO:HD2	1:A:287:PRO:HG2	1.75	0.68
1:B:359:GLU:CD	1:B:648:ARG:HH22	2.01	0.67
1:A:368:PRO:HG3	1:A:634:MET:CE	2.24	0.67
1:B:189:LEU:HD22	1:B:189:LEU:O	1.95	0.67
1:B:94:HIS:HD2	1:B:96:LEU:H	1.42	0.67
1:B:621:PHE:CE2	1:B:634:MET:HE1	2.27	0.67
1:A:368:PRO:HG3	1:A:634:MET:HE3	1.75	0.66
1:B:109:GLU:HG2	4:B:1514:HOH:O	1.94	0.66
1:A:723:LEU:HD23	1:B:298:ARG:HD3	1.76	0.66
1:B:723:LEU:HD11	1:B:725:LYS:HD2	1.76	0.66
1:A:126:ILE:HG12	1:A:154:VAL:HG13	1.76	0.65
1:B:272:GLN:HE21	1:B:274:LYS:HG2	1.62	0.65
1:A:237:LYS:HG2	4:A:1146:HOH:O	1.97	0.64
1:B:241:ARG:HG2	1:B:270:LEU:HB2	1.80	0.64
1:A:7:MET:HA	1:A:70:VAL:O	1.98	0.64
1:B:503:GLU:HG2	4:B:1569:HOH:O	1.97	0.64
1:B:477:ASN:HD22	1:B:477:ASN:C	2.06	0.64
1:B:644:HIS:HB2	1:B:647:GLU:HG3	1.79	0.64
1:B:65:ASP:O	1:B:66:ASN:CB	2.45	0.64
1:A:341:MET:HE2	4:A:995:HOH:O	1.98	0.63
1:A:260:PRO:HD2	1:A:287:PRO:CD	2.29	0.63
1:A:477:ASN:C	1:A:477:ASN:HD22	2.07	0.63
1:B:572:ASN:ND2	1:B:671:ASN:HD21	1.96	0.63
1:A:298:ARG:HA	1:B:722:ALA:O	1.99	0.62
1:A:38:TYR:N	1:A:51:ASN:HD21	1.93	0.62
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.13	0.62
1:A:260:PRO:HD2	1:A:287:PRO:HD2	1.82	0.62
1:A:299:VAL:HG23	1:B:724:LYS:HG2	1.82	0.62
1:B:272:GLN:NE2	1:B:274:LYS:HD3	2.15	0.62
1:A:233:LYS:HG3	4:A:1370:HOH:O	2.00	0.61
1:B:307:GLN:NE2	4:B:1533:HOH:O	2.33	0.61
1:B:580:PHE:H	1:B:637:GLN:HE21	1.47	0.61
1:B:581:ASP:HB3	1:B:584:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ASN:ND2	1:A:555:ALA:H	1.98	0.61
1:A:574:GLN:H	1:A:671:ASN:ND2	1.99	0.60
1:A:539:GLU:HG2	1:A:678:ASP:HB2	1.83	0.60
1:A:439:LYS:NZ	1:A:447:ASN:ND2	2.47	0.60
1:B:101:ALA:O	1:B:105:LYS:HG3	2.00	0.60
1:A:322:MET:HG2	4:A:1278:HOH:O	2.01	0.60
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.32	0.60
1:A:368:PRO:CG	1:A:634:MET:CE	2.80	0.59
1:A:600:PRO:HB3	4:A:1136:HOH:O	2.02	0.59
1:A:595:ASN:ND2	1:A:599:ASN:H	2.01	0.59
1:B:574:GLN:H	1:B:671:ASN:HD22	1.50	0.59
1:B:229:TYR:CD1	1:B:238:GLN:NE2	2.70	0.58
1:A:209:VAL:HG13	1:A:214:ILE:HB	1.85	0.58
1:B:539:GLU:HB2	4:B:1352:HOH:O	2.03	0.58
1:A:260:PRO:HD2	1:A:287:PRO:CG	2.34	0.58
1:B:259:HIS:HE1	1:B:289:THR:O	1.86	0.58
1:B:545:ALA:O	1:B:567:GLN:HA	2.04	0.58
1:B:40:LYS:HE2	4:B:1501:HOH:O	2.03	0.58
1:B:95:PRO:HB3	1:B:146:VAL:HG21	1.86	0.58
1:A:326:ARG:HH12	1:B:303:VAL:HG21	1.69	0.57
1:A:574:GLN:HG2	1:A:671:ASN:HB2	1.85	0.57
1:B:669:LYS:HE3	1:B:669:LYS:O	2.04	0.57
1:A:42:LYS:HB3	1:A:42:LYS:HZ2	1.69	0.57
1:B:263:ASN:CA	1:B:374:ILE:HD11	2.34	0.57
1:B:38:TYR:CE1	1:B:40:LYS:HE3	2.37	0.57
1:B:366:ILE:HA	1:B:381:TYR:O	2.04	0.57
1:A:121:THR:HG23	1:A:156:MET:HB2	1.87	0.57
1:A:63:MET:HE3	1:A:66:ASN:HA	1.85	0.57
1:B:210:LYS:CE	1:B:217:ALA:HB2	2.16	0.57
1:B:578:GLN:HA	1:B:636:LYS:HD3	1.86	0.57
1:A:366:ILE:HG23	1:A:527:ILE:HB	1.86	0.57
1:B:629:HIS:C	1:B:629:HIS:CD2	2.82	0.57
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.40	0.57
1:B:271:GLU:HA	1:B:271:GLU:OE1	2.05	0.57
1:B:196:GLN:HE22	1:B:222:THR:H	1.51	0.57
1:B:595:ASN:HB3	1:B:712:ASN:O	2.05	0.57
1:A:117:PHE:CZ	1:A:121:THR:HB	2.40	0.56
1:B:7:MET:HE3	1:B:59:VAL:HG12	1.87	0.56
1:B:628:TYR:CD1	1:B:628:TYR:C	2.83	0.56
1:A:582:PRO:C	1:B:615:VAL:HG12	2.30	0.56
1:B:263:ASN:C	1:B:374:ILE:HD11	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD21	1:A:427:ILE:HG21	1.88	0.56
1:A:237:LYS:CE	1:A:239:ASP:HB2	2.35	0.56
1:B:10:MET:HG2	1:B:14:LEU:HD12	1.88	0.56
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.19	0.56
1:A:717:THR:HG21	1:B:698:ILE:HG23	1.88	0.56
1:B:111:VAL:O	1:B:114:SER:HB3	2.05	0.56
1:B:168:ASP:HB2	1:B:175:LEU:HD11	1.87	0.56
1:B:133:LYS:NZ	1:B:533:ASP:OD2	2.39	0.55
1:B:596:ARG:HB3	1:B:597:MET:CE	2.35	0.55
1:A:331:HIS:CE1	1:A:333:SER:HB3	2.41	0.55
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.20	0.55
1:A:243:LEU:HD12	1:A:270:LEU:HD11	1.89	0.55
1:B:7:MET:HE3	1:B:59:VAL:HG11	1.87	0.55
1:B:17:PHE:HB2	1:B:75:ILE:HD13	1.89	0.55
1:A:326:ARG:NH1	1:B:303:VAL:HG21	2.21	0.55
1:A:324:HIS:HD2	1:A:329:ASP:OD1	1.90	0.55
1:A:539:GLU:HB2	4:A:1423:HOH:O	2.05	0.55
1:A:308:ILE:HG12	1:B:308:ILE:HG12	1.88	0.55
1:A:610:GLY:HA3	1:B:610:GLY:HA3	1.89	0.55
1:B:111:VAL:O	1:B:117:PHE:HB2	2.06	0.55
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.15	0.54
4:A:1438:HOH:O	1:B:46:GLN:HG2	2.07	0.54
1:B:541:ASN:ND2	4:B:1496:HOH:O	2.41	0.54
1:A:299:VAL:HG23	1:B:724:LYS:CG	2.37	0.54
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.43	0.54
1:B:596:ARG:HB3	1:B:597:MET:HE1	1.88	0.54
1:B:642:ARG:HD2	1:B:672:GLU:HB2	1.90	0.54
1:B:263:ASN:HA	1:B:374:ILE:HD11	1.89	0.53
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.90	0.53
1:B:143:ASN:ND2	1:B:143:ASN:O	2.41	0.53
1:B:596:ARG:NH2	4:B:1112:HOH:O	2.42	0.53
1:A:89:VAL:HG12	4:A:909:HOH:O	2.08	0.53
1:B:269:ASP:CB	1:B:276:VAL:HG11	2.36	0.53
1:B:322:MET:CE	1:B:330:PHE:C	2.80	0.53
1:A:326:ARG:HD3	1:A:476:GLU:CD	2.34	0.53
1:B:8:VAL:HG12	1:B:13:THR:OG1	2.09	0.53
1:A:8:VAL:HB	1:A:9:PRO:HD2	1.91	0.52
1:B:286:VAL:O	1:B:288:MET:HG2	2.09	0.52
1:B:574:GLN:H	1:B:671:ASN:ND2	2.07	0.52
1:B:36:GLY:HA2	1:B:314:LYS:HE2	1.92	0.52
1:A:38:TYR:N	1:A:51:ASN:ND2	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HB	1:A:245:VAL:HG13	1.92	0.52
1:B:10:MET:CG	1:B:14:LEU:HD12	2.39	0.52
1:B:272:GLN:HE21	1:B:274:LYS:CG	2.22	0.52
1:A:263:ASN:HB3	1:A:281:GLY:HA3	1.93	0.51
1:A:724:LYS:HE3	1:B:298:ARG:O	2.10	0.51
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.92	0.51
1:A:196:GLN:HE22	1:A:222:THR:H	1.59	0.51
1:A:291:ARG:NH2	1:B:596:ARG:HH12	2.09	0.51
1:B:642:ARG:HD2	1:B:672:GLU:CB	2.40	0.51
1:B:291:ARG:HD2	1:B:516:ASP:OD2	2.11	0.51
1:A:559:ARG:HG2	1:B:377:TYR:HB2	1.93	0.51
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.41	0.51
1:B:536:VAL:H	1:B:541:ASN:HD21	1.59	0.50
1:A:439:LYS:NZ	1:A:447:ASN:HD21	2.08	0.50
1:B:7:MET:HE2	1:B:70:VAL:CA	2.41	0.50
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.93	0.50
1:B:460:ILE:HA	1:B:468:TYR:O	2.12	0.50
1:A:723:LEU:HD23	1:B:298:ARG:CD	2.42	0.50
1:B:21:VAL:HG22	1:B:32:LEU:HD22	1.92	0.50
1:B:243:LEU:CD1	1:B:270:LEU:HD11	2.42	0.50
1:A:321:ASP:HB3	1:A:332:LEU:O	2.12	0.49
1:A:592:ASN:ND2	1:A:676:ASN:HD21	1.87	0.49
1:B:152:ALA:HB3	1:B:167:VAL:HG22	1.95	0.49
1:B:157:LEU:HG	1:B:159:GLY:O	2.13	0.49
1:A:121:THR:CG2	1:A:156:MET:HB2	2.42	0.49
1:A:580:PHE:HA	4:A:1387:HOH:O	2.12	0.49
1:B:243:LEU:HD12	1:B:270:LEU:HD11	1.93	0.49
1:A:291:ARG:HH21	1:A:516:ASP:CG	2.20	0.49
1:A:384:SER:HB3	1:A:389:MET:SD	2.53	0.49
1:A:342:ILE:HG22	1:A:345:VAL:CG2	2.43	0.49
1:A:204:GLU:O	1:A:207:ALA:HB3	2.12	0.49
1:A:595:ASN:HD22	1:A:595:ASN:C	2.20	0.49
1:B:91:LYS:HE3	4:B:1507:HOH:O	2.12	0.49
1:B:366:ILE:HD11	1:B:380:ALA:HB1	1.95	0.49
1:B:387:TYR:CZ	1:B:466:PAQ:H5	2.48	0.49
1:A:511:TYR:HB3	4:A:1311:HOH:O	2.14	0.48
1:B:588:LEU:HB2	1:B:605:ILE:HD11	1.94	0.48
1:A:71:SER:C	1:A:73:THR:H	2.21	0.48
1:A:613:HIS:CE1	1:A:702:GLU:HG3	2.48	0.48
1:B:210:LYS:N	1:B:210:LYS:HD2	2.28	0.48
1:B:229:TYR:CZ	1:B:231:ASP:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLN:HE22	1:B:620:GLN:H	1.59	0.48
1:A:439:LYS:HZ1	1:A:447:ASN:HD21	1.60	0.48
1:B:112:LYS:HG2	1:B:117:PHE:CE2	2.49	0.48
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.96	0.48
1:A:367:VAL:HG13	1:A:525:GLN:O	2.14	0.48
1:B:119:PRO:O	1:B:120:ASN:HB2	2.12	0.48
1:B:99:LEU:HA	1:B:103:GLU:OE1	2.14	0.48
1:A:348:ASN:ND2	1:A:351:GLY:H	2.12	0.48
1:A:716:GLU:HA	1:B:693:ALA:O	2.13	0.48
1:A:119:PRO:O	1:A:120:ASN:HB2	2.14	0.48
1:A:532:LEU:HD11	1:A:683:MET:HE2	1.95	0.48
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.96	0.48
1:B:629:HIS:CD2	1:B:630:ARG:N	2.81	0.48
1:A:209:VAL:CG1	1:A:214:ILE:HB	2.44	0.48
1:B:164:GLU:OE2	1:B:653:LYS:HE2	2.14	0.48
1:A:368:PRO:CG	1:A:634:MET:HE1	2.44	0.47
1:A:515:ILE:HG21	1:A:691:ALA:HB1	1.96	0.47
1:A:389:MET:HE3	1:A:468:TYR:CD2	2.50	0.47
1:A:560:THR:OG1	1:B:624:ASP:OD1	2.24	0.47
1:A:620:GLN:HB3	1:B:563:MET:HG2	1.96	0.47
1:B:76:ASN:OD1	1:B:80:GLN:NE2	2.48	0.47
1:B:262:GLU:O	1:B:263:ASN:HB2	2.14	0.47
1:B:717:THR:HB	1:B:720:LEU:HG	1.97	0.47
1:A:348:ASN:HD22	1:A:348:ASN:C	2.23	0.47
1:B:383:ASP:OD1	1:B:466:PAQ:N3	2.47	0.47
1:A:188:LEU:O	1:A:191:ASP:HB2	2.15	0.47
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.97	0.47
1:B:87:PHE:HA	1:B:318:ILE:O	2.15	0.47
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.78	0.47
1:B:410:ASN:OD1	1:B:424:PRO:HA	2.15	0.47
1:A:485:GLY:HA2	1:A:702:GLU:O	2.15	0.47
1:A:545:ALA:O	1:A:567:GLN:HA	2.15	0.47
1:B:595:ASN:C	1:B:595:ASN:ND2	2.72	0.47
1:A:7:MET:HE2	1:A:59:VAL:HG11	1.97	0.47
1:A:365:MET:HE1	1:A:528:TYR:CE1	2.50	0.47
1:B:95:PRO:CB	1:B:146:VAL:HG21	2.44	0.47
1:A:574:GLN:HG2	1:A:671:ASN:CB	2.44	0.47
1:B:460:ILE:HG12	1:B:469:ILE:HG23	1.96	0.47
1:A:441:GLN:NE2	1:A:445:GLN:O	2.46	0.47
1:A:516:ASP:HB2	1:A:696:TRP:CD1	2.50	0.47
1:B:368:PRO:CB	1:B:621:PHE:CZ	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:HA	1:A:468:TYR:O	2.14	0.46
1:A:595:ASN:ND2	1:A:595:ASN:C	2.71	0.46
1:B:197:ASN:ND2	4:B:1521:HOH:O	2.43	0.46
1:A:14:LEU:HD11	1:A:32:LEU:HD13	1.97	0.46
1:A:40:LYS:HB2	1:A:40:LYS:HE2	1.80	0.46
1:A:402:ALA:HB1	1:A:403:PRO:HD2	1.97	0.46
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.81	0.46
1:A:408:LEU:HD12	1:A:425:ARG:HD2	1.96	0.46
1:A:574:GLN:CG	1:A:671:ASN:HB2	2.45	0.46
1:A:617:LYS:O	1:A:637:GLN:NE2	2.47	0.46
1:A:629:HIS:HD2	4:A:1264:HOH:O	1.98	0.46
1:B:218:LYS:HD3	1:B:218:LYS:N	2.31	0.46
1:A:391:THR:HA	1:A:413:ILE:CD1	2.46	0.46
1:A:551:LYS:O	1:A:562:THR:N	2.41	0.46
1:B:210:LYS:HE2	1:B:214:ILE:O	2.15	0.46
1:B:476:GLU:OE1	4:B:1301:HOH:O	2.21	0.46
1:B:629:HIS:HD2	1:B:630:ARG:N	2.14	0.46
1:B:322:MET:HE2	4:B:1195:HOH:O	2.14	0.46
1:B:24:ASP:O	1:B:28:GLN:N	2.49	0.46
1:B:67:LYS:HD2	1:B:69:TRP:CZ2	2.51	0.45
1:B:253:ASP:O	1:B:292:PRO:HB3	2.16	0.45
1:B:129:LEU:HA	1:B:130:PRO:HD2	1.68	0.45
1:B:67:LYS:HD2	1:B:69:TRP:CE2	2.51	0.45
1:B:110:ILE:HD11	1:B:172:ASN:HA	1.97	0.45
1:B:164:GLU:HG3	1:B:180:ILE:CG1	2.47	0.45
1:B:545:ALA:HB3	1:B:568:TYR:CE2	2.52	0.45
1:B:129:LEU:HD23	1:B:129:LEU:C	2.42	0.45
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.17	0.45
1:B:699:MET:HA	1:B:700:PRO:HD3	1.71	0.45
1:A:326:ARG:NH2	1:B:303:VAL:CG1	2.75	0.45
1:B:469:ILE:O	1:B:484:ALA:HA	2.17	0.45
1:B:679:ALA:HB2	4:B:1380:HOH:O	2.17	0.45
1:B:229:TYR:CE1	1:B:238:GLN:NE2	2.85	0.45
1:B:487:THR:OG1	1:B:699:MET:O	2.29	0.45
1:A:377:TYR:HB2	1:B:559:ARG:HG2	1.98	0.45
1:B:29:LEU:HD12	1:B:42:LYS:HG3	1.98	0.45
1:B:559:ARG:HA	1:B:559:ARG:HD2	1.86	0.45
1:A:222:THR:HB	1:A:245:VAL:CG1	2.46	0.45
1:A:371:ASP:HB3	1:A:376:TRP:HB3	1.98	0.45
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.88	0.45
1:B:225:LEU:CD1	1:B:246:ILE:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ASN:C	1:B:595:ASN:HD22	2.24	0.45
1:A:636:LYS:HB2	1:A:639:TRP:CE2	2.51	0.44
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.81	0.44
1:B:445:GLN:CB	1:B:446:PRO:CD	2.85	0.44
1:B:532:LEU:HD11	1:B:683:MET:HE2	1.98	0.44
1:B:547:ASP:HA	1:B:548:PRO:HD3	1.74	0.44
1:A:434:ALA:HB3	1:A:452:ARG:HG2	2.00	0.44
1:B:9:PRO:HB3	1:B:67:LYS:HD3	1.99	0.44
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.52	0.44
1:A:45:ALA:O	1:A:60:PRO:HB3	2.16	0.44
1:A:563:MET:HE2	1:B:620:GLN:HB2	1.99	0.44
1:A:653:LYS:O	1:A:655:PRO:HD3	2.18	0.44
1:B:38:TYR:N	1:B:51:ASN:HD21	2.08	0.44
1:B:123:PHE:O	1:B:416:TYR:HA	2.17	0.44
1:B:225:LEU:HD12	1:B:246:ILE:HG12	1.99	0.44
1:B:553:ASN:ND2	1:B:555:ALA:H	2.14	0.44
1:A:240:ALA:HB1	1:A:242:LEU:HD21	1.99	0.44
1:B:8:VAL:CG1	1:B:9:PRO:HD2	2.48	0.44
1:A:243:LEU:CD1	1:A:270:LEU:HD11	2.48	0.44
1:A:273:LYS:HD2	4:A:1250:HOH:O	2.17	0.44
1:B:165:ALA:HA	1:B:176:SER:O	2.18	0.44
1:B:437:GLU:HA	1:B:452:ARG:HB2	2.00	0.44
1:B:496:LYS:NZ	4:B:1519:HOH:O	2.41	0.44
1:A:77:ASP:O	1:A:81:SER:HB3	2.18	0.44
1:A:449:SER:O	1:B:400:LYS:HE2	2.18	0.44
1:B:387:TYR:CE1	1:B:466:PAQ:H5	2.52	0.44
1:B:644:HIS:HB2	1:B:647:GLU:CG	2.48	0.44
1:A:388:GLY:HA3	4:A:1137:HOH:O	2.17	0.44
1:A:286:VAL:HA	1:A:287:PRO:HD3	1.78	0.43
1:B:419:VAL:HA	1:B:420:PRO:HD3	1.91	0.43
1:B:574:GLN:CG	1:B:671:ASN:HB2	2.48	0.43
1:A:91:LYS:HG3	4:A:1405:HOH:O	2.18	0.43
1:A:395:PRO:HB3	1:A:424:PRO:O	2.17	0.43
1:A:230:PHE:O	1:A:231:ASP:HB3	2.18	0.43
1:A:382:LEU:HD13	1:A:655:PRO:HB2	2.01	0.43
1:B:578:GLN:OE1	4:B:1483:HOH:O	2.21	0.43
1:A:8:VAL:C	1:A:69:TRP:CE3	2.97	0.43
1:A:130:PRO:HA	1:A:131:PRO:HD3	1.78	0.43
1:A:269:ASP:CG	1:A:272:GLN:HG3	2.44	0.43
1:A:331:HIS:HE1	1:A:333:SER:HB3	1.81	0.43
1:B:7:MET:CE	1:B:71:SER:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ALA:O	1:B:210:LYS:CD	2.66	0.43
1:B:398:ARG:HG3	1:B:408:LEU:HD11	2.01	0.43
1:A:620:GLN:HB2	1:B:563:MET:HE2	2.00	0.43
1:A:14:LEU:CD1	1:A:32:LEU:HD22	2.49	0.43
1:A:214:ILE:HD11	1:A:261:ILE:CG1	2.46	0.43
1:A:619:ALA:C	1:A:621:PHE:H	2.27	0.43
1:B:723:LEU:HG	1:B:725:LYS:HG3	2.01	0.43
1:A:308:ILE:O	1:A:405:ASN:HB3	2.19	0.43
1:A:324:HIS:CD2	1:A:329:ASP:OD1	2.72	0.42
1:A:593:LYS:O	1:A:600:PRO:HA	2.18	0.42
1:A:699:MET:HB3	4:A:1421:HOH:O	2.18	0.42
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.85	0.42
1:B:194:SER:O	1:B:198:ILE:HG13	2.19	0.42
1:B:210:LYS:HE3	1:B:217:ALA:CB	2.18	0.42
1:B:619:ALA:HB1	1:B:621:PHE:CD2	2.55	0.42
1:B:627:ILE:CD1	1:B:631:LEU:HD12	2.49	0.42
1:A:437:GLU:HA	1:A:452:ARG:HB2	2.02	0.42
1:A:500:MET:HG3	1:B:599:ASN:ND2	2.34	0.42
1:B:337:ARG:HD3	1:B:649:PHE:CE1	2.54	0.42
1:A:131:PRO:HA	4:A:1245:HOH:O	2.19	0.42
1:A:366:ILE:CG2	1:A:527:ILE:HB	2.47	0.42
1:A:391:THR:HA	1:A:413:ILE:HD11	2.01	0.42
1:B:692:ARG:HG3	1:B:694:GLU:OE1	2.19	0.42
1:A:366:ILE:HG13	1:A:368:PRO:HG3	2.02	0.42
1:A:241:ARG:HB2	4:A:1317:HOH:O	2.19	0.42
1:A:640:VAL:HA	1:A:680:VAL:O	2.20	0.42
1:B:260:PRO:HD2	1:B:287:PRO:HD2	2.01	0.42
1:B:595:ASN:ND2	1:B:597:MET:H	2.17	0.42
1:B:665:GLY:HA2	4:B:1441:HOH:O	2.19	0.42
1:A:529:ASN:HA	1:A:683:MET:O	2.20	0.42
1:A:611:GLY:HA2	1:A:703:TRP:O	2.20	0.42
1:B:366:ILE:HD11	1:B:627:ILE:HD11	2.01	0.42
1:B:516:ASP:HB3	1:B:519:ILE:HB	2.01	0.42
1:B:525:GLN:NE2	1:B:620:GLN:H	2.18	0.42
1:A:207:ALA:O	1:A:210:LYS:HB3	2.20	0.42
1:A:216:ASP:HB3	1:A:219:LYS:CD	2.43	0.42
1:B:629:HIS:HD2	1:B:630:ARG:HA	1.85	0.42
1:B:272:GLN:HB3	1:B:274:LYS:HG2	2.02	0.41
1:B:644:HIS:HD2	1:B:647:GLU:CD	2.27	0.41
1:A:531:ARG:HD2	1:A:682:TRP:CH2	2.55	0.41
1:B:45:ALA:O	1:B:60:PRO:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:THR:HA	1:B:413:ILE:HD11	2.02	0.41
1:A:326:ARG:NH2	1:B:303:VAL:HG13	2.34	0.41
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.66	0.41
1:B:230:PHE:HB3	1:B:233:LYS:HB2	2.02	0.41
1:B:238:GLN:NE2	1:B:238:GLN:HA	2.35	0.41
1:B:249:LEU:O	1:B:259:HIS:HB2	2.19	0.41
1:B:546:MET:HE2	1:B:567:GLN:NE2	2.36	0.41
1:B:644:HIS:CD2	4:B:1279:HOH:O	2.73	0.41
1:A:445:GLN:HB3	1:A:446:PRO:HD2	2.02	0.41
1:A:465:ASN:HB2	1:A:489:ILE:O	2.21	0.41
1:B:229:TYR:HD1	1:B:238:GLN:HE22	1.67	0.41
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.55	0.41
1:B:477:ASN:C	1:B:477:ASN:ND2	2.77	0.41
1:A:574:GLN:H	1:A:671:ASN:HD22	1.68	0.41
1:B:104:ILE:HB	1:B:420:PRO:HG3	2.01	0.41
1:B:339:GLY:HA3	1:B:340:PRO:HD2	1.87	0.41
1:A:108:VAL:HG12	1:A:112:LYS:HD2	2.03	0.41
1:B:139:PHE:CD1	1:B:139:PHE:C	2.98	0.41
1:A:200:ASN:HD22	1:A:200:ASN:HA	1.63	0.41
1:B:75:ILE:O	1:B:79:PHE:HB2	2.20	0.41
1:B:141:LEU:HD21	1:B:346:THR:HG21	2.02	0.41
1:B:163:ILE:HG21	1:B:177:TRP:CE2	2.56	0.41
1:A:191:ASP:O	1:A:195:VAL:HG23	2.20	0.41
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.36	0.41
1:A:365:MET:HB2	1:A:365:MET:HE3	1.55	0.41
1:B:8:VAL:HG12	1:B:9:PRO:HD2	2.02	0.41
1:B:189:LEU:HD22	1:B:189:LEU:C	2.46	0.41
1:B:269:ASP:HB2	1:B:276:VAL:CG1	2.43	0.41
1:B:366:ILE:HG12	1:B:367:VAL:N	2.35	0.41
1:B:572:ASN:CB	1:B:672:GLU:O	2.69	0.41
1:B:723:LEU:HD11	1:B:725:LYS:CD	2.49	0.41
1:A:130:PRO:C	1:A:131:PRO:O	2.60	0.41
1:A:720:LEU:HD11	1:B:697:PRO:HG2	2.03	0.41
1:B:545:ALA:HB2	1:B:570:ILE:HD11	2.02	0.41
1:A:401:ASP:OD1	1:B:449:SER:OG	2.33	0.40
1:A:699:MET:HA	1:A:700:PRO:HD3	1.94	0.40
1:B:627:ILE:HG23	1:B:628:TYR:N	2.36	0.40
1:B:412:THR:HA	1:B:421:MET:O	2.21	0.40
1:A:114:SER:HB2	1:A:174:LEU:HD22	2.02	0.40
1:A:583:GLY:N	1:B:615:VAL:HG12	2.36	0.40
1:B:300:ALA:HA	1:B:301:PRO:HD2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ASP:HB3	1:B:584:THR:CG2	2.50	0.40
1:A:197:ASN:HD22	1:A:197:ASN:HA	1.58	0.40
1:A:210:LYS:HE3	1:A:210:LYS:HA	2.03	0.40
1:A:627:ILE:HD12	1:A:627:ILE:HA	1.80	0.40
1:B:46:GLN:NE2	4:B:1505:HOH:O	2.54	0.40
1:B:184:HIS:HB2	1:B:656:ASN:O	2.22	0.40
1:B:619:ALA:HB2	1:B:634:MET:HB3	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	715/727 (98%)	684 (96%)	31 (4%)	0	100	100
1	B	717/727 (99%)	691 (96%)	26 (4%)	0	100	100
All	All	1432/1454 (98%)	1375 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/615 (99%)	579 (95%)	30 (5%)	22	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	611/615 (99%)	570 (93%)	41 (7%)	15	11
All	All	1220/1230 (99%)	1149 (94%)	71 (6%)	18	15

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	11	ASP
1	A	22	GLN
1	A	40	LYS
1	A	64	LYS
1	A	80	GLN
1	A	89	VAL
1	A	128	LEU
1	A	132	ASP
1	A	151	LYS
1	A	156	MET
1	A	199	ILE
1	A	201	ASN
1	A	210	LYS
1	A	215	THR
1	A	239	ASP
1	A	348	ASN
1	A	362	LEU
1	A	365	MET
1	A	377	TYR
1	A	477	ASN
1	A	496	LYS
1	A	506	LYS
1	A	532	LEU
1	A	595	ASN
1	A	613	HIS
1	A	636	LYS
1	A	638	LEU
1	A	669	LYS
1	A	723	LEU
1	B	7	MET
1	B	11	ASP
1	B	15	LYS
1	B	66	ASN
1	B	67	LYS
1	B	91	LYS

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Mol	Chain	Res	Type
1	B	92	ARG
1	B	129	LEU
1	B	132	ASP
1	B	143	ASN
1	B	144	LYS
1	B	156	MET
1	B	167	VAL
1	B	173	LYS
1	B	189	LEU
1	B	203	GLU
1	B	209	VAL
1	B	210	LYS
1	B	233	LYS
1	B	237	LYS
1	B	271	GLU
1	B	291	ARG
1	B	322	MET
1	B	342	ILE
1	B	469	ILE
1	B	477	ASN
1	B	551	LYS
1	B	559	ARG
1	B	565	VAL
1	B	566	ASN
1	B	572	ASN
1	B	595	ASN
1	B	599	ASN
1	B	613	HIS
1	B	620	GLN
1	B	629	HIS
1	B	635	ASP
1	B	636	LYS
1	B	648	ARG
1	B	669	LYS
1	B	692	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	97	ASN
1	A	120	ASN

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	196	GLN
1	A	197	ASN
1	A	200	ASN
1	A	201	ASN
1	A	263	ASN
1	A	272	GLN
1	A	324	HIS
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	540	ASN
1	A	541	ASN
1	A	553	ASN
1	A	567	GLN
1	A	595	ASN
1	A	599	ASN
1	A	604	GLN
1	A	656	ASN
1	A	671	ASN
1	A	676	ASN
1	B	46	GLN
1	B	51	ASN
1	B	53	GLN
1	B	66	ASN
1	B	76	ASN
1	B	80	GLN
1	B	94	HIS
1	B	143	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	315	ASN
1	B	327	ASN
1	B	350	ASN

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Mol	Chain	Res	Type
1	B	477	ASN
1	B	501	HIS
1	B	525	GLN
1	B	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	564	GLN
1	B	567	GLN
1	B	572	ASN
1	B	592	ASN
1	B	595	ASN
1	B	599	ASN
1	B	620	GLN
1	B	629	HIS
1	B	637	GLN
1	B	644	HIS
1	B	656	ASN
1	B	671	ASN
1	B	676	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PAQ	B	466	1	19,22,23	2.59	7 (36%)	18,29,31	2.78	3 (16%)
1	PAQ	A	466	1	19,22,23	2.52	6 (31%)	18,29,31	2.76	6 (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	PAQ	B	466	1	1/1/5/10	2/8/27/29	0/2/2/2
1	PAQ	A	466	1	1/1/5/10	3/8/27/29	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	PAQ	CG-CD2	-5.51	1.40	1.50
1	B	466	PAQ	CG-CD2	-5.40	1.40	1.50
1	A	466	PAQ	CE2-N1	-5.14	1.19	1.33
1	B	466	PAQ	CE2-N1	-5.07	1.19	1.33
1	B	466	PAQ	C3-C2	-4.80	1.30	1.38
1	A	466	PAQ	C3-C2	-4.50	1.31	1.38
1	A	466	PAQ	CE1-CD1	-3.49	1.39	1.46
1	B	466	PAQ	CB-CG	-3.27	1.50	1.54
1	B	466	PAQ	OH-CZ	-3.10	1.25	1.33
1	B	466	PAQ	CE1-CD1	-2.75	1.41	1.46
1	A	466	PAQ	CB-CG	-2.72	1.51	1.54
1	B	466	PAQ	CE1-CZ	2.19	1.40	1.36
1	A	466	PAQ	CE1-CZ	2.13	1.39	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	PAQ	CB-CG-CD1	9.00	123.70	111.13
1	A	466	PAQ	CB-CA-C	-6.30	101.29	110.99
1	A	466	PAQ	CD2-CG-CD1	6.20	118.87	104.64
1	B	466	PAQ	CD2-CG-CD1	5.74	117.81	104.64
1	A	466	PAQ	CB-CG-CD1	5.20	118.40	111.13
1	A	466	PAQ	O2-CD1-CE1	-3.16	116.22	121.46
1	A	466	PAQ	CB-CA-N	2.99	117.02	110.48
1	B	466	PAQ	CB-CA-C	-2.90	106.52	110.99
1	A	466	PAQ	CE2-N1-N2	-2.04	116.45	121.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	466	PAQ	CG
1	B	466	PAQ	CG

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	PAQ	N-CA-CB-CG
1	A	466	PAQ	CE2-N1-N2-C1
1	B	466	PAQ	CE2-N1-N2-C1
1	A	466	PAQ	CA-CB-CG-CD2
1	B	466	PAQ	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	PAQ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	717/727 (98%)	-0.30	10 (1%) 73 73	8, 21, 53, 82	0
1	B	719/727 (98%)	-0.19	21 (2%) 53 52	11, 24, 60, 99	0
All	All	1436/1454 (98%)	-0.25	31 (2%) 62 61	8, 23, 58, 99	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	725	LYS	4.0
1	B	644	HIS	3.7
1	A	217	ALA	3.5
1	B	628	TYR	3.4
1	A	66	ASN	3.4
1	B	301	PRO	3.4
1	B	629	HIS	3.3
1	B	65	ASP	3.3
1	A	148	GLN	3.0
1	B	143	ASN	2.9
1	B	6	HIS	2.9
1	B	146	VAL	2.9
1	B	147	ASP	2.9
1	B	302	ALA	2.9
1	A	130	PRO	2.7
1	A	239	ASP	2.5
1	B	215	THR	2.5
1	B	148	GLN	2.4
1	B	178	GLN	2.3
1	B	233	LYS	2.3
1	A	644	HIS	2.3
1	B	92	ARG	2.3
1	A	213	GLY	2.3
1	B	66	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	67	LYS	2.2
1	A	132	ASP	2.2
1	B	239	ASP	2.2
1	B	8	VAL	2.1
1	A	617	LYS	2.1
1	B	11	ASP	2.0
1	B	211	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PAQ	A	466	21/22	0.95	0.08	9,23,34,38	0
1	PAQ	B	466	21/22	0.95	0.07	10,29,33,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	B	802	1/1	0.59	0.25	71,71,71,71	0
3	CA	A	802	1/1	0.94	0.09	56,56,56,56	0
3	CA	A	801	1/1	0.99	0.02	19,19,19,19	0
2	CU	A	800	1/1	0.99	0.02	25,25,25,25	0
2	CU	B	800	1/1	0.99	0.01	20,20,20,20	0
3	CA	B	801	1/1	1.00	0.01	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.