



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2017 – 11:16 PM EST

PDB ID : 5N4L  
Title : Rat ceruloplasmin trigonal form  
Authors : Samygina, V.R.; Sokolov, A.V.; Bourenkov, G.; Vasilyev, V.B.  
Deposited on : unknown  
Resolution : 3.20 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

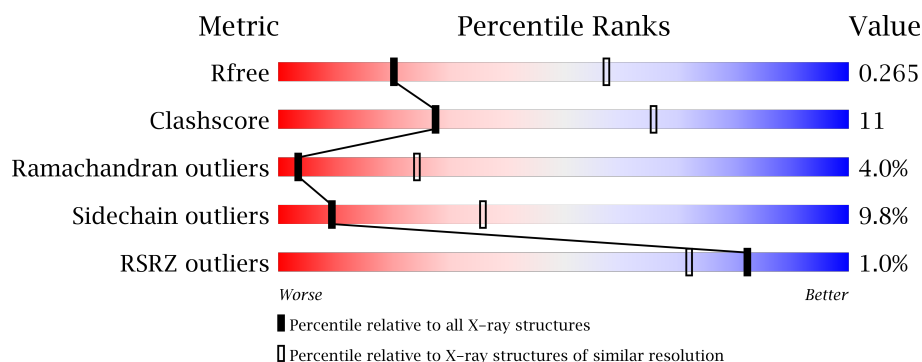
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	1034	<div> <div></div> <div>65%</div> <div>30%</div> <div>5%</div> </div>
1	B	1034	<div> <div></div> <div>66%</div> <div>28%</div> <div>5%</div> </div>

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
2	CU	B	1102	-	-	X	-
4	NA	A	1107	-	-	-	X
4	NA	B	1108	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16660 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 Ceruloplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1034	Total	C	N	O	S	0	0	0
			8312	5284	1387	1600	41			
1	B	1034	Total	C	N	O	S	0	0	0
			8312	5284	1387	1600	41			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Cu	0	0
			6	6		
2	A	5	Total	Cu	0	0
			5	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

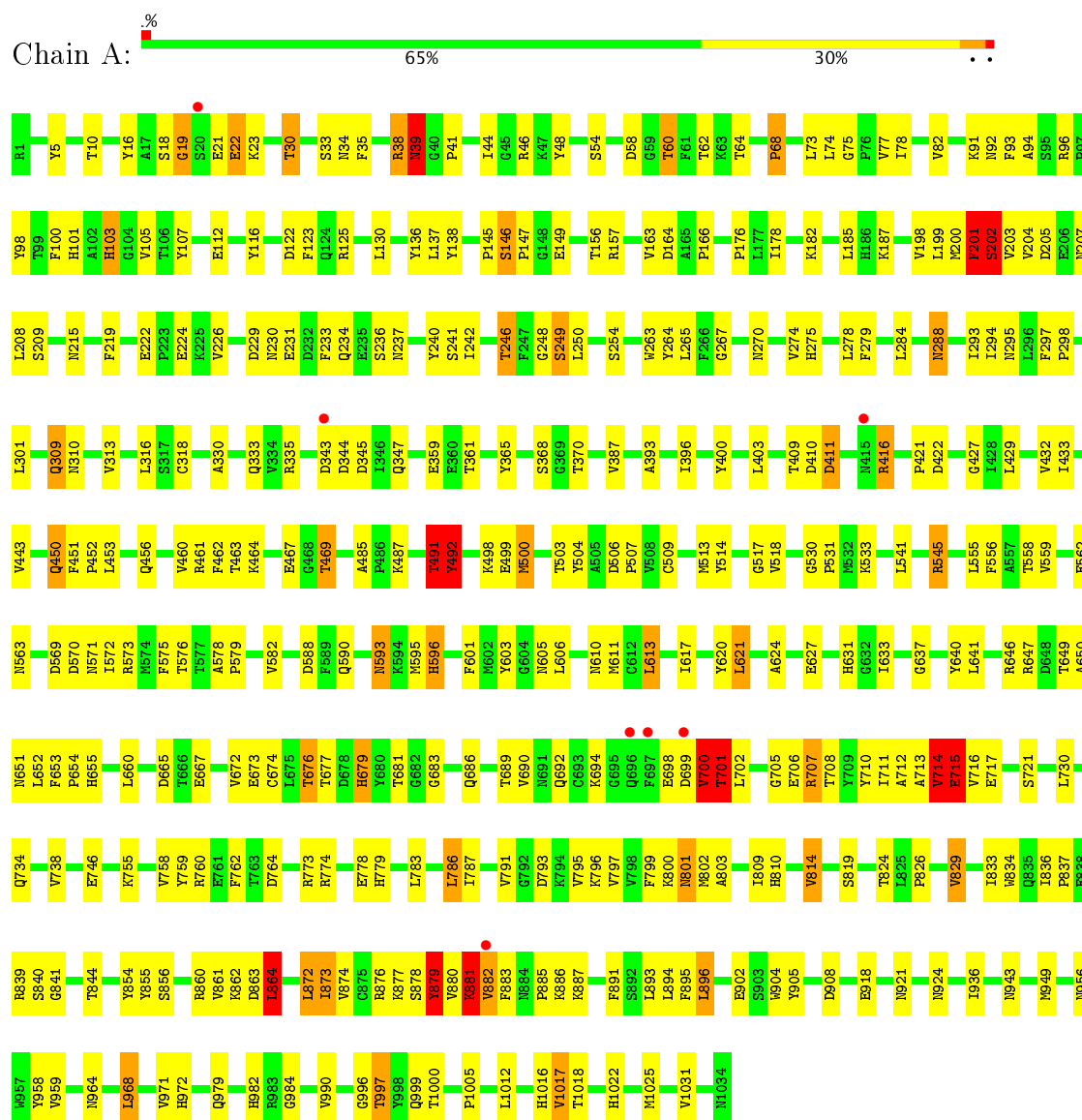
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	11	Total 11	O 11	0	0

### 3 Residue-property plots

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



#### • Molecule 1: Ceruloplasmin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.23Å 128.23Å 407.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.99 – 3.20 14.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (14.99-3.20) 99.4 (14.99-3.20)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.193 , 0.265 0.201 , 0.265	Depositor DCC
$R_{free}$ test set	3198 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	118.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 87.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.83	5/8536 (0.1%)	1.00	13/11570 (0.1%)
1	B	0.83	4/8536 (0.0%)	1.01	20/11570 (0.2%)
All	All	0.83	9/17072 (0.1%)	1.00	33/23140 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	13
All	All	0	23

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	705	GLY	N-CA	6.89	1.56	1.46
1	B	706	GLU	N-CA	6.34	1.59	1.46
1	A	904	TRP	CB-CG	-5.68	1.40	1.50
1	B	1016	HIS	N-CA	5.08	1.56	1.46
1	B	701	THR	N-CA	5.07	1.56	1.46
1	A	879	TYR	CB-CG	5.07	1.59	1.51
1	A	701	THR	N-CA	5.03	1.56	1.46
1	A	706	GLU	N-CA	5.03	1.56	1.46
1	A	16	TYR	CE1-CZ	5.01	1.45	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	B	702	LEU	N-CA-C	7.10	130.17	111.00
1	A	202	SER	N-CA-C	6.30	128.01	111.00
1	B	125	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	491	THR	C-N-CA	6.08	136.90	121.70
1	A	361	THR	N-CA-CB	5.83	121.39	110.30
1	A	492	TYR	N-CA-CB	5.77	120.98	110.60
1	B	646	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	573	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	760	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	714	VAL	C-N-CA	5.66	135.84	121.70
1	A	968	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	19	GLY	N-CA-C	5.64	127.20	113.10
1	B	201	PHE	CA-C-N	5.61	129.54	117.20
1	B	701	THR	N-CA-C	5.59	126.11	111.00
1	A	802	MET	CG-SD-CE	5.57	109.11	100.20
1	B	127	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	760	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	96	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	715	GLU	N-CA-C	-5.41	96.40	111.00
1	B	269	GLY	N-CA-C	5.38	126.56	113.10
1	A	864	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	201	PHE	O-C-N	-5.24	114.31	122.70
1	B	333	GLN	CB-CA-C	5.22	120.83	110.40
1	A	491	THR	C-N-CA	5.15	134.58	121.70
1	B	935	ALA	N-CA-C	5.14	124.87	111.00
1	A	701	THR	N-CA-C	5.11	124.81	111.00
1	A	96	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	238	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	38	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	573	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	702	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	364	ASP	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	PRO	Peptide
1	A	19	GLY	Peptide
1	A	201	PHE	Peptide
1	A	202	SER	Peptide
1	A	343	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	39	ASN	Peptide
1	A	491	THR	Peptide
1	A	714	VAL	Peptide
1	A	879	TYR	Peptide
1	A	881	LYS	Peptide
1	B	1014	HIS	Peptide
1	B	145	PRO	Peptide
1	B	19	GLY	Peptide
1	B	20	SER	Peptide
1	B	201	PHE	Peptide
1	B	223	PRO	Peptide
1	B	332	PHE	Peptide
1	B	38	ARG	Peptide
1	B	714	VAL	Peptide
1	B	847	SER	Peptide
1	B	879	TYR	Peptide
1	B	880	VAL	Peptide
1	B	881	LYS	Peptide

## 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	8312	0	7919	190	0
1	B	8312	0	7920	179	0
2	A	5	0	0	0	0
2	B	6	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	1	0
5	B	11	0	0	1	0
All	All	16660	0	15839	368	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 11.

All (368) 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:A:674:CYS:SG	1:A:676:THR:OG1	2.26	0.92
1:B:318:CYS:HG	2:B:1102:CU:CU	0.75	0.91
1:B:129:LYS:NZ	1:B:733:LEU:O	2.12	0.79
1:A:674:CYS:SG	1:A:679:HIS:CD2	2.76	0.77
1:A:58:ASP:HB2	1:A:60:THR:OG1	1.87	0.75
1:A:403:LEU:HD23	1:A:453:LEU:HD11	1.70	0.74
1:B:908:ASP:O	1:B:912:THR:OG1	2.04	0.74
1:B:111:ASN:ND2	1:B:139:VAL:HG23	2.02	0.72
1:B:503:THR:HG22	1:B:506:ASP:OD2	1.92	0.70
1:A:878:SER:OG	1:A:879:TYR:N	2.23	0.69
1:A:801:ASN:HD21	1:A:803:ALA:HB3	1.59	0.68
1:B:131:PHE:HB2	1:B:134:GLN:HE21	1.59	0.68
1:A:156:THR:HG22	1:A:264:TYR:HB3	1.76	0.68
1:A:265:LEU:HD22	1:A:294:ILE:HG21	1.75	0.68
1:A:503:THR:HG22	1:A:506:ASP:OD2	1.94	0.67
1:A:246:THR:O	1:A:249:SER:OG	2.13	0.67
1:B:695:GLY:HA3	1:B:696:GLN:HB2	1.75	0.67
1:B:156:THR:HG22	1:B:264:TYR:HB3	1.76	0.67
1:A:640:TYR:CE2	1:A:660:LEU:HD22	2.29	0.67
1:B:21:GLU:HB3	1:B:22:GLU:HA	1.78	0.66
1:A:344:ASP:HA	1:A:345:ASP:CB	2.24	0.66
1:B:724:ARG:O	1:B:726:TRP:N	2.30	0.65
1:A:921:ASN:HB3	1:A:924:ASN:HB2	1.79	0.65
1:B:715:GLU:H	1:B:757:VAL:HA	1.62	0.65
1:B:106:THR:HG22	1:B:144:GLU:OE2	1.99	0.63
1:A:344:ASP:HA	1:A:345:ASP:HB3	1.80	0.63
1:B:116:TYR:O	1:B:125:ARG:NH2	2.31	0.63
1:B:640:TYR:CE2	1:B:660:LEU:HD22	2.33	0.62
1:B:485:ALA:HB3	1:B:488:GLU:HG3	1.81	0.62
1:A:309:GLN:HA	1:A:309:GLN:HE21	1.64	0.62
1:B:344:ASP:HA	1:B:345:ASP:CB	2.29	0.62
1:B:317:SER:OG	1:B:319:GLN:NE2	2.33	0.62
1:A:368:SER:OG	1:A:605:ASN:ND2	2.32	0.62
1:A:674:CYS:SG	1:A:679:HIS:HD2	2.23	0.61
1:B:58:ASP:HB2	1:B:60:THR:OG1	2.00	0.61
1:A:646:ARG:HD2	1:A:841:GLY:O	2.01	0.61
1:A:801:ASN:ND2	1:A:803:ALA:HB3	2.15	0.61
1:B:200:MET:HG2	1:B:202:SER:HB2	1.82	0.61
1:B:646:ARG:HD2	1:B:841:GLY:O	2.01	0.60
1:B:1033:PRO:O	1:B:1034:ASN:HB2	2.01	0.60
1:A:572:ILE:HG23	1:A:582:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ARG:HG3	5:A:1207:HOH:O	2.02	0.60
1:B:791:VAL:HG13	1:B:837:PRO:O	2.02	0.60
1:A:795:VAL:HG23	1:A:836:ILE:HD11	1.84	0.59
1:B:718:TRP:HB3	1:B:756:LYS:HG3	1.83	0.59
1:B:278:LEU:HD23	1:B:279:PHE:N	2.17	0.59
1:A:267:GLY:HA3	1:A:297:PHE:O	2.02	0.59
1:A:710:TYR:HB2	1:A:762:PHE:O	2.02	0.59
1:B:701:THR:HG22	1:B:702:LEU:CD2	2.33	0.58
1:B:116:TYR:CE2	1:B:1012:LEU:HB2	2.38	0.58
1:B:711:ILE:HD11	1:B:785:PRO:HD2	1.85	0.58
1:A:611:MET:HB2	1:A:617:ILE:HD11	1.86	0.58
1:A:77:VAL:HG22	1:A:176:PRO:HG2	1.85	0.58
1:A:38:ARG:HA	1:A:39:ASN:CB	2.33	0.58
1:A:555:LEU:HB2	1:A:621:LEU:HD22	1.84	0.58
1:A:677:THR:HG23	1:A:861:VAL:HG11	1.84	0.57
1:B:310:ASN:HD22	1:B:461:ARG:HD2	1.70	0.57
1:B:677:THR:HG23	1:B:861:VAL:CG1	2.34	0.57
1:B:719:ASP:O	1:B:722:PRO:HD3	2.04	0.57
1:A:559:VAL:HG13	1:A:596:HIS:CD2	2.39	0.57
1:B:514:TYR:CZ	1:B:530:GLY:HA3	2.39	0.57
1:A:38:ARG:HA	1:A:39:ASN:HB2	1.86	0.57
1:A:716:VAL:HG22	1:A:717:GLU:N	2.20	0.57
1:A:203:VAL:HG12	1:A:203:VAL:O	2.05	0.57
1:A:631:HIS:ND1	1:A:679:HIS:CD2	2.73	0.57
1:A:130:LEU:HD21	1:A:136:TYR:HB2	1.86	0.57
1:A:226:VAL:HG13	1:A:226:VAL:O	2.05	0.56
1:B:496:VAL:HG12	1:B:496:VAL:O	2.06	0.56
1:A:164:ASP:OD1	1:A:166:PRO:HD2	2.05	0.56
1:B:757:VAL:HG21	1:B:807:TYR:CE2	2.40	0.56
1:B:862:LYS:O	1:B:866:SER:OG	2.19	0.56
1:A:248:GLY:HA2	1:A:330:ALA:HA	1.87	0.56
1:A:712:ALA:HB3	1:A:762:PHE:CE1	2.41	0.56
1:B:649:THR:HG21	1:B:996:GLY:HA3	1.87	0.56
1:A:711:ILE:HD11	1:A:787:ILE:HD11	1.87	0.56
1:A:699:ASP:O	1:A:701:THR:N	2.39	0.55
1:B:1011:TRP:O	1:B:1028:THR:HB	2.06	0.55
1:A:396:ILE:HG23	1:A:575:PHE:HB2	1.88	0.55
1:A:714:VAL:HA	1:A:715:GLU:HB2	1.88	0.55
1:A:787:ILE:CG2	1:A:872:LEU:HD12	2.36	0.55
1:B:110:ALA:O	1:B:127:ASP:HB3	2.05	0.55
1:B:647:ARG:NH1	1:B:999:GLN:HE22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:HIS:NE2	1:B:292:ASP:OD2	2.39	0.55
1:A:30:THR:O	1:A:34:ASN:ND2	2.41	0.54
1:A:288:ASN:O	1:A:503:THR:HG21	2.08	0.54
1:A:881:LYS:HE3	1:A:882:VAL:HG13	1.89	0.54
1:A:491:THR:HA	1:A:492:TYR:HB2	1.89	0.54
1:A:541:LEU:HD12	1:A:545:ARG:HB2	1.89	0.54
1:B:117:PRO:HD2	1:B:726:TRP:CZ2	2.42	0.54
1:A:673:GLU:OE2	1:A:860:ARG:NE	2.40	0.54
1:A:755:LYS:HG2	1:A:905:TYR:HD1	1.73	0.54
1:B:634:TYR:HB2	1:B:649:THR:HG23	1.89	0.54
1:B:833:ILE:O	1:B:833:ILE:HG22	2.07	0.54
1:A:603:TYR:CE1	1:A:683:GLY:HA3	2.42	0.54
1:B:309:GLN:HE21	1:B:309:GLN:HA	1.73	0.54
1:A:432:VAL:HG22	1:A:531:PRO:HG2	1.90	0.54
1:B:676:THR:O	1:B:677:THR:C	2.46	0.54
1:A:400:TYR:CD2	1:A:562:GLU:HG3	2.43	0.54
1:B:677:THR:HG23	1:B:861:VAL:HG11	1.89	0.54
1:B:111:ASN:HD21	1:B:139:VAL:HG23	1.70	0.53
1:B:344:ASP:HA	1:B:345:ASP:HB2	1.89	0.53
1:A:631:HIS:CE1	1:A:679:HIS:CD2	2.96	0.53
1:A:759:TYR:CE1	1:A:809:ILE:HD12	2.43	0.53
1:B:318:CYS:SG	2:B:1102:CU:CU	1.88	0.53
1:B:724:ARG:O	1:B:727:GLU:N	2.40	0.53
1:B:1033:PRO:O	1:B:1034:ASN:CB	2.56	0.53
1:A:365:TYR:CE2	1:A:595:MET:HG3	2.44	0.53
1:B:432:VAL:HG22	1:B:531:PRO:HG2	1.91	0.53
1:B:606:LEU:HD23	1:B:686:GLN:HG3	1.90	0.53
1:A:365:TYR:CD2	1:A:595:MET:HG3	2.42	0.53
1:B:14:TRP:HB3	1:B:50:LYS:HG3	1.90	0.53
1:B:313:VAL:O	1:B:464:LYS:HE2	2.08	0.52
1:A:810:HIS:O	1:A:854:TYR:HA	2.10	0.52
1:B:757:VAL:HG21	1:B:807:TYR:CD2	2.45	0.52
1:A:201:PHE:O	1:A:275:HIS:NE2	2.42	0.52
1:A:278:LEU:HD23	1:A:279:PHE:N	2.24	0.52
1:A:840:SER:O	1:A:874:VAL:HG11	2.10	0.52
1:A:103:HIS:CE1	1:A:972:HIS:CE1	2.97	0.52
1:B:748:PHE:CD1	1:B:919:LYS:O	2.63	0.52
1:A:708:THR:HG22	1:A:796:LYS:HD2	1.92	0.52
1:B:422:ASP:O	1:B:425:HIS:ND1	2.41	0.52
1:A:879:TYR:HB3	1:A:881:LYS:N	2.25	0.52
1:B:299:ALA:HB2	1:B:1016:HIS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:THR:CG2	1:B:1032:LEU:HD12	2.40	0.52
1:A:433:ILE:HD12	1:A:514:TYR:CD2	2.44	0.51
1:A:677:THR:HG23	1:A:861:VAL:CG1	2.41	0.51
1:B:796:LYS:HA	1:B:832:TYR:O	2.10	0.51
1:B:117:PRO:HD2	1:B:726:TRP:CE2	2.45	0.51
1:A:48:TYR:HB3	1:A:215:ASN:ND2	2.26	0.51
1:A:156:THR:HG22	1:A:264:TYR:CB	2.40	0.51
1:A:864:LEU:HD11	1:A:896:LEU:HD11	1.92	0.51
1:B:677:THR:HG1	1:B:865:TYR:HE2	1.59	0.51
1:A:631:HIS:HD1	1:A:679:HIS:HD2	1.57	0.51
1:B:146:SER:HB3	1:B:147:PRO:HD3	1.93	0.51
1:B:618:VAL:HG22	1:B:661:LEU:HD23	1.93	0.50
1:B:110:ALA:HB2	1:B:124:GLN:HA	1.93	0.50
1:B:491:THR:HA	1:B:492:TYR:HB2	1.92	0.50
1:B:647:ARG:HH12	1:B:999:GLN:HE22	1.60	0.50
1:B:297:PHE:HB3	1:B:298:PRO:CD	2.42	0.50
1:B:403:LEU:HD23	1:B:453:LEU:HD11	1.93	0.50
1:B:864:LEU:HD11	1:B:896:LEU:HD11	1.92	0.50
1:A:198:VAL:O	1:A:199:LEU:HD23	2.11	0.50
1:B:814:VAL:HG23	1:B:872:LEU:HD21	1.93	0.50
1:B:515:TYR:CG	1:B:524:ILE:HD11	2.47	0.50
1:A:298:PRO:HG2	1:A:1017:VAL:HG12	1.94	0.50
1:B:1008:PRO:HA	1:B:1031:VAL:HG12	1.94	0.50
1:A:613:LEU:HD11	1:A:665:ASP:O	2.12	0.49
1:B:873:ILE:HD12	1:B:958:TYR:CD1	2.47	0.49
1:B:676:THR:HG22	1:B:995:PRO:HG2	1.93	0.49
1:A:359:GLU:OE1	1:A:416:ARG:NH2	2.45	0.49
1:A:621:LEU:HB3	1:A:652:LEU:HD11	1.94	0.49
1:B:299:ALA:HB2	1:B:1016:HIS:CD2	2.45	0.49
1:A:146:SER:HB3	1:A:147:PRO:HD3	1.95	0.49
1:A:297:PHE:N	1:A:297:PHE:CD1	2.80	0.49
1:B:572:ILE:CG2	1:B:582:VAL:HG21	2.42	0.49
1:A:469:THR:HG23	1:A:517:GLY:O	2.13	0.49
1:B:555:LEU:HB2	1:B:621:LEU:HD22	1.95	0.49
1:B:891:PHE:CE2	1:B:949:MET:HE1	2.47	0.49
1:A:611:MET:O	1:A:690:VAL:HA	2.13	0.49
1:A:610:ASN:OD1	1:A:689:THR:HB	2.13	0.49
1:B:756:LYS:HD3	1:B:782:ILE:HD11	1.94	0.49
1:A:48:TYR:HB3	1:A:215:ASN:HD21	1.77	0.49
1:A:98:TYR:O	1:A:130:LEU:HB2	2.12	0.49
1:A:201:PHE:O	1:A:275:HIS:CD2	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:HG2	1:B:185:LEU:HD22	1.95	0.48
1:B:783:LEU:HD11	1:B:937:ASN:OD1	2.12	0.48
1:A:60:THR:HB	1:A:62:THR:HG23	1.95	0.48
1:A:640:TYR:CD2	1:A:660:LEU:HD22	2.48	0.48
1:A:230:ASN:O	1:A:233:PHE:N	2.46	0.48
1:A:556:PHE:CE2	1:A:558:THR:HG21	2.47	0.48
1:B:396:ILE:HG23	1:B:575:PHE:HB2	1.94	0.48
1:A:265:LEU:N	1:A:265:LEU:HD12	2.28	0.48
1:A:971:VAL:O	1:A:990:VAL:HA	2.13	0.48
1:B:226:VAL:O	1:B:226:VAL:HG13	2.14	0.48
1:A:116:TYR:CZ	1:A:1012:LEU:HB2	2.48	0.48
1:A:207:ASN:ND2	1:A:237:ASN:HB2	2.28	0.48
1:A:541:LEU:HD12	1:A:545:ARG:CB	2.44	0.48
1:A:880:VAL:O	1:A:881:LYS:O	2.32	0.48
1:B:750:ILE:HG23	1:B:913:TYR:HB2	1.95	0.48
1:B:92:ASN:HD21	1:B:94:ALA:HB3	1.79	0.48
1:B:717:GLU:OE1	1:B:913:TYR:OH	2.29	0.48
1:B:878:SER:O	1:B:879:TYR:HB2	2.12	0.48
1:B:937:ASN:HD22	1:B:944:LEU:HD21	1.79	0.48
1:B:757:VAL:O	1:B:868:LEU:HG	2.11	0.48
1:B:71:LEU:CD2	1:B:74:LEU:HB2	2.44	0.48
1:A:464:LYS:NZ	1:A:467:GLU:OE1	2.47	0.47
1:A:563:ASN:HD21	1:A:590:GLN:CA	2.28	0.47
1:B:266:PHE:C	1:B:296:LEU:HD13	2.35	0.47
1:B:71:LEU:HD23	1:B:74:LEU:HB2	1.96	0.47
1:A:30:THR:HA	1:A:33:SER:HB3	1.95	0.47
1:A:949:MET:CG	1:A:1031:VAL:HG22	2.44	0.47
1:B:631:HIS:HB2	1:B:652:LEU:HB2	1.95	0.47
1:B:745:LYS:O	1:B:749:PHE:HB2	2.13	0.47
1:A:166:PRO:HB3	1:A:1018:THR:HG23	1.96	0.47
1:B:425:HIS:HA	1:B:607:PRO:O	2.15	0.47
1:B:649:THR:HG21	1:B:996:GLY:CA	2.44	0.47
1:A:100:PHE:HB3	1:A:138:TYR:CE1	2.50	0.47
1:A:429:LEU:HD22	1:A:531:PRO:HD3	1.96	0.47
1:A:82:VAL:HG22	1:A:146:SER:HB2	1.97	0.47
1:A:893:LEU:HB2	1:A:959:VAL:HG12	1.97	0.47
1:B:540:LEU:HD23	1:B:545:ARG:O	2.15	0.47
1:B:457:PRO:HA	1:B:514:TYR:HA	1.96	0.47
1:A:787:ILE:HG21	1:A:872:LEU:HD12	1.97	0.47
1:B:797:VAL:O	1:B:831:THR:HG23	2.15	0.47
1:B:4:HIS:ND1	1:B:87:SER:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:ND2	1:A:1018:THR:HB	2.30	0.47
1:A:166:PRO:HG2	1:A:1022:HIS:CD2	2.50	0.47
1:A:1005:PRO:HB3	1:A:1031:VAL:HG21	1.96	0.46
1:A:207:ASN:HD21	1:A:234:GLN:HA	1.81	0.46
1:A:460:VAL:HA	1:A:500:MET:HG2	1.96	0.46
1:A:707:ARG:NE	1:A:793:ASP:OD2	2.47	0.46
1:B:670:PHE:HB2	1:B:688:TYR:CE1	2.50	0.46
1:A:803:ALA:O	1:A:826:PRO:HB3	2.15	0.46
1:B:1024:GLY:O	1:B:1026:VAL:N	2.44	0.46
1:A:263:TRP:HB3	1:A:265:LEU:HD11	1.97	0.46
1:A:443:VAL:O	1:A:492:TYR:HB2	2.15	0.46
1:A:450:GLN:HE21	1:A:450:GLN:CA	2.29	0.46
1:A:509:CYS:HB2	1:A:620:TYR:OH	2.16	0.46
1:A:721:SER:HA	1:A:943:ASN:HD22	1.81	0.46
1:B:166:PRO:HG3	1:B:1021:ILE:HD12	1.96	0.46
1:A:514:TYR:CZ	1:A:530:GLY:HA3	2.51	0.46
1:A:58:ASP:CB	1:A:60:THR:OG1	2.59	0.46
1:B:450:GLN:HG2	1:B:451:PHE:CD1	2.51	0.46
1:A:711:ILE:CD1	1:A:787:ILE:HD11	2.45	0.46
1:A:240:TYR:O	1:A:246:THR:HG23	2.16	0.46
1:B:450:GLN:HE21	1:B:450:GLN:H	1.64	0.46
1:A:295:ASN:ND2	1:A:653:PHE:HD2	2.14	0.45
1:B:109:LYS:O	1:B:127:ASP:OD2	2.34	0.45
1:B:703:TYR:O	1:B:704:GLN:OE1	2.33	0.45
1:B:1010:THR:HG23	1:B:1030:THR:OG1	2.16	0.45
1:B:249:SER:O	1:B:251:PRO:HD3	2.17	0.45
1:B:806:PRO:HB2	1:B:858:VAL:HG11	1.98	0.45
1:B:77:VAL:HG22	1:B:176:PRO:HG2	1.99	0.45
1:B:4:HIS:CE1	1:B:87:SER:HB2	2.52	0.45
1:A:649:THR:HG21	1:A:996:GLY:HA3	1.98	0.45
1:B:556:PHE:CE2	1:B:558:THR:HG21	2.52	0.45
1:A:572:ILE:CG2	1:A:582:VAL:HG21	2.46	0.45
1:B:934:HIS:CG	1:B:1023:ALA:CB	2.99	0.45
1:B:242:ILE:O	1:B:243:ASN:HB2	2.16	0.45
1:B:516:SER:HB3	1:B:523:ASP:HB3	1.97	0.45
1:B:646:ARG:N	1:B:846:ASP:OD2	2.48	0.45
1:A:313:VAL:HG22	1:A:333:GLN:HA	1.97	0.45
1:A:451:PHE:HB3	1:A:452:PRO:HD2	1.97	0.45
1:A:5:TYR:CE1	1:A:78:ILE:HG23	2.52	0.45
1:B:265:LEU:HD23	1:B:294:ILE:HG21	1.98	0.45
1:B:715:GLU:HG2	1:B:905:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ASN:ND2	1:B:997:THR:OG1	2.47	0.45
1:B:634:TYR:CE1	1:B:812:HIS:CD2	3.05	0.45
1:B:726:TRP:HB3	1:B:941:PHE:O	2.16	0.45
1:A:101:HIS:HA	1:A:112:GLU:O	2.17	0.45
1:B:814:VAL:HG23	1:B:872:LEU:CD2	2.47	0.45
1:A:294:ILE:O	1:A:294:ILE:HG22	2.16	0.44
1:A:713:ALA:HB2	1:A:799:PHE:CE1	2.52	0.44
1:A:773:ARG:NH2	1:A:783:LEU:O	2.49	0.44
1:A:21:GLU:HA	1:A:22:GLU:CB	2.48	0.44
1:A:274:VAL:O	1:A:274:VAL:HG12	2.18	0.44
1:A:562:GLU:HB2	1:A:593:ASN:HB3	1.98	0.44
1:B:443:VAL:O	1:B:492:TYR:HB2	2.16	0.44
1:A:310:ASN:HD22	1:A:461:ARG:HD2	1.83	0.44
1:A:485:ALA:O	1:A:487:LYS:N	2.51	0.44
1:B:503:THR:O	1:B:504:TYR:C	2.55	0.44
1:A:801:ASN:HB2	1:A:824:THR:HG22	1.99	0.44
1:B:787:ILE:HG22	1:B:872:LEU:HD12	1.99	0.44
1:B:712:ALA:HB3	1:B:762:PHE:CE1	2.52	0.44
1:A:801:ASN:HD22	1:A:801:ASN:C	2.21	0.44
1:A:714:VAL:O	1:A:758:VAL:HG22	2.18	0.44
1:B:694:LYS:C	1:B:694:LYS:HD3	2.38	0.44
1:A:44:ILE:HG23	1:A:219:PHE:HB2	2.00	0.44
1:A:631:HIS:ND1	1:A:679:HIS:HD2	2.13	0.44
1:A:651:ASN:ND2	1:A:997:THR:OG1	2.50	0.44
1:B:402:LYS:NZ	1:B:562:GLU:OE2	2.44	0.44
1:B:756:LYS:NZ	1:B:900:GLU:OE1	2.50	0.44
1:B:263:TRP:HB2	1:B:304:VAL:HG22	2.00	0.44
1:B:297:PHE:N	1:B:297:PHE:CD1	2.85	0.44
1:B:288:ASN:O	1:B:503:THR:HG21	2.18	0.43
1:A:606:LEU:HD23	1:A:686:GLN:HG3	2.00	0.43
1:A:204:VAL:HG23	1:A:241:SER:OG	2.19	0.43
1:A:833:ILE:HG22	1:A:833:ILE:O	2.18	0.43
1:B:414:THR:HB	1:B:415:ASN:HD22	1.82	0.43
1:A:41:PRO:HB2	1:A:222:GLU:HB2	2.00	0.43
1:A:637:GLY:O	1:A:839:ARG:NH2	2.51	0.43
1:B:1010:THR:HG22	1:B:1028:THR:HB	2.01	0.43
1:B:74:LEU:HD21	1:B:200:MET:SD	2.59	0.43
1:A:157:ARG:HD3	1:A:301:LEU:HD13	2.00	0.43
1:A:58:ASP:HB2	1:A:60:THR:HG1	1.80	0.43
1:A:879:TYR:HB3	1:A:881:LYS:H	1.84	0.43
1:A:92:ASN:HD21	1:A:94:ALA:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:ASN:O	1:B:924:ASN:HB3	2.18	0.43
1:A:21:GLU:HB3	1:A:23:LYS:HG3	1.99	0.43
1:A:533:LYS:HD2	1:A:620:TYR:CE2	2.54	0.43
1:A:107:TYR:CE1	1:A:112:GLU:HG3	2.54	0.43
1:B:706:GLU:HG3	1:B:794:LYS:HB2	2.00	0.42
1:B:356:ILE:O	1:B:445:PHE:HA	2.19	0.42
1:B:915:ASP:OD1	1:B:915:ASP:N	2.52	0.42
1:A:716:VAL:CG2	1:A:717:GLU:N	2.83	0.42
1:B:941:PHE:CZ	1:B:1024:GLY:HA2	2.55	0.42
1:B:270:ASN:ND2	1:B:1018:THR:HB	2.34	0.42
1:B:816:THR:HG22	1:B:833:ILE:O	2.19	0.42
1:A:786:LEU:HD11	1:A:873:ILE:CG1	2.49	0.42
1:B:833:ILE:O	1:B:833:ILE:CG2	2.67	0.42
1:B:840:SER:O	1:B:874:VAL:HG11	2.19	0.42
1:A:779:HIS:CE1	1:A:891:PHE:HD1	2.37	0.42
1:B:677:THR:HG23	1:B:861:VAL:HG13	2.00	0.42
1:B:750:ILE:HD11	1:B:927:PHE:HE1	1.85	0.42
1:A:400:TYR:CD2	1:A:562:GLU:CG	3.03	0.42
1:A:700:VAL:O	1:A:701:THR:HG23	2.20	0.42
1:B:428:ILE:HG22	1:B:599:ASN:C	2.39	0.42
1:B:934:HIS:CG	1:B:1023:ALA:HB1	2.55	0.42
1:A:224:GLU:N	1:A:224:GLU:CD	2.74	0.42
1:B:958:TYR:CD1	1:B:1000:THR:HG23	2.55	0.42
1:A:224:GLU:OE2	1:A:224:GLU:N	2.53	0.41
1:A:41:PRO:HD3	1:B:38:ARG:HD3	2.01	0.41
1:B:267:GLY:HA3	1:B:297:PHE:O	2.20	0.41
1:B:344:ASP:CA	1:B:345:ASP:CB	2.98	0.41
1:B:856:SER:HB2	1:B:868:LEU:HD13	2.02	0.41
1:A:73:LEU:HD12	1:A:73:LEU:C	2.40	0.41
1:A:800:LYS:HA	1:A:829:VAL:HB	2.01	0.41
1:A:814:VAL:HG11	1:A:834:TRP:CD1	2.56	0.41
1:B:621:LEU:HB3	1:B:652:LEU:HD11	2.03	0.41
1:B:694:LYS:HD3	1:B:695:GLY:N	2.35	0.41
1:A:34:ASN:O	1:A:35:PHE:C	2.55	0.41
1:A:578:ALA:N	1:A:579:PRO:HD3	2.35	0.41
1:A:163:VAL:O	1:A:734:GLN:HG2	2.21	0.41
1:B:368:SER:OG	1:B:605:ASN:ND2	2.53	0.41
1:A:427:GLY:HA3	1:A:601:PHE:HE2	1.85	0.41
1:A:714:VAL:O	1:A:758:VAL:O	2.39	0.41
1:A:711:ILE:HD12	1:A:797:VAL:CG1	2.51	0.41
1:A:862:LYS:NZ	1:A:902:GLU:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ALA:O	1:B:52:LEU:HD23	2.20	0.41
1:A:91:LYS:HE3	1:A:93:PHE:CE1	2.56	0.41
1:B:754:TYR:CD2	1:B:900:GLU:HG3	2.55	0.41
1:A:74:LEU:HD21	1:A:200:MET:SD	2.61	0.41
1:A:711:ILE:HD12	1:A:797:VAL:HG13	2.02	0.41
1:B:878:SER:O	1:B:879:TYR:CB	2.67	0.41
1:B:431:PRO:O	1:B:514:TYR:OH	2.32	0.41
1:B:555:LEU:HD12	1:B:621:LEU:CD2	2.51	0.41
1:B:5:TYR:CE2	1:B:78:ILE:HA	2.55	0.41
1:A:242:ILE:HG22	1:A:250:LEU:HD22	2.03	0.41
1:A:624:ALA:HA	1:A:654:PRO:HA	2.02	0.41
1:B:101:HIS:HA	1:B:112:GLU:O	2.20	0.41
1:A:295:ASN:ND2	1:A:653:PHE:CD2	2.89	0.41
1:A:463:THR:O	1:A:464:LYS:C	2.59	0.41
1:B:620:TYR:CE1	1:B:659:THR:HG23	2.56	0.41
1:B:933:MET:HB3	1:B:940:MET:CE	2.51	0.41
1:B:162:HIS:O	1:B:162:HIS:ND1	2.51	0.41
1:B:825:LEU:HB3	1:B:826:PRO:CD	2.51	0.41
1:B:907:ASP:HA	1:B:910:ILE:HD12	2.03	0.41
1:A:207:ASN:ND2	1:A:234:GLN:O	2.51	0.40
1:A:801:ASN:HD22	1:A:803:ALA:H	1.68	0.40
1:A:856:SER:HB3	1:A:863:ASP:HB3	2.04	0.40
1:B:838:GLU:N	5:B:1202:HOH:O	2.54	0.40
1:A:344:ASP:CA	1:A:345:ASP:CB	2.99	0.40
1:A:396:ILE:HD13	1:A:571:ASN:HB3	2.02	0.40
1:A:293:ILE:HD13	1:A:655:HIS:HB2	2.02	0.40
1:A:613:LEU:HD13	1:A:667:GLU:HB2	2.03	0.40
1:A:895:PHE:CD2	1:A:936:ILE:HG23	2.56	0.40
1:B:285:THR:HG22	1:B:290:HIS:HA	2.03	0.40
1:B:499:GLU:H	1:B:499:GLU:CD	2.25	0.40
1:B:813:GLY:O	1:B:839:ARG:NH1	2.54	0.40
1:A:631:HIS:CE1	1:A:679:HIS:NE2	2.90	0.40
1:A:633:ILE:HB	1:A:650:ALA:HB3	2.03	0.40
1:B:298:PRO:HG2	1:B:1017:VAL:HB	2.04	0.40
1:A:958:TYR:CE1	1:A:1000:THR:HG23	2.57	0.40
1:A:711:ILE:O	1:A:799:PHE:HA	2.21	0.40
1:B:156:THR:HG22	1:B:264:TYR:CB	2.47	0.40
1:B:30:THR:HA	1:B:33:SER:HB3	2.02	0.40
1:B:815:LYS:HB3	1:B:835:GLN:HB2	2.04	0.40
1:B:785:PRO:HD2	1:B:854:TYR:OH	2.21	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	1032/1034 (100%)	869 (84%)	122 (12%)	41 (4%)	3	24
1	B	1032/1034 (100%)	874 (85%)	117 (11%)	41 (4%)	3	24
All	All	2064/2068 (100%)	1743 (84%)	239 (12%)	82 (4%)	3	24

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	146	SER
1	A	393	ALA
1	A	411	ASP
1	A	492	TYR
1	A	698	GLU
1	A	700	VAL
1	A	701	THR
1	A	715	GLU
1	A	738	VAL
1	A	774	ARG
1	A	814	VAL
1	A	881	LYS
1	A	885	PRO
1	B	21	GLU
1	B	40	GLY
1	B	202	SER
1	B	498	LYS
1	B	701	THR
1	B	725	ASP
1	B	814	VAL
1	B	837	PRO
1	B	878	SER
1	B	880	VAL
1	A	18	SER

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Mol	Chain	Res	Type
1	A	39	ASN
1	A	209	SER
1	A	231	GLU
1	A	387	VAL
1	A	627	GLU
1	A	837	PRO
1	A	877	LYS
1	B	19	GLY
1	B	20	SER
1	B	108	THR
1	B	129	LYS
1	B	345	ASP
1	B	492	TYR
1	B	697	PHE
1	B	738	VAL
1	B	779	HIS
1	B	793	ASP
1	B	877	LYS
1	B	1025	MET
1	A	202	SER
1	A	498	LYS
1	A	596	HIS
1	A	705	GLY
1	B	146	SER
1	B	507	PRO
1	B	627	GLU
1	B	677	THR
1	B	879	TYR
1	A	75	GLY
1	A	416	ARG
1	A	984	GLY
1	B	226	VAL
1	B	387	VAL
1	B	411	ASP
1	B	694	LYS
1	B	881	LYS
1	B	882	VAL
1	B	1016	HIS
1	A	68	PRO
1	A	569	ASP
1	A	819	SER
1	A	887	LYS

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Mol	Chain	Res	Type
1	A	1025	MET
1	B	125	ARG
1	B	772	LYS
1	B	828	GLU
1	B	848	PRO
1	A	205	ASP
1	A	570	ASP
1	B	75	GLY
1	B	176	PRO
1	A	507	PRO
1	A	518	VAL
1	A	791	VAL
1	A	19	GLY
1	A	421	PRO
1	B	910	ILE

### 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	909/909 (100%)	815 (90%)	94 (10%)	8	33
1	B	909/909 (100%)	824 (91%)	85 (9%)	10	38
All	All	1818/1818 (100%)	1639 (90%)	179 (10%)	9	36

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	22	GLU
1	A	30	THR
1	A	38	ARG
1	A	46	ARG
1	A	54	SER
1	A	60	THR
1	A	64	THR

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Mol	Chain	Res	Type
1	A	68	PRO
1	A	103	HIS
1	A	105	VAL
1	A	123	PHE
1	A	125	ARG
1	A	137	LEU
1	A	149	GLU
1	A	178	ILE
1	A	182	LYS
1	A	185	LEU
1	A	187	LYS
1	A	201	PHE
1	A	202	SER
1	A	208	LEU
1	A	229	ASP
1	A	236	SER
1	A	246	THR
1	A	249	SER
1	A	254	SER
1	A	284	LEU
1	A	288	ASN
1	A	309	GLN
1	A	316	LEU
1	A	318	CYS
1	A	335	ARG
1	A	347	GLN
1	A	370	THR
1	A	409	THR
1	A	410	ASP
1	A	411	ASP
1	A	422	ASP
1	A	450	GLN
1	A	456	GLN
1	A	462	PHE
1	A	469	THR
1	A	492	TYR
1	A	499	GLU
1	A	500	MET
1	A	504	TYR
1	A	513	MET
1	A	545	ARG
1	A	576	THR

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Mol	Chain	Res	Type
1	A	588	ASP
1	A	593	ASN
1	A	613	LEU
1	A	621	LEU
1	A	641	LEU
1	A	672	VAL
1	A	676	THR
1	A	679	HIS
1	A	681	THR
1	A	692	GLN
1	A	694	LYS
1	A	700	VAL
1	A	707	ARG
1	A	714	VAL
1	A	715	GLU
1	A	730	LEU
1	A	746	GLU
1	A	764	ASP
1	A	778	GLU
1	A	786	LEU
1	A	801	ASN
1	A	829	VAL
1	A	844	THR
1	A	855	TYR
1	A	864	LEU
1	A	872	LEU
1	A	873	ILE
1	A	876	ARG
1	A	882	VAL
1	A	883	PHE
1	A	886	LYS
1	A	894	LEU
1	A	896	LEU
1	A	908	ASP
1	A	918	GLU
1	A	956	ASN
1	A	964	ASN
1	A	968	LEU
1	A	979	GLN
1	A	982	HIS
1	A	997	THR
1	A	999	GLN

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Mol	Chain	Res	Type
1	A	1016	HIS
1	A	1017	VAL
1	B	2	GLU
1	B	30	THR
1	B	38	ARG
1	B	50	LYS
1	B	71	LEU
1	B	108	THR
1	B	115	ILE
1	B	121	THR
1	B	123	PHE
1	B	125	ARG
1	B	137	LEU
1	B	185	LEU
1	B	187	LYS
1	B	229	ASP
1	B	231	GLU
1	B	232	ASP
1	B	246	THR
1	B	260	ARG
1	B	265	LEU
1	B	284	LEU
1	B	303	ASP
1	B	309	GLN
1	B	318	CYS
1	B	328	LEU
1	B	361	THR
1	B	363	TRP
1	B	395	ARG
1	B	414	THR
1	B	450	GLN
1	B	456	GLN
1	B	462	PHE
1	B	474	ASP
1	B	498	LYS
1	B	500	MET
1	B	504	TYR
1	B	545	ARG
1	B	567	LEU
1	B	576	THR
1	B	588	ASP
1	B	597	SER

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Mol	Chain	Res	Type
1	B	634	TYR
1	B	641	LEU
1	B	647	ARG
1	B	663	THR
1	B	672	VAL
1	B	692	GLN
1	B	694	LYS
1	B	697	PHE
1	B	699	ASP
1	B	701	THR
1	B	708	THR
1	B	711	ILE
1	B	730	LEU
1	B	737	ASN
1	B	746	GLU
1	B	755	LYS
1	B	773	ARG
1	B	776	GLU
1	B	829	VAL
1	B	833	ILE
1	B	839	ARG
1	B	844	THR
1	B	855	TYR
1	B	864	LEU
1	B	878	SER
1	B	879	TYR
1	B	883	PHE
1	B	894	LEU
1	B	896	LEU
1	B	907	ASP
1	B	908	ASP
1	B	915	ASP
1	B	918	GLU
1	B	929	GLU
1	B	956	ASN
1	B	968	LEU
1	B	979	GLN
1	B	983	ARG
1	B	998	TYR
1	B	999	GLN
1	B	1000	THR
1	B	1007	THR

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Mol	Chain	Res	Type
1	B	1013	LEU
1	B	1016	HIS
1	B	1017	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	111	ASN
1	A	186	HIS
1	A	295	ASN
1	A	309	GLN
1	A	310	ASN
1	A	319	GLN
1	A	329	GLN
1	A	347	GLN
1	A	450	GLN
1	A	456	GLN
1	A	483	HIS
1	A	546	GLN
1	A	596	HIS
1	A	605	ASN
1	A	651	ASN
1	A	679	HIS
1	A	770	GLN
1	A	801	ASN
1	A	810	HIS
1	A	835	GLN
1	A	956	ASN
1	A	979	GLN
1	A	999	GLN
1	B	34	ASN
1	B	92	ASN
1	B	111	ASN
1	B	134	GLN
1	B	186	HIS
1	B	295	ASN
1	B	309	GLN
1	B	310	ASN
1	B	319	GLN
1	B	329	GLN
1	B	391	GLN

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Mol	Chain	Res	Type
1	B	415	ASN
1	B	450	GLN
1	B	456	GLN
1	B	466	ASN
1	B	605	ASN
1	B	651	ASN
1	B	655	HIS
1	B	736	GLN
1	B	770	GLN
1	B	801	ASN
1	B	810	HIS
1	B	999	GLN
1	B	1022	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 15 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	1034/1034 (100%)	-0.54	7 (0%) 87 80	95, 144, 188, 256	0
1	B	1034/1034 (100%)	-0.48	14 (1%) 75 63	98, 153, 202, 285	0
All	All	2068/2068 (100%)	-0.51	21 (1%) 82 72	95, 148, 199, 285	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	884	ASN	5.4
1	A	697	PHE	4.9
1	B	885	PRO	4.7
1	A	696	GLN	4.5
1	B	697	PHE	4.4
1	B	699	ASP	4.3
1	B	698	GLU	4.0
1	B	696	GLN	3.9
1	B	883	PHE	3.8
1	A	882	VAL	3.5
1	B	882	VAL	3.0
1	A	415	ASN	2.9
1	B	712	ALA	2.8
1	B	415	ASN	2.6
1	B	381	LEU	2.6
1	A	20	SER	2.5
1	B	225	LYS	2.5
1	A	699	ASP	2.5
1	B	345	ASP	2.2
1	A	343	ASP	2.1
1	B	391	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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	NA	A	1107	1/1	0.92	0.41	4.66	120,120,120,120	0
4	NA	B	1108	1/1	0.98	0.29	2.48	95,95,95,95	0
3	CA	A	1106	1/1	0.99	0.18	0.57	143,143,143,143	0
3	CA	B	1107	1/1	0.99	0.14	-0.09	132,132,132,132	0
2	CU	A	1103	1/1	0.99	0.15	-0.74	125,125,125,125	0
2	CU	B	1102	1/1	1.00	0.13	-0.82	120,120,120,120	0
2	CU	A	1102	1/1	1.00	0.12	-1.12	130,130,130,130	0
2	CU	A	1105	1/1	0.97	0.09	-1.38	146,146,146,146	0
2	CU	B	1104	1/1	0.99	0.13	-1.50	176,176,176,176	0
2	CU	B	1106	1/1	0.94	0.10	-2.06	155,155,155,155	0
2	CU	B	1101	1/1	0.99	0.10	-2.30	140,140,140,140	0
2	CU	B	1105	1/1	0.98	0.06	-4.07	131,131,131,131	0
2	CU	B	1103	1/1	0.99	0.07	-4.42	131,131,131,131	0
2	CU	A	1101	1/1	0.97	0.05	-5.58	149,149,149,149	0
2	CU	A	1104	1/1	0.99	0.03	-5.92	116,116,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.