



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 AM GMT

PDB ID : 2VNC  
Title : CRYSTAL STRUCTURE OF GLYCOGEN DEBRANCHING ENZYME  
TREX FROM SULFOLOBUS SOLFATARICUS  
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Deposited on : 2008-02-04  
Resolution : 3.00 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](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

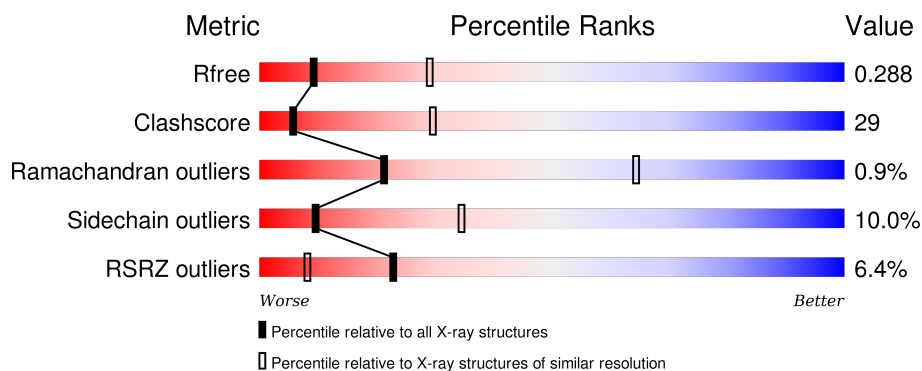
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

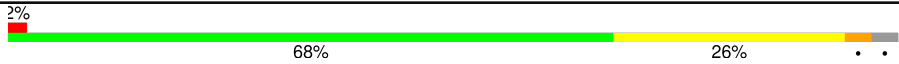

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	718	 2% 68% 26% • •
1	B	718	 10% 47% 36% 8% • 7%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11284 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 GLYCOGEN OPERON PROTEIN GLGX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5711	3661	959	1073	18			
1	B	666	Total	C	N	O	S	0	0	0
			5443	3490	919	1018	16			

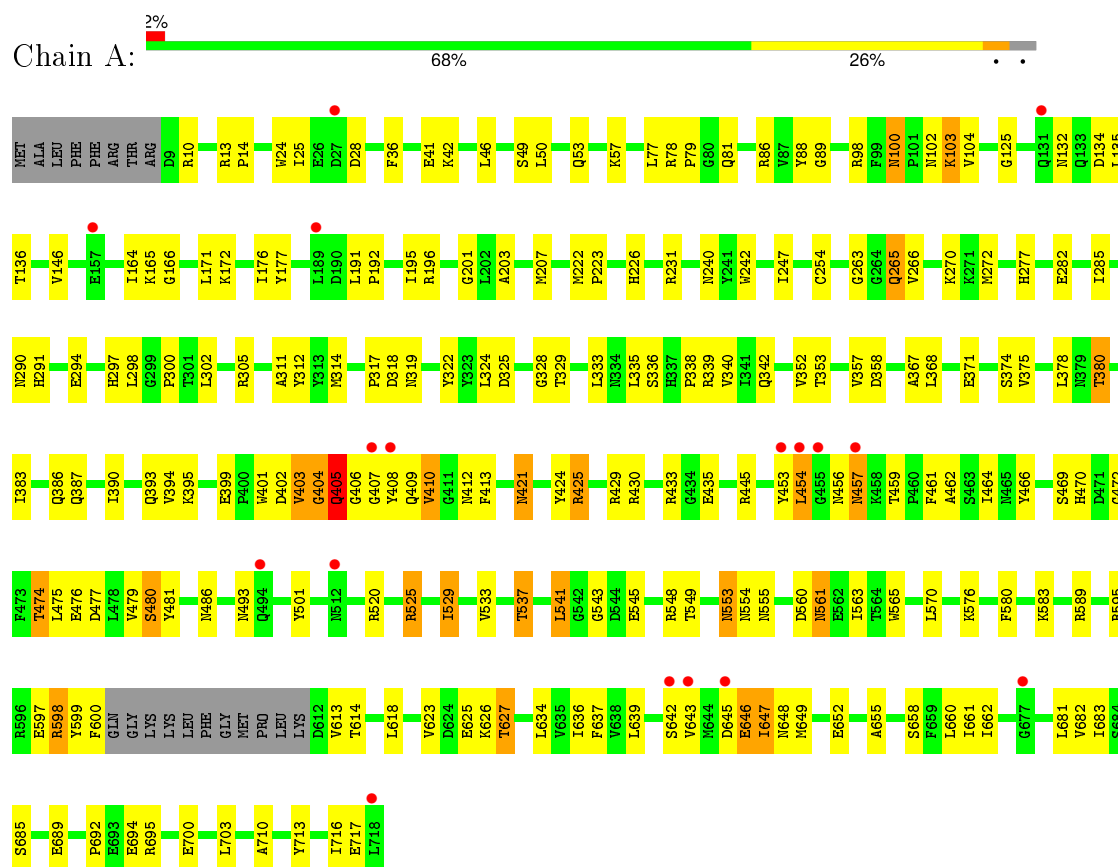
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	30	Total	O	0	0
			30	30		

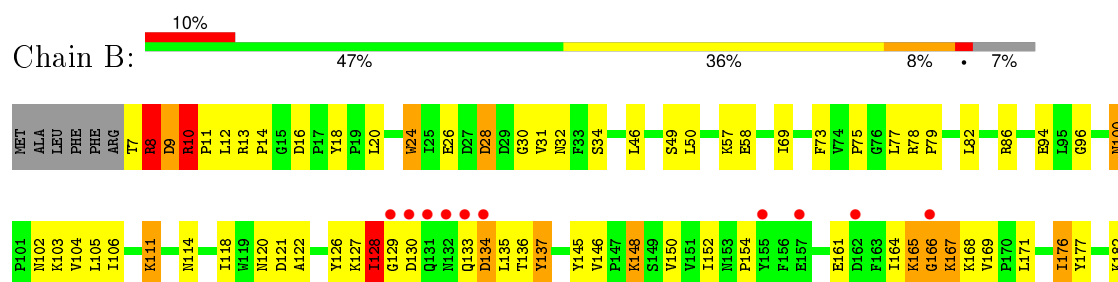
### 3 Residue-property plots

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

#### • Molecule 1: GLYCOGEN OPERON PROTEIN GLGX



#### • Molecule 1: GLYCOGEN OPERON PROTEIN GLGX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.08Å 136.08Å 173.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 3.00 29.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-3.00) 99.8 (29.91-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.12 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.287 0.221 , 0.288	Depositor DCC
$R_{free}$ test set	1909 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.0	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37652 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

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	0.51	0/5860	0.64	0/7948
1	B	0.47	0/5582	0.59	2/7566 (0.0%)
All	All	0.49	0/11442	0.62	2/15514 (0.0%)

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	3
1	B	0	23
All	All	0	26

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	459	THR	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	VAL	Peptide
1	A	404	GLY	Peptide
1	A	405	GLN	Peptide
1	B	10	ARG	Peptide
1	B	166	GLY	Peptide
1	B	231	ARG	Peptide
1	B	232	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	474	THR	Peptide
1	B	475	LEU	Peptide
1	B	476	GLU	Peptide
1	B	477	ASP	Peptide
1	B	478	LEU	Peptide
1	B	480	SER	Peptide
1	B	481	TYR	Peptide
1	B	540	ILE	Peptide
1	B	571	ASP	Peptide
1	B	573	ARG	Peptide
1	B	574	LYS	Peptide
1	B	614	THR	Peptide
1	B	625	GLU	Peptide
1	B	626	LYS	Peptide
1	B	664	ASN	Peptide
1	B	665	ALA	Peptide
1	B	708	ARG	Peptide
1	B	710	ALA	Peptide
1	B	8	ARG	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	5711	0	5508	157	1
1	B	5443	0	5242	486	12
2	A	100	0	0	4	0
2	B	30	0	0	6	0
All	All	11284	0	10750	635	13

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 29.

All (635) 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:473:PHE:HB3	1:B:478:LEU:CD2	1.54	1.35
1:B:476:GLU:CG	1:B:479:VAL:HG13	1.58	1.31
1:B:9:ASP:CB	1:B:10:ARG:HA	1.63	1.25
1:B:476:GLU:HG2	1:B:479:VAL:CG1	1.72	1.18
1:B:9:ASP:HB3	1:B:10:ARG:CA	1.71	1.18
1:B:614:THR:OG1	1:B:637:PHE:HA	1.44	1.16
1:B:475:LEU:H	1:B:476:GLU:C	1.48	1.15
1:B:691:LYS:HG2	1:B:692:PRO:CD	1.75	1.15
1:B:472:GLY:HA2	1:B:554:ASN:HA	1.24	1.14
1:B:231:ARG:CB	1:B:232:PHE:HB2	1.76	1.14
1:B:543:GLY:O	1:B:548:ARG:HB2	1.47	1.14
1:B:473:PHE:O	1:B:474:THR:HG22	1.46	1.13
1:B:10:ARG:HG3	1:B:10:ARG:HH21	1.03	1.12
1:B:691:LYS:HG2	1:B:692:PRO:HD3	1.17	1.11
1:B:559:GLN:HE21	1:B:563:ILE:HD12	1.11	1.11
1:B:231:ARG:HB3	1:B:232:PHE:HB2	1.15	1.10
1:B:473:PHE:HB3	1:B:478:LEU:HD21	1.25	1.10
1:B:482:ASN:OD1	1:B:502:SER:O	1.70	1.09
1:B:615:PHE:CD1	1:B:636:ILE:O	2.06	1.08
1:B:7:THR:HG22	1:B:8:ARG:H	1.12	1.07
1:B:458:LYS:HG3	1:B:458:LYS:O	1.54	1.07
1:B:665:ALA:HB3	1:B:666:ASN:HB3	1.34	1.07
1:B:473:PHE:HB3	1:B:478:LEU:HD22	1.29	1.05
1:B:574:LYS:HD3	1:B:574:LYS:N	1.59	1.05
1:B:614:THR:HG1	1:B:637:PHE:HA	1.12	1.05
1:B:10:ARG:O	1:B:10:ARG:HG3	1.57	1.04
1:B:476:GLU:OE1	1:B:520:ARG:HG3	1.56	1.04
1:B:7:THR:HG22	1:B:8:ARG:N	1.67	1.04
1:B:231:ARG:HB3	1:B:232:PHE:CB	1.86	1.04
1:B:476:GLU:CG	1:B:479:VAL:CG1	2.30	1.03
1:B:710:ALA:O	1:B:711:LEU:HD13	1.59	1.02
1:B:10:ARG:H	1:B:11:PRO:HA	1.23	1.02
1:B:476:GLU:OE2	1:B:479:VAL:HG11	1.60	1.01
1:B:471:ASP:O	1:B:554:ASN:O	1.80	0.99
1:B:476:GLU:HG2	1:B:479:VAL:HG13	1.33	0.99
1:B:615:PHE:HE1	1:B:636:ILE:H	1.00	0.98
1:B:230:GLN:O	1:B:233:LEU:N	1.97	0.98
1:B:481:TYR:H	1:B:482:ASN:HB2	1.30	0.96
1:B:559:GLN:NE2	1:B:563:ILE:HD12	1.80	0.96
1:B:231:ARG:CA	1:B:232:PHE:HB2	1.94	0.96
1:B:231:ARG:N	1:B:232:PHE:HB2	1.83	0.94
1:B:618:LEU:O	1:B:618:LEU:HD13	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:THR:OG1	1:B:637:PHE:CA	2.16	0.93
1:B:480:SER:HG	1:B:481:TYR:HD1	0.94	0.93
1:B:473:PHE:HD2	1:B:474:THR:H	1.09	0.92
1:B:468:THR:CB	1:B:473:PHE:HE2	1.82	0.92
1:B:473:PHE:HA	1:B:478:LEU:HD13	1.49	0.91
1:B:468:THR:HB	1:B:473:PHE:HE2	1.31	0.91
1:B:473:PHE:CB	1:B:478:LEU:HD22	1.99	0.91
1:B:708:ARG:N	1:B:709:THR:HG22	1.86	0.91
1:B:708:ARG:N	1:B:709:THR:CG2	2.34	0.90
1:B:476:GLU:CD	1:B:479:VAL:HG13	1.91	0.90
1:B:479:VAL:HG22	1:B:479:VAL:O	1.71	0.89
1:B:476:GLU:CB	1:B:479:VAL:HG13	2.03	0.89
1:B:480:SER:OG	1:B:481:TYR:HD1	1.55	0.88
1:B:571:ASP:HB3	1:B:574:LYS:HE3	1.55	0.88
1:B:473:PHE:CB	1:B:478:LEU:CD2	2.48	0.88
1:B:529:ILE:CD1	1:B:710:ALA:CB	2.50	0.88
1:B:10:ARG:CG	1:B:10:ARG:HH21	1.85	0.87
1:B:476:GLU:OE2	1:B:523:GLN:HB2	1.75	0.86
1:B:10:ARG:NH2	1:B:10:ARG:HG3	1.84	0.86
1:B:475:LEU:N	1:B:476:GLU:O	2.07	0.86
1:B:476:GLU:CD	1:B:479:VAL:CG1	2.43	0.86
1:B:573:ARG:C	1:B:574:LYS:HD3	1.96	0.86
1:B:26:GLU:O	1:B:26:GLU:HG2	1.74	0.85
1:B:10:ARG:N	1:B:11:PRO:HA	1.92	0.85
1:B:503:TRP:HD1	1:B:504:ASN:H	1.23	0.84
1:B:475:LEU:N	1:B:476:GLU:C	2.31	0.84
1:B:615:PHE:CD1	1:B:616:TYR:N	2.44	0.84
1:B:472:GLY:HA2	1:B:554:ASN:CA	2.07	0.83
1:B:665:ALA:HB3	1:B:666:ASN:CB	2.08	0.83
1:B:529:ILE:HD11	1:B:710:ALA:CB	2.08	0.83
1:A:380:THR:HG22	1:B:380:THR:HG22	1.59	0.83
1:B:476:GLU:HA	1:B:479:VAL:H	1.42	0.83
1:B:9:ASP:CB	1:B:10:ARG:CA	2.41	0.83
1:B:478:LEU:N	1:B:478:LEU:HD13	1.93	0.83
1:B:615:PHE:O	1:B:616:TYR:CD2	2.32	0.83
1:B:529:ILE:HD13	1:B:710:ALA:HB1	1.60	0.83
1:B:478:LEU:H	1:B:478:LEU:HD13	1.42	0.82
1:B:473:PHE:O	1:B:474:THR:CG2	2.27	0.82
1:A:265:GLN:H	1:A:265:GLN:HE21	1.26	0.81
1:B:626:LYS:CB	1:B:627:THR:HB	2.11	0.81
1:B:529:ILE:HD13	1:B:710:ALA:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:LYS:CD	1:B:574:LYS:N	2.41	0.80
1:B:476:GLU:OE2	1:B:479:VAL:CG1	2.30	0.80
1:B:297:HIS:O	1:B:298:LEU:HB2	1.81	0.80
1:B:468:THR:HG22	1:B:473:PHE:CE2	2.17	0.79
1:B:529:ILE:CD1	1:B:710:ALA:HB3	2.10	0.79
1:B:674:PHE:HZ	1:B:703:LEU:HD12	1.48	0.79
1:B:482:ASN:ND2	1:B:502:SER:C	2.34	0.79
1:B:684:SER:HB2	1:B:711:LEU:CD1	2.12	0.79
1:B:78:ARG:HB2	1:B:79:PRO:HD2	1.64	0.79
1:B:529:ILE:HD11	1:B:710:ALA:HB3	1.65	0.79
1:B:10:ARG:HB3	1:B:12:LEU:HG	1.63	0.78
1:B:472:GLY:O	1:B:473:PHE:CG	2.36	0.78
1:B:691:LYS:HG3	1:B:692:PRO:HG3	1.65	0.78
1:B:478:LEU:HA	1:B:480:SER:H	1.49	0.78
1:B:480:SER:OG	1:B:481:TYR:CD1	2.35	0.78
1:B:231:ARG:HB3	1:B:232:PHE:CG	2.18	0.78
1:B:473:PHE:CD2	1:B:474:THR:N	2.51	0.77
1:B:321:ARG:HD3	1:B:322:TYR:HE2	1.49	0.77
1:A:560:ASP:OD1	1:A:565:TRP:HH2	1.66	0.77
1:B:482:ASN:CG	1:B:502:SER:C	2.43	0.77
1:B:231:ARG:N	1:B:232:PHE:CB	2.48	0.77
1:B:458:LYS:CG	1:B:458:LYS:O	2.32	0.77
1:A:297:HIS:O	1:A:298:LEU:HB2	1.85	0.77
1:B:292:THR:H	1:B:331:ASN:HD21	1.31	0.76
1:B:16:ASP:H	1:B:32:ASN:HD21	1.33	0.76
1:B:626:LYS:H	1:B:627:THR:HB	1.50	0.76
1:B:191:LEU:HD21	1:B:206:GLN:NE2	2.01	0.76
1:B:168:LYS:HB3	1:B:282:GLU:OE2	1.86	0.76
1:B:10:ARG:H	1:B:11:PRO:CA	1.96	0.75
1:B:671:LYS:HA	1:B:704:GLU:HG3	1.67	0.75
1:A:560:ASP:OD1	1:A:565:TRP:CH2	2.40	0.75
1:A:265:GLN:H	1:A:265:GLN:NE2	1.84	0.74
1:B:666:ASN:O	1:B:708:ARG:NH2	2.07	0.74
1:B:49:SER:HB3	1:B:57:LYS:HD3	1.67	0.74
1:B:691:LYS:CG	1:B:692:PRO:HD3	2.10	0.74
1:B:134:ASP:HB3	1:B:298:LEU:HD12	1.68	0.74
1:B:708:ARG:H	1:B:709:THR:HG22	1.49	0.74
1:B:9:ASP:HB3	1:B:10:ARG:HA	0.79	0.73
1:B:468:THR:CB	1:B:473:PHE:CE2	2.70	0.73
1:B:707:GLY:C	1:B:709:THR:HG23	2.09	0.73
1:B:710:ALA:O	1:B:711:LEU:CD1	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:PHE:CZ	1:B:703:LEU:HD12	2.23	0.73
1:A:476:GLU:O	1:A:480:SER:OG	2.06	0.73
1:B:612:ASP:OD2	1:B:641:GLY:CA	2.37	0.72
1:B:468:THR:HB	1:B:473:PHE:CE2	2.22	0.72
1:B:321:ARG:HD3	1:B:322:TYR:CE2	2.24	0.72
1:B:616:TYR:O	1:B:636:ILE:HD12	1.89	0.72
1:A:77:LEU:HD22	1:A:81:GLN:HE21	1.54	0.72
1:B:127:LYS:H	1:B:136:THR:HG23	1.55	0.71
1:B:570:LEU:H	1:B:570:LEU:HD23	1.54	0.71
1:B:230:GLN:H	1:B:230:GLN:NE2	1.87	0.71
1:B:223:PRO:HB2	1:B:243:GLY:HA3	1.73	0.71
1:B:479:VAL:CG2	1:B:479:VAL:O	2.39	0.70
1:B:703:LEU:HB3	1:B:704:GLU:HA	1.74	0.70
1:B:626:LYS:H	1:B:627:THR:CG2	2.04	0.70
1:B:193:GLU:HA	1:B:196:ARG:HH11	1.56	0.70
1:B:133:GLN:O	1:B:134:ASP:CG	2.30	0.70
1:B:482:ASN:CG	1:B:502:SER:O	2.30	0.69
1:B:626:LYS:N	1:B:627:THR:HB	2.07	0.69
1:B:472:GLY:C	1:B:473:PHE:CD1	2.66	0.69
1:B:472:GLY:C	1:B:473:PHE:CG	2.66	0.69
1:B:615:PHE:CE1	1:B:636:ILE:O	2.45	0.69
1:B:684:SER:CB	1:B:711:LEU:HD12	2.23	0.69
1:A:405:GLN:C	1:A:405:GLN:OE1	2.31	0.69
1:B:478:LEU:HA	1:B:480:SER:N	2.07	0.69
1:B:7:THR:CG2	1:B:8:ARG:H	1.88	0.69
1:B:193:GLU:HA	1:B:196:ARG:NH1	2.07	0.68
1:B:290:ASN:OD1	1:B:291:HIS:HD2	1.75	0.68
1:A:561:ASN:HD22	1:A:563:ILE:H	1.40	0.68
1:B:615:PHE:HD1	1:B:636:ILE:O	1.72	0.68
1:A:403:VAL:O	1:A:406:GLY:CA	2.41	0.68
1:B:476:GLU:HA	1:B:479:VAL:N	2.09	0.68
1:B:626:LYS:H	1:B:627:THR:CB	2.06	0.68
1:A:371:GLU:O	1:A:374:SER:HB3	1.93	0.68
1:B:708:ARG:N	1:B:709:THR:HG23	2.08	0.68
1:B:614:THR:OG1	1:B:637:PHE:CB	2.41	0.67
1:A:380:THR:HG22	1:B:380:THR:CG2	2.25	0.67
1:B:626:LYS:CA	1:B:627:THR:HB	2.23	0.67
1:B:684:SER:HB2	1:B:711:LEU:HD12	1.74	0.67
1:A:380:THR:HB	1:B:380:THR:HB	1.77	0.67
1:B:468:THR:HG22	1:B:473:PHE:CD2	2.29	0.67
1:B:618:LEU:HD22	1:B:618:LEU:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:VAL:O	1:B:713:TYR:CG	2.47	0.67
1:A:403:VAL:O	1:A:406:GLY:HA2	1.95	0.67
1:B:478:LEU:CD2	1:B:478:LEU:O	2.43	0.67
1:B:712:VAL:O	1:B:713:TYR:CD1	2.47	0.67
1:B:7:THR:CG2	1:B:8:ARG:N	2.42	0.66
1:B:191:LEU:HD22	1:B:195:ILE:HD11	1.77	0.66
1:B:430:ARG:HB3	1:B:437:LEU:HD21	1.77	0.66
1:B:468:THR:CG2	1:B:473:PHE:CE2	2.78	0.66
1:B:541:LEU:HD13	1:B:542:GLY:N	2.10	0.66
1:A:192:PRO:HG2	1:A:195:ILE:HG12	1.77	0.66
1:B:475:LEU:CD1	1:B:544:ASP:HB3	2.26	0.66
1:B:691:LYS:CG	1:B:692:PRO:CD	2.64	0.66
1:B:336:SER:HB3	1:B:375:VAL:HB	1.78	0.66
1:B:474:THR:HG23	1:B:474:THR:O	1.94	0.66
1:A:649:MET:HA	1:B:14:PRO:HG2	1.77	0.66
1:B:691:LYS:CG	1:B:692:PRO:HG3	2.27	0.65
1:B:247:ILE:O	1:B:247:ILE:HD13	1.96	0.65
1:B:221:LEU:O	1:B:286:ASP:HB2	1.96	0.65
1:A:486:ASN:H	1:A:493:ASN:ND2	1.94	0.65
1:B:242:TRP:HA	2:B:2013:HOH:O	1.96	0.65
1:B:285:ILE:HG12	1:B:357:VAL:HG11	1.79	0.65
1:B:540:ILE:HG22	1:B:541:LEU:O	1.97	0.65
1:A:649:MET:HA	1:B:14:PRO:CG	2.27	0.65
1:B:365:ALA:CB	1:B:398:ALA:HB1	2.27	0.64
1:B:389:PRO:O	1:B:393:GLN:NE2	2.30	0.64
1:B:473:PHE:HA	1:B:478:LEU:CD1	2.26	0.64
1:B:478:LEU:HD22	1:B:478:LEU:O	1.97	0.64
1:B:665:ALA:O	1:B:708:ARG:HD3	1.97	0.64
1:B:614:THR:HG23	1:B:638:VAL:O	1.97	0.64
1:B:188:ARG:HH11	1:B:188:ARG:HG3	1.63	0.64
1:A:407:GLY:O	1:A:409:GLN:N	2.30	0.64
1:B:440:SER:HB3	1:B:628:TRP:CD1	2.33	0.64
1:A:291:HIS:ND1	1:A:329:THR:HG21	2.12	0.64
1:B:615:PHE:HE1	1:B:636:ILE:N	1.84	0.64
1:B:233:LEU:O	1:B:235:ASP:N	2.30	0.64
1:B:633:GLN:HB3	1:B:665:ALA:CB	2.28	0.64
1:B:705:ILE:HG22	1:B:706:GLU:H	1.63	0.64
1:A:36:PHE:CE1	1:A:339:ARG:HG3	2.33	0.63
1:B:134:ASP:HB3	1:B:298:LEU:CD1	2.28	0.63
1:B:571:ASP:O	1:B:573:ARG:N	2.32	0.63
1:A:472:GLY:HA2	1:A:554:ASN:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:PHE:HE2	1:B:713:TYR:CE1	2.16	0.63
1:A:525:ARG:HG2	1:A:580:PHE:CE2	2.34	0.63
1:B:615:PHE:HD1	1:B:616:TYR:H	1.40	0.62
1:B:429:ARG:NH2	1:B:473:PHE:CZ	2.68	0.62
1:B:466:TYR:CE2	1:B:469:SER:HB3	2.34	0.62
1:B:633:GLN:HG2	1:B:665:ALA:CB	2.28	0.62
1:A:477:ASP:O	1:A:481:TYR:HB2	1.99	0.62
1:A:453:TYR:HB2	1:A:600:PHE:CE1	2.34	0.62
1:B:529:ILE:CD1	1:B:710:ALA:HB1	2.23	0.62
1:A:692:PRO:HA	1:A:695:ARG:HD2	1.82	0.61
2:A:2010:HOH:O	1:B:415:TYR:HE1	1.83	0.61
1:B:475:LEU:H	1:B:477:ASP:N	1.95	0.61
1:B:706:GLU:HG2	1:B:707:GLY:N	2.14	0.61
1:B:473:PHE:HA	1:B:478:LEU:H	1.66	0.61
1:B:230:GLN:H	1:B:230:GLN:HE21	1.48	0.61
1:B:134:ASP:C	1:B:134:ASP:OD2	2.38	0.61
1:B:439:TYR:OH	1:B:634:LEU:N	2.34	0.61
1:B:10:ARG:HB3	1:B:12:LEU:CG	2.30	0.61
1:B:188:ARG:HH11	1:B:188:ARG:CG	2.14	0.61
1:B:636:ILE:HG12	1:B:662:ILE:HG23	1.83	0.61
1:B:263:GLY:H	1:B:265:GLN:NE2	1.98	0.61
1:B:476:GLU:HG2	1:B:479:VAL:HG12	1.80	0.61
1:B:710:ALA:C	1:B:711:LEU:HD13	2.21	0.61
1:A:623:VAL:HG13	1:A:627:THR:HB	1.83	0.61
1:B:233:LEU:HD23	1:B:234:THR:H	1.66	0.61
1:B:190:ASP:O	1:B:191:LEU:HG	2.01	0.61
1:A:474:THR:O	1:A:477:ASP:N	2.34	0.61
1:A:561:ASN:ND2	1:A:563:ILE:H	1.99	0.61
1:B:476:GLU:OE2	1:B:523:GLN:CB	2.48	0.60
1:B:616:TYR:HB2	1:B:636:ILE:HB	1.81	0.60
1:B:127:LYS:O	1:B:129:GLY:N	2.34	0.60
1:A:425:ARG:HB3	1:A:466:TYR:O	2.01	0.60
1:B:684:SER:HB2	1:B:711:LEU:HD11	1.82	0.60
1:B:666:ASN:N	1:B:708:ARG:HE	1.99	0.60
1:B:310:THR:CG2	2:B:2004:HOH:O	2.49	0.60
1:B:573:ARG:O	1:B:574:LYS:HD3	2.01	0.60
1:B:26:GLU:O	1:B:26:GLU:CG	2.44	0.60
1:B:222:MET:HB3	1:B:223:PRO:HD2	1.83	0.60
1:B:126:TYR:HA	1:B:136:THR:O	2.02	0.60
1:A:285:ILE:HG12	1:A:357:VAL:HG11	1.83	0.60
1:B:171:LEU:H	1:B:171:LEU:HD12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HG	1:B:372:LEU:CD1	2.30	0.60
1:B:111:LYS:HB2	1:B:152:ILE:HG12	1.83	0.60
1:B:352:VAL:HG21	1:B:394:VAL:HG11	1.84	0.60
1:B:627:THR:HG22	1:B:628:TRP:N	2.17	0.59
1:B:230:GLN:HE21	1:B:233:LEU:HD22	1.66	0.59
1:A:353:THR:HG23	1:A:390:ILE:HD12	1.83	0.59
1:B:146:VAL:O	1:B:148:LYS:HE2	2.02	0.59
1:B:78:ARG:HB2	1:B:79:PRO:CD	2.32	0.59
1:B:234:THR:HA	1:B:238:LEU:O	2.03	0.59
1:A:642:SER:HB3	1:A:655:ALA:HB1	1.85	0.59
1:B:535:GLN:HE22	1:B:594:PHE:HA	1.67	0.59
1:A:317:PRO:O	1:A:318:ASP:HB2	2.03	0.58
1:A:265:GLN:HE21	1:A:265:GLN:N	1.99	0.58
1:B:10:ARG:N	1:B:11:PRO:CA	2.57	0.58
1:B:335:LEU:HG	1:B:372:LEU:HD12	1.86	0.58
1:A:410:VAL:CG1	1:A:413:PHE:CE1	2.85	0.58
1:B:596:ARG:HH22	1:B:639:LEU:HD21	1.68	0.58
1:B:472:GLY:O	1:B:473:PHE:CD2	2.56	0.58
1:B:665:ALA:HB3	1:B:666:ASN:CA	2.33	0.58
1:A:297:HIS:CD2	1:A:298:LEU:HD13	2.39	0.58
1:A:290:ASN:OD1	1:A:291:HIS:HD2	1.87	0.58
1:B:10:ARG:NE	1:B:58:GLU:OE1	2.36	0.58
1:A:454:LEU:H	1:A:454:LEU:HD22	1.68	0.58
1:B:618:LEU:CD1	1:B:618:LEU:O	2.47	0.58
1:B:618:LEU:H	1:B:618:LEU:HD12	1.69	0.57
1:B:525:ARG:O	1:B:529:ILE:HG13	2.04	0.57
1:A:339:ARG:NH1	1:A:342:GLN:HE22	2.02	0.57
1:B:215:GLY:HA3	1:B:585:ILE:HD11	1.85	0.57
1:B:82:LEU:HD23	1:B:150:VAL:HG22	1.85	0.57
1:A:410:VAL:HG11	1:A:413:PHE:CE1	2.39	0.57
1:A:561:ASN:HD21	1:A:563:ILE:HB	1.69	0.57
1:B:625:GLU:O	1:B:625:GLU:HG3	2.04	0.57
1:A:399:GLU:O	1:A:401:TRP:CD1	2.57	0.57
1:B:614:THR:OG1	1:B:615:PHE:HA	2.05	0.57
1:A:405:GLN:OE1	1:A:405:GLN:CA	2.53	0.57
1:A:410:VAL:HG12	1:A:410:VAL:O	2.04	0.57
1:A:647:ILE:HG23	1:A:648:ASN:N	2.20	0.57
1:A:453:TYR:HB2	1:A:600:PHE:HE1	1.70	0.56
1:B:633:GLN:HB3	1:B:665:ALA:HB2	1.85	0.56
1:A:263:GLY:H	1:A:265:GLN:HE22	1.52	0.56
1:B:176:ILE:HG13	1:B:539:MET:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ASP:HB3	1:B:516:VAL:H	1.71	0.56
1:A:380:THR:CG2	1:B:380:THR:HG22	2.35	0.56
1:B:705:ILE:HG22	1:B:706:GLU:N	2.20	0.56
1:A:100:ASN:HD21	1:A:102:ASN:HD22	1.54	0.56
1:B:691:LYS:HG2	1:B:692:PRO:CG	2.34	0.56
1:B:209:SER:O	1:B:213:ASP:HB2	2.05	0.56
1:B:473:PHE:CA	1:B:478:LEU:HD13	2.31	0.55
1:B:691:LYS:CG	1:B:692:PRO:CG	2.84	0.55
1:B:234:THR:O	1:B:237:GLY:N	2.31	0.55
1:A:646:GLU:HB3	1:A:652:GLU:O	2.06	0.55
1:B:311:ALA:O	1:B:312:TYR:HB2	2.05	0.55
1:B:478:LEU:N	1:B:478:LEU:CD1	2.66	0.55
1:B:231:ARG:H	1:B:232:PHE:HB2	1.71	0.55
1:A:694:GLU:HG2	1:A:703:LEU:HD11	1.89	0.55
1:A:424:TYR:HA	1:A:445:ARG:HD2	1.87	0.55
1:B:618:LEU:H	1:B:618:LEU:CD1	2.20	0.55
1:B:401:TRP:HZ3	1:B:408:TYR:O	1.89	0.55
1:B:50:LEU:HD23	1:B:50:LEU:H	1.72	0.55
1:A:13:ARG:HH11	1:A:14:PRO:HD2	1.72	0.55
1:B:473:PHE:HD2	1:B:474:THR:N	1.92	0.55
1:B:615:PHE:HD1	1:B:616:TYR:N	2.00	0.55
1:B:24:TRP:CD2	1:B:79:PRO:HD3	2.42	0.55
1:B:365:ALA:HB3	1:B:399:GLU:HG2	1.88	0.55
1:A:525:ARG:HG2	1:A:580:PHE:CD2	2.42	0.55
1:B:634:LEU:HD22	1:B:664:ASN:OD1	2.06	0.54
1:B:421:ASN:C	1:B:421:ASN:HD22	2.09	0.54
1:B:470:HIS:CD2	1:B:470:HIS:O	2.61	0.54
1:A:525:ARG:O	1:A:529:ILE:HG23	2.07	0.54
1:B:469:SER:H	1:B:473:PHE:HZ	1.56	0.54
1:B:265:GLN:H	1:B:265:GLN:HE21	1.55	0.54
1:B:82:LEU:CD2	1:B:150:VAL:HG22	2.37	0.54
1:A:103:LYS:NZ	1:A:125:GLY:H	2.06	0.54
1:A:403:VAL:O	1:A:406:GLY:HA3	2.06	0.54
1:B:24:TRP:CH2	1:B:26:GLU:HB2	2.43	0.54
1:A:336:SER:HB3	1:A:375:VAL:HB	1.88	0.54
1:B:135:LEU:HD11	1:B:321:ARG:HH21	1.71	0.54
1:B:20:LEU:HD21	1:B:69:ILE:HD12	1.88	0.54
1:B:481:TYR:N	1:B:482:ASN:HB2	2.11	0.54
1:A:425:ARG:O	1:A:429:ARG:HG3	2.08	0.53
1:B:424:TYR:HA	1:B:445:ARG:HD2	1.90	0.53
1:B:482:ASN:CB	1:B:504:ASN:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:PHE:CA	1:B:478:LEU:CD1	2.86	0.53
1:B:242:TRP:CD1	1:B:557:PHE:HA	2.43	0.53
1:B:480:SER:HA	1:B:520:ARG:NH2	2.23	0.53
1:B:505:CYS:HB2	1:B:520:ARG:HE	1.74	0.53
1:B:191:LEU:HD11	1:B:206:GLN:CG	2.38	0.53
1:B:13:ARG:HB2	1:B:73:PHE:HB3	1.91	0.53
1:B:310:THR:HG22	2:B:2004:HOH:O	2.07	0.53
1:A:685:SER:HG	1:A:710:ALA:H	1.56	0.53
1:B:118:ILE:O	1:B:145:TYR:HB3	2.09	0.53
1:B:13:ARG:O	1:B:73:PHE:HB3	2.09	0.53
1:B:482:ASN:OD1	1:B:502:SER:C	2.42	0.53
1:A:46:LEU:HD21	1:A:86:ARG:HD2	1.89	0.53
1:B:626:LYS:HB2	1:B:627:THR:HB	1.88	0.52
1:A:98:ARG:NH2	1:A:134:ASP:O	2.42	0.52
1:B:521:GLU:HG3	1:B:525:ARG:HE	1.74	0.52
1:A:297:HIS:O	1:A:298:LEU:CB	2.56	0.52
1:B:486:ASN:HD21	1:B:555:ASN:HB3	1.74	0.52
1:B:103:LYS:HD2	1:B:103:LYS:N	2.24	0.52
1:B:524:LYS:NZ	1:B:547:SER:HB3	2.24	0.52
1:B:627:THR:CG2	1:B:628:TRP:N	2.72	0.52
1:B:20:LEU:HA	1:B:34:SER:OG	2.09	0.52
1:A:410:VAL:HG12	1:A:413:PHE:CE1	2.45	0.52
1:B:472:GLY:O	1:B:473:PHE:CD1	2.63	0.52
1:A:401:TRP:HZ3	1:A:408:TYR:O	1.92	0.52
1:B:495:ASP:OD2	1:B:555:ASN:ND2	2.42	0.51
1:B:692:PRO:O	1:B:693:GLU:C	2.48	0.51
1:A:367:ALA:O	1:A:371:GLU:HG3	2.11	0.51
1:B:265:GLN:NE2	1:B:265:GLN:H	2.09	0.51
1:B:10:ARG:CG	1:B:10:ARG:NH2	2.52	0.51
1:B:712:VAL:HG13	1:B:713:TYR:N	2.25	0.51
1:B:243:GLY:N	2:B:2013:HOH:O	2.34	0.51
1:B:373:TYR:CE1	1:B:404:GLY:HA3	2.46	0.51
1:A:480:SER:HB3	1:A:520:ARG:CZ	2.41	0.50
1:A:646:GLU:HB2	1:A:647:ILE:CA	2.41	0.50
1:A:410:VAL:CG1	1:A:410:VAL:O	2.58	0.50
1:B:349:ARG:HA	1:B:390:ILE:HD11	1.92	0.50
1:B:126:TYR:CE2	1:B:298:LEU:HA	2.46	0.50
1:B:276:LEU:HD22	1:B:281:ILE:HD11	1.93	0.50
1:A:682:VAL:HG23	1:A:683:ILE:HG22	1.93	0.50
1:A:469:SER:HA	1:A:541:LEU:HG	1.92	0.50
1:A:294:GLU:O	1:A:305:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:THR:HA	1:B:473:PHE:CE2	2.47	0.50
1:B:135:LEU:HD11	1:B:321:ARG:NH2	2.26	0.50
1:A:36:PHE:CD1	1:A:339:ARG:HG3	2.47	0.50
1:A:430:ARG:HD2	1:A:435:GLU:OE2	2.12	0.50
1:A:553:ASN:HD22	1:A:555:ASN:H	1.60	0.50
1:A:401:TRP:CZ3	1:A:408:TYR:O	2.65	0.50
1:B:703:LEU:HB3	1:B:704:GLU:CA	2.42	0.49
1:B:476:GLU:HB3	1:B:479:VAL:HG13	1.89	0.49
1:B:541:LEU:CD1	1:B:542:GLY:O	2.60	0.49
1:A:598:ARG:HD2	1:A:598:ARG:O	2.11	0.49
1:B:231:ARG:HB3	1:B:232:PHE:CD2	2.47	0.49
1:B:300:PRO:HB2	1:B:302:LEU:HG	1.95	0.49
1:B:13:ARG:HD2	1:B:13:ARG:N	2.27	0.49
1:A:300:PRO:HB2	1:A:302:LEU:HG	1.95	0.49
1:B:134:ASP:OD2	1:B:134:ASP:O	2.30	0.49
1:A:42:LYS:HB3	1:A:88:TYR:HB2	1.95	0.49
1:B:327:THR:HG22	1:B:364:LEU:HD23	1.94	0.49
1:B:476:GLU:OE1	1:B:520:ARG:CG	2.44	0.49
1:B:674:PHE:CE2	1:B:713:TYR:CE1	2.99	0.49
1:B:121:ASP:CG	1:B:128:ILE:HG12	2.33	0.49
1:B:473:PHE:N	1:B:478:LEU:HD11	2.27	0.49
1:A:689:GLU:H	1:A:689:GLU:CD	2.16	0.49
1:B:494:GLN:O	1:B:494:GLN:HG2	2.13	0.49
1:B:106:ILE:HD12	1:B:302:LEU:O	2.13	0.49
1:B:619:GLU:OE1	1:B:673:LYS:N	2.39	0.48
1:B:614:THR:OG1	1:B:637:PHE:HB2	2.12	0.48
1:B:633:GLN:HB3	1:B:665:ALA:HB3	1.94	0.48
1:B:133:GLN:O	1:B:134:ASP:CB	2.59	0.48
1:B:127:LYS:N	1:B:136:THR:HG23	2.25	0.48
1:B:468:THR:CA	1:B:473:PHE:HE2	2.26	0.48
1:B:692:PRO:O	1:B:694:GLU:HG3	2.12	0.48
1:A:408:TYR:O	1:A:409:GLN:HB2	2.13	0.48
1:B:524:LYS:O	1:B:526:ASN:N	2.37	0.48
1:B:526:ASN:CG	1:B:527:PHE:H	2.17	0.48
1:B:349:ARG:HD3	1:B:388:ASP:OD2	2.13	0.48
1:B:475:LEU:HD12	1:B:544:ASP:HB3	1.94	0.48
1:B:662:ILE:O	1:B:711:LEU:O	2.31	0.48
1:B:294:GLU:HB3	1:B:305:ARG:NH2	2.28	0.48
1:B:440:SER:HB3	1:B:628:TRP:NE1	2.29	0.48
1:B:191:LEU:HD11	1:B:206:GLN:HG3	1.95	0.48
1:B:10:ARG:O	1:B:10:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:LEU:HB2	1:B:713:TYR:CE2	2.48	0.48
1:B:195:ILE:HD12	1:B:201:GLY:HA2	1.96	0.48
1:B:612:ASP:OD2	1:B:641:GLY:HA2	2.13	0.48
1:B:219:VAL:HG23	1:B:281:ILE:HD13	1.95	0.48
1:B:708:ARG:H	1:B:709:THR:CG2	2.15	0.48
1:A:561:ASN:HD22	1:A:563:ILE:N	2.10	0.48
1:B:229:ASP:OD1	1:B:255:ARG:NH2	2.47	0.48
1:A:543:GLY:HA3	1:A:548:ARG:HD3	1.95	0.48
1:B:468:THR:CA	1:B:473:PHE:CE2	2.97	0.48
1:A:195:ILE:HD12	1:A:201:GLY:HA2	1.96	0.48
1:B:441:GLU:O	1:B:444:ASN:HB2	2.13	0.48
1:B:461:PHE:CZ	1:B:597:GLU:HB3	2.49	0.48
1:B:263:GLY:H	1:B:265:GLN:HE22	1.62	0.47
1:B:100:ASN:ND2	1:B:137:TYR:HE1	2.11	0.47
1:B:467:VAL:HG13	1:B:531:LEU:HD13	1.95	0.47
1:B:535:GLN:NE2	1:B:594:PHE:HA	2.29	0.47
1:B:378:LEU:O	1:B:382:PHE:HD2	1.97	0.47
1:B:228:ILE:HG12	1:B:293:ALA:HB1	1.95	0.47
1:B:543:GLY:HA2	1:B:545:GLU:OE2	2.14	0.47
1:B:666:ASN:O	1:B:708:ARG:CZ	2.60	0.47
1:B:666:ASN:C	1:B:708:ARG:CZ	2.63	0.47
1:B:503:TRP:CD1	1:B:504:ASN:N	2.78	0.47
1:B:666:ASN:C	1:B:708:ARG:HE	2.16	0.47
1:B:203:ALA:HB2	1:B:272:MET:HG3	1.95	0.47
1:B:694:GLU:HB3	1:B:703:LEU:HD21	1.95	0.47
1:B:540:ILE:H	1:B:540:ILE:HD12	1.80	0.47
1:A:405:GLN:OE1	1:A:405:GLN:O	2.32	0.47
1:A:290:ASN:OD1	1:A:291:HIS:CD2	2.67	0.47
1:A:464:ILE:HD13	1:A:537:THR:HG23	1.95	0.47
1:A:242:TRP:CZ2	1:A:470:HIS:O	2.67	0.47
1:B:519:CYS:O	1:B:523:GLN:N	2.45	0.47
1:B:465:ASN:O	1:B:538:PRO:HA	2.14	0.47
1:B:184:PHE:CE2	1:B:207:MET:HG3	2.49	0.47
1:B:666:ASN:C	1:B:708:ARG:NE	2.68	0.47
1:B:612:ASP:OD2	1:B:641:GLY:C	2.53	0.47
1:B:467:VAL:HG22	1:B:531:LEU:HD22	1.97	0.47
1:A:132:ASN:HB2	1:A:136:THR:HG23	1.96	0.47
1:A:433:ARG:CZ	1:A:501:TYR:HA	2.45	0.47
1:B:233:LEU:HG	1:B:234:THR:N	2.29	0.46
1:A:24:TRP:CD2	1:A:79:PRO:HD3	2.50	0.46
1:B:473:PHE:CB	1:B:478:LEU:HD21	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:THR:HG1	1:B:615:PHE:HA	1.79	0.46
1:B:241:TYR:CE2	1:B:564:THR:HG21	2.49	0.46
1:A:649:MET:HA	1:B:14:PRO:HG3	1.95	0.46
1:A:49:SER:OG	1:A:57:LYS:HD2	2.15	0.46
1:A:266:VAL:HG12	1:A:270:LYS:HD2	1.97	0.46
1:B:482:ASN:HB3	1:B:504:ASN:HA	1.96	0.46
1:B:614:THR:CG2	1:B:638:VAL:O	2.61	0.46
1:A:393:GLN:HG2	1:B:18:TYR:CD1	2.51	0.46
1:B:362:PHE:HE1	1:B:396:LEU:HD22	1.80	0.46
1:A:402:ASP:OD1	1:A:405:GLN:O	2.34	0.46
1:B:624:ASP:C	1:B:627:THR:HG21	2.35	0.46
1:B:242:TRP:CG	1:B:557:PHE:HA	2.51	0.46
1:B:13:ARG:O	1:B:73:PHE:N	2.42	0.46
1:B:161:GLU:HA	1:B:164:ILE:HD12	1.97	0.46
1:B:705:ILE:CG2	1:B:706:GLU:H	2.26	0.46
1:B:230:GLN:HB3	1:B:232:PHE:O	2.16	0.46
1:B:444:ASN:HB3	1:B:445:ARG:NH1	2.30	0.46
1:B:120:ASN:HD22	1:B:122:ALA:H	1.64	0.46
1:B:219:VAL:HG12	1:B:221:LEU:HD12	1.98	0.46
1:B:152:ILE:O	1:B:154:PRO:HD3	2.16	0.46
1:B:225:PHE:CZ	1:B:287:VAL:HG12	2.51	0.46
1:B:626:LYS:H	1:B:627:THR:HG22	1.81	0.45
1:A:104:VAL:O	1:A:146:VAL:HG11	2.16	0.45
1:A:41:GLU:HG2	1:A:89:GLY:HA2	1.97	0.45
1:B:574:LYS:O	1:B:576:LYS:N	2.49	0.45
1:A:103:LYS:HD3	1:A:125:GLY:HA2	1.99	0.45
1:B:537:THR:HA	1:B:538:PRO:HD3	1.85	0.45
1:A:402:ASP:OD1	1:A:406:GLY:CA	2.65	0.45
1:A:525:ARG:HG2	1:A:580:PHE:CZ	2.50	0.45
1:B:482:ASN:CB	1:B:504:ASN:CA	2.94	0.45
1:B:96:GLY:O	1:B:309:ASN:ND2	2.38	0.45
1:B:619:GLU:CD	1:B:672:VAL:HA	2.37	0.45
1:B:317:PRO:O	1:B:318:ASP:HB2	2.16	0.45
1:B:165:LYS:HA	1:B:166:GLY:HA2	1.56	0.45
1:B:388:ASP:HB3	1:B:391:LEU:HB2	1.98	0.45
1:B:429:ARG:NH2	1:B:467:VAL:O	2.49	0.45
1:A:339:ARG:HH11	1:A:342:GLN:HE22	1.64	0.45
1:A:645:ASP:HA	1:A:646:GLU:HA	1.74	0.45
1:A:553:ASN:ND2	1:A:555:ASN:H	2.14	0.45
1:B:542:GLY:O	1:B:548:ARG:HD3	2.17	0.45
1:B:46:LEU:HD21	1:B:86:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:PRO:O	1:B:75:PRO:HG2	2.17	0.44
1:B:233:LEU:O	1:B:234:THR:C	2.55	0.44
1:B:665:ALA:CB	1:B:666:ASN:CA	2.95	0.44
1:A:352:VAL:HG21	1:A:394:VAL:HG11	2.00	0.44
1:A:172:LYS:HB3	1:A:597:GLU:OE1	2.17	0.44
1:B:593:ALA:HB1	1:B:639:LEU:HG	1.99	0.44
1:B:432:TRP:CZ3	1:B:664:ASN:O	2.70	0.44
1:B:310:THR:HG21	2:B:2004:HOH:O	2.13	0.44
1:A:103:LYS:HZ3	1:A:125:GLY:H	1.65	0.44
1:A:583:LYS:HD2	1:A:683:ILE:HD12	1.99	0.44
1:B:679:TRP:HZ3	1:B:694:GLU:O	2.00	0.44
1:B:708:ARG:HA	1:B:708:ARG:HD3	1.67	0.44
1:B:626:LYS:N	1:B:627:THR:CB	2.75	0.44
1:B:570:LEU:H	1:B:570:LEU:CD2	2.22	0.44
1:B:570:LEU:N	1:B:570:LEU:HD23	2.28	0.44
1:A:403:VAL:N	1:A:406:GLY:HA3	2.33	0.44
1:A:694:GLU:HG2	1:A:703:LEU:HD21	1.99	0.44
1:A:472:GLY:CA	1:A:554:ASN:O	2.65	0.44
1:A:191:LEU:O	1:A:196:ARG:NE	2.51	0.44
1:A:456:ASN:O	1:A:456:ASN:ND2	2.51	0.44
1:A:314:MET:HB3	1:A:324:LEU:HD12	1.98	0.44
1:B:230:GLN:C	1:B:232:PHE:C	2.77	0.44
1:A:479:VAL:O	1:A:520:ARG:HG2	2.18	0.44
1:B:633:GLN:CG	1:B:665:ALA:HB2	2.48	0.44
1:B:571:ASP:O	1:B:571:ASP:OD2	2.35	0.44
1:B:182:LYS:HA	1:B:197:GLY:HA2	2.00	0.44
1:B:614:THR:HG22	1:B:638:VAL:HB	1.47	0.43
1:B:171:LEU:O	1:B:537:THR:HG22	2.17	0.43
1:A:647:ILE:CG2	1:A:648:ASN:N	2.80	0.43
1:A:277:HIS:HE1	1:A:358:ASP:OD2	2.01	0.43
1:B:707:GLY:C	1:B:709:THR:CG2	2.75	0.43
1:B:195:ILE:O	1:B:201:GLY:HA3	2.17	0.43
1:B:430:ARG:HA	1:B:433:ARG:HB3	2.00	0.43
1:A:461:PHE:HZ	1:A:595:ARG:HA	1.83	0.43
1:B:230:GLN:O	1:B:231:ARG:C	2.57	0.43
1:B:191:LEU:HD11	1:B:206:GLN:HG2	2.00	0.43
1:B:28:ASP:OD2	1:B:28:ASP:N	2.50	0.43
1:B:708:ARG:C	1:B:709:THR:HG22	2.39	0.43
1:A:171:LEU:HD22	1:A:537:THR:HG21	1.99	0.43
1:B:126:TYR:CZ	1:B:298:LEU:HA	2.53	0.43
1:B:559:GLN:O	1:B:564:THR:OG1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:GLN:CG	1:B:665:ALA:CB	2.96	0.43
1:B:102:ASN:HB2	1:B:103:LYS:HZ2	1.84	0.43
1:B:473:PHE:C	1:B:474:THR:HG22	2.29	0.43
1:B:475:LEU:HD11	1:B:544:ASP:HB3	1.98	0.43
1:B:711:LEU:HD12	1:B:711:LEU:HA	1.81	0.43
1:A:383:ILE:O	1:A:387:GLN:HG3	2.18	0.43
1:A:681:LEU:HD23	1:A:713:TYR:CE1	2.53	0.43
1:B:638:VAL:HG12	1:B:639:LEU:N	2.34	0.43
1:B:222:MET:HE2	2:B:2013:HOH:O	2.17	0.43
1:A:639:LEU:HA	1:A:639:LEU:HD23	1.86	0.43
1:B:169:VAL:HG11	1:B:217:THR:HB	2.00	0.43
1:B:618:LEU:CD1	1:B:618:LEU:N	2.79	0.43
1:B:703:LEU:CB	1:B:704:GLU:HA	2.46	0.43
1:B:591:HIS:HA	1:B:592:PRO:HD3	1.83	0.43
1:B:347:SER:O	1:B:351:TRP:HD1	2.02	0.43
1:A:222:MET:HB3	1:A:223:PRO:HD2	2.00	0.42
1:B:612:ASP:OD2	1:B:641:GLY:HA3	2.18	0.42
1:B:444:ASN:HB3	1:B:445:ARG:HH12	1.83	0.42
1:A:625:GLU:O	1:A:626:LYS:HB3	2.20	0.42
1:A:176:ILE:HG22	1:A:177:TYR:N	2.34	0.42
1:A:637:PHE:CE1	1:A:661:ILE:HD13	2.54	0.42
1:B:232:PHE:HA	1:B:232:PHE:HD1	1.71	0.42
1:A:410:VAL:HG11	1:A:413:PHE:CZ	2.55	0.42
1:A:226:HIS:O	1:A:247:ILE:HG22	2.19	0.42
1:A:333:LEU:HB3	1:A:340:VAL:HG11	2.01	0.42
1:B:618:LEU:HA	1:B:619:GLU:HA	1.53	0.42
1:A:319:ASN:ND2	1:A:322:TYR:CE2	2.88	0.42
1:B:541:LEU:CD1	1:B:548:ARG:HE	2.32	0.42
1:B:188:ARG:CG	1:B:188:ARG:NH1	2.77	0.42
1:A:474:THR:O	1:A:475:LEU:C	2.58	0.42
1:B:424:TYR:CD1	1:B:445:ARG:HB3	2.55	0.42
1:B:514:GLN:HB3	1:B:514:GLN:HE21	1.74	0.42
1:B:671:LYS:CA	1:B:704:GLU:HG3	2.44	0.42
1:B:230:GLN:O	1:B:232:PHE:C	2.56	0.42
1:B:666:ASN:O	1:B:708:ARG:NE	2.53	0.42
1:A:78:ARG:O	1:A:79:PRO:C	2.57	0.42
1:A:165:LYS:HA	1:A:166:GLY:HA2	1.74	0.42
1:B:121:ASP:CB	1:B:128:ILE:HG12	2.50	0.42
1:A:405:GLN:HB2	2:A:2066:HOH:O	2.19	0.42
1:B:530:THR:O	1:B:533:VAL:HG12	2.20	0.42
1:A:311:ALA:O	1:A:312:TYR:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HG2	1:B:12:LEU:HD21	2.02	0.42
1:B:486:ASN:ND2	1:B:495:ASP:OD2	2.52	0.42
1:B:30:GLY:HA3	1:B:73:PHE:CZ	2.55	0.42
1:B:105:LEU:HA	1:B:302:LEU:O	2.20	0.42
1:A:636:ILE:HG23	1:A:662:ILE:HG12	2.02	0.42
1:B:680:GLU:HB2	1:B:714:ARG:HG2	2.02	0.42
1:B:614:THR:HG21	1:B:638:VAL:HG23	2.02	0.41
1:B:618:LEU:CD2	1:B:618:LEU:O	2.64	0.41
1:B:526:ASN:CG	1:B:527:PHE:N	2.73	0.41
1:B:167:LYS:HD2	1:B:167:LYS:HA	1.79	0.41
1:B:233:LEU:C	1:B:235:ASP:N	2.72	0.41
1:A:10:ARG:HA	2:A:2001:HOH:O	2.20	0.41
1:B:666:ASN:HB2	1:B:667:PRO:CD	2.50	0.41
1:B:24:TRP:HA	1:B:31:VAL:HA	2.02	0.41
1:B:365:ALA:HB1	1:B:398:ALA:HB1	1.99	0.41
1:A:46:LEU:HD21	1:A:86:ARG:HH11	1.86	0.41
1:A:634:LEU:CD2	1:A:636:ILE:HD11	2.51	0.41
1:A:462:ALA:HB1	2:A:2075:HOH:O	2.20	0.41
1:A:282:GLU:OE1	1:A:395:LYS:HE3	2.20	0.41
1:B:468:THR:CG2	1:B:473:PHE:CD2	3.01	0.41
1:B:127:LYS:O	1:B:128:ILE:C	2.58	0.41
1:B:188:ARG:NH1	1:B:190:ASP:OD2	2.54	0.41
1:B:312:TYR:O	1:B:333:LEU:HA	2.20	0.41
1:A:421:ASN:ND2	1:A:424:TYR:H	2.19	0.41
1:A:263:GLY:H	1:A:265:GLN:NE2	2.16	0.41
1:B:128:ILE:HD12	1:B:129:GLY:N	2.36	0.41
1:A:553:ASN:C	1:A:553:ASN:HD22	2.24	0.41
1:B:233:LEU:CG	1:B:234:THR:N	2.83	0.41
1:B:31:VAL:HG23	1:B:77:LEU:HB2	2.02	0.41
1:B:331:ASN:HD22	1:B:331:ASN:C	2.24	0.41
1:B:290:ASN:OD1	1:B:291:HIS:CD2	2.64	0.41
1:B:700:GLU:O	1:B:701:LYS:HG3	2.21	0.41
1:A:338:PRO:O	1:A:342:GLN:HB2	2.21	0.41
1:B:261:CYS:C	1:B:265:GLN:HE22	2.25	0.41
1:B:114:ASN:ND2	1:B:261:CYS:O	2.48	0.41
1:A:429:ARG:O	1:A:433:ARG:HB2	2.21	0.41
1:B:104:VAL:O	1:B:146:VAL:HG11	2.21	0.41
1:B:581:VAL:O	1:B:585:ILE:HG23	2.21	0.41
1:A:41:GLU:CG	1:A:89:GLY:HA2	2.51	0.41
1:A:10:ARG:HB3	1:A:10:ARG:HE	1.69	0.41
1:A:386:GLN:HE22	1:A:412:ASN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:OD1	1:A:328:GLY:N	2.53	0.41
1:B:230:GLN:O	1:B:233:LEU:HD23	2.21	0.41
1:B:431:PHE:CE1	1:B:633:GLN:HA	2.56	0.41
1:B:612:ASP:O	1:B:612:ASP:OD1	2.38	0.41
1:A:561:ASN:HD22	1:A:561:ASN:C	2.23	0.41
1:B:207:MET:O	1:B:208:ILE:HB	2.21	0.41
1:B:177:TYR:HD1	1:B:216:ILE:HG21	1.86	0.41
1:A:25:ILE:HG21	1:A:28:ASP:OD2	2.20	0.41
1:B:233:LEU:O	1:B:236:LYS:N	2.30	0.40
1:B:559:GLN:NE2	1:B:561:ASN:HD22	2.19	0.40
1:B:478:LEU:O	1:B:478:LEU:HD23	2.18	0.40
1:A:474:THR:O	1:A:476:GLU:N	2.54	0.40
1:B:349:ARG:HG2	1:B:390:ILE:HD11	2.04	0.40
1:B:672:VAL:N	1:B:704:GLU:HG3	2.36	0.40
1:B:524:LYS:HZ3	1:B:547:SER:HB3	1.85	0.40
1:A:716:ILE:O	1:A:717:GLU:HG3	2.21	0.40
1:B:9:ASP:HB2	1:B:10:ARG:HB2	2.04	0.40
1:A:203:ALA:HB2	1:A:272:MET:HG3	2.04	0.40
1:B:324:LEU:O	1:B:332:THR:HG22	2.20	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ASN:C	1:B:572:GLU:OE2[5_554]	0.89	1.31
1:B:571:ASP:OD1	1:B:571:ASP:OD1[5_554]	1.34	0.86
1:B:569:ASN:CA	1:B:572:GLU:OE2[5_554]	1.47	0.73
1:B:569:ASN:ND2	1:B:572:GLU:OE1[5_554]	1.58	0.62
1:B:569:ASN:O	1:B:572:GLU:OE2[5_554]	1.61	0.59
1:A:336:SER:OG	1:A:404:GLY:O[6_554]	1.68	0.52
1:B:570:LEU:N	1:B:572:GLU:OE2[5_554]	1.75	0.45
1:B:569:ASN:CB	1:B:572:GLU:OE2[5_554]	1.91	0.29
1:B:569:ASN:C	1:B:572:GLU:CD[5_554]	2.05	0.15
1:B:571:ASP:CG	1:B:571:ASP:OD1[5_554]	2.09	0.11
1:B:569:ASN:CG	1:B:572:GLU:OE1[5_554]	2.09	0.11
1:B:569:ASN:CB	1:B:572:GLU:OE1[5_554]	2.10	0.10
1:B:569:ASN:CB	1:B:572:GLU:CD[5_554]	2.16	0.04



## 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	695/718 (97%)	629 (90%)	62 (9%)	4 (1%)	30	72
1	B	652/718 (91%)	531 (81%)	113 (17%)	8 (1%)	16	56
All	All	1347/1436 (94%)	1160 (86%)	175 (13%)	12 (1%)	21	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	ILE
1	B	517	VAL
1	B	234	THR
1	B	190	ASP
1	B	420	TRP
1	B	675	PRO
1	B	231	ARG
1	A	457	ASN
1	B	10	ARG
1	A	164	ILE
1	A	643	VAL
1	B	128	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	617/636 (97%)	572 (93%)	45 (7%)	17	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	589/636 (93%)	513 (87%)	76 (13%)	5	23
All	All	1206/1272 (95%)	1085 (90%)	121 (10%)	9	34

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	53	GLN
1	A	100	ASN
1	A	103	LYS
1	A	135	LEU
1	A	207	MET
1	A	231	ARG
1	A	240	ASN
1	A	254	CYS
1	A	265	GLN
1	A	335	LEU
1	A	368	LEU
1	A	378	LEU
1	A	380	THR
1	A	405	GLN
1	A	410	VAL
1	A	421	ASN
1	A	425	ARG
1	A	454	LEU
1	A	457	ASN
1	A	459	THR
1	A	474	THR
1	A	480	SER
1	A	525	ARG
1	A	529	ILE
1	A	533	VAL
1	A	537	THR
1	A	541	LEU
1	A	545	GLU
1	A	549	THR
1	A	553	ASN
1	A	561	ASN
1	A	570	LEU
1	A	576	LYS
1	A	589	ARG
1	A	598	ARG

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Mol	Chain	Res	Type
1	A	599	TYR
1	A	613	VAL
1	A	614	THR
1	A	618	LEU
1	A	627	THR
1	A	646	GLU
1	A	658	SER
1	A	660	LEU
1	A	700	GLU
1	B	8	ARG
1	B	9	ASP
1	B	10	ARG
1	B	24	TRP
1	B	28	ASP
1	B	94	GLU
1	B	100	ASN
1	B	111	LYS
1	B	128	ILE
1	B	130	ASP
1	B	134	ASP
1	B	137	TYR
1	B	148	LYS
1	B	165	LYS
1	B	167	LYS
1	B	176	ILE
1	B	188	ARG
1	B	193	GLU
1	B	206	GLN
1	B	207	MET
1	B	217	THR
1	B	230	GLN
1	B	232	PHE
1	B	245	ASP
1	B	247	ILE
1	B	265	GLN
1	B	281	ILE
1	B	297	HIS
1	B	315	LEU
1	B	327	THR
1	B	331	ASN
1	B	372	LEU
1	B	380	THR

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Mol	Chain	Res	Type
1	B	421	ASN
1	B	447	LEU
1	B	452	ILE
1	B	457	ASN
1	B	461	PHE
1	B	464	ILE
1	B	475	LEU
1	B	478	LEU
1	B	479	VAL
1	B	481	TYR
1	B	491	PHE
1	B	493	ASN
1	B	504	ASN
1	B	520	ARG
1	B	533	VAL
1	B	545	GLU
1	B	558	CYS
1	B	564	THR
1	B	570	LEU
1	B	572	GLU
1	B	573	ARG
1	B	574	LYS
1	B	583	LYS
1	B	584	MET
1	B	596	ARG
1	B	613	VAL
1	B	618	LEU
1	B	619	GLU
1	B	626	LYS
1	B	627	THR
1	B	634	LEU
1	B	663	LEU
1	B	666	ASN
1	B	682	VAL
1	B	686	TYR
1	B	690	ILE
1	B	691	LYS
1	B	702	GLU
1	B	704	GLU
1	B	708	ARG
1	B	709	THR
1	B	711	LEU

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Mol	Chain	Res	Type
1	B	712	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	71	HIS
1	A	102	ASN
1	A	120	ASN
1	A	133	GLN
1	A	240	ASN
1	A	265	GLN
1	A	291	HIS
1	A	297	HIS
1	A	342	GLN
1	A	421	ASN
1	A	456	ASN
1	A	465	ASN
1	A	489	ASN
1	A	493	ASN
1	A	494	GLN
1	A	553	ASN
1	A	559	GLN
1	A	561	ASN
1	A	591	HIS
1	A	633	GLN
1	A	668	ASN
1	A	669	ASN
1	B	32	ASN
1	B	102	ASN
1	B	120	ASN
1	B	230	GLN
1	B	265	GLN
1	B	277	HIS
1	B	291	HIS
1	B	331	ASN
1	B	356	HIS
1	B	376	ASN
1	B	409	GLN
1	B	421	ASN
1	B	465	ASN
1	B	486	ASN

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Mol	Chain	Res	Type
1	B	500	ASN
1	B	504	ASN
1	B	514	GLN
1	B	535	GLN
1	B	559	GLN
1	B	666	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	699/718 (97%)	-0.15	17 (2%) 62 32	25, 52, 83, 92	3 (0%)
1	B	666/718 (92%)	0.39	70 (10%) 8 3	34, 82, 122, 128	2 (0%)
All	All	1365/1436 (95%)	0.11	87 (6%) 23 8	25, 61, 118, 128	5 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	LEU	4.9
1	A	455	GLY	4.9
1	B	631	PRO	4.7
1	A	718	LEU	4.5
1	B	506	GLY	4.3
1	B	706	GLU	4.2
1	B	436	ALA	4.1
1	B	166	GLY	3.8
1	A	645	ASP	3.8
1	B	133	GLN	3.7
1	B	515	ASN	3.7
1	A	642	SER	3.6
1	B	131	GLN	3.6
1	B	690	ILE	3.5
1	A	453	TYR	3.4
1	B	632	THR	3.4
1	B	408	TYR	3.2
1	B	553	ASN	3.2
1	B	627	THR	3.1
1	B	516	VAL	3.1
1	A	512	ASN	3.1
1	B	628	TRP	3.1
1	B	476	GLU	3.1
1	B	700	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	491	PHE	3.0
1	B	707	GLY	3.0
1	B	157	GLU	3.0
1	B	569	ASN	2.9
1	B	583	LYS	2.9
1	B	502	SER	2.9
1	A	457	ASN	2.8
1	B	567	ASP	2.7
1	B	503	TRP	2.7
1	B	237	GLY	2.7
1	B	482	ASN	2.7
1	B	703	LEU	2.7
1	B	434	GLY	2.6
1	B	562	GLU	2.6
1	A	408	TYR	2.6
1	A	131	GLN	2.6
1	B	458	LYS	2.5
1	B	513	ASP	2.5
1	B	155	TYR	2.5
1	B	232	PHE	2.5
1	B	437	LEU	2.5
1	B	461	PHE	2.5
1	B	132	ASN	2.5
1	B	438	PRO	2.5
1	B	591	HIS	2.5
1	B	236	LYS	2.5
1	B	676	LYS	2.5
1	B	699	GLY	2.4
1	B	238	LEU	2.4
1	B	640	GLU	2.4
1	A	407	GLY	2.4
1	A	677	GLY	2.4
1	B	190	ASP	2.3
1	B	189	LEU	2.3
1	B	134	ASP	2.3
1	B	239	THR	2.3
1	B	572	GLU	2.3
1	B	534	SER	2.3
1	B	514	GLN	2.3
1	B	715	ARG	2.3
1	B	701	LYS	2.3
1	B	624	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	598	ARG	2.2
1	B	592	PRO	2.2
1	A	494	GLN	2.2
1	B	685	SER	2.1
1	B	130	ASP	2.1
1	B	162	ASP	2.1
1	A	189	LEU	2.1
1	B	710	ALA	2.1
1	B	459	THR	2.1
1	B	497	MET	2.1
1	A	27	ASP	2.1
1	A	157	GLU	2.1
1	A	643	VAL	2.1
1	B	541	LEU	2.1
1	B	702	GLU	2.1
1	B	129	GLY	2.1
1	B	641	GLY	2.0
1	B	691	LYS	2.0
1	B	693	GLU	2.0
1	B	478	LEU	2.0
1	B	679	TRP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.