



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 2VUY / pdb_00002vuy
Title : Crystal structure of Glycogen Debranching exzyme TreX from Sulfolobus solfatarius
Authors : Song, H.-N.; Yoon, S.-M.; Cha, H.-J.; Park, K.-H.; Woo, E.-J.
Deposited on : 2008-06-02
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

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
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

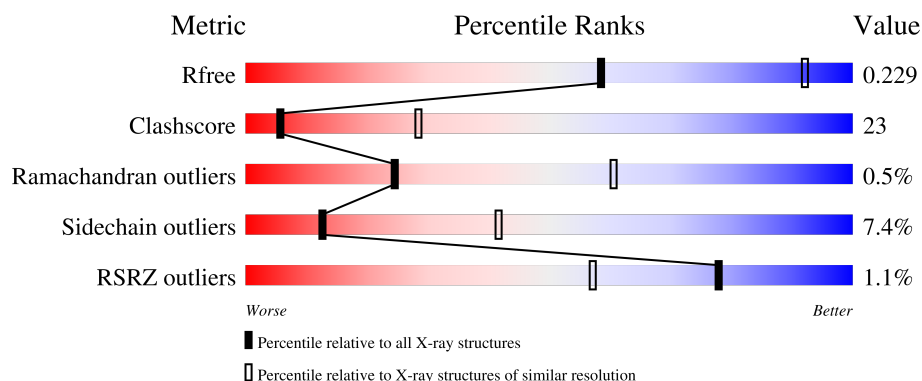
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	718	61% 33% 6%
1	B	718	61% 32% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11634 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.

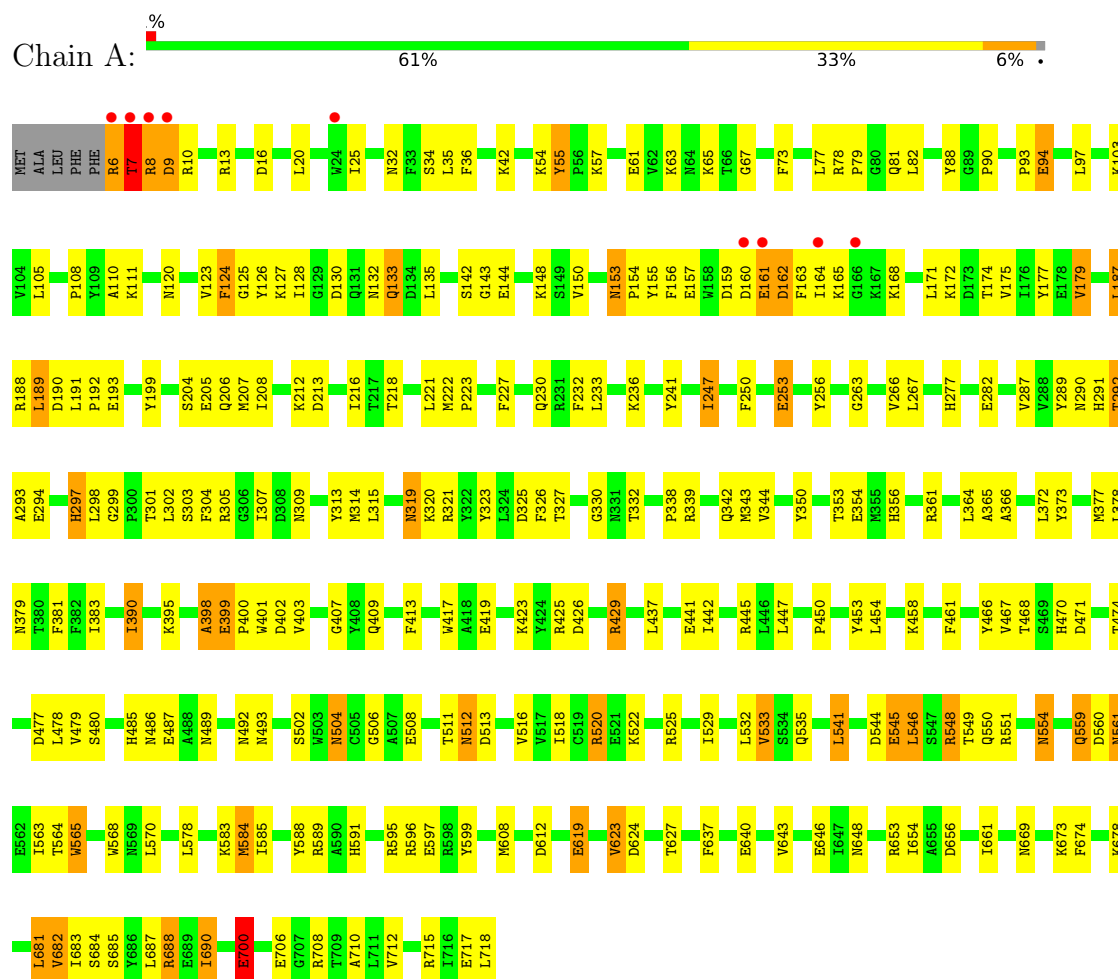
- Molecule 1 is a protein called GLYCOGEN OPERON PROTEIN GLGX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	0	0
			5826	3735	983	1089	19			
1	B	711	Total	C	N	O	S	0	0	0
			5808	3725	978	1086	19			

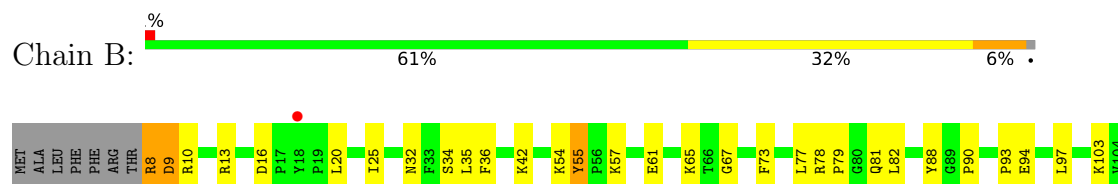
3 Residue-property plots [i](#)

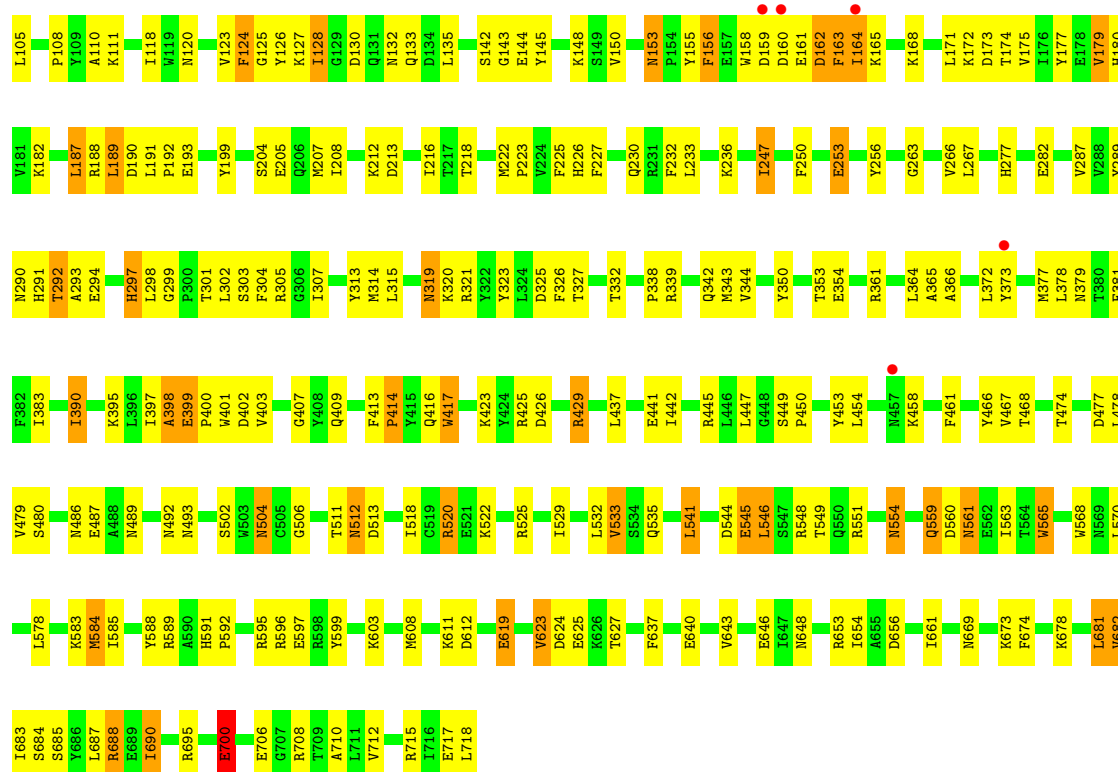
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GLYCOGEN OPERON PROTEIN GLGX



• Molecule 1: GLYCOGEN OPERON PROTEIN GLGX





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.63Å 203.63Å 89.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 3.00 29.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.86-3.00) 92.9 (29.86-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.56 (at 3.01Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.206 , 0.231 0.204 , 0.229	Depositor DCC
R_{free} test set	2004 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11634	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

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	0.38	0/5978	0.89	13/8104 (0.2%)
1	B	0.37	0/5960	0.89	13/8080 (0.2%)
All	All	0.37	0/11938	0.89	26/16184 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	3
All	All	1	5

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	HIS	N-CA-C	-7.84	100.77	110.41
1	A	297	HIS	N-CA-C	-7.69	100.95	110.41
1	A	373	TYR	N-CA-C	6.59	120.42	112.38
1	B	373	TYR	N-CA-C	6.59	120.42	112.38
1	B	474	THR	N-CA-C	-6.56	100.27	110.17
1	B	321	ARG	N-CA-C	-6.49	104.05	112.23
1	A	321	ARG	N-CA-C	-6.48	104.06	112.23
1	A	7	THR	CB-CA-C	-6.46	109.13	116.63
1	A	474	THR	N-CA-C	-6.42	100.47	110.17
1	B	128	ILE	N-CA-C	6.29	116.97	110.36
1	B	124	PHE	N-CA-C	6.26	121.98	113.97
1	A	124	PHE	N-CA-C	6.23	121.95	113.97
1	A	512	ASN	N-CA-C	-6.19	105.52	114.12
1	B	512	ASN	N-CA-C	-5.92	105.89	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	LYS	N-CA-C	-5.90	106.09	113.28
1	A	57	LYS	N-CA-C	-5.82	106.19	113.28
1	B	674	PHE	N-CA-C	5.42	115.83	109.60
1	B	287	VAL	N-CA-C	5.29	116.33	108.46
1	A	287	VAL	N-CA-C	5.26	116.29	108.46
1	A	674	PHE	N-CA-C	5.23	115.61	109.60
1	B	570	LEU	N-CA-C	5.14	117.61	109.24
1	A	570	LEU	N-CA-C	5.12	117.58	109.24
1	B	390	ILE	N-CA-C	5.10	115.77	110.82
1	A	390	ILE	N-CA-C	5.09	115.75	110.82
1	B	625	GLU	N-CA-C	5.08	117.21	111.02
1	A	309	ASN	N-CA-C	5.05	117.17	111.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	THR	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	ALA	Peptide
1	A	7	THR	Peptide
1	B	398	ALA	Peptide
1	B	417	TRP	Peptide
1	B	9	ASP	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	5826	0	5642	280	0
1	B	5808	0	5622	258	0
All	All	11634	0	11264	534	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 23.

All (534) 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:6:ARG:NH1	1:A:7:THR:HG22	1.29	1.43
1:A:6:ARG:CG	1:A:7:THR:H	1.59	1.15
1:A:511:THR:HG22	1:A:513:ASP:H	1.13	1.10
1:B:8:ARG:O	1:B:8:ARG:HG2	1.51	1.10
1:B:292:THR:HG22	1:B:294:GLU:H	1.17	1.08
1:B:511:THR:HG22	1:B:513:ASP:H	1.16	1.07
1:A:6:ARG:HG2	1:A:7:THR:N	1.51	1.07
1:A:292:THR:HG22	1:A:294:GLU:H	1.16	1.06
1:A:6:ARG:NH1	1:A:7:THR:CG2	2.19	1.05
1:A:6:ARG:CZ	1:A:7:THR:HG22	1.85	1.05
1:A:8:ARG:HH11	1:A:8:ARG:CG	1.75	0.99
1:A:161:GLU:OE2	1:A:356:HIS:ND1	1.95	0.99
1:A:549:THR:HG22	1:A:551:ARG:H	1.30	0.97
1:B:549:THR:HG22	1:B:551:ARG:H	1.30	0.96
1:B:400:PRO:HA	1:B:413:PHE:CE1	2.02	0.94
1:B:339:ARG:HH11	1:B:342:GLN:HE22	1.16	0.92
1:A:690:ILE:HD13	1:A:690:ILE:H	1.38	0.89
1:A:339:ARG:HH11	1:A:342:GLN:HE22	1.16	0.89
1:B:690:ILE:HD13	1:B:690:ILE:H	1.39	0.88
1:A:8:ARG:HH11	1:A:8:ARG:HG3	1.39	0.87
1:A:6:ARG:HG2	1:A:7:THR:H	0.71	0.86
1:B:682:VAL:HG22	1:B:683:ILE:HG13	1.56	0.85
1:A:230:GLN:HB2	1:A:233:LEU:HD23	1.59	0.85
1:A:561:ASN:HD22	1:A:563:ILE:H	1.22	0.84
1:A:161:GLU:OE1	1:A:277:HIS:ND1	2.10	0.83
1:A:682:VAL:HG22	1:A:683:ILE:HG13	1.58	0.83
1:A:623:VAL:HG22	1:A:627:THR:HG23	1.60	0.83
1:B:230:GLN:HB2	1:B:233:LEU:HD23	1.59	0.83
1:B:561:ASN:HD22	1:B:563:ILE:H	1.23	0.82
1:A:584:MET:CE	1:A:683:ILE:HD13	2.10	0.81
1:A:193:GLU:O	1:A:193:GLU:HG2	1.80	0.81
1:A:715:ARG:HD3	1:A:718:LEU:HB2	1.63	0.81
1:B:584:MET:CE	1:B:683:ILE:HD13	2.11	0.80
1:B:715:ARG:HD3	1:B:718:LEU:HB2	1.64	0.80
1:A:16:ASP:H	1:A:32:ASN:HD21	1.27	0.80
1:B:193:GLU:O	1:B:193:GLU:HG2	1.81	0.80
1:B:8:ARG:NH2	1:B:61:GLU:H	1.78	0.80
1:A:338:PRO:HG3	1:B:383:ILE:HD12	1.64	0.80
1:B:623:VAL:HG22	1:B:627:THR:HG23	1.62	0.79
1:B:453:TYR:HB3	1:B:458:LYS:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:GLU:HB3	1:B:643:VAL:HG22	1.65	0.79
1:A:453:TYR:HB3	1:A:458:LYS:HB2	1.65	0.78
1:A:640:GLU:HB3	1:A:643:VAL:HG22	1.65	0.78
1:B:479:VAL:O	1:B:520:ARG:HD2	1.83	0.78
1:A:511:THR:HG22	1:A:513:ASP:N	1.97	0.78
1:B:16:ASP:H	1:B:32:ASN:HD21	1.29	0.77
1:B:222:MET:HB3	1:B:223:PRO:CD	2.14	0.77
1:A:13:ARG:HB2	1:A:73:PHE:HB3	1.66	0.77
1:A:161:GLU:O	1:A:165:LYS:HG2	1.84	0.77
1:A:383:ILE:HD12	1:B:338:PRO:HG3	1.66	0.77
1:B:13:ARG:HB2	1:B:73:PHE:HB3	1.67	0.77
1:A:400:PRO:HA	1:A:413:PHE:CE1	2.20	0.77
1:A:77:LEU:HD22	1:A:81:GLN:HE21	1.50	0.76
1:A:153:ASN:HD22	1:A:153:ASN:C	1.91	0.76
1:A:8:ARG:HG3	1:A:8:ARG:NH1	1.95	0.76
1:A:479:VAL:O	1:A:520:ARG:HD2	1.85	0.76
1:A:477:ASP:OD2	1:A:549:THR:HG23	1.85	0.75
1:A:339:ARG:HH11	1:A:342:GLN:NE2	1.83	0.75
1:B:339:ARG:HH11	1:B:342:GLN:NE2	1.83	0.75
1:A:191:LEU:HB3	1:A:192:PRO:HD2	1.67	0.74
1:A:339:ARG:NH1	1:A:342:GLN:HE22	1.85	0.74
1:B:511:THR:HG22	1:B:513:ASP:N	1.99	0.74
1:B:339:ARG:NH1	1:B:342:GLN:HE22	1.85	0.74
1:A:624:ASP:H	1:A:627:THR:CG2	2.01	0.73
1:B:477:ASP:OD2	1:B:549:THR:HG23	1.88	0.73
1:B:624:ASP:H	1:B:627:THR:CG2	2.02	0.73
1:B:292:THR:HG22	1:B:294:GLU:N	2.00	0.72
1:A:292:THR:HG22	1:A:294:GLU:N	2.00	0.72
1:A:153:ASN:HD22	1:A:154:PRO:N	1.86	0.72
1:B:77:LEU:HD22	1:B:81:GLN:HE21	1.52	0.72
1:B:222:MET:HB3	1:B:223:PRO:HD2	1.71	0.71
1:B:624:ASP:OD2	1:B:627:THR:HG22	1.89	0.71
1:A:6:ARG:C	1:A:7:THR:HG23	2.14	0.71
1:A:624:ASP:OD2	1:A:627:THR:HG22	1.90	0.71
1:B:585:ILE:O	1:B:589:ARG:HG3	1.89	0.71
1:B:648:ASN:HB3	1:B:654:ILE:HD11	1.73	0.71
1:A:379:ASN:ND2	1:A:381:PHE:HB3	2.06	0.71
1:A:511:THR:HG22	1:A:512:ASN:N	2.06	0.71
1:B:297:HIS:O	1:B:298:LEU:HB2	1.91	0.71
1:B:559:GLN:CG	1:B:563:ILE:HD12	2.21	0.71
1:B:379:ASN:ND2	1:B:381:PHE:HB3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ILE:O	1:A:589:ARG:HG3	1.90	0.70
1:B:218:THR:HG22	1:B:282:GLU:HB2	1.74	0.70
1:A:297:HIS:O	1:A:298:LEU:HB2	1.92	0.70
1:A:8:ARG:HH11	1:A:8:ARG:HG2	1.57	0.70
1:B:511:THR:HG22	1:B:512:ASN:N	2.07	0.70
1:B:559:GLN:HG2	1:B:563:ILE:HD12	1.73	0.70
1:A:559:GLN:CG	1:A:563:ILE:HD12	2.21	0.69
1:A:153:ASN:HD22	1:A:154:PRO:CD	2.04	0.69
1:A:648:ASN:HB3	1:A:654:ILE:HD11	1.74	0.69
1:B:398:ALA:HB2	1:B:417:TRP:CE3	2.28	0.68
1:A:6:ARG:NH2	1:A:7:THR:OG1	2.26	0.68
1:B:191:LEU:HB3	1:B:192:PRO:HD2	1.75	0.68
1:A:218:THR:HG22	1:A:282:GLU:HB2	1.75	0.68
1:A:303:SER:O	1:A:307:ILE:HG13	1.93	0.68
1:A:379:ASN:HD21	1:A:381:PHE:HB3	1.59	0.68
1:A:559:GLN:HG2	1:A:563:ILE:HD12	1.75	0.67
1:A:619:GLU:CD	1:A:619:GLU:H	2.02	0.67
1:B:301:THR:HG22	1:B:301:THR:O	1.94	0.67
1:B:326:PHE:O	1:B:403:VAL:HG22	1.94	0.67
1:A:172:LYS:HB3	1:A:461:PHE:CZ	2.30	0.67
1:A:584:MET:HE3	1:A:683:ILE:HD13	1.76	0.67
1:B:400:PRO:HA	1:B:413:PHE:HE1	1.56	0.67
1:A:222:MET:HB3	1:A:223:PRO:HD2	1.78	0.66
1:B:172:LYS:HB3	1:B:461:PHE:CZ	2.30	0.66
1:B:379:ASN:HD21	1:B:381:PHE:HB3	1.60	0.66
1:B:584:MET:HE3	1:B:683:ILE:HD13	1.77	0.66
1:A:518:ILE:HG23	1:A:687:LEU:HD12	1.78	0.66
1:A:8:ARG:CG	1:A:8:ARG:NH1	2.44	0.66
1:A:54:LYS:C	1:A:55:TYR:HD2	2.04	0.65
1:B:518:ILE:HG23	1:B:687:LEU:HD12	1.78	0.65
1:A:153:ASN:HD22	1:A:154:PRO:HD2	1.61	0.65
1:A:511:THR:HG22	1:A:512:ASN:H	1.62	0.65
1:B:511:THR:HG22	1:B:512:ASN:H	1.62	0.65
1:A:468:THR:HG21	1:A:544:ASP:OD2	1.97	0.65
1:A:486:ASN:HB3	1:A:489:ASN:ND2	2.12	0.65
1:B:54:LYS:C	1:B:55:TYR:HD2	2.05	0.65
1:A:222:MET:HB3	1:A:223:PRO:CD	2.28	0.64
1:A:161:GLU:CD	1:A:356:HIS:HD1	2.04	0.64
1:B:619:GLU:CD	1:B:619:GLU:H	2.03	0.64
1:A:301:THR:O	1:A:301:THR:HG22	1.96	0.64
1:A:690:ILE:H	1:A:690:ILE:CD1	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:SER:O	1:B:307:ILE:HG13	1.99	0.63
1:A:425:ARG:O	1:A:429:ARG:HB2	1.98	0.63
1:B:153:ASN:C	1:B:153:ASN:HD22	2.07	0.63
1:B:682:VAL:HG13	1:B:712:VAL:O	1.99	0.63
1:B:486:ASN:HB3	1:B:489:ASN:ND2	2.13	0.62
1:A:365:ALA:HB3	1:A:399:GLU:O	1.99	0.62
1:B:425:ARG:O	1:B:429:ARG:HB2	1.98	0.62
1:A:153:ASN:C	1:A:153:ASN:ND2	2.54	0.62
1:B:171:LEU:HD23	1:B:395:LYS:HE3	1.82	0.62
1:B:193:GLU:O	1:B:193:GLU:CG	2.47	0.62
1:B:8:ARG:O	1:B:8:ARG:CG	2.34	0.62
1:A:193:GLU:O	1:A:193:GLU:CG	2.47	0.62
1:A:584:MET:HE1	1:A:683:ILE:HD13	1.82	0.61
1:A:6:ARG:CG	1:A:7:THR:N	2.31	0.61
1:B:584:MET:HE1	1:B:683:ILE:HD13	1.83	0.61
1:A:171:LEU:HD23	1:A:395:LYS:HE3	1.83	0.61
1:B:468:THR:HG21	1:B:544:ASP:OD2	2.00	0.61
1:B:554:ASN:C	1:B:554:ASN:ND2	2.58	0.60
1:B:305:ARG:HD3	1:B:323:TYR:OH	2.02	0.60
1:A:338:PRO:HG3	1:B:383:ILE:CD1	2.31	0.60
1:A:398:ALA:HB2	1:A:417:TRP:CZ3	2.37	0.60
1:B:365:ALA:HB3	1:B:399:GLU:O	2.01	0.60
1:A:561:ASN:ND2	1:A:563:ILE:H	1.96	0.60
1:B:554:ASN:C	1:B:554:ASN:HD22	2.09	0.60
1:A:247:ILE:HD12	1:A:247:ILE:H	1.66	0.59
1:A:624:ASP:H	1:A:627:THR:HG22	1.67	0.59
1:A:6:ARG:CZ	1:A:7:THR:CG2	2.69	0.59
1:B:105:LEU:HD12	1:B:302:LEU:O	2.02	0.59
1:B:450:PRO:HG3	1:B:599:TYR:CD2	2.38	0.59
1:B:164:ILE:HG12	1:B:164:ILE:O	2.02	0.59
1:A:560:ASP:OD2	1:A:565:TRP:HH2	1.86	0.59
1:B:425:ARG:HD2	1:B:466:TYR:CE2	2.38	0.59
1:B:624:ASP:H	1:B:627:THR:HG22	1.68	0.59
1:B:105:LEU:HA	1:B:302:LEU:O	2.02	0.59
1:A:682:VAL:HG13	1:A:712:VAL:O	2.03	0.58
1:B:8:ARG:HH22	1:B:61:GLU:H	1.49	0.58
1:A:105:LEU:HA	1:A:302:LEU:O	2.02	0.58
1:A:560:ASP:OD2	1:A:565:TRP:CH2	2.56	0.58
1:A:690:ILE:HD13	1:A:690:ILE:N	2.14	0.58
1:B:608:MET:HG3	1:B:643:VAL:HG12	1.85	0.58
1:B:247:ILE:H	1:B:247:ILE:HD12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ASN:ND2	1:B:563:ILE:H	1.97	0.58
1:A:305:ARG:HD3	1:A:323:TYR:OH	2.04	0.58
1:B:163:PHE:C	1:B:165:LYS:H	2.12	0.58
1:B:690:ILE:HD13	1:B:690:ILE:N	2.16	0.58
1:B:461:PHE:CE2	1:B:597:GLU:HG3	2.39	0.58
1:A:36:PHE:CE1	1:A:339:ARG:HG3	2.39	0.57
1:B:560:ASP:OD2	1:B:565:TRP:CH2	2.57	0.57
1:A:6:ARG:HH11	1:A:7:THR:HG22	1.54	0.57
1:A:153:ASN:ND2	1:A:154:PRO:HD2	2.20	0.57
1:A:554:ASN:C	1:A:554:ASN:HD22	2.13	0.57
1:B:126:TYR:CZ	1:B:298:LEU:HA	2.40	0.57
1:A:398:ALA:HB2	1:A:417:TRP:CE3	2.40	0.57
1:A:36:PHE:CD1	1:A:339:ARG:HG3	2.40	0.57
1:A:126:TYR:CZ	1:A:298:LEU:HA	2.39	0.57
1:A:425:ARG:NH1	1:A:426:ASP:OD2	2.38	0.57
1:A:450:PRO:HG3	1:A:599:TYR:CD2	2.40	0.57
1:A:554:ASN:C	1:A:554:ASN:ND2	2.61	0.57
1:A:292:THR:HG21	1:A:313:TYR:OH	2.05	0.57
1:A:326:PHE:O	1:A:403:VAL:HG22	2.05	0.57
1:B:158:TRP:HB3	1:B:161:GLU:HB3	1.87	0.57
1:A:584:MET:HE3	1:A:683:ILE:HG21	1.87	0.56
1:A:608:MET:HG3	1:A:643:VAL:HG12	1.86	0.56
1:A:425:ARG:HD2	1:A:466:TYR:CE2	2.40	0.56
1:B:36:PHE:CD1	1:B:339:ARG:HG3	2.40	0.56
1:A:461:PHE:CE2	1:A:597:GLU:HG3	2.40	0.56
1:B:690:ILE:H	1:B:690:ILE:CD1	2.11	0.56
1:A:6:ARG:HH22	1:A:63:LYS:NZ	2.04	0.56
1:B:160:ASP:O	1:B:163:PHE:HB2	2.05	0.56
1:B:425:ARG:NH1	1:B:426:ASP:OD2	2.39	0.56
1:B:216:ILE:HD12	1:B:216:ILE:C	2.31	0.55
1:B:437:LEU:HB2	1:B:442:ILE:HD11	1.88	0.55
1:B:560:ASP:OD2	1:B:565:TRP:HH2	1.87	0.55
1:A:188:ARG:HG3	1:A:190:ASP:HB3	1.88	0.55
1:B:416:GLN:O	1:B:416:GLN:HG2	2.06	0.55
1:A:127:LYS:HB2	1:A:130:ASP:HB2	1.89	0.55
1:B:189:LEU:HD22	1:B:189:LEU:H	1.72	0.55
1:B:36:PHE:CE1	1:B:339:ARG:HG3	2.42	0.55
1:A:120:ASN:O	1:A:123:VAL:HG22	2.07	0.55
1:B:504:ASN:C	1:B:504:ASN:HD22	2.15	0.55
1:A:216:ILE:C	1:A:216:ILE:HD12	2.32	0.55
1:B:216:ILE:HD12	1:B:216:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:C	1:A:190:ASP:H	2.16	0.54
1:B:486:ASN:HD21	1:B:554:ASN:ND2	2.05	0.54
1:A:486:ASN:HD21	1:A:554:ASN:ND2	2.05	0.54
1:A:504:ASN:C	1:A:504:ASN:HD22	2.14	0.54
1:B:584:MET:HE3	1:B:683:ILE:HG21	1.89	0.54
1:A:16:ASP:N	1:A:32:ASN:HD21	2.02	0.54
1:A:640:GLU:HB3	1:A:643:VAL:CG2	2.36	0.54
1:A:189:LEU:H	1:A:189:LEU:HD22	1.73	0.53
1:A:437:LEU:HB2	1:A:442:ILE:HD11	1.89	0.53
1:A:105:LEU:HD12	1:A:302:LEU:O	2.08	0.53
1:A:294:GLU:O	1:A:305:ARG:NH2	2.41	0.53
1:B:400:PRO:CA	1:B:413:PHE:CE1	2.85	0.53
1:A:132:ASN:O	1:A:133:GLN:C	2.52	0.53
1:B:681:LEU:HD22	1:B:682:VAL:H	1.74	0.53
1:A:93:PRO:HB2	1:A:135:LEU:HD23	1.91	0.53
1:B:159:ASP:C	1:B:161:GLU:H	2.17	0.53
1:B:162:ASP:C	1:B:165:LYS:HG2	2.34	0.53
1:A:55:TYR:N	1:A:55:TYR:CD2	2.76	0.53
1:B:54:LYS:HG3	1:B:144:GLU:HB2	1.90	0.53
1:B:640:GLU:HB3	1:B:643:VAL:CG2	2.37	0.53
1:A:216:ILE:HD12	1:A:216:ILE:O	2.10	0.52
1:A:681:LEU:HD22	1:A:682:VAL:H	1.74	0.52
1:B:127:LYS:HB2	1:B:130:ASP:HB2	1.91	0.52
1:B:478:LEU:HD12	1:B:502:SER:HB3	1.90	0.52
1:B:529:ILE:O	1:B:533:VAL:HB	2.10	0.52
1:A:366:ALA:HB3	1:A:402:ASP:N	2.25	0.52
1:B:55:TYR:N	1:B:55:TYR:CD2	2.77	0.52
1:B:161:GLU:C	1:B:163:PHE:H	2.15	0.52
1:A:208:ILE:O	1:A:212:LYS:HG2	2.10	0.52
1:B:619:GLU:O	1:B:673:LYS:HB3	2.10	0.52
1:B:16:ASP:N	1:B:32:ASN:HD21	2.04	0.52
1:B:400:PRO:CA	1:B:413:PHE:HE1	2.21	0.52
1:A:6:ARG:C	1:A:7:THR:CG2	2.82	0.52
1:B:164:ILE:O	1:B:168:LYS:HE2	2.10	0.52
1:A:504:ASN:ND2	1:A:506:GLY:H	2.08	0.51
1:B:93:PRO:HB2	1:B:135:LEU:HD23	1.92	0.51
1:A:161:GLU:OE2	1:A:356:HIS:CE1	2.60	0.51
1:A:161:GLU:O	1:A:165:LYS:CG	2.56	0.51
1:A:478:LEU:HD12	1:A:502:SER:HB3	1.92	0.51
1:B:208:ILE:O	1:B:212:LYS:HG2	2.10	0.51
1:A:222:MET:O	1:A:223:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:CE2	1:A:253:GLU:HG3	2.46	0.51
1:A:678:LYS:HB3	1:A:717:GLU:HB3	1.93	0.51
1:A:164:ILE:HG12	1:A:164:ILE:O	2.10	0.51
1:B:504:ASN:ND2	1:B:506:GLY:H	2.08	0.51
1:B:596:ARG:NE	1:B:646:GLU:HG2	2.26	0.51
1:A:383:ILE:CD1	1:B:338:PRO:HG3	2.37	0.51
1:B:133:GLN:O	1:B:135:LEU:N	2.43	0.51
1:A:205:GLU:N	1:A:205:GLU:OE1	2.44	0.51
1:A:619:GLU:O	1:A:673:LYS:HB3	2.10	0.51
1:B:294:GLU:O	1:B:305:ARG:NH2	2.43	0.51
1:A:105:LEU:HD12	1:A:302:LEU:C	2.35	0.51
1:A:511:THR:CG2	1:A:512:ASN:N	2.74	0.51
1:A:8:ARG:C	1:A:10:ARG:H	2.17	0.51
1:A:160:ASP:O	1:A:162:ASP:N	2.37	0.50
1:A:314:MET:CE	1:A:332:THR:HG21	2.41	0.50
1:B:292:THR:HG21	1:B:313:TYR:OH	2.11	0.50
1:A:304:PHE:HE2	1:A:343:MET:HE1	1.76	0.50
1:A:353:THR:CG2	1:A:390:ILE:HD13	2.40	0.50
1:A:529:ILE:O	1:A:533:VAL:HB	2.11	0.50
1:B:353:THR:CG2	1:B:390:ILE:HD13	2.42	0.50
1:B:398:ALA:HB2	1:B:417:TRP:HE3	1.72	0.50
1:B:304:PHE:HE2	1:B:343:MET:HE1	1.76	0.50
1:B:398:ALA:HB2	1:B:417:TRP:CZ3	2.47	0.50
1:A:290:ASN:OD1	1:A:291:HIS:HD2	1.95	0.50
1:B:227:PHE:CE2	1:B:253:GLU:HG3	2.46	0.50
1:B:297:HIS:C	1:B:299:GLY:H	2.20	0.50
1:B:511:THR:CG2	1:B:512:ASN:N	2.75	0.50
1:B:678:LYS:HB3	1:B:717:GLU:HB3	1.94	0.49
1:B:103:LYS:HE3	1:B:125:GLY:H	1.76	0.49
1:B:105:LEU:HD12	1:B:302:LEU:C	2.36	0.49
1:B:290:ASN:OD1	1:B:291:HIS:HD2	1.94	0.49
1:B:205:GLU:N	1:B:205:GLU:OE1	2.46	0.49
1:A:353:THR:HG21	1:A:390:ILE:HD13	1.94	0.49
1:B:55:TYR:HD2	1:B:55:TYR:N	2.10	0.49
1:B:290:ASN:ND2	1:B:364:LEU:HB2	2.28	0.49
1:B:684:SER:HA	1:B:710:ALA:O	2.12	0.49
1:B:132:ASN:O	1:B:133:GLN:C	2.55	0.49
1:A:164:ILE:O	1:A:168:LYS:HE2	2.13	0.49
1:B:546:LEU:HD21	1:B:568:TRP:CZ3	2.48	0.49
1:A:126:TYR:CE2	1:A:298:LEU:HA	2.48	0.49
1:B:222:MET:CB	1:B:223:PRO:CD	2.88	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HB3	1:A:88:TYR:HB2	1.95	0.48
1:B:681:LEU:HD22	1:B:682:VAL:N	2.28	0.48
1:A:681:LEU:HD22	1:A:682:VAL:N	2.28	0.48
1:B:120:ASN:O	1:B:123:VAL:HG22	2.12	0.48
1:B:190:ASP:OD1	1:B:190:ASP:C	2.56	0.48
1:A:6:ARG:HH12	1:A:7:THR:CG2	2.20	0.48
1:A:20:LEU:HD23	1:A:34:SER:OG	2.14	0.48
1:A:290:ASN:ND2	1:A:364:LEU:HB2	2.28	0.48
1:A:669:ASN:N	1:A:669:ASN:HD22	2.11	0.48
1:A:441:GLU:O	1:A:445:ARG:HG2	2.13	0.48
1:A:596:ARG:NE	1:A:646:GLU:HG2	2.28	0.48
1:B:108:PRO:HB3	1:B:343:MET:CE	2.43	0.48
1:A:108:PRO:HB3	1:A:343:MET:CE	2.42	0.48
1:A:189:LEU:HD13	1:A:189:LEU:N	2.26	0.48
1:A:400:PRO:HA	1:A:413:PHE:HE1	1.75	0.48
1:A:468:THR:HG23	1:A:541:LEU:CB	2.43	0.48
1:A:177:TYR:CE2	1:A:179:VAL:HG13	2.48	0.48
1:B:133:GLN:C	1:B:135:LEU:H	2.21	0.48
1:B:315:LEU:HB3	1:B:320:LYS:HA	1.95	0.48
1:B:365:ALA:CB	1:B:398:ALA:HB1	2.44	0.48
1:A:319:ASN:O	1:A:320:LYS:HB2	2.13	0.48
1:B:468:THR:HG23	1:B:541:LEU:CB	2.44	0.48
1:A:315:LEU:HB3	1:A:320:LYS:HA	1.95	0.48
1:A:682:VAL:C	1:A:683:ILE:HG13	2.38	0.48
1:B:155:TYR:O	1:B:156:PHE:HB2	2.12	0.48
1:B:177:TYR:CE2	1:B:179:VAL:HG13	2.49	0.48
1:A:54:LYS:HG3	1:A:144:GLU:HB2	1.96	0.48
1:A:103:LYS:HE3	1:A:125:GLY:H	1.79	0.48
1:A:546:LEU:HD21	1:A:568:TRP:CZ3	2.49	0.47
1:B:204:SER:OG	1:B:207:MET:HG2	2.14	0.47
1:A:637:PHE:CE1	1:A:661:ILE:HD12	2.49	0.47
1:B:289:TYR:CD2	1:B:344:VAL:HG13	2.49	0.47
1:B:297:HIS:O	1:B:298:LEU:CB	2.59	0.47
1:B:441:GLU:O	1:B:445:ARG:HG2	2.15	0.47
1:A:684:SER:HA	1:A:710:ALA:O	2.15	0.47
1:A:688:ARG:NH1	1:A:706:GLU:OE2	2.44	0.47
1:B:290:ASN:OD1	1:B:291:HIS:CD2	2.67	0.47
1:B:292:THR:CG2	1:B:293:ALA:N	2.78	0.47
1:A:6:ARG:O	1:A:7:THR:HG23	2.15	0.47
1:A:174:THR:HG22	1:A:175:VAL:N	2.29	0.47
1:A:204:SER:OG	1:A:207:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:HIS:C	1:A:299:GLY:H	2.21	0.47
1:A:365:ALA:CB	1:A:398:ALA:HB1	2.45	0.47
1:B:20:LEU:HD23	1:B:34:SER:OG	2.15	0.47
1:B:230:GLN:HB2	1:B:233:LEU:CD2	2.40	0.47
1:B:314:MET:CE	1:B:332:THR:HG21	2.44	0.47
1:B:174:THR:HG22	1:B:175:VAL:N	2.30	0.47
1:B:42:LYS:HB3	1:B:88:TYR:HB2	1.97	0.47
1:B:669:ASN:N	1:B:669:ASN:HD22	2.13	0.47
1:A:8:ARG:NH2	1:A:61:GLU:H	2.12	0.47
1:B:353:THR:HG21	1:B:390:ILE:HD13	1.96	0.47
1:A:133:GLN:O	1:A:135:LEU:N	2.47	0.46
1:A:172:LYS:HB3	1:A:461:PHE:HZ	1.79	0.46
1:B:189:LEU:HD13	1:B:189:LEU:N	2.30	0.46
1:B:511:THR:CG2	1:B:512:ASN:H	2.27	0.46
1:A:559:GLN:HG3	1:A:561:ASN:HD21	1.80	0.46
1:B:65:LYS:HE2	1:B:67:GLY:O	2.16	0.46
1:B:126:TYR:CE2	1:B:298:LEU:HA	2.50	0.46
1:B:153:ASN:C	1:B:153:ASN:ND2	2.73	0.46
1:A:468:THR:HG23	1:A:541:LEU:HB2	1.97	0.46
1:B:163:PHE:C	1:B:165:LYS:N	2.73	0.46
1:B:182:LYS:HZ3	1:B:565:TRP:HH2	1.63	0.46
1:A:612:ASP:HA	1:A:643:VAL:HG23	1.97	0.46
1:A:163:PHE:C	1:A:165:LYS:H	2.24	0.46
1:A:504:ASN:C	1:A:504:ASN:ND2	2.74	0.46
1:B:522:LYS:HG3	1:B:685:SER:O	2.16	0.46
1:A:55:TYR:HD2	1:A:55:TYR:N	2.11	0.46
1:A:290:ASN:OD1	1:A:291:HIS:CD2	2.67	0.46
1:B:143:GLY:O	1:B:148:LYS:NZ	2.49	0.46
1:A:325:ASP:OD2	1:A:330:GLY:N	2.39	0.46
1:B:82:LEU:HD23	1:B:150:VAL:HG22	1.98	0.46
1:A:511:THR:CG2	1:A:512:ASN:H	2.27	0.46
1:B:263:GLY:O	1:B:266:VAL:HG12	2.16	0.46
1:A:187:LEU:HD22	1:A:565:TRP:CB	2.46	0.46
1:B:103:LYS:HA	1:B:142:SER:OG	2.16	0.46
1:A:413:PHE:HB2	1:A:419:GLU:OE2	2.16	0.45
1:B:172:LYS:HB3	1:B:461:PHE:CE1	2.51	0.45
1:B:319:ASN:O	1:B:320:LYS:HB2	2.16	0.45
1:B:682:VAL:C	1:B:683:ILE:HG13	2.39	0.45
1:A:161:GLU:C	1:A:163:PHE:H	2.23	0.45
1:A:199:TYR:CZ	1:A:256:TYR:HB2	2.50	0.45
1:A:230:GLN:HB2	1:A:233:LEU:CD2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HG3	1:A:685:SER:O	2.16	0.45
1:B:447:LEU:C	1:B:535:GLN:HB2	2.40	0.45
1:B:591:HIS:HB3	1:B:656:ASP:OD1	2.16	0.45
1:B:199:TYR:CZ	1:B:256:TYR:HB2	2.51	0.45
1:B:361:ARG:HD3	1:B:361:ARG:C	2.41	0.45
1:A:164:ILE:HG21	1:A:277:HIS:HB3	1.98	0.45
1:A:535:GLN:NE2	1:A:596:ARG:HB2	2.32	0.45
1:B:188:ARG:C	1:B:190:ASP:H	2.23	0.45
1:B:187:LEU:HD22	1:B:565:TRP:CB	2.47	0.45
1:B:325:ASP:OD1	1:B:325:ASP:C	2.59	0.45
1:B:504:ASN:C	1:B:504:ASN:ND2	2.74	0.45
1:A:187:LEU:HD22	1:A:565:TRP:HB3	1.99	0.45
1:B:437:LEU:N	1:B:437:LEU:HD12	2.32	0.45
1:B:559:GLN:HG3	1:B:561:ASN:HD21	1.82	0.45
1:A:103:LYS:HA	1:A:142:SER:OG	2.17	0.45
1:A:513:ASP:O	1:A:516:VAL:N	2.47	0.45
1:B:161:GLU:C	1:B:163:PHE:N	2.75	0.45
1:A:177:TYR:CE2	1:A:179:VAL:CG1	3.00	0.45
1:A:361:ARG:HD3	1:A:361:ARG:C	2.42	0.45
1:A:172:LYS:HB3	1:A:461:PHE:CE1	2.51	0.45
1:B:612:ASP:HA	1:B:643:VAL:HG23	1.98	0.45
1:A:172:LYS:O	1:A:595:ARG:HB3	2.17	0.45
1:A:297:HIS:O	1:A:298:LEU:CB	2.59	0.45
1:A:578:LEU:HD12	1:A:578:LEU:O	2.17	0.45
1:A:153:ASN:ND2	1:A:155:TYR:H	2.15	0.44
1:B:549:THR:HG22	1:B:551:ARG:N	2.13	0.44
1:A:161:GLU:C	1:A:163:PHE:N	2.75	0.44
1:A:289:TYR:CD2	1:A:344:VAL:HG13	2.52	0.44
1:B:480:SER:HA	1:B:520:ARG:NH1	2.30	0.44
1:A:7:THR:HB	1:A:8:ARG:H	1.69	0.44
1:A:437:LEU:HD12	1:A:437:LEU:N	2.33	0.44
1:B:177:TYR:CE2	1:B:179:VAL:CG1	3.00	0.44
1:A:65:LYS:HE2	1:A:67:GLY:O	2.17	0.44
1:A:263:GLY:O	1:A:266:VAL:HG12	2.18	0.44
1:B:603:LYS:HA	1:B:611:LYS:HG2	2.00	0.44
1:B:108:PRO:HB3	1:B:343:MET:HE2	1.98	0.44
1:B:450:PRO:O	1:B:454:LEU:HB3	2.18	0.44
1:B:637:PHE:CE1	1:B:661:ILE:HD12	2.52	0.44
1:A:157:GLU:O	1:A:157:GLU:HG3	2.18	0.44
1:A:160:ASP:C	1:A:162:ASP:H	2.23	0.44
1:A:108:PRO:HB3	1:A:343:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASP:C	1:B:161:GLU:N	2.76	0.44
1:B:314:MET:HE2	1:B:332:THR:CG2	2.48	0.44
1:B:588:TYR:CZ	1:B:595:ARG:HG2	2.53	0.44
1:A:82:LEU:HD23	1:A:150:VAL:HG22	1.99	0.44
1:A:143:GLY:O	1:A:148:LYS:NZ	2.51	0.44
1:A:292:THR:CG2	1:A:293:ALA:N	2.78	0.44
1:A:398:ALA:O	1:A:400:PRO:HD3	2.17	0.44
1:B:103:LYS:O	1:B:105:LEU:HD22	2.18	0.44
1:A:111:LYS:HD2	1:A:350:TYR:CZ	2.53	0.43
1:A:325:ASP:OD1	1:A:325:ASP:C	2.61	0.43
1:B:297:HIS:CD2	1:B:298:LEU:HG	2.52	0.43
1:B:525:ARG:O	1:B:529:ILE:HG13	2.18	0.43
1:B:591:HIS:HA	1:B:592:PRO:HD3	1.82	0.43
1:A:35:LEU:HD11	1:A:307:ILE:HD13	1.99	0.43
1:A:297:HIS:CD2	1:A:298:LEU:HG	2.53	0.43
1:B:164:ILE:HG21	1:B:277:HIS:HB3	2.00	0.43
1:B:103:LYS:HE3	1:B:125:GLY:N	2.33	0.43
1:B:172:LYS:HB3	1:B:461:PHE:HZ	1.79	0.43
1:B:187:LEU:HD22	1:B:565:TRP:HB3	1.99	0.43
1:B:673:LYS:HE2	1:B:700:GLU:HB2	1.99	0.43
1:A:78:ARG:HB3	1:A:79:PRO:CD	2.49	0.43
1:A:447:LEU:C	1:A:535:GLN:HB2	2.43	0.43
1:A:673:LYS:HE2	1:A:700:GLU:HB2	2.01	0.43
1:A:16:ASP:H	1:A:32:ASN:ND2	2.06	0.43
1:B:111:LYS:HD2	1:B:350:TYR:CZ	2.54	0.43
1:B:372:LEU:HD12	1:B:372:LEU:HA	1.77	0.43
1:A:191:LEU:CD2	1:A:206:GLN:OE1	2.67	0.43
1:B:398:ALA:O	1:B:400:PRO:HD3	2.18	0.43
1:B:695:ARG:HH11	1:B:695:ARG:HG2	1.83	0.43
1:A:13:ARG:HD2	1:A:73:PHE:CD2	2.54	0.43
1:A:450:PRO:O	1:A:454:LEU:HB3	2.18	0.43
1:A:480:SER:HA	1:A:520:ARG:NH1	2.33	0.43
1:B:25:ILE:O	1:B:25:ILE:HG22	2.18	0.43
1:B:401:TRP:HA	1:B:407:GLY:O	2.19	0.43
1:B:688:ARG:NH1	1:B:706:GLU:OE2	2.46	0.43
1:B:232:PHE:CE1	1:B:233:LEU:HD22	2.54	0.43
1:B:688:ARG:HG2	1:B:688:ARG:HH11	1.83	0.43
1:B:156:PHE:C	1:B:156:PHE:CD2	2.96	0.43
1:B:291:HIS:HB3	1:B:327:THR:HG21	2.01	0.43
1:B:35:LEU:HD11	1:B:307:ILE:HD13	2.00	0.42
1:A:103:LYS:O	1:A:105:LEU:HD22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CD2	1:A:156:PHE:C	2.97	0.42
1:B:468:THR:HG23	1:B:541:LEU:HB2	1.99	0.42
1:A:8:ARG:C	1:A:10:ARG:N	2.77	0.42
1:A:188:ARG:C	1:A:190:ASP:N	2.77	0.42
1:A:314:MET:HE2	1:A:332:THR:CG2	2.48	0.42
1:B:535:GLN:NE2	1:B:596:ARG:HB2	2.34	0.42
1:A:377:MET:CE	1:A:409:GLN:HB3	2.49	0.42
1:B:8:ARG:HH21	1:B:61:GLU:HB3	1.84	0.42
1:B:78:ARG:HB3	1:B:79:PRO:CD	2.49	0.42
1:B:90:PRO:HB2	1:B:97:LEU:HD13	2.01	0.42
1:A:163:PHE:C	1:A:165:LYS:N	2.78	0.42
1:B:118:ILE:O	1:B:145:TYR:HB3	2.20	0.42
1:A:6:ARG:HH22	1:A:63:LYS:HZ3	1.67	0.42
1:A:532:LEU:HD12	1:A:584:MET:HB3	2.02	0.42
1:A:549:THR:HG22	1:A:551:ARG:N	2.13	0.42
1:B:13:ARG:HD2	1:B:73:PHE:CD2	2.55	0.42
1:B:172:LYS:O	1:B:595:ARG:HB3	2.19	0.42
1:B:222:MET:O	1:B:223:PRO:C	2.62	0.42
1:B:437:LEU:N	1:B:437:LEU:CD1	2.83	0.42
1:A:222:MET:HE3	1:A:470:HIS:CG	2.55	0.42
1:B:361:ARG:HA	1:B:397:ILE:O	2.20	0.42
1:A:232:PHE:CE1	1:A:233:LEU:HD22	2.54	0.42
1:A:584:MET:HA	1:A:584:MET:HE2	2.02	0.42
1:B:110:ALA:O	1:B:250:PHE:HB2	2.20	0.42
1:B:148:LYS:HD2	1:B:148:LYS:N	2.35	0.42
1:B:173:ASP:HA	1:B:595:ARG:HD2	2.02	0.42
1:A:103:LYS:HE3	1:A:125:GLY:HA2	2.00	0.42
1:B:105:LEU:CD1	1:B:302:LEU:O	2.68	0.42
1:B:124:PHE:CG	1:B:128:ILE:HD11	2.55	0.42
1:B:366:ALA:HB3	1:B:402:ASP:N	2.35	0.42
1:B:545:GLU:CD	1:B:545:GLU:H	2.28	0.42
1:A:423:LYS:HB2	1:A:423:LYS:HE2	1.85	0.41
1:A:525:ARG:O	1:A:529:ILE:HG13	2.21	0.41
1:A:160:ASP:O	1:A:162:ASP:CG	2.63	0.41
1:A:401:TRP:HA	1:A:407:GLY:O	2.20	0.41
1:B:159:ASP:O	1:B:159:ASP:OD2	2.38	0.41
1:B:708:ARG:HH11	1:B:708:ARG:HG2	1.84	0.41
1:A:437:LEU:N	1:A:437:LEU:CD1	2.83	0.41
1:A:588:TYR:CZ	1:A:595:ARG:HG2	2.54	0.41
1:A:708:ARG:HH11	1:A:708:ARG:HG2	1.84	0.41
1:B:103:LYS:HE3	1:B:125:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:ND2	1:B:155:TYR:H	2.18	0.41
1:A:168:LYS:HB2	1:A:168:LYS:HE3	1.77	0.41
1:A:221:LEU:HD12	1:A:221:LEU:N	2.35	0.41
1:B:16:ASP:H	1:B:32:ASN:ND2	2.07	0.41
1:B:402:ASP:OD2	1:B:402:ASP:C	2.64	0.41
1:A:124:PHE:CG	1:A:128:ILE:HD11	2.56	0.41
1:A:160:ASP:C	1:A:162:ASP:N	2.78	0.41
1:B:413:PHE:O	1:B:414:PRO:O	2.38	0.41
1:B:423:LYS:HE2	1:B:423:LYS:HB2	1.84	0.41
1:B:532:LEU:HD12	1:B:584:MET:HB3	2.01	0.41
1:A:624:ASP:H	1:A:627:THR:HG21	1.84	0.41
1:B:377:MET:CE	1:B:409:GLN:HB3	2.51	0.41
1:B:479:VAL:HG23	1:B:520:ARG:HG3	2.01	0.41
1:A:94:GLU:CD	1:A:94:GLU:H	2.29	0.41
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.78	0.41
1:B:126:TYR:OH	1:B:298:LEU:HA	2.21	0.41
1:A:110:ALA:O	1:A:250:PHE:HB2	2.21	0.41
1:A:485:HIS:HE1	1:A:508:GLU:OE2	2.04	0.41
1:A:545:GLU:CD	1:A:545:GLU:H	2.27	0.41
1:A:561:ASN:ND2	1:A:563:ILE:HG13	2.36	0.41
1:A:591:HIS:HB3	1:A:656:ASP:OD1	2.21	0.41
1:A:688:ARG:HH11	1:A:688:ARG:HG2	1.86	0.41
1:A:291:HIS:HB3	1:A:327:THR:HG21	2.03	0.41
1:A:559:GLN:HG3	1:A:563:ILE:HD12	2.01	0.41
1:B:225:PHE:O	1:B:226:HIS:C	2.64	0.41
1:B:559:GLN:HG3	1:B:563:ILE:HD12	2.03	0.41
1:A:90:PRO:HB2	1:A:97:LEU:HD13	2.02	0.40
1:A:583:LYS:HE2	1:A:583:LYS:HB3	1.86	0.40
1:B:449:SER:N	1:B:450:PRO:HD3	2.37	0.40
1:B:453:TYR:HB3	1:B:458:LYS:CB	2.41	0.40
1:B:487:GLU:H	1:B:487:GLU:CD	2.29	0.40
1:A:218:THR:CG2	1:A:282:GLU:HB2	2.46	0.40
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.81	0.40
1:B:583:LYS:HE2	1:B:583:LYS:HB3	1.87	0.40
1:A:25:ILE:O	1:A:25:ILE:HG22	2.19	0.40
1:A:148:LYS:HD2	1:A:148:LYS:N	2.36	0.40
1:A:564:THR:O	1:A:565:TRP:C	2.64	0.40
1:B:180:HIS:CE1	1:B:182:LYS:HB3	2.57	0.40
1:B:578:LEU:HD12	1:B:578:LEU:O	2.21	0.40
1:A:191:LEU:CB	1:A:192:PRO:HD2	2.37	0.40
1:A:487:GLU:CD	1:A:487:GLU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:CE1	1:A:565:TRP:HZ3	2.39	0.40
1:A:548:ARG:NH1	1:A:550:GLN:HE21	2.20	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	711/718 (99%)	644 (91%)	64 (9%)	3 (0%)	30 65
1	B	709/718 (99%)	643 (91%)	62 (9%)	4 (1%)	21 56
All	All	1420/1436 (99%)	1287 (91%)	126 (9%)	7 (0%)	24 60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	700	GLU
1	B	156	PHE
1	B	414	PRO
1	B	700	GLU
1	A	133	GLN
1	B	164	ILE

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	629/636 (99%)	581 (92%)	48 (8%)	12	41
1	B	627/636 (99%)	582 (93%)	45 (7%)	13	43
All	All	1256/1272 (99%)	1163 (93%)	93 (7%)	13	42

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	THR
1	A	8	ARG
1	A	9	ASP
1	A	55	TYR
1	A	94	GLU
1	A	153	ASN
1	A	159	ASP
1	A	161	GLU
1	A	162	ASP
1	A	179	VAL
1	A	187	LEU
1	A	189	LEU
1	A	213	ASP
1	A	236	LYS
1	A	247	ILE
1	A	253	GLU
1	A	267	LEU
1	A	292	THR
1	A	319	ASN
1	A	354	GLU
1	A	378	LEU
1	A	399	GLU
1	A	429	ARG
1	A	467	VAL
1	A	471	ASP
1	A	492	ASN
1	A	493	ASN
1	A	504	ASN
1	A	520	ARG
1	A	533	VAL
1	A	541	LEU
1	A	545	GLU
1	A	546	LEU
1	A	548	ARG

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Mol	Chain	Res	Type
1	A	554	ASN
1	A	559	GLN
1	A	561	ASN
1	A	565	TRP
1	A	584	MET
1	A	619	GLU
1	A	623	VAL
1	A	653	ARG
1	A	681	LEU
1	A	682	VAL
1	A	688	ARG
1	A	690	ILE
1	A	700	GLU
1	B	8	ARG
1	B	9	ASP
1	B	10	ARG
1	B	55	TYR
1	B	94	GLU
1	B	153	ASN
1	B	162	ASP
1	B	163	PHE
1	B	179	VAL
1	B	187	LEU
1	B	189	LEU
1	B	213	ASP
1	B	236	LYS
1	B	247	ILE
1	B	253	GLU
1	B	267	LEU
1	B	292	THR
1	B	319	ASN
1	B	354	GLU
1	B	378	LEU
1	B	399	GLU
1	B	429	ARG
1	B	467	VAL
1	B	492	ASN
1	B	493	ASN
1	B	504	ASN
1	B	520	ARG
1	B	533	VAL
1	B	541	LEU

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Mol	Chain	Res	Type
1	B	545	GLU
1	B	546	LEU
1	B	548	ARG
1	B	554	ASN
1	B	559	GLN
1	B	561	ASN
1	B	565	TRP
1	B	584	MET
1	B	619	GLU
1	B	623	VAL
1	B	653	ARG
1	B	681	LEU
1	B	682	VAL
1	B	688	ARG
1	B	690	ILE
1	B	700	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	ASN
1	A	53	GLN
1	A	114	ASN
1	A	131	GLN
1	A	153	ASN
1	A	194	ASN
1	A	226	HIS
1	A	274	ASN
1	A	278	ASN
1	A	291	HIS
1	A	309	ASN
1	A	334	ASN
1	A	342	GLN
1	A	376	ASN
1	A	379	ASN
1	A	412	ASN
1	A	485	HIS
1	A	492	ASN
1	A	493	ASN
1	A	500	ASN
1	A	504	ASN

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Mol	Chain	Res	Type
1	A	523	GLN
1	A	526	ASN
1	A	550	GLN
1	A	554	ASN
1	A	555	ASN
1	A	559	GLN
1	A	561	ASN
1	A	601	GLN
1	A	633	GLN
1	A	668	ASN
1	A	669	ASN
1	B	32	ASN
1	B	53	GLN
1	B	114	ASN
1	B	131	GLN
1	B	132	ASN
1	B	153	ASN
1	B	194	ASN
1	B	226	HIS
1	B	278	ASN
1	B	291	HIS
1	B	309	ASN
1	B	319	ASN
1	B	334	ASN
1	B	342	GLN
1	B	376	ASN
1	B	379	ASN
1	B	412	ASN
1	B	485	HIS
1	B	492	ASN
1	B	493	ASN
1	B	500	ASN
1	B	504	ASN
1	B	523	GLN
1	B	550	GLN
1	B	554	ASN
1	B	555	ASN
1	B	559	GLN
1	B	561	ASN
1	B	601	GLN
1	B	633	GLN
1	B	668	ASN

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Mol	Chain	Res	Type
1	B	669	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	713/718 (99%)	-0.17	9 (1%) 75 53	16, 32, 53, 100	0
1	B	711/718 (99%)	-0.15	6 (0%) 82 64	13, 34, 58, 83	0
All	All	1424/1436 (99%)	-0.16	15 (1%) 78 57	13, 33, 55, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	THR	7.9
1	B	164	ILE	3.3
1	A	6	ARG	3.2
1	B	159	ASP	3.1
1	B	160	ASP	2.9
1	A	164	ILE	2.8
1	A	160	ASP	2.7
1	A	161	GLU	2.5
1	B	373	TYR	2.5
1	B	18	TYR	2.4
1	A	166	GLY	2.3
1	A	8	ARG	2.2
1	A	24	TRP	2.1
1	B	457	ASN	2.0
1	A	9	ASP	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 oligosaccharides 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.