



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:28 PM UTC

PDB ID : 1NL3 / pdb_00001nl3
Title : CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION
ATPASE FROM MYCOBACTERIUM TUBERCULOSIS in APO FORM
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Consortium (TBSGC)
Deposited on : 2003-01-06
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

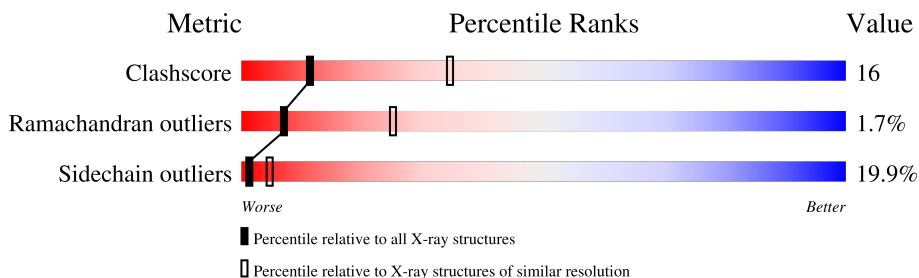
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	922	
1	B	922	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14209 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 PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6639	4157	1169	1288	25			
1	B	838	Total	C	N	O	S	0	0	0
			6640	4157	1171	1287	25			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	cloning artifact	UNP P0A5Y8
A	-28	LYS	-	cloning artifact	UNP P0A5Y8
A	-27	GLU	-	cloning artifact	UNP P0A5Y8
A	-26	THR	-	cloning artifact	UNP P0A5Y8
A	-25	ALA	-	cloning artifact	UNP P0A5Y8
A	-24	ALA	-	cloning artifact	UNP P0A5Y8
A	-23	ALA	-	cloning artifact	UNP P0A5Y8
A	-22	LYS	-	cloning artifact	UNP P0A5Y8
A	-21	PHE	-	cloning artifact	UNP P0A5Y8
A	-20	GLU	-	cloning artifact	UNP P0A5Y8
A	-19	ARG	-	cloning artifact	UNP P0A5Y8
A	-18	GLN	-	cloning artifact	UNP P0A5Y8
A	-17	HIS	-	cloning artifact	UNP P0A5Y8
A	-16	MET	-	cloning artifact	UNP P0A5Y8
A	-15	ASP	-	cloning artifact	UNP P0A5Y8
A	-14	SER	-	cloning artifact	UNP P0A5Y8
A	-13	PRO	-	cloning artifact	UNP P0A5Y8
A	-12	ASP	-	cloning artifact	UNP P0A5Y8
A	-11	LEU	-	cloning artifact	UNP P0A5Y8
A	-10	GLY	-	cloning artifact	UNP P0A5Y8
A	-9	THR	-	cloning artifact	UNP P0A5Y8
A	-8	LEU	-	cloning artifact	UNP P0A5Y8
A	-7	VAL	-	cloning artifact	UNP P0A5Y8
A	-6	PRO	-	cloning artifact	UNP P0A5Y8
A	-5	ARG	-	cloning artifact	UNP P0A5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	cloning artifact	UNP P0A5Y8
A	-3	SER	-	cloning artifact	UNP P0A5Y8
A	-2	MET	-	cloning artifact	UNP P0A5Y8
A	-1	ALA	-	cloning artifact	UNP P0A5Y8
A	0	ASP	-	cloning artifact	UNP P0A5Y8
A	1	ILE	-	cloning artifact	UNP P0A5Y8
B	-29	MET	-	cloning artifact	UNP P0A5Y8
B	-28	LYS	-	cloning artifact	UNP P0A5Y8
B	-27	GLU	-	cloning artifact	UNP P0A5Y8
B	-26	THR	-	cloning artifact	UNP P0A5Y8
B	-25	ALA	-	cloning artifact	UNP P0A5Y8
B	-24	ALA	-	cloning artifact	UNP P0A5Y8
B	-23	ALA	-	cloning artifact	UNP P0A5Y8
B	-22	LYS	-	cloning artifact	UNP P0A5Y8
B	-21	PHE	-	cloning artifact	UNP P0A5Y8
B	-20	GLU	-	cloning artifact	UNP P0A5Y8
B	-19	ARG	-	cloning artifact	UNP P0A5Y8
B	-18	GLN	-	cloning artifact	UNP P0A5Y8
B	-17	HIS	-	cloning artifact	UNP P0A5Y8
B	-16	MET	-	cloning artifact	UNP P0A5Y8
B	-15	ASP	-	cloning artifact	UNP P0A5Y8
B	-14	SER	-	cloning artifact	UNP P0A5Y8
B	-13	PRO	-	cloning artifact	UNP P0A5Y8
B	-12	ASP	-	cloning artifact	UNP P0A5Y8
B	-11	LEU	-	cloning artifact	UNP P0A5Y8
B	-10	GLY	-	cloning artifact	UNP P0A5Y8
B	-9	THR	-	cloning artifact	UNP P0A5Y8
B	-8	LEU	-	cloning artifact	UNP P0A5Y8
B	-7	VAL	-	cloning artifact	UNP P0A5Y8
B	-6	PRO	-	cloning artifact	UNP P0A5Y8
B	-5	ARG	-	cloning artifact	UNP P0A5Y8
B	-4	GLY	-	cloning artifact	UNP P0A5Y8
B	-3	SER	-	cloning artifact	UNP P0A5Y8
B	-2	MET	-	cloning artifact	UNP P0A5Y8
B	-1	ALA	-	cloning artifact	UNP P0A5Y8
B	0	ASP	-	cloning artifact	UNP P0A5Y8
B	1	ILE	-	cloning artifact	UNP P0A5Y8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	475	Total O 475 475	0	0

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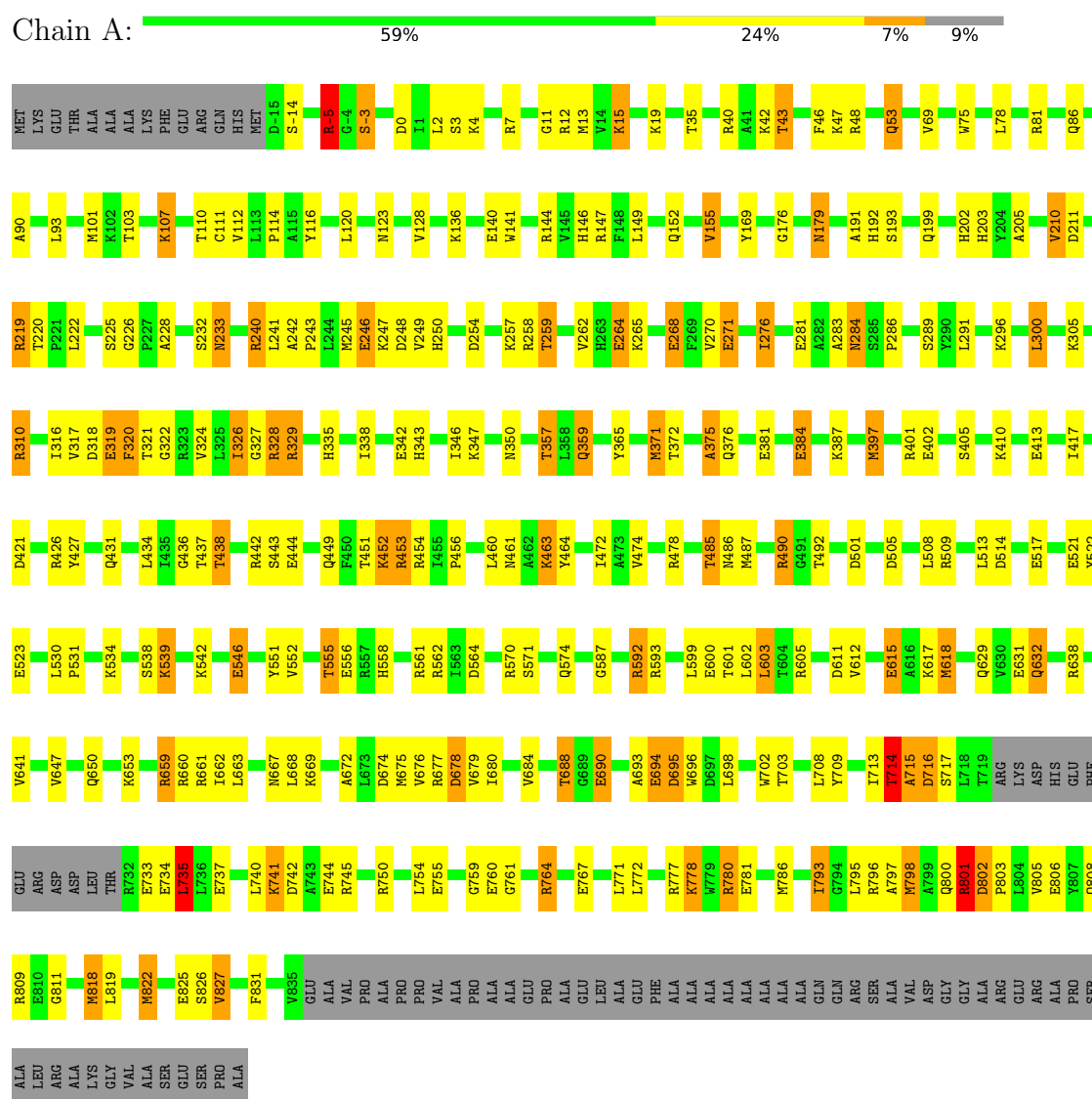
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	455	Total 455	O 455	0	0

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT



• Molecule 1: PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	206.20 Å 206.20 Å 295.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.4 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.193 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14209	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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	0.74	4/6743 (0.1%)	1.06	10/9116 (0.1%)
1	B	0.73	2/6744 (0.0%)	1.05	12/9116 (0.1%)
All	All	0.74	6/13487 (0.0%)	1.05	22/18232 (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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	MET	SD-CE	6.05	1.94	1.79
1	B	326	ILE	CA-CB	5.61	1.60	1.54
1	B	113	LEU	CA-C	5.52	1.58	1.52
1	A	474	VAL	CA-CB	5.43	1.60	1.54
1	A	714	THR	CA-CB	5.41	1.62	1.53
1	A	346	ILE	CA-CB	5.26	1.60	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	THR	N-CA-C	-11.71	99.53	114.04
1	B	486	ASN	CA-C-N	-8.97	109.01	122.83
1	B	486	ASN	C-N-CA	-8.97	109.01	122.83
1	A	486	ASN	CA-C-N	-8.85	109.98	123.17
1	A	486	ASN	C-N-CA	-8.85	109.98	123.17
1	A	210	VAL	CB-CA-C	-8.02	101.62	111.88
1	B	210	VAL	CB-CA-C	-7.22	102.39	112.14
1	A	431	GLN	N-CA-C	7.18	118.40	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	VAL	CB-CA-C	-6.87	100.93	110.96
1	A	210	VAL	N-CA-CB	6.53	117.76	110.51
1	B	5	LEU	N-CA-C	-6.45	105.51	113.19
1	B	39	LEU	N-CA-C	-6.33	102.17	110.53
1	A	320	PHE	N-CA-C	6.11	120.01	107.37
1	B	41	ALA	N-CA-C	-6.08	104.77	111.82
1	B	331	ASN	N-CA-C	6.02	119.52	109.95
1	B	216	ASP	N-CA-C	5.92	118.24	111.02
1	A	155	VAL	CB-CA-C	-5.66	101.79	110.50
1	B	155	VAL	CB-CA-C	-5.47	101.24	110.71
1	A	375	ALA	N-CA-C	-5.42	107.31	114.04
1	B	734	GLU	N-CA-C	5.29	122.06	110.80
1	A	759	GLY	N-CA-C	5.18	120.48	112.81
1	B	695	ASP	N-CA-C	5.03	121.52	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	PHE	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	6639	0	6576	208	0
1	B	6640	0	6585	229	0
2	A	475	0	0	57	0
2	B	455	0	0	66	0
All	All	14209	0	13161	429	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 16.

All (429) 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:615:GLU:HG3	1:B:323:ARG:HG3	1.37	1.06
1:B:775:ILE:HG12	1:B:822:MET:HE3	1.33	1.06
1:A:702:TRP:NE1	1:A:714:THR:HA	1.73	1.03
1:A:660:ARG:HG2	2:A:1748:HOH:O	1.60	1.01
1:B:359:GLN:H	1:B:359:GLN:HE21	1.08	1.00
1:A:734:GLU:O	1:A:735:LEU:HB3	1.64	0.94
1:B:141:TRP:HZ2	1:B:501:ASP:HB3	1.29	0.94
1:B:101:MET:HE1	1:B:371:MET:HE2	1.49	0.94
1:A:436:GLY:O	1:A:555:THR:HB	1.69	0.93
1:A:101:MET:HE1	1:A:371:MET:HE2	1.49	0.92
1:B:780:ARG:HD2	2:B:1298:HOH:O	1.70	0.92
1:A:702:TRP:HE1	1:A:714:THR:HA	1.34	0.91
1:A:359:GLN:H	1:A:359:GLN:HE21	1.04	0.91
1:A:777:ARG:NH2	1:A:825:GLU:OE1	2.03	0.90
1:B:755:GLU:HA	1:B:759:GLY:HA3	1.53	0.89
1:B:53:GLN:H	1:B:53:GLN:HE21	1.22	0.87
1:B:777:ARG:NH2	1:B:825:GLU:OE1	2.07	0.87
1:A:101:MET:HE1	1:A:371:MET:CE	2.05	0.86
1:A:328:ARG:HG3	1:A:328:ARG:HH11	1.40	0.86
1:B:141:TRP:CZ2	1:B:501:ASP:HB3	2.11	0.86
1:A:421:ASP:OD1	1:A:453:ARG:NH2	2.09	0.85
1:A:806:GLU:HG3	2:A:1885:HOH:O	1.77	0.85
1:A:328:ARG:HH11	1:A:328:ARG:CG	1.92	0.82
1:B:447:SER:HB2	1:B:457:HIS:NE2	1.95	0.82
1:B:453:ARG:HG3	2:B:1847:HOH:O	1.81	0.81
1:A:384:GLU:HG3	2:A:1788:HOH:O	1.81	0.81
1:A:780:ARG:HD3	2:A:1593:HOH:O	1.79	0.80
1:A:246:GLU:H	1:A:250:HIS:HD2	1.29	0.80
1:B:3:SER:HB3	2:B:1795:HOH:O	1.82	0.80
1:B:558:HIS:HD2	1:B:564:ASP:OD2	1.65	0.79
2:A:1362:HOH:O	1:B:615:GLU:HG3	1.80	0.79
1:B:227:PRO:HD2	2:B:1863:HOH:O	1.83	0.79
1:B:683:TYR:HE2	2:B:1094:HOH:O	1.64	0.79
1:A:733:GLU:HA	2:A:1533:HOH:O	1.83	0.79
1:B:650:GLN:HG3	2:B:1306:HOH:O	1.81	0.79
1:B:93:LEU:HD11	1:B:371:MET:HE3	1.65	0.78
1:A:734:GLU:HA	2:A:1698:HOH:O	1.84	0.77
1:A:246:GLU:H	1:A:250:HIS:CD2	2.03	0.76
1:B:191:ALA:O	1:B:659:ARG:NH2	2.18	0.76
1:B:558:HIS:CD2	1:B:564:ASP:OD2	2.39	0.76
1:A:93:LEU:HD11	1:A:371:MET:HE3	1.67	0.75
1:A:558:HIS:HD2	1:A:564:ASP:OD2	1.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:GLY:O	1:B:760:GLU:HB2	1.85	0.75
1:A:86:GLN:HG2	1:A:110:THR:OG1	1.87	0.74
1:B:141:TRP:HE3	2:B:1713:HOH:O	1.71	0.73
1:B:705:LEU:HD23	1:B:709:TYR:CE1	2.24	0.73
1:B:705:LEU:HD23	1:B:709:TYR:HE1	1.52	0.73
1:B:636:GLU:HG3	2:B:1560:HOH:O	1.89	0.72
1:B:801:ARG:HD2	1:B:802:ASP:H	1.54	0.72
1:A:780:ARG:CD	2:A:1593:HOH:O	2.35	0.72
1:B:507:ARG:CG	1:B:507:ARG:HH11	2.03	0.71
1:B:592:ARG:HD2	2:B:1682:HOH:O	1.90	0.71
1:A:40:ARG:HG2	2:A:1665:HOH:O	1.90	0.71
1:A:144:ARG:HD2	1:A:523:GLU:OE2	1.91	0.70
1:A:780:ARG:HD2	2:A:1503:HOH:O	1.90	0.70
1:A:461:ASN:OD1	1:A:485:THR:HG21	1.92	0.69
1:A:611:ASP:HB3	2:A:1380:HOH:O	1.92	0.69
1:A:801:ARG:H	1:A:801:ARG:HE	1.38	0.69
1:A:461:ASN:HA	1:A:485:THR:HG23	1.73	0.69
1:A:381:GLU:OE1	1:A:638:ARG:NH1	2.25	0.69
1:A:75:TRP:HB2	1:A:81:ARG:HB2	1.75	0.69
1:B:101:MET:HE1	1:B:371:MET:CE	2.23	0.69
1:A:669:LYS:HD3	1:A:764:ARG:NH2	2.08	0.68
1:B:246:GLU:HB3	1:B:249:VAL:HB	1.75	0.68
1:B:507:ARG:HD3	2:B:1832:HOH:O	1.91	0.68
1:A:819:LEU:HD23	1:A:822:MET:HE2	1.75	0.68
1:A:764:ARG:HA	1:A:767:GLU:OE1	1.94	0.67
1:B:507:ARG:HH11	1:B:507:ARG:CB	2.07	0.67
1:B:714:THR:O	1:B:717:SER:HB2	1.93	0.67
1:A:615:GLU:CG	1:B:323:ARG:HG3	2.21	0.67
1:B:660:ARG:HG3	2:B:1740:HOH:O	1.94	0.67
1:B:570:ARG:HD2	2:B:1063:HOH:O	1.95	0.67
1:A:318:ASP:OD1	1:A:319:GLU:N	2.28	0.66
1:B:178:ASN:ND2	2:B:1702:HOH:O	2.23	0.66
1:A:741:LYS:HE3	2:A:1715:HOH:O	1.95	0.66
1:B:229:ASP:HB2	2:B:1746:HOH:O	1.96	0.66
1:B:179:ASN:HB2	2:B:1749:HOH:O	1.94	0.66
1:A:801:ARG:HE	1:A:801:ARG:N	1.92	0.66
1:A:15:LYS:HD3	2:A:1869:HOH:O	1.95	0.65
1:A:248:ASP:HA	2:A:1609:HOH:O	1.96	0.65
1:A:708:LEU:HD13	1:A:827:VAL:CG2	2.26	0.65
1:B:4:LYS:C	1:B:6:LEU:H	2.01	0.65
1:B:257:LYS:HG3	2:B:1639:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HD13	1:B:608:LEU:HD12	1.79	0.65
1:A:546:GLU:HG3	2:A:1763:HOH:O	1.95	0.65
1:B:559:GLU:HG2	1:B:630:VAL:CG1	2.27	0.65
1:B:101:MET:CE	1:B:371:MET:HE2	2.26	0.65
1:B:359:GLN:H	1:B:359:GLN:NE2	1.90	0.64
1:A:688:THR:O	1:A:688:THR:HG22	1.98	0.64
1:A:801:ARG:HD2	1:A:802:ASP:N	2.12	0.64
1:B:141:TRP:CD1	1:B:142:MET:HE2	2.33	0.63
1:A:798:MET:HA	1:B:621:ARG:HH12	1.63	0.63
1:B:309:VAL:O	1:B:310:ARG:HD3	1.98	0.63
1:A:322:GLY:HA3	2:A:1642:HOH:O	1.98	0.63
1:B:490:ARG:HA	2:B:1818:HOH:O	1.99	0.63
1:B:801:ARG:HD2	1:B:802:ASP:N	2.14	0.63
1:B:511:ARG:NH2	1:B:529:GLU:OE2	2.32	0.62
1:A:668:LEU:HD13	1:A:771:LEU:HD12	1.80	0.62
1:B:80:GLN:HG2	2:B:1209:HOH:O	1.98	0.62
1:B:254:ASP:CG	1:B:257:LYS:HB2	2.25	0.61
1:B:53:GLN:HE21	1:B:53:GLN:N	1.93	0.61
1:A:228:ALA:HB3	2:A:1405:HOH:O	2.00	0.61
1:A:326:ILE:HG13	1:A:327:GLY:N	2.15	0.61
1:A:632:GLN:HA	1:A:632:GLN:NE2	2.16	0.61
1:B:806:GLU:HG2	2:B:1188:HOH:O	2.00	0.61
1:A:618:MET:HG3	2:B:1389:HOH:O	1.99	0.61
1:A:508:LEU:O	1:A:513:LEU:HB2	2.01	0.60
1:B:639:LYS:HD3	2:B:1438:HOH:O	1.99	0.60
1:A:101:MET:CE	1:A:371:MET:HE2	2.30	0.60
1:B:683:TYR:CE2	2:B:1094:HOH:O	2.47	0.60
1:B:530:LEU:HB3	1:B:531:PRO:HD3	1.83	0.60
1:B:520:GLU:HG2	2:B:1911:HOH:O	2.02	0.60
1:B:429:LYS:HG2	2:B:1606:HOH:O	2.01	0.59
1:B:436:GLY:O	1:B:555:THR:HB	2.02	0.59
1:A:521:GLU:OE1	2:A:1766:HOH:O	2.16	0.59
1:B:440:VAL:O	1:B:444:GLU:HG2	2.03	0.59
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.14	0.59
1:A:246:GLU:HG3	2:A:1358:HOH:O	2.03	0.59
1:A:259:THR:HG23	2:A:1346:HOH:O	2.01	0.59
1:A:514:ASP:HB3	1:A:517:GLU:HB2	1.84	0.59
1:B:112:VAL:HG13	1:B:146:HIS:CE1	2.38	0.59
1:B:248:ASP:HA	2:B:1725:HOH:O	2.02	0.59
1:A:112:VAL:HG13	1:A:146:HIS:CE1	2.38	0.58
1:B:116:TYR:HD1	1:B:151:LEU:HD11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HB3	2:A:1874:HOH:O	2.02	0.58
1:A:461:ASN:HA	1:A:485:THR:CG2	2.34	0.58
1:B:797:ALA:HB1	1:B:801:ARG:HD3	1.86	0.58
1:B:116:TYR:CD1	1:B:151:LEU:HD11	2.39	0.58
1:B:357:THR:HB	1:B:359:GLN:NE2	2.18	0.58
1:B:4:LYS:C	1:B:6:LEU:N	2.62	0.58
1:B:426:ARG:HA	2:B:1813:HOH:O	2.03	0.58
1:A:539:LYS:HE2	2:A:1814:HOH:O	2.05	0.57
1:A:680:ILE:O	1:A:684:VAL:HG23	2.04	0.57
1:A:650:GLN:HG3	2:A:1371:HOH:O	2.05	0.57
1:B:144:ARG:HD2	1:B:523:GLU:OE2	2.05	0.57
1:B:235:TYR:CE2	1:B:336:GLN:HG2	2.39	0.57
1:A:141:TRP:HZ2	2:A:1786:HOH:O	1.88	0.56
1:A:742:ASP:OD1	1:A:745:ARG:NH1	2.37	0.56
1:B:256:ARG:CB	1:B:256:ARG:HH11	2.18	0.56
1:B:39:LEU:HD23	1:B:148:PHE:HE1	1.70	0.56
1:A:410:LYS:HD2	1:A:603:LEU:HB3	1.86	0.56
1:B:108:THR:HG23	2:B:1651:HOH:O	2.04	0.56
1:B:256:ARG:HH11	1:B:256:ARG:HB2	1.71	0.56
1:A:53:GLN:H	1:A:53:GLN:CD	2.14	0.55
1:A:245:MET:CE	1:A:270:VAL:HG22	2.37	0.55
1:A:693:ALA:C	1:A:695:ASP:H	2.15	0.55
1:B:649:ASN:HD22	1:B:652:ARG:HE	1.52	0.55
1:B:799:ALA:O	1:B:800:GLN:HB2	2.05	0.55
1:B:318:ASP:HB3	1:B:321:THR:HB	1.88	0.55
1:A:140:GLU:HA	1:A:147:ARG:HH22	1.71	0.55
1:B:359:GLN:HE21	1:B:359:GLN:N	1.92	0.55
1:B:137:ARG:HD2	2:B:1836:HOH:O	2.05	0.55
1:A:192:HIS:HD2	2:A:1694:HOH:O	1.89	0.55
1:A:233:ASN:HB3	2:A:1057:HOH:O	2.06	0.55
1:A:472:ILE:HG21	1:A:492:THR:HB	1.87	0.55
1:A:764:ARG:HD3	1:A:767:GLU:OE1	2.06	0.54
1:B:460:LEU:HB3	1:B:468:GLU:HG2	1.89	0.54
1:B:422:ASP:O	1:B:426:ARG:HG2	2.06	0.54
1:A:233:ASN:N	1:A:233:ASN:HD22	2.04	0.54
1:A:612:VAL:HG13	1:B:323:ARG:HH22	1.71	0.54
1:B:507:ARG:HH11	1:B:507:ARG:HG3	1.71	0.54
1:A:501:ASP:HB3	2:A:1786:HOH:O	2.07	0.54
1:A:243:PRO:HG2	2:A:1382:HOH:O	2.07	0.54
1:B:425:GLU:HG2	2:B:1707:HOH:O	2.07	0.54
1:B:675:MET:HE1	1:B:771:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HG3	1:A:328:ARG:NH1	2.17	0.54
1:A:793:ILE:HG22	2:A:1117:HOH:O	2.08	0.54
1:A:437:THR:HG22	1:A:555:THR:HG21	1.89	0.54
1:A:755:GLU:HB3	2:A:1925:HOH:O	2.08	0.54
1:B:429:LYS:HG3	2:B:1893:HOH:O	2.08	0.54
1:B:251:TYR:OH	1:B:299:GLU:OE2	2.18	0.53
1:A:662:ILE:HG21	1:A:772:LEU:HB2	1.90	0.53
1:B:303:ARG:O	1:B:304:ASP:HB2	2.08	0.53
1:B:53:GLN:H	1:B:53:GLN:NE2	2.00	0.53
1:B:694:GLU:O	1:B:696:TRP:N	2.41	0.53
1:B:801:ARG:HB3	2:B:1437:HOH:O	2.09	0.53
1:A:558:HIS:CD2	1:A:564:ASP:OD2	2.56	0.53
1:A:669:LYS:HD3	1:A:764:ARG:HH21	1.74	0.53
1:A:81:ARG:HD3	2:A:1319:HOH:O	2.08	0.53
1:B:801:ARG:NH2	2:B:1899:HOH:O	2.41	0.52
1:A:-14:SER:H	1:A:-3:SER:HB2	1.72	0.52
1:B:246:GLU:OE2	1:B:249:VAL:HG21	2.08	0.52
1:B:2:LEU:C	1:B:4:LYS:H	2.18	0.52
1:B:527:HIS:HB2	2:B:1513:HOH:O	2.08	0.52
1:B:447:SER:HA	1:B:450:PHE:HB2	1.91	0.52
1:B:684:VAL:O	1:B:688:THR:HB	2.10	0.52
1:B:372:THR:HG21	1:B:375:ALA:HB2	1.91	0.52
1:A:733:GLU:CB	2:A:1739:HOH:O	2.58	0.52
1:B:559:GLU:HG2	1:B:630:VAL:HG11	1.92	0.52
1:A:463:LYS:HB2	2:A:1859:HOH:O	2.09	0.52
1:B:246:GLU:H	1:B:250:HIS:HD2	1.57	0.51
1:A:329:ARG:HB3	1:A:335:HIS:CE1	2.45	0.51
1:A:490:ARG:NH1	2:A:1802:HOH:O	2.44	0.51
1:A:667:ASN:ND2	1:A:764:ARG:HD2	2.26	0.51
1:B:227:PRO:HA	1:B:349:GLU:O	2.10	0.51
1:B:243:PRO:HG2	2:B:1347:HOH:O	2.10	0.51
1:A:359:GLN:H	1:A:359:GLN:NE2	1.89	0.51
1:A:602:LEU:HD11	1:B:791:GLU:O	2.11	0.51
1:A:669:LYS:HE2	2:A:1860:HOH:O	2.10	0.51
1:B:775:ILE:CG1	1:B:822:MET:HE3	2.23	0.51
1:A:708:LEU:HD13	1:A:827:VAL:HG22	1.92	0.51
1:B:13:MET:HE2	1:B:17:LEU:HG	1.92	0.51
1:A:289:SER:HB3	2:A:1842:HOH:O	2.09	0.51
1:A:240:ARG:O	1:A:243:PRO:HD2	2.11	0.51
1:A:675:MET:O	1:A:679:VAL:HG23	2.11	0.51
1:B:228:ALA:HB3	2:B:1706:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ASP:O	1:B:717:SER:C	2.54	0.50
1:A:372:THR:CG2	1:A:375:ALA:HB2	2.40	0.50
1:B:278:ASN:HD21	1:B:832:ASN:ND2	2.09	0.50
1:B:118:ASN:HD21	1:B:367:LYS:NZ	2.10	0.50
1:B:129:THR:HB	2:B:1366:HOH:O	2.11	0.50
1:A:702:TRP:HE1	1:A:714:THR:CA	2.17	0.50
1:B:341:LYS:HE2	1:B:342:GLU:OE2	2.11	0.50
1:A:140:GLU:HA	1:A:147:ARG:NH2	2.26	0.50
1:A:328:ARG:CG	1:A:328:ARG:NH1	2.61	0.50
1:A:15:LYS:CD	2:A:1869:HOH:O	2.57	0.50
1:A:793:ILE:CG2	2:A:1117:HOH:O	2.60	0.50
1:B:810:GLU:O	1:B:814:MET:HG2	2.12	0.50
1:B:593:ARG:HD2	2:B:1701:HOH:O	2.10	0.50
1:B:660:ARG:CG	2:B:1740:HOH:O	2.57	0.50
1:B:136:LYS:HA	1:B:155:VAL:HG11	1.93	0.50
1:B:677:ARG:HD3	2:B:1289:HOH:O	2.11	0.50
1:B:775:ILE:HG12	1:B:822:MET:CE	2.24	0.50
1:A:254:ASP:HB3	1:A:259:THR:HG22	1.94	0.50
1:B:78:LEU:O	1:B:79:ASP:HB2	2.12	0.50
1:A:558:HIS:HE1	2:A:1297:HOH:O	1.93	0.49
1:A:258:ARG:HA	1:A:300:LEU:HD11	1.93	0.49
1:B:784:TYR:CE2	1:B:788:TYR:HE2	2.30	0.49
1:B:5:LEU:N	2:B:1569:HOH:O	2.45	0.49
1:B:42:LYS:NZ	2:B:1195:HOH:O	2.44	0.49
1:B:223:ILE:HG12	1:B:355:THR:HG22	1.95	0.49
1:A:786:MET:HE1	1:A:811:GLY:HA3	1.94	0.49
1:B:733:GLU:O	1:B:735:LEU:N	2.46	0.49
1:A:715:ALA:O	1:A:717:SER:N	2.46	0.48
1:A:128:VAL:HA	1:A:176:GLY:O	2.13	0.48
1:B:254:ASP:HB3	1:B:259:THR:HG22	1.95	0.48
1:A:42:LYS:NZ	2:A:1285:HOH:O	2.46	0.48
1:A:490:ARG:HG2	2:A:1751:HOH:O	2.11	0.48
1:A:674:ASP:OD1	1:A:677:ARG:NH1	2.46	0.48
1:A:276:ILE:HG13	1:A:281:GLU:OE2	2.12	0.48
1:A:688:THR:HG23	1:A:696:TRP:CZ2	2.48	0.48
1:B:421:ASP:OD1	1:B:453:ARG:NH2	2.46	0.48
1:A:11:GLY:HA2	2:A:1133:HOH:O	2.13	0.48
1:A:357:THR:HB	1:A:359:GLN:NE2	2.29	0.48
1:B:453:ARG:CG	1:B:453:ARG:NH1	2.77	0.48
1:A:169:TYR:CZ	1:A:199:GLN:HG2	2.49	0.48
1:A:778:LYS:HE2	2:A:1431:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:THR:C	1:A:453:ARG:H	2.22	0.47
1:B:328:ARG:HH11	1:B:796:ARG:HD2	1.79	0.47
1:B:372:THR:CG2	1:B:375:ALA:HB2	2.43	0.47
1:A:116:TYR:CZ	1:A:149:LEU:HD13	2.50	0.47
1:B:714:THR:O	1:B:717:SER:CB	2.61	0.47
1:B:472:ILE:HG13	1:B:489:GLY:HA3	1.97	0.47
1:B:764:ARG:HD3	1:B:764:ARG:HA	1.45	0.47
1:B:328:ARG:HG2	2:B:1598:HOH:O	2.14	0.47
1:B:648:MET:HG3	2:B:1537:HOH:O	2.14	0.47
1:A:505:ASP:OD1	1:A:522:TYR:OH	2.31	0.47
1:B:345:GLU:HG3	2:B:1412:HOH:O	2.13	0.47
1:A:246:GLU:OE1	1:A:249:VAL:HG21	2.14	0.47
1:A:397:MET:HE3	1:A:397:MET:HB3	1.87	0.47
1:A:672:ALA:O	1:A:676:VAL:HG23	2.14	0.47
1:A:677:ARG:HD3	2:A:1341:HOH:O	2.14	0.47
1:B:24:VAL:HG22	1:B:64:PRO:HA	1.96	0.47
1:A:326:ILE:HG21	2:B:1884:HOH:O	2.14	0.47
1:B:15:LYS:HD3	2:B:1434:HOH:O	2.14	0.47
1:B:141:TRP:HD1	1:B:142:MET:HE2	1.79	0.47
1:B:190:MET:HE2	1:B:224:ILE:HD12	1.96	0.47
1:A:245:MET:HE2	1:A:270:VAL:HG22	1.96	0.47
1:A:381:GLU:CD	1:A:638:ARG:HH11	2.23	0.47
1:A:713:ILE:O	1:A:714:THR:O	2.32	0.47
1:B:321:THR:HG22	1:B:323:ARG:HB2	1.96	0.47
1:B:546:GLU:OE2	1:B:546:GLU:HA	2.15	0.47
1:A:245:MET:HE1	1:A:270:VAL:CG2	2.45	0.47
1:A:509:ARG:HD2	2:A:1828:HOH:O	2.14	0.47
1:A:819:LEU:HD23	1:A:822:MET:CE	2.41	0.47
1:A:310:ARG:HA	1:A:310:ARG:HE	1.79	0.47
1:B:543:GLU:HB3	2:B:1692:HOH:O	2.14	0.47
1:A:426:ARG:HD3	1:A:551:TYR:CD2	2.50	0.46
1:A:463:LYS:HE2	2:A:1768:HOH:O	2.14	0.46
1:B:6:LEU:C	1:B:8:LEU:N	2.73	0.46
1:A:75:TRP:CE2	2:A:1783:HOH:O	2.56	0.46
1:A:660:ARG:O	1:A:661:ARG:C	2.58	0.46
1:A:123:ASN:HB3	1:A:203:HIS:CD2	2.51	0.46
1:B:793:ILE:HG12	1:B:807:TYR:HB2	1.97	0.46
1:A:-5:ARG:HD3	1:A:-5:ARG:HA	1.65	0.46
1:A:2:LEU:HB3	1:A:13:MET:HE3	1.98	0.46
1:A:233:ASN:H	1:A:233:ASN:ND2	2.14	0.46
1:A:647:VAL:HG22	1:A:808:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:O	1:A:659:ARG:NH2	2.38	0.46
1:B:6:LEU:C	1:B:8:LEU:H	2.24	0.46
1:A:247:LYS:C	1:A:249:VAL:H	2.23	0.45
1:B:12:ARG:NH1	2:B:1295:HOH:O	2.48	0.45
1:B:258:ARG:HG2	2:B:1493:HOH:O	2.15	0.45
1:B:662:ILE:HG23	1:B:768:ARG:HG2	1.97	0.45
1:A:226:GLY:O	1:A:350:ASN:HA	2.17	0.45
1:A:587:GLY:O	1:A:592:ARG:NH1	2.48	0.45
1:B:163:ASP:OD1	1:B:166:ARG:NH1	2.50	0.45
1:B:323:ARG:HD2	1:B:323:ARG:HA	1.73	0.45
1:B:39:LEU:O	1:B:40:ARG:CB	2.64	0.45
1:B:276:ILE:HG13	1:B:281:GLU:OE2	2.16	0.45
1:A:211:ASP:OD2	1:A:562:ARG:NH1	2.46	0.45
1:A:427:TYR:CZ	1:A:456:PRO:HD2	2.51	0.45
1:B:129:THR:CB	2:B:1366:HOH:O	2.64	0.45
1:B:444:GLU:HG2	1:B:444:GLU:H	1.64	0.45
1:A:372:THR:HG21	1:A:375:ALA:HB2	1.99	0.45
1:A:552:VAL:HG23	1:A:571:SER:HB2	1.97	0.45
1:B:4:LYS:HG3	2:B:1069:HOH:O	2.16	0.45
1:A:46:PHE:HB3	1:A:120:LEU:HD13	1.99	0.45
1:A:270:VAL:HG21	1:A:291:LEU:HD22	1.99	0.45
1:B:510:GLU:HG2	2:B:1916:HOH:O	2.17	0.45
1:A:359:GLN:HE21	1:A:359:GLN:N	1.89	0.45
1:A:546:GLU:HB3	2:A:1726:HOH:O	2.17	0.45
1:B:246:GLU:N	1:B:250:HIS:HD2	2.14	0.45
1:A:179:ASN:HB2	2:A:1827:HOH:O	2.16	0.45
1:A:605:ARG:NH1	1:B:791:GLU:OE2	2.49	0.45
1:B:532:ILE:O	1:B:535:GLU:HB2	2.15	0.45
1:B:585:SER:C	1:B:587:GLY:H	2.25	0.45
1:B:615:GLU:HA	2:B:1514:HOH:O	2.17	0.45
1:A:463:LYS:HB3	1:A:464:TYR:CD1	2.52	0.44
1:A:617:LYS:HB2	2:A:1872:HOH:O	2.17	0.44
1:B:586:LEU:HD21	1:B:619:VAL:HG13	1.98	0.44
1:B:671:GLN:CD	1:B:671:GLN:H	2.25	0.44
1:A:764:ARG:HA	1:A:764:ARG:HD3	1.62	0.44
1:B:270:VAL:HG21	1:B:291:LEU:HD22	1.98	0.44
1:B:505:ASP:OD1	1:B:522:TYR:OH	2.21	0.44
1:A:802:ASP:HA	1:A:803:PRO:HD2	1.87	0.44
1:B:698:LEU:O	1:B:702:TRP:HB2	2.18	0.44
1:B:709:TYR:HB3	1:B:831:PHE:CD2	2.52	0.44
1:B:205:ALA:HB2	1:B:365:TYR:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:VAL:HG11	1:B:450:PHE:CZ	2.53	0.44
1:A:286:PRO:HG3	1:A:777:ARG:NH2	2.31	0.44
1:B:81:ARG:HG2	2:B:1378:HOH:O	2.18	0.44
1:A:219:ARG:HD2	2:A:1678:HOH:O	2.16	0.44
1:A:709:TYR:HB3	1:A:831:PHE:CD2	2.53	0.44
1:A:798:MET:HG2	2:A:1385:HOH:O	2.17	0.44
1:A:451:THR:C	1:A:453:ARG:N	2.74	0.43
1:B:367:LYS:HA	2:B:1557:HOH:O	2.18	0.43
1:B:669:LYS:HB2	1:B:764:ARG:NH1	2.33	0.43
1:B:694:GLU:H	1:B:694:GLU:HG2	1.61	0.43
1:A:530:LEU:HB3	1:A:531:PRO:HD3	2.00	0.43
1:A:661:ARG:NH2	2:A:1576:HOH:O	2.51	0.43
1:B:242:ALA:N	1:B:243:PRO:HD2	2.33	0.43
1:B:519:PRO:HD2	2:B:1374:HOH:O	2.18	0.43
1:B:531:PRO:HB3	2:B:1584:HOH:O	2.17	0.43
1:B:4:LYS:CG	2:B:1069:HOH:O	2.66	0.43
1:B:559:GLU:HG2	1:B:630:VAL:HG12	2.01	0.43
1:B:200:ARG:O	1:B:200:ARG:HG3	2.19	0.43
1:B:430:GLY:O	1:B:478:ARG:HB2	2.19	0.43
1:A:241:LEU:O	1:A:245:MET:HG3	2.18	0.43
1:B:205:ALA:HB2	1:B:365:TYR:CD2	2.53	0.43
1:B:260:VAL:HG11	1:B:295:LEU:HB2	2.00	0.43
1:B:442:ARG:HA	1:B:442:ARG:HD2	1.59	0.43
1:B:687:ALA:HB3	1:B:701:LEU:HD13	2.00	0.43
1:A:246:GLU:N	1:A:250:HIS:HD2	2.08	0.43
1:B:328:ARG:NH1	1:B:796:ARG:HD2	2.34	0.43
1:B:463:LYS:HB3	1:B:464:TYR:CD1	2.53	0.43
1:B:678:ASP:OD1	1:B:823:LYS:HE2	2.18	0.43
1:A:90:ALA:HB1	1:A:114:PRO:HD3	2.00	0.43
1:A:233:ASN:N	1:A:233:ASN:ND2	2.66	0.43
1:A:761:GLY:O	1:A:764:ARG:HB2	2.19	0.43
1:A:798:MET:O	1:A:801:ARG:HG3	2.18	0.43
1:B:40:ARG:HD3	2:B:1825:HOH:O	2.18	0.43
1:A:371:MET:HE2	1:A:371:MET:HB3	1.62	0.42
1:A:438:THR:HB	1:A:556:GLU:CG	2.49	0.42
1:A:329:ARG:HB3	1:A:335:HIS:ND1	2.34	0.42
1:A:233:ASN:HD22	1:A:233:ASN:H	1.65	0.42
1:A:818:MET:HE3	1:A:818:MET:HB3	1.86	0.42
1:B:464:TYR:CD1	1:B:464:TYR:N	2.87	0.42
1:B:809:ARG:HD3	2:B:1189:HOH:O	2.20	0.42
1:A:612:VAL:CG1	1:B:323:ARG:HH22	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ILE:HG12	1:B:355:THR:CG2	2.49	0.42
1:B:559:GLU:CG	1:B:630:VAL:HG11	2.49	0.42
1:B:617:LYS:HB3	2:B:1908:HOH:O	2.19	0.42
1:B:693:ALA:O	1:B:694:GLU:C	2.62	0.42
1:A:103:THR:HA	2:A:1132:HOH:O	2.18	0.42
1:A:169:TYR:CE1	1:A:199:GLN:HG2	2.55	0.42
1:A:797:ALA:HA	1:A:801:ARG:HD3	2.01	0.42
1:B:410:LYS:HD2	1:B:603:LEU:HB3	2.02	0.42
1:A:205:ALA:HB2	1:A:365:TYR:CE2	2.54	0.42
1:B:107:LYS:HD3	2:B:1001:HOH:O	2.18	0.42
1:B:540:GLU:O	1:B:540:GLU:HG3	2.19	0.42
1:B:770:VAL:O	1:B:774:VAL:HG23	2.20	0.42
1:A:674:ASP:O	1:A:678:ASP:HB2	2.20	0.42
1:B:655:ILE:HD13	1:B:655:ILE:HA	1.87	0.42
1:B:-5:ARG:HD3	1:B:-5:ARG:HA	1.65	0.42
1:B:39:LEU:HD23	1:B:148:PHE:CE1	2.53	0.42
1:A:342:GLU:O	1:A:343:HIS:C	2.62	0.41
1:A:561:ARG:O	1:A:561:ARG:HG3	2.19	0.41
1:B:222:LEU:O	1:B:355:THR:HG22	2.20	0.41
1:B:223:ILE:HG23	1:B:352:THR:HG23	2.02	0.41
1:A:438:THR:HB	1:A:556:GLU:CD	2.44	0.41
1:A:660:ARG:NH1	2:A:1929:HOH:O	2.51	0.41
1:B:133:TYR:CZ	1:B:137:ARG:HD3	2.55	0.41
1:B:453:ARG:HG3	1:B:453:ARG:HH11	1.84	0.41
1:A:796:ARG:HG2	2:A:1785:HOH:O	2.19	0.41
1:B:21:ALA:HB2	1:B:88:MET:HG3	2.03	0.41
1:A:202:HIS:O	1:A:365:TYR:HA	2.21	0.41
1:B:116:TYR:HD1	1:B:151:LEU:CD1	2.31	0.41
1:B:424:ALA:HB2	1:B:455:ILE:HD11	2.01	0.41
1:B:802:ASP:HA	1:B:803:PRO:HD2	1.95	0.41
1:B:381:GLU:OE2	1:B:638:ARG:HD2	2.20	0.41
1:B:507:ARG:CG	1:B:507:ARG:NH1	2.75	0.41
1:B:754:LEU:HD13	1:B:763:MET:SD	2.61	0.41
1:B:143:GLY:O	1:B:147:ARG:HB2	2.20	0.41
1:A:796:ARG:HD3	2:A:1885:HOH:O	2.21	0.41
1:A:268:GLU:HA	1:A:271:GLU:HB2	2.03	0.41
1:A:381:GLU:OE2	1:A:638:ARG:HD2	2.21	0.41
1:B:152:GLN:HG2	2:B:1365:HOH:O	2.21	0.41
1:B:552:VAL:HG23	1:B:571:SER:HB2	2.03	0.41
1:B:556:GLU:HG2	2:B:1862:HOH:O	2.21	0.41
1:A:242:ALA:N	1:A:243:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:LEU:HD23	1:B:771:LEU:HA	1.84	0.40
1:A:43:THR:HG1	1:A:116:TYR:HH	1.68	0.40
1:A:245:MET:CE	1:A:270:VAL:CG2	2.98	0.40
1:A:801:ARG:NE	1:A:802:ASP:H	2.20	0.40
1:B:186:LEU:HD22	1:B:354:ALA:HB1	2.03	0.40
1:B:326:ILE:HG13	1:B:795:LEU:HD13	2.04	0.40
1:B:653:LYS:HE3	2:B:1235:HOH:O	2.21	0.40
1:A:245:MET:HE1	1:A:270:VAL:HG22	2.03	0.40
1:B:325:LEU:HD13	1:B:328:ARG:NH2	2.36	0.40
1:B:514:ASP:HB3	1:B:517:GLU:HB2	2.03	0.40
1:A:283:ALA:O	1:A:284:ASN:CB	2.68	0.40
1:B:551:TYR:HD1	1:B:579:GLU:HB3	1.86	0.40
1:B:785:GLU:HG3	2:B:1130:HOH:O	2.20	0.40
1:A:53:GLN:CD	1:A:53:GLN:N	2.78	0.40
1:A:317:VAL:HG12	1:A:324:VAL:HA	2.04	0.40
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.96	0.40
1:A:702:TRP:CD1	1:A:714:THR:HG23	2.57	0.40
1:B:672:ALA:HB2	1:B:767:GLU:HG2	2.03	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	835/922 (91%)	765 (92%)	57 (7%)	13 (2%)	7	27
1	B	834/922 (90%)	758 (91%)	60 (7%)	16 (2%)	6	22
All	All	1669/1844 (90%)	1523 (91%)	117 (7%)	29 (2%)	7	25

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLU
1	A	714	THR
1	A	715	ALA
1	A	716	ASP
1	B	695	ASP
1	B	734	GLU
1	B	760	GLU
1	A	735	LEU
1	B	229	ASP
1	B	693	ALA
1	A	-5	ARG
1	A	452	LYS
1	B	3	SER
1	B	111	CYS
1	B	717	SER
1	B	758	ALA
1	B	799	ALA
1	B	800	GLN
1	A	107	LYS
1	A	574	GLN
1	A	801	ARG
1	A	802	ASP
1	A	690	GLU
1	A	694	GLU
1	B	311	ASP
1	B	802	ASP
1	B	-4	GLY
1	B	694	GLU
1	B	324	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	696/755 (92%)	565 (81%)	131 (19%)	1	5
1	B	697/755 (92%)	551 (79%)	146 (21%)	1	4
All	All	1393/1510 (92%)	1116 (80%)	277 (20%)	1	5

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	ARG
1	A	-3	SER
1	A	0	ASP
1	A	3	SER
1	A	4	LYS
1	A	7	ARG
1	A	12	ARG
1	A	15	LYS
1	A	19	LYS
1	A	35	THR
1	A	43	THR
1	A	47	LYS
1	A	48	ARG
1	A	53	GLN
1	A	69	VAL
1	A	78	LEU
1	A	107	LYS
1	A	111	CYS
1	A	136	LYS
1	A	152	GLN
1	A	155	VAL
1	A	179	ASN
1	A	193	SER
1	A	210	VAL
1	A	219	ARG
1	A	220	THR
1	A	222	LEU
1	A	225	SER
1	A	232	SER
1	A	233	ASN
1	A	240	ARG
1	A	246	GLU
1	A	257	LYS
1	A	259	THR
1	A	262	VAL
1	A	264	GLU
1	A	265	LYS
1	A	268	GLU
1	A	271	GLU
1	A	276	ILE
1	A	284	ASN
1	A	296	LYS

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	305	LYS
1	A	310	ARG
1	A	316	ILE
1	A	319	GLU
1	A	326	ILE
1	A	328	ARG
1	A	329	ARG
1	A	338	ILE
1	A	347	LYS
1	A	357	THR
1	A	359	GLN
1	A	371	MET
1	A	376	GLN
1	A	384	GLU
1	A	387	LYS
1	A	401	ARG
1	A	402	GLU
1	A	405	SER
1	A	413	GLU
1	A	417	ILE
1	A	434	LEU
1	A	438	THR
1	A	442	ARG
1	A	443	SER
1	A	444	GLU
1	A	449	GLN
1	A	452	LYS
1	A	453	ARG
1	A	454	ARG
1	A	460	LEU
1	A	463	LYS
1	A	478	ARG
1	A	485	THR
1	A	487	MET
1	A	490	ARG
1	A	534	LYS
1	A	538	SER
1	A	539	LYS
1	A	542	LYS
1	A	546	GLU
1	A	555	THR

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Mol	Chain	Res	Type
1	A	570	ARG
1	A	592	ARG
1	A	593	ARG
1	A	599	LEU
1	A	600	GLU
1	A	601	THR
1	A	603	LEU
1	A	615	GLU
1	A	618	MET
1	A	629	GLN
1	A	631	GLU
1	A	632	GLN
1	A	641	VAL
1	A	653	LYS
1	A	659	ARG
1	A	663	LEU
1	A	678	ASP
1	A	688	THR
1	A	690	GLU
1	A	694	GLU
1	A	695	ASP
1	A	698	LEU
1	A	703	THR
1	A	716	ASP
1	A	735	LEU
1	A	737	GLU
1	A	740	LEU
1	A	741	LYS
1	A	744	GLU
1	A	750	ARG
1	A	754	LEU
1	A	760	GLU
1	A	764	ARG
1	A	778	LYS
1	A	780	ARG
1	A	781	GLU
1	A	793	ILE
1	A	795	LEU
1	A	798	MET
1	A	800	GLN
1	A	801	ARG
1	A	805	VAL

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Mol	Chain	Res	Type
1	A	809	ARG
1	A	818	MET
1	A	822	MET
1	A	826	SER
1	A	827	VAL
1	B	-14	SER
1	B	-5	ARG
1	B	3	SER
1	B	4	LYS
1	B	7	ARG
1	B	8	LEU
1	B	12	ARG
1	B	18	LYS
1	B	26	THR
1	B	31	VAL
1	B	33	LYS
1	B	35	THR
1	B	39	LEU
1	B	40	ARG
1	B	47	LYS
1	B	48	ARG
1	B	50	LEU
1	B	52	ASP
1	B	53	GLN
1	B	54	LYS
1	B	55	ASN
1	B	107	LYS
1	B	108	THR
1	B	130	VAL
1	B	152	GLN
1	B	155	VAL
1	B	210	VAL
1	B	212	SER
1	B	219	ARG
1	B	225	SER
1	B	232	SER
1	B	233	ASN
1	B	236	THR
1	B	256	ARG
1	B	257	LYS
1	B	258	ARG
1	B	259	THR

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Mol	Chain	Res	Type
1	B	265	LYS
1	B	276	ILE
1	B	284	ASN
1	B	289	SER
1	B	293	ASN
1	B	296	LYS
1	B	305	LYS
1	B	308	ILE
1	B	310	ARG
1	B	311	ASP
1	B	319	GLU
1	B	320	PHE
1	B	323	ARG
1	B	326	ILE
1	B	328	ARG
1	B	329	ARG
1	B	338	ILE
1	B	344	VAL
1	B	347	LYS
1	B	355	THR
1	B	359	GLN
1	B	371	MET
1	B	372	THR
1	B	384	GLU
1	B	391	VAL
1	B	397	MET
1	B	400	ILE
1	B	410	LYS
1	B	411	THR
1	B	413	GLU
1	B	417	ILE
1	B	421	ASP
1	B	425	GLU
1	B	429	LYS
1	B	433	VAL
1	B	434	LEU
1	B	438	THR
1	B	441	GLU
1	B	442	ARG
1	B	444	GLU
1	B	449	GLN
1	B	452	LYS

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Mol	Chain	Res	Type
1	B	453	ARG
1	B	454	ARG
1	B	460	LEU
1	B	463	LYS
1	B	478	ARG
1	B	493	ASP
1	B	507	ARG
1	B	510	GLU
1	B	517	GLU
1	B	534	LYS
1	B	536	GLU
1	B	538	SER
1	B	539	LYS
1	B	540	GLU
1	B	546	GLU
1	B	555	THR
1	B	556	GLU
1	B	566	GLN
1	B	573	ARG
1	B	599	LEU
1	B	600	GLU
1	B	601	THR
1	B	605	ARG
1	B	617	LYS
1	B	618	MET
1	B	621	ARG
1	B	623	ILE
1	B	629	GLN
1	B	636	GLU
1	B	659	ARG
1	B	663	LEU
1	B	664	GLU
1	B	669	LYS
1	B	671	GLN
1	B	680	ILE
1	B	683	TYR
1	B	688	THR
1	B	694	GLU
1	B	698	LEU
1	B	705	LEU
1	B	713	ILE
1	B	717	SER

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Mol	Chain	Res	Type
1	B	718	LEU
1	B	737	GLU
1	B	740	LEU
1	B	744	GLU
1	B	750	ARG
1	B	754	LEU
1	B	755	GLU
1	B	756	GLU
1	B	760	GLU
1	B	764	ARG
1	B	766	LEU
1	B	767	GLU
1	B	770	VAL
1	B	778	LYS
1	B	796	ARG
1	B	798	MET
1	B	800	GLN
1	B	801	ARG
1	B	806	GLU
1	B	810	GLU
1	B	814	MET
1	B	822	MET
1	B	824	GLU
1	B	827	VAL
1	B	835	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	146	HIS
1	A	192	HIS
1	A	203	HIS
1	A	233	ASN
1	A	250	HIS
1	A	284	ASN
1	A	293	ASN
1	A	350	ASN
1	A	359	GLN
1	A	396	ASN
1	A	458	ASN
1	A	486	ASN

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Mol	Chain	Res	Type
1	A	506	GLN
1	A	558	HIS
1	A	607	ASN
1	A	632	GLN
1	A	649	ASN
1	B	53	GLN
1	B	118	ASN
1	B	146	HIS
1	B	250	HIS
1	B	293	ASN
1	B	359	GLN
1	B	396	ASN
1	B	458	ASN
1	B	461	ASN
1	B	558	HIS
1	B	649	ASN
1	B	671	GLN
1	B	765	GLN
1	B	773	ASN
1	B	808	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.