



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:48 PM UTC

PDB ID : 1L7D / pdb_0000117d
Title : Crystal Structure of R. rubrum Transhydrogenase Domain I without Bound NAD(H)
Authors : Prasad, G.S.; Wahlberg, M.; Sridhar, V.; Yamaguchi, M.; Hatefi, Y.; Stout, C.D.
Deposited on : 2002-03-14
Resolution : 1.81 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

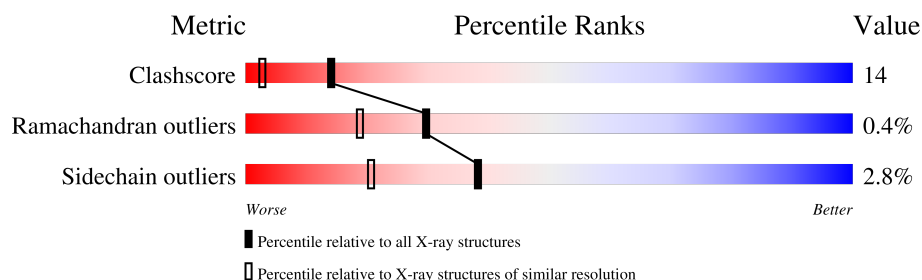
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)

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	384	
1	B	384	
1	C	384	
1	D	384	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11344 atoms, of which 0 are hydrogens and 0 are deuteriums.

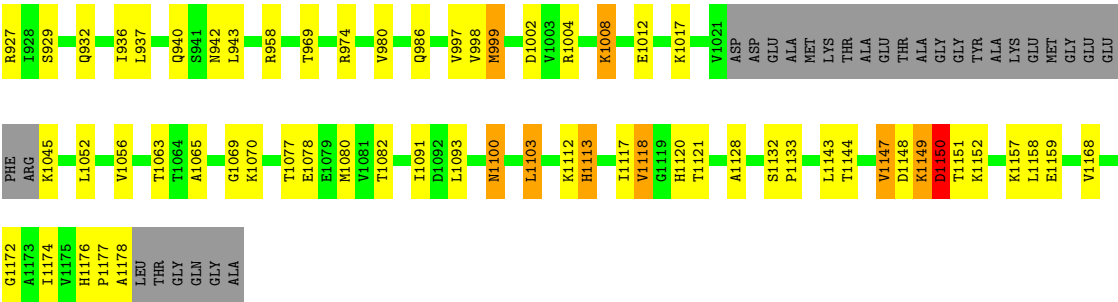
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called nicotinamide nucleotide Transhydrogenase, subunit alpha 1.

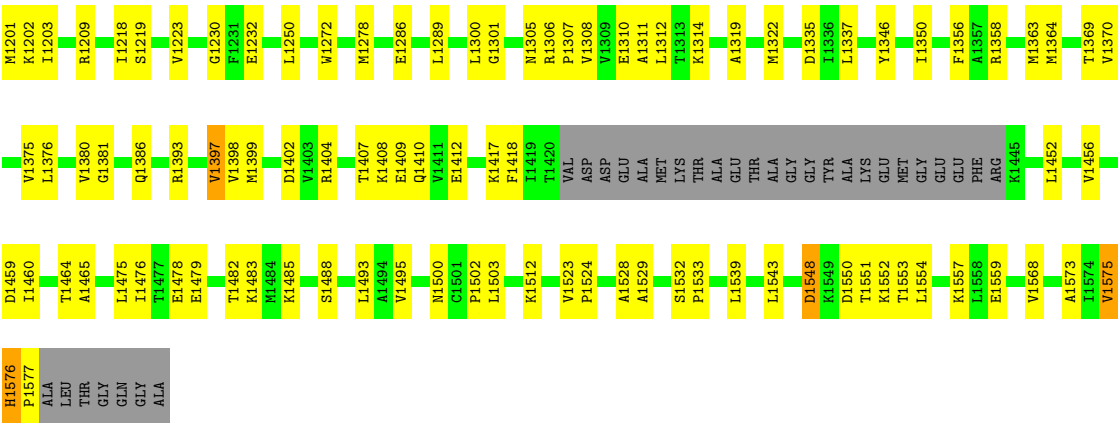
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2589	1638	448	487	16			
1	B	358	Total	C	N	O	S	0	0	0
			2620	1656	454	494	16			
1	C	355	Total	C	N	O	S	0	0	0
			2604	1648	451	489	16			
1	D	353	Total	C	N	O	S	0	0	0
			2592	1640	449	487	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total	O	0	0
			184	184		
2	B	243	Total	O	0	0
			243	243		
2	C	291	Total	O	0	0
			291	291		
2	D	221	Total	O	0	0
			221	221		



● Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.96Å 117.13Å 94.23Å 90.00° 108.26° 90.00°	Depositor
Resolution (Å)	50.00 – 1.81	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.81)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11344	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.73	4/2623 (0.2%)	1.08	22/3560 (0.6%)
1	B	0.41	0/2654	0.93	9/3600 (0.2%)
1	C	0.51	2/2638 (0.1%)	0.97	13/3578 (0.4%)
1	D	0.46	2/2626 (0.1%)	0.98	15/3561 (0.4%)
All	All	0.54	8/10541 (0.1%)	0.99	59/14299 (0.4%)

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	3	6
1	B	1	0
All	All	4	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	ASP	CA-C	-21.14	1.26	1.52
1	A	348	ASP	C-N	14.64	1.54	1.33
1	C	1147	VAL	C-N	-9.51	1.21	1.33
1	A	347	VAL	C-N	-8.45	1.21	1.33
1	C	1150	ASP	C-N	8.13	1.47	1.33
1	A	377	PRO	N-CD	6.47	1.56	1.47
1	D	1576	HIS	C-N	5.38	1.43	1.34
1	D	1577	PRO	N-CD	5.24	1.55	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	O-C-N	13.08	138.13	123.22
1	D	1576	HIS	CA-C-O	10.32	128.13	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	HIS	O-C-N	-10.19	109.61	121.32
1	C	1150	ASP	O-C-N	9.16	134.78	122.59
1	D	1575	VAL	CA-C-O	8.94	127.16	119.38
1	A	377	PRO	CA-N-CD	-8.77	99.72	112.00
1	D	1575	VAL	O-C-N	-8.76	113.39	122.06
1	C	1113	HIS	CA-C-O	8.39	131.22	120.81
1	A	375	VAL	N-CA-C	8.29	119.90	106.72
1	B	432	GLU	N-CA-C	-8.07	96.08	109.24
1	C	1113	HIS	CA-CB-CG	7.98	121.78	113.80
1	B	721	THR	N-CA-C	7.89	121.42	111.24
1	D	1232	GLU	N-CA-C	-7.89	96.38	109.24
1	A	377	PRO	N-CA-CB	7.65	111.42	103.00
1	D	1528	ALA	N-CA-C	7.01	119.81	111.33
1	A	348	ASP	CA-C-O	6.96	127.80	120.36
1	A	328	ALA	N-CA-C	6.92	118.82	111.28
1	C	1128	ALA	N-CA-C	6.86	119.63	111.33
1	D	1381	GLY	N-CA-C	-6.63	103.12	112.60
1	A	374	ILE	CA-C-N	6.54	132.00	123.10
1	A	374	ILE	C-N-CA	6.54	132.00	123.10
1	D	1577	PRO	CA-N-CD	-6.53	102.86	112.00
1	A	347	VAL	CA-C-N	6.51	131.42	122.77
1	A	347	VAL	C-N-CA	6.51	131.42	122.77
1	B	597	VAL	N-CA-C	-6.15	98.82	108.23
1	B	598	VAL	N-CA-C	6.09	116.70	108.17
1	B	499	HIS	N-CA-C	-6.08	97.77	108.23
1	C	997	VAL	N-CA-C	-6.05	98.97	108.23
1	A	198	VAL	N-CA-C	5.84	116.27	107.80
1	A	181	GLY	N-CA-C	-5.81	104.29	112.60
1	B	679	GLU	N-CA-C	-5.80	105.04	111.36
1	C	1147	VAL	O-C-N	5.79	129.16	122.97
1	A	197	VAL	N-CA-C	-5.76	99.41	108.23
1	A	371	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	1397	VAL	N-CA-C	-5.70	99.50	108.23
1	C	998	VAL	N-CA-C	5.68	116.06	108.11
1	C	1151	THR	N-CA-C	-5.64	104.98	113.89
1	D	1576	HIS	C-N-CD	5.61	148.01	125.00
1	D	1301	GLY	N-CA-C	-5.59	103.70	113.76
1	A	99	HIS	N-CA-C	-5.58	100.03	108.67
1	C	1100	ASN	N-CA-C	-5.45	106.59	113.18
1	D	1500	ASN	N-CA-C	-5.42	106.63	113.18
1	B	502	ALA	N-CA-C	5.34	117.52	111.11
1	A	376	HIS	N-CA-CB	5.33	119.86	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLN	N-CA-C	-5.30	105.67	111.82
1	D	1398	VAL	N-CA-C	5.24	115.40	107.80
1	D	1335	ASP	N-CA-C	5.23	116.77	108.67
1	C	832	GLU	N-CA-C	-5.21	99.29	108.20
1	A	352	LYS	CA-C-O	5.18	127.18	120.55
1	A	265	ALA	N-CA-C	5.16	117.15	109.25
1	A	375	VAL	CA-CB-CG2	5.15	119.15	110.40
1	C	1113	HIS	O-C-N	-5.15	113.31	122.21
1	D	1543	LEU	N-CA-C	5.13	118.00	111.69
1	A	135	ASP	N-CA-C	5.10	117.01	108.23
1	B	401	MET	CB-CA-C	5.08	119.76	110.10
1	B	529	SER	N-CA-C	5.06	117.19	111.11
1	D	1495	VAL	N-CA-C	5.06	116.39	110.62
1	C	1065	ALA	N-CA-C	5.04	116.99	109.59
1	C	833	VAL	N-CA-C	5.02	115.31	107.99

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	374	ILE	CB
1	A	375	VAL	CA
1	A	376	HIS	CA
1	B	401	MET	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	VAL	Mainchain
1	A	350	ASP	Mainchain
1	A	375	VAL	Mainchain,Peptide
1	A	376	HIS	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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	2589	0	2715	91	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2620	0	2754	70	0
1	C	2604	0	2744	85	0
1	D	2592	0	2730	69	0
2	A	184	0	0	3	0
2	B	243	0	0	5	1
2	C	291	0	0	7	0
2	D	221	0	0	1	0
All	All	11344	0	10943	306	1

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 14.

All (306) 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:564:MET:HE3	1:B:569:THR:HG21	1.46	0.96
1:A:281:VAL:HA	1:A:284:MET:HE2	1.49	0.95
1:A:284:MET:HE1	1:A:290:ILE:HD11	1.49	0.95
1:A:127:ARG:H	1:A:127:ARG:HH21	1.11	0.94
1:C:999:MET:HE3	1:C:1017:LYS:HB2	1.50	0.93
1:B:401:MET:N	1:B:469:ASP:OD2	2.07	0.85
1:C:837:GLN:HE21	1:C:859:SER:HA	1.41	0.84
1:D:1286:GLU:HA	1:D:1289:LEU:HD23	1.60	0.83
1:D:1308:VAL:O	1:D:1312:LEU:HD23	1.79	0.82
1:B:542:ASN:HD21	1:B:586:GLN:HE21	1.23	0.81
1:A:351:THR:CB	1:A:353:THR:HG22	2.11	0.81
1:B:678:GLU:O	1:B:681:VAL:HG12	1.82	0.80
1:C:923:GLU:HA	1:C:937:LEU:HD11	1.65	0.78
1:A:127:ARG:H	1:A:127:ARG:NH2	1.81	0.78
1:C:942:ASN:HD21	1:C:986:GLN:HE21	1.32	0.76
1:D:1397:VAL:HG12	1:D:1399:MET:HE1	1.67	0.75
1:C:958:ARG:HG3	1:D:1529:ALA:HB3	1.67	0.75
1:B:421:GLU:OE1	1:B:737:LYS:HE2	1.87	0.74
1:B:526:PRO:HA	1:B:527:ARG:HH21	1.53	0.73
1:B:401:MET:HE1	1:B:754:LEU:N	2.03	0.73
1:D:1364:MET:HA	1:D:1369:THR:HG22	1.71	0.72
1:A:1:MET:HE1	1:A:354:LEU:HB2	1.71	0.72
1:D:1306:ARG:O	1:D:1310:GLU:HG3	1.90	0.72
1:B:691:ILE:HD13	1:B:718:VAL:CG1	2.20	0.71
1:A:253:LYS:HE2	1:A:253:LYS:HA	1.74	0.70
1:D:1306:ARG:N	1:D:1307:PRO:HD2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1201:MET:HE3	1:D:1554:LEU:N	2.06	0.70
1:C:911:ALA:O	1:C:914:LYS:HG3	1.92	0.70
1:A:329:ALA:HB3	1:B:558:ARG:HG3	1.74	0.70
1:A:221:VAL:CG1	1:A:250:ALA:HB2	2.23	0.69
1:B:605:ALA:O	1:B:608:LYS:HG2	1.94	0.67
1:A:199:MET:HE1	1:A:217:LYS:HD3	1.75	0.67
1:A:346:HIS:ND1	1:A:357:LYS:HG2	2.10	0.67
1:A:80:ALA:CA	1:A:85:ASP:HB3	2.25	0.66
1:A:2:LYS:HD2	1:A:34:ILE:HD11	1.76	0.66
1:C:906:ARG:H	1:C:907:PRO:CD	2.09	0.66
1:B:691:ILE:HD13	1:B:718:VAL:HG11	1.78	0.65
1:B:401:MET:HE1	1:B:754:LEU:H	1.60	0.65
1:C:903:LEU:HD12	1:C:904:THR:HG23	1.78	0.65
1:D:1557:LYS:HE3	1:D:1559:GLU:OE1	1.96	0.64
1:B:732:SER:HB2	1:B:733:PRO:HD3	1.78	0.64
1:C:802:LYS:HD3	1:C:834:ILE:HD12	1.79	0.64
1:B:690:ILE:HD12	1:B:717:ILE:HD12	1.79	0.63
1:D:1380:VAL:HG22	1:D:1402:ASP:CB	2.28	0.63
1:D:1568:VAL:HA	1:D:1576:HIS:HB2	1.81	0.63
1:D:1408:LYS:HE2	1:D:1412:GLU:OE2	1.99	0.63
1:B:527:ARG:HE	1:B:527:ARG:N	1.97	0.62
1:C:923:GLU:HA	1:C:937:LEU:CD1	2.29	0.62
1:C:999:MET:HE3	1:C:1017:LYS:CB	2.29	0.61
1:B:563:MET:HB2	1:B:570:VAL:HB	1.82	0.61
1:A:158:ARG:HG2	1:B:729:ALA:HB3	1.82	0.61
1:A:348:ASP:OD2	1:A:350:ASP:HB2	2.00	0.61
1:D:1230:GLY:HA3	1:D:1552:LYS:HD2	1.81	0.60
1:D:1386:GLN:HE22	1:D:1393:ARG:HH12	1.48	0.60
1:B:690:ILE:HD12	1:B:717:ILE:CD1	2.31	0.59
1:C:1077:THR:OG1	1:C:1080:MET:HE3	2.02	0.59
1:A:375:VAL:HG23	1:A:376:HIS:HB3	1.83	0.59
1:C:1069:GLY:O	1:C:1070:LYS:HG3	2.01	0.59
1:A:21:GLU:HG3	1:C:1159:GLU:OE1	2.03	0.58
1:A:88:ALA:C	1:A:115:ARG:NH1	2.62	0.58
1:D:1356:PHE:CE2	1:D:1358:ARG:HB2	2.39	0.58
1:D:1375:VAL:HG22	1:D:1460:ILE:HB	1.85	0.58
1:B:678:GLU:O	1:B:682:THR:HG23	2.03	0.58
1:C:923:GLU:CA	1:C:937:LEU:HD11	2.33	0.57
1:D:1311:ALA:HA	1:D:1314:LYS:HE2	1.86	0.57
1:A:21:GLU:HG3	1:C:1159:GLU:CD	2.29	0.57
1:C:1149:LYS:HA	1:C:1152:LYS:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:MET:HE3	1:B:742:PHE:HD1	1.70	0.56
1:D:1322:MET:HE2	1:D:1539:LEU:HD23	1.86	0.56
1:D:1380:VAL:HG23	1:D:1407:THR:HG21	1.87	0.56
1:C:906:ARG:H	1:C:907:PRO:HD2	1.71	0.56
1:A:221:VAL:HG13	1:A:250:ALA:HB2	1.86	0.56
1:C:1147:VAL:HG22	1:C:1148:ASP:N	2.21	0.56
1:B:497:MET:CE	1:B:742:PHE:HD1	2.19	0.56
1:C:1178:ALA:HB2	2:C:1713:HOH:O	2.06	0.56
1:B:592:LYS:HE2	1:B:615:GLY:O	2.06	0.55
1:A:158:ARG:HD2	1:B:730:ASP:OD1	2.06	0.55
1:B:564:MET:HE3	1:B:569:THR:CG2	2.27	0.55
1:C:936:ILE:HG13	1:C:937:LEU:HD12	1.87	0.55
1:A:332:SER:HB2	1:A:333:PRO:HD3	1.89	0.55
1:B:491:LYS:HE3	2:B:2460:HOH:O	2.07	0.55
1:C:845:ILE:HG22	1:C:850:LEU:HD21	1.89	0.55
1:C:845:ILE:HG22	1:C:850:LEU:CD2	2.37	0.55
1:C:1157:LYS:NZ	1:C:1157:LYS:HB3	2.21	0.55
1:A:284:MET:HE1	1:A:290:ILE:CD1	2.31	0.54
1:B:497:MET:HE3	1:B:742:PHE:CD1	2.42	0.54
1:B:667:ILE:HD11	1:B:670:LYS:HG2	1.89	0.54
1:A:186:GLN:HE22	1:A:193:ARG:HH12	1.54	0.54
1:A:348:ASP:OD2	1:A:351:THR:N	2.37	0.54
1:A:2:LYS:HD2	1:A:34:ILE:CD1	2.36	0.54
1:C:900:LEU:CD2	1:C:1168:VAL:HG21	2.38	0.54
1:C:999:MET:HG3	2:C:2387:HOH:O	2.07	0.54
1:C:1008:LYS:HD3	1:C:1012:GLU:CD	2.33	0.54
1:C:1063:THR:CB	1:C:1100:ASN:HD22	2.20	0.54
1:B:691:ILE:HA	1:B:718:VAL:HG13	1.90	0.54
1:D:1452:LEU:HD23	1:D:1452:LEU:O	2.08	0.54
1:C:1149:LYS:HA	1:C:1152:LYS:CA	2.38	0.53
1:B:497:MET:HE2	1:B:739:LEU:HD22	1.90	0.53
1:B:768:VAL:C	1:B:775:VAL:HG22	2.33	0.53
1:B:523:GLU:HB2	1:B:537:LEU:HD11	1.89	0.53
1:B:580:VAL:HG12	1:B:580:VAL:O	2.09	0.53
1:C:1148:ASP:HB3	1:C:1150:ASP:HB2	1.89	0.53
1:A:76:ARG:HG2	1:A:76:ARG:HH21	1.73	0.53
1:A:278:GLU:O	1:A:282:THR:HG23	2.08	0.53
1:A:329:ALA:CB	1:B:558:ARG:HG3	2.39	0.53
1:A:106:ARG:N	1:A:107:PRO:CD	2.72	0.53
1:D:1550:ASP:OD1	1:D:1551:THR:HG23	2.09	0.53
1:A:221:VAL:HG22	1:A:247:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1311:ALA:HA	1:D:1314:LYS:CE	2.39	0.53
1:C:837:GLN:HE21	1:C:859:SER:CA	2.17	0.52
1:C:1120:HIS:HD2	2:C:2118:HOH:O	1.92	0.52
1:D:1459:ASP:CB	1:D:1460:ILE:HD12	2.39	0.52
1:D:1346:TYR:O	1:D:1350:ILE:HD13	2.10	0.52
1:A:80:ALA:N	1:A:85:ASP:HB3	2.25	0.52
1:A:264:THR:HG22	1:A:293:LEU:HD12	1.92	0.52
1:A:221:VAL:HG22	1:A:247:GLN:NE2	2.24	0.52
1:C:1143:LEU:C	1:C:1143:LEU:HD23	2.34	0.52
1:C:1144:THR:O	1:C:1147:VAL:HG12	2.08	0.52
1:A:80:ALA:HB2	1:A:85:ASP:HB3	1.91	0.52
1:B:535:ASP:OD2	1:B:538:SER:HB2	2.11	0.51
1:C:1002:ASP:OD1	1:C:1004:ARG:HG2	2.10	0.51
1:D:1203:ILE:HD11	1:D:1272:TRP:CD2	2.45	0.51
1:D:1380:VAL:HG21	1:D:1407:THR:OG1	2.10	0.51
1:A:194:LEU:HA	1:B:593:ARG:HD3	1.91	0.51
1:D:1286:GLU:HA	1:D:1289:LEU:CD2	2.37	0.51
1:C:818:ILE:HG13	1:C:819:SER:N	2.25	0.51
1:C:905:ASN:OD1	1:C:908:VAL:HG12	2.10	0.51
1:A:208:LYS:HG3	1:A:218:PHE:CB	2.40	0.51
1:D:1408:LYS:O	1:D:1412:GLU:HG3	2.10	0.51
1:A:267:ILE:HG23	1:A:268:PRO:HD2	1.93	0.51
1:C:980:VAL:O	1:C:980:VAL:HG12	2.10	0.51
1:C:1132:SER:HB2	1:C:1133:PRO:HD3	1.92	0.51
1:C:1103:LEU:HB3	1:C:1117:ILE:HD13	1.91	0.51
1:A:91:LYS:HD2	1:A:92:GLU:O	2.11	0.50
1:A:104:THR:C	1:A:105:ASN:HD22	2.19	0.50
1:B:608:LYS:HB3	1:B:618:PHE:CD2	2.46	0.50
1:B:617:LYS:HD2	1:C:1174:ILE:HD12	1.94	0.50
1:B:556:PHE:CE2	1:B:558:ARG:HB2	2.46	0.50
1:B:425:LYS:CD	1:B:740:LEU:HD21	2.42	0.50
1:D:1399:MET:SD	1:D:1417:LYS:HD2	2.51	0.50
1:A:199:MET:SD	1:A:217:LYS:HB3	2.52	0.50
1:A:343:LEU:C	1:A:343:LEU:HD23	2.37	0.50
1:C:892:GLU:O	1:C:915:ARG:O	2.30	0.49
1:D:1300:LEU:HD11	1:D:1319:ALA:HB1	1.94	0.49
1:B:667:ILE:HG13	1:B:670:LYS:HB3	1.93	0.49
1:A:89:LEU:HD22	1:A:89:LEU:N	2.27	0.49
1:C:885:ASP:O	1:C:889:LEU:HD13	2.12	0.49
1:C:1078:GLU:O	1:C:1082:THR:HG23	2.11	0.49
1:C:1120:HIS:HE1	2:C:2279:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1459:ASP:HB2	1:D:1460:ILE:HD12	1.95	0.49
1:A:106:ARG:HB2	1:A:107:PRO:HD3	1.94	0.49
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.47	0.49
1:D:1464:THR:HG22	1:D:1493:LEU:HD12	1.94	0.49
1:D:1306:ARG:N	1:D:1307:PRO:CD	2.74	0.49
1:A:18:ILE:HG13	1:A:19:SER:N	2.28	0.48
1:A:122:MET:HE1	1:A:342:PHE:CE2	2.48	0.48
1:A:180:VAL:HG23	1:A:202:ASP:HB2	1.95	0.48
1:A:317:ILE:N	1:A:317:ILE:HD12	2.29	0.48
1:D:1523:VAL:N	1:D:1524:PRO:HD2	2.28	0.48
1:C:1077:THR:HG23	1:C:1080:MET:HE3	1.96	0.48
1:D:1532:SER:HB2	1:D:1533:PRO:HD3	1.95	0.48
1:C:1112:LYS:HD2	2:C:2241:HOH:O	2.13	0.48
1:A:302:PRO:HG3	2:A:2119:HOH:O	2.13	0.48
1:B:646:LYS:O	1:B:649:GLU:HB3	2.14	0.48
1:B:667:ILE:CD1	1:B:670:LYS:HG2	2.44	0.48
1:B:678:GLU:HB3	1:B:703:LEU:HD13	1.96	0.48
1:C:1103:LEU:HB3	1:C:1117:ILE:CD1	2.44	0.48
1:B:685:LYS:HG2	2:B:1983:HOH:O	2.13	0.47
1:C:927:ARG:HD2	1:C:927:ARG:N	2.29	0.47
1:A:156:PHE:CZ	1:A:259:ASP:HB3	2.50	0.47
1:D:1305:ASN:O	1:D:1308:VAL:HG12	2.15	0.47
1:B:425:LYS:HD3	1:B:740:LEU:HD21	1.96	0.47
1:B:580:VAL:CG1	1:B:585:LEU:HD13	2.45	0.47
1:C:1063:THR:HB	1:C:1100:ASN:HD22	1.78	0.47
1:A:358:LEU:N	1:A:358:LEU:HD22	2.30	0.47
1:B:556:PHE:CZ	1:B:659:ASP:HB3	2.49	0.47
1:C:1149:LYS:HB2	1:C:1152:LYS:HE3	1.95	0.47
1:D:1201:MET:CE	1:D:1554:LEU:HB2	2.45	0.47
1:D:1459:ASP:C	1:D:1460:ILE:HD12	2.40	0.47
1:C:1052:LEU:HD23	1:C:1052:LEU:O	2.15	0.47
1:A:76:ARG:NE	1:A:105:ASN:OD1	2.47	0.47
1:A:122:MET:HE2	1:A:122:MET:HA	1.96	0.47
1:D:1363:MET:HB2	1:D:1370:VAL:HB	1.96	0.47
1:C:1158:LEU:N	1:C:1158:LEU:HD12	2.31	0.46
1:C:1177:PRO:O	1:C:1178:ALA:HB2	2.15	0.46
1:A:281:VAL:CA	1:A:284:MET:HE2	2.34	0.46
1:C:887:VAL:HG12	1:C:915:ARG:HD3	1.98	0.46
1:A:80:ALA:CB	1:A:85:ASP:HB3	2.46	0.46
1:A:203:VAL:HG23	1:A:204:ARG:HD3	1.97	0.46
1:D:1460:ILE:HD12	1:D:1460:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE1	1:A:354:LEU:CB	2.41	0.46
1:B:430:GLY:HA3	1:B:752:LYS:HG2	1.98	0.46
1:B:712:LYS:HG2	2:B:2342:HOH:O	2.15	0.46
1:C:829:LEU:HD13	1:C:1147:VAL:HG11	1.98	0.46
1:C:929:SER:O	1:C:932:GLN:HG3	2.15	0.46
1:A:2:LYS:NZ	1:A:67:GLN:HE21	2.13	0.46
1:B:463:GLN:NE2	2:B:1925:HOH:O	2.49	0.46
1:C:1045:LYS:N	2:C:1879:HOH:O	2.48	0.46
1:B:506:ARG:O	1:B:510:GLU:HG3	2.15	0.46
1:C:867:GLN:O	1:C:867:GLN:HG3	2.16	0.46
1:C:1147:VAL:CG2	1:C:1148:ASP:N	2.79	0.46
1:C:1149:LYS:HB2	1:C:1152:LYS:CE	2.45	0.46
1:A:348:ASP:C	1:A:350:ASP:H	2.24	0.46
1:C:974:ARG:HD3	2:C:1842:HOH:O	2.15	0.46
1:A:104:THR:HG23	2:A:2457:HOH:O	2.15	0.45
1:D:1553:THR:HG22	1:D:1554:LEU:N	2.31	0.45
1:C:1157:LYS:HB3	1:C:1157:LYS:HZ3	1.80	0.45
1:B:647:GLN:HA	1:B:647:GLN:NE2	2.31	0.45
1:B:647:GLN:HA	1:B:647:GLN:HE21	1.80	0.45
1:A:73:LYS:NZ	1:A:73:LYS:HB3	2.31	0.45
1:A:344:THR:HB	1:A:345:PRO:HD3	1.96	0.45
1:D:1218:ILE:HG13	1:D:1219:SER:N	2.32	0.45
1:D:1573:ALA:O	1:D:1575:VAL:HG13	2.16	0.45
1:A:246:LYS:CD	1:A:249:GLU:HB2	2.47	0.45
1:B:652:LEU:HD13	1:B:652:LEU:O	2.17	0.45
1:D:1380:VAL:HG21	1:D:1407:THR:CB	2.46	0.45
1:B:552:GLY:HA2	1:B:691:ILE:HD11	1.99	0.45
1:C:1082:THR:HG22	1:C:1113:HIS:CD2	2.51	0.45
1:C:818:ILE:HG13	1:C:819:SER:H	1.82	0.45
1:C:910:GLU:O	1:C:914:LYS:HG2	2.17	0.45
1:C:1052:LEU:HD23	1:C:1056:VAL:HG13	1.98	0.45
1:D:1350:ILE:HD12	1:D:1350:ILE:N	2.31	0.45
1:D:1209:ARG:HB2	1:D:1278:MET:HE2	1.99	0.45
1:A:351:THR:C	1:A:353:THR:N	2.72	0.45
1:D:1503:LEU:HB3	1:D:1512:LYS:HD2	1.99	0.44
1:D:1551:THR:O	1:D:1552:LYS:C	2.59	0.44
1:D:1380:VAL:HG23	1:D:1380:VAL:O	2.18	0.44
1:A:284:MET:HE3	1:A:315:VAL:HG21	1.99	0.44
1:B:664:THR:HG22	1:B:693:LEU:HD22	1.98	0.44
1:A:357:LYS:HD3	2:A:2477:HOH:O	2.16	0.44
1:D:1408:LYS:HD2	1:D:1418:PHE:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD22	1:A:358:LEU:H	1.83	0.44
1:C:900:LEU:HD23	1:C:1168:VAL:HG21	2.00	0.44
1:C:1063:THR:HB	1:C:1100:ASN:ND2	2.33	0.44
1:C:1168:VAL:HA	1:C:1176:HIS:HB2	2.00	0.44
1:D:1219:SER:O	1:D:1223:VAL:HG23	2.18	0.44
1:D:1479:GLU:OE2	1:D:1483:LYS:HD2	2.17	0.44
1:D:1404:ARG:NH1	2:D:2400:HOH:O	2.50	0.43
1:A:284:MET:CE	1:A:290:ILE:HD11	2.35	0.43
1:C:913:THR:HG23	1:C:1172:GLY:C	2.43	0.43
1:C:937:LEU:HD12	1:C:937:LEU:N	2.33	0.43
1:A:204:ARG:HG2	1:A:204:ARG:HH21	1.83	0.43
1:B:660:ILE:HD13	1:B:689:VAL:HB	1.99	0.43
1:A:3:ILE:HA	1:A:70:VAL:O	2.18	0.43
1:D:1452:LEU:HD23	1:D:1456:VAL:HG13	1.99	0.43
1:A:161:PRO:HG2	1:A:163:MET:HE3	1.99	0.43
1:C:1158:LEU:N	1:C:1158:LEU:CD1	2.82	0.43
1:D:1202:LYS:HE3	1:D:1202:LYS:HB2	1.87	0.43
1:A:80:ALA:HA	1:A:85:ASP:HB3	1.97	0.43
1:A:253:LYS:HE2	1:A:253:LYS:CA	2.46	0.43
1:C:908:VAL:HG13	1:C:909:VAL:N	2.33	0.43
1:C:906:ARG:HG3	1:C:906:ARG:HH11	1.83	0.43
1:C:1077:THR:CG2	1:C:1080:MET:HE3	2.48	0.43
1:B:693:LEU:N	1:B:693:LEU:HD12	2.34	0.43
1:C:823:VAL:O	1:C:827:VAL:HG23	2.18	0.43
1:D:1465:ALA:CB	1:D:1475:LEU:HD11	2.49	0.42
1:A:221:VAL:HG13	1:A:250:ALA:CB	2.49	0.42
1:B:493:GLY:HA2	1:B:516:LYS:O	2.19	0.42
1:C:1045:LYS:HD2	1:C:1045:LYS:O	2.19	0.42
1:D:1203:ILE:HD11	1:D:1272:TRP:CE2	2.53	0.42
1:D:1409:GLU:HG3	1:D:1410:GLN:N	2.34	0.42
1:A:323:VAL:N	1:A:324:PRO:HD2	2.35	0.42
1:B:655:LEU:HD22	1:B:680:MET:HE2	2.02	0.42
1:A:91:LYS:HE2	1:A:91:LYS:HB3	1.95	0.42
1:B:767:CYS:O	1:B:775:VAL:CG2	2.68	0.42
1:C:1091:ILE:HA	1:C:1118:VAL:HG22	2.01	0.42
1:D:1363:MET:O	1:D:1369:THR:HA	2.19	0.42
1:D:1478:GLU:O	1:D:1482:THR:HG23	2.19	0.42
1:A:24:LYS:HB2	1:A:24:LYS:NZ	2.34	0.42
1:B:590:THR:HA	1:B:593:ARG:HG2	2.01	0.42
1:C:879:THR:OG1	1:C:882:GLU:HG3	2.20	0.42
1:D:1356:PHE:CZ	1:D:1358:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ARG:HE	1:B:527:ARG:H	1.66	0.42
1:D:1485:LYS:HG2	1:D:1488:SER:OG	2.20	0.42
1:C:1045:LYS:HD2	1:C:1045:LYS:C	2.44	0.42
1:D:1356:PHE:CZ	1:D:1459:ASP:HB3	2.55	0.42
1:D:1548:ASP:HB3	1:D:1551:THR:OG1	2.19	0.42
1:A:160:PHE:N	1:A:161:PRO:HD2	2.35	0.41
1:D:1408:LYS:HD2	1:D:1418:PHE:HB3	2.01	0.41
1:A:88:ALA:HA	1:A:115:ARG:NH1	2.35	0.41
1:C:801:MET:HE2	1:C:869:ASP:HB3	2.03	0.41
1:A:19:SER:O	1:A:23:VAL:HG23	2.20	0.41
1:D:1380:VAL:HG22	1:D:1402:ASP:HB2	2.02	0.41
1:B:666:LEU:O	1:B:666:LEU:HG	2.21	0.41
1:A:2:LYS:NZ	1:A:67:GLN:NE2	2.68	0.41
1:A:23:VAL:O	1:A:27:VAL:HG23	2.21	0.41
1:A:106:ARG:O	1:A:110:GLU:HG3	2.21	0.41
1:A:205:ALA:C	1:A:207:THR:H	2.29	0.41
1:B:679:GLU:O	1:B:683:LYS:HG3	2.21	0.41
1:B:691:ILE:CD1	1:B:718:VAL:HG11	2.48	0.41
1:C:867:GLN:NE2	1:C:891:LYS:HD3	2.36	0.41
1:A:5:ILE:HD12	1:A:5:ILE:N	2.35	0.41
1:A:88:ALA:O	1:A:115:ARG:NH1	2.54	0.41
1:B:608:LYS:HE2	2:B:1985:HOH:O	2.21	0.40
1:D:1476:ILE:O	1:D:1502:PRO:HD2	2.22	0.40
1:A:208:LYS:O	1:A:212:GLU:HG3	2.22	0.40
1:C:802:LYS:NZ	1:C:834:ILE:HD11	2.36	0.40
1:A:10:ARG:HH21	1:A:76:ARG:HG3	1.86	0.40
1:B:563:MET:O	1:B:569:THR:HA	2.21	0.40
1:D:1465:ALA:HB3	1:D:1475:LEU:HD11	2.03	0.40
1:A:357:LYS:HG2	1:A:357:LYS:H	1.62	0.40
1:B:663:THR:O	1:B:693:LEU:HD13	2.22	0.40
1:B:707:GLY:N	1:B:721:THR:HG23	2.37	0.40
1:C:936:ILE:O	1:C:940:GLN:HG2	2.22	0.40
1:A:10:ARG:HA	1:A:11:PRO:HD3	1.88	0.40
1:D:1452:LEU:HD23	1:D:1452:LEU:C	2.46	0.40

All (1) 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:A:377:PRO:O	2:B:2379:HOH:O[2_545]	1.71	0.49

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	350/384 (91%)	329 (94%)	20 (6%)	1 (0%)	36	26
1	B	354/384 (92%)	340 (96%)	14 (4%)	0	100	100
1	C	351/384 (91%)	332 (95%)	14 (4%)	5 (1%)	9	2
1	D	349/384 (91%)	337 (97%)	12 (3%)	0	100	100
All	All	1404/1536 (91%)	1338 (95%)	60 (4%)	6 (0%)	30	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	HIS
1	C	1150	ASP
1	C	866	SER
1	C	892	GLU
1	C	906	ARG
1	C	1121	THR

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	274/296 (93%)	268 (98%)	6 (2%)	45	30
1	B	278/296 (94%)	267 (96%)	11 (4%)	28	10
1	C	277/296 (94%)	267 (96%)	10 (4%)	31	13
1	D	276/296 (93%)	272 (99%)	4 (1%)	59	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1105/1184 (93%)	1074 (97%)	31 (3%)	38 21

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	24	LYS
1	A	127	ARG
1	A	253	LYS
1	A	350	ASP
1	A	376	HIS
1	B	450	LEU
1	B	527	ARG
1	B	564	MET
1	B	576	LEU
1	B	585	LEU
1	B	652	LEU
1	B	679	GLU
1	B	685	LYS
1	B	703	LEU
1	B	718	VAL
1	B	749	LYS
1	C	850	LEU
1	C	943	LEU
1	C	969	THR
1	C	999	MET
1	C	1008	LYS
1	C	1093	LEU
1	C	1103	LEU
1	C	1118	VAL
1	C	1149	LYS
1	C	1150	ASP
1	D	1250	LEU
1	D	1337	LEU
1	D	1376	LEU
1	D	1548	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	67	GLN
1	A	99	HIS
1	A	142	ASN
1	A	186	GLN
1	A	210	GLN
1	A	247	GLN
1	A	313	HIS
1	A	341	ASN
1	B	437	GLN
1	B	463	GLN
1	B	499	HIS
1	B	532	GLN
1	B	542	ASN
1	B	586	GLN
1	B	647	GLN
1	B	720	HIS
1	B	722	ASN
1	B	741	ASN
1	B	782	GLN
1	C	837	GLN
1	C	867	GLN
1	C	942	ASN
1	C	986	GLN
1	C	1100	ASN
1	C	1120	HIS
1	C	1122	ASN
1	C	1141	ASN
1	D	1237	GLN
1	D	1263	GLN
1	D	1267	GLN
1	D	1332	GLN
1	D	1342	ASN
1	D	1386	GLN
1	D	1410	GLN
1	D	1520	HIS

5.3.3 RNA ⓘ

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

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.