



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:28 PM UTC

PDB ID : 1KIT / pdb_00001kit
Title : VIBRIO CHOLERAЕ NEURAMINIDASE
Authors : Taylor, G.L.; Crennell, S.J.; Garman, E.F.; Vimr, E.R.; Laver, W.G.
Deposited on : 1996-06-21
Resolution : 2.30 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
Xtrriage (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

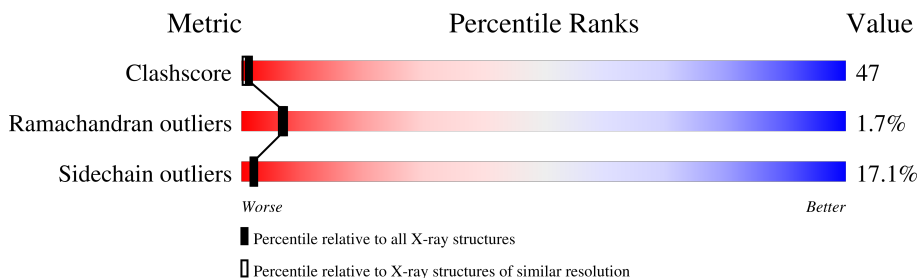
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	757	 34% 52% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6560 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	757	5859	3669	1012	1166	12	0	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

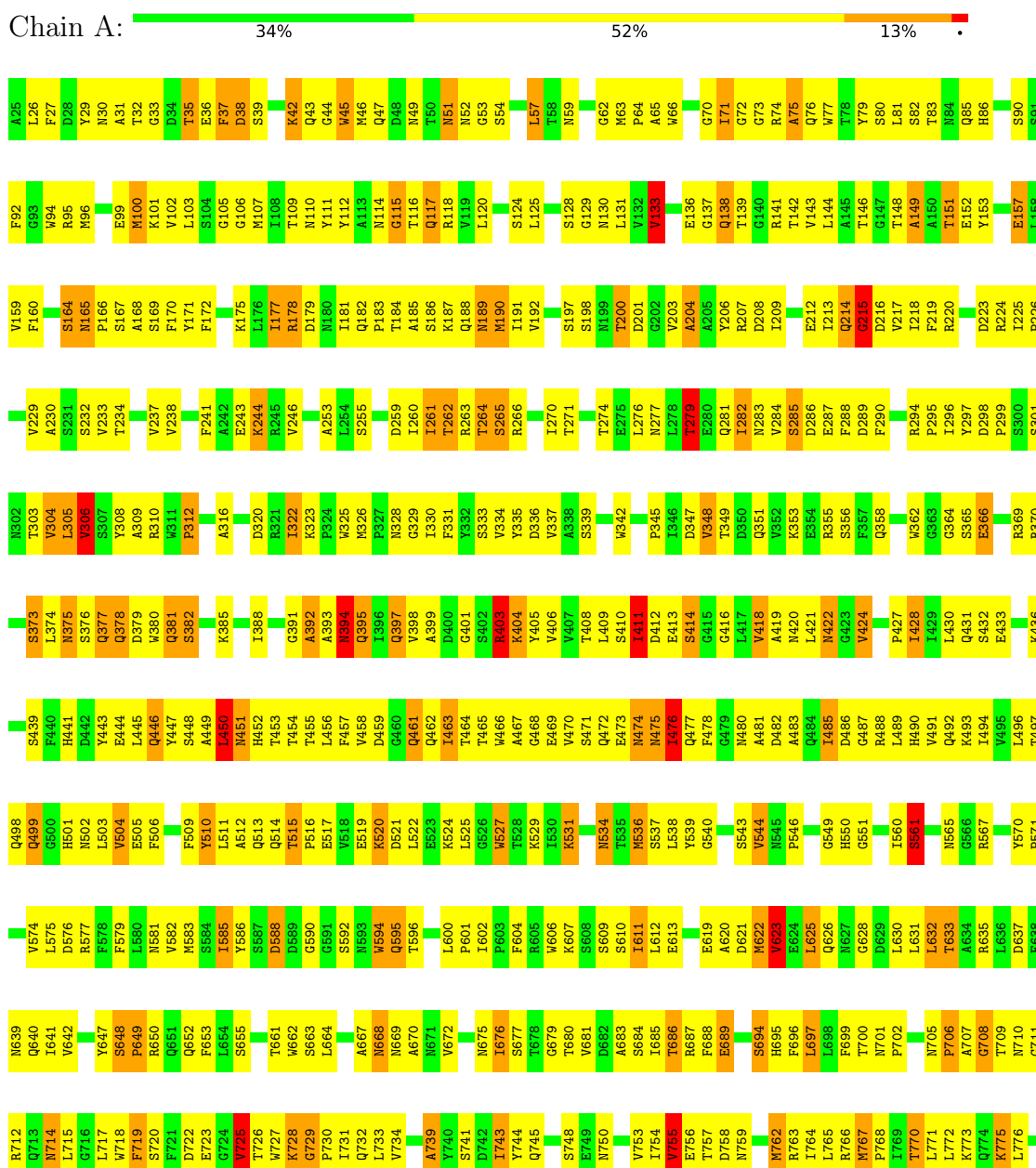
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	699	Total	O	0	0
			699	699		

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. 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: SIALIDASE



0780
0910

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.30Å 78.90Å 164.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5C	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	1.00	8/5987 (0.1%)	1.23	58/8151 (0.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	MET	SD-CE	-6.58	1.63	1.79
1	A	762	MET	SD-CE	6.25	1.95	1.79
1	A	316	ALA	CA-CB	6.01	1.60	1.54
1	A	373	SER	C-O	-5.95	1.15	1.23
1	A	411	ILE	CA-CB	5.73	1.61	1.54
1	A	485	ILE	CA-CB	-5.63	1.47	1.54
1	A	536	MET	SD-CE	5.58	1.93	1.79
1	A	622	MET	CG-SD	5.26	1.94	1.80

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	637	ASP	N-CA-C	14.02	128.94	111.69
1	A	164	SER	N-CA-C	-9.70	100.78	111.36
1	A	649	PRO	N-CA-C	-9.46	103.67	114.92
1	A	725	VAL	N-CA-C	-9.26	101.84	110.82
1	A	395	GLN	N-CA-C	8.50	121.99	109.07
1	A	279	THR	N-CA-C	7.78	123.09	112.90
1	A	475	ASN	N-CA-C	7.70	120.86	109.24
1	A	750	ASN	N-CA-C	6.98	120.89	109.72
1	A	143	VAL	CB-CA-C	-6.86	103.06	111.08
1	A	42	LYS	N-CA-C	-6.80	104.98	113.55
1	A	767	MET	N-CA-C	6.58	118.09	109.93
1	A	149	ALA	N-CA-C	-6.50	104.39	112.90
1	A	213	ILE	CB-CA-C	-6.49	103.11	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ALA	N-CA-C	6.47	120.61	110.32
1	A	232	SER	N-CA-C	-6.34	105.67	113.41
1	A	413	GLU	N-CA-C	-6.34	105.40	113.01
1	A	187	LYS	N-CA-C	-6.28	103.97	113.89
1	A	37	PHE	N-CA-C	6.27	121.06	113.17
1	A	394	ASN	N-CA-C	-6.26	99.04	109.24
1	A	588	ASP	N-CA-C	-6.26	105.28	113.17
1	A	120	LEU	N-CA-C	6.25	122.34	108.27
1	A	133	VAL	CB-CA-C	-6.15	100.85	110.69
1	A	510	TYR	N-CA-C	6.09	117.72	111.14
1	A	204	ALA	N-CA-C	6.00	118.27	108.55
1	A	301	SER	N-CA-C	-5.99	106.01	113.38
1	A	312	PRO	N-CA-C	-5.99	102.47	111.57
1	A	75	ALA	N-CA-C	-5.92	98.63	108.34
1	A	214	GLN	N-CA-C	5.89	123.34	110.80
1	A	100	MET	N-CA-C	5.82	117.07	108.86
1	A	527	TRP	N-CA-C	5.70	118.25	110.55
1	A	175	LYS	N-CA-C	-5.65	102.16	110.52
1	A	306	VAL	CB-CA-C	-5.63	103.04	110.98
1	A	244	LYS	N-CA-C	-5.57	101.40	109.59
1	A	594	TRP	N-CA-C	5.56	118.61	109.72
1	A	44	GLY	N-CA-C	5.49	122.64	115.40
1	A	392	ALA	N-CA-C	5.45	115.32	108.45
1	A	623	VAL	CB-CA-C	-5.44	102.39	110.33
1	A	571	PRO	CB-CA-C	-5.39	107.34	111.87
1	A	422	ASN	N-CA-C	5.27	118.08	110.28
1	A	403	ARG	N-CA-C	5.27	117.41	109.41
1	A	476	ILE	N-CA-C	-5.26	99.99	107.77
1	A	377	GLN	N-CA-C	-5.23	106.29	113.30
1	A	590	GLY	N-CA-C	-5.18	108.17	115.32
1	A	397	GLN	N-CA-C	5.18	116.83	108.34
1	A	561	SER	N-CA-C	5.16	117.17	109.59
1	A	289	ASP	N-CA-C	-5.16	100.63	109.24
1	A	694	SER	N-CA-C	5.14	117.16	110.43
1	A	739	ALA	N-CA-C	5.12	115.86	108.34
1	A	105	GLY	N-CA-C	5.11	118.85	111.24
1	A	45	TRP	N-CA-C	5.11	116.69	110.41
1	A	585	ILE	N-CA-C	-5.08	98.71	107.24
1	A	379	ASP	N-CA-C	5.05	117.04	110.43
1	A	298	ASP	CA-C-N	5.04	126.14	119.84
1	A	298	ASP	C-N-CA	5.04	126.14	119.84
1	A	428	ILE	CB-CA-C	-5.04	103.62	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	PHE	N-CA-C	-5.03	101.76	109.41
1	A	755	VAL	CB-CA-C	-5.02	102.64	110.52
1	A	215	GLY	N-CA-C	5.01	125.06	113.18

There are no chirality outliers.

There are no planarity outliers.

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	5859	0	5619	544	0
2	A	2	0	0	0	0
3	A	699	0	0	90	0
All	All	6560	0	5619	544	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 47.

All (544) 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:626:GLN:NE2	1:A:687:ARG:HH22	1.42	1.17
1:A:304:VAL:HG22	1:A:335:TYR:HB3	1.24	1.16
1:A:356:SER:H	1:A:540:GLY:HA2	1.24	1.02
1:A:206:TYR:HD2	1:A:209:ILE:HD11	1.28	0.95
1:A:206:TYR:CD2	1:A:209:ILE:HD11	2.02	0.94
1:A:303:THR:HG21	1:A:334:VAL:HG13	1.48	0.94
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.28	0.94
1:A:497:THR:HB	1:A:502:ASN:HD22	1.32	0.91
1:A:626:GLN:HE21	1:A:687:ARG:HH22	1.13	0.90
1:A:138:GLN:HE21	1:A:138:GLN:HA	1.35	0.90
1:A:496:LEU:HB3	1:A:504:VAL:HG22	1.53	0.89
1:A:403:ARG:HG3	1:A:470:VAL:HA	1.55	0.89
1:A:375:ASN:ND2	1:A:378:GLN:HB3	1.88	0.88
1:A:282:ILE:HD11	1:A:345:PRO:CB	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG11	1:A:297:TYR:HB2	1.54	0.87
1:A:374:LEU:H	1:A:474:ASN:HD21	1.18	0.86
1:A:170:PHE:CD2	1:A:177:ILE:HD13	2.09	0.86
1:A:355:ARG:CZ	1:A:513:GLN:HG3	2.06	0.85
1:A:652:GLN:HE21	1:A:668:ASN:HD22	1.21	0.85
1:A:244:LYS:HB2	1:A:261:ILE:HD13	1.57	0.85
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.42	0.84
1:A:626:GLN:NE2	1:A:687:ARG:NH2	2.25	0.84
1:A:497:THR:HB	1:A:502:ASN:ND2	1.92	0.84
1:A:172:PHE:N	1:A:177:ILE:HD11	1.93	0.84
1:A:476:ILE:HD12	1:A:477:GLN:N	1.94	0.83
1:A:488:ARG:HE	1:A:490:HIS:HE1	1.23	0.81
1:A:414:SER:HB2	3:A:899:HOH:O	1.81	0.81
1:A:330:ILE:H	1:A:349:THR:HG22	1.45	0.81
1:A:421:LEU:HB2	1:A:424:VAL:HG21	1.63	0.81
1:A:331:PHE:CE2	1:A:347:ASP:HB2	2.15	0.81
1:A:705:ASN:OD1	1:A:706:PRO:HD3	1.81	0.81
1:A:446:GLN:HA	1:A:446:GLN:NE2	1.94	0.79
1:A:279:THR:HG21	1:A:290:PHE:CG	2.18	0.78
1:A:606:TRP:CE2	1:A:612:LEU:HD13	2.19	0.77
1:A:282:ILE:HD11	1:A:345:PRO:HB2	1.66	0.77
1:A:57:LEU:HD23	1:A:66:TRP:HZ3	1.49	0.77
1:A:369:ARG:HD3	1:A:477:GLN:NE2	1.99	0.77
1:A:719:PHE:HE1	1:A:731:ILE:HD12	1.50	0.76
1:A:648:SER:OG	1:A:669:ASN:HB2	1.84	0.76
1:A:303:THR:CG2	1:A:334:VAL:HG13	2.14	0.76
1:A:241:PHE:CE2	1:A:262:THR:HG23	2.19	0.75
1:A:57:LEU:HD22	3:A:1428:HOH:O	1.86	0.75
1:A:229:VAL:CG1	1:A:297:TYR:HB2	2.16	0.75
1:A:241:PHE:CD2	1:A:262:THR:HG23	2.21	0.74
1:A:476:ILE:HD12	1:A:477:GLN:H	1.51	0.74
1:A:304:VAL:CG2	1:A:335:TYR:HB3	2.11	0.74
1:A:392:ALA:HB2	3:A:869:HOH:O	1.85	0.74
1:A:586:TYR:CZ	1:A:595:GLN:HB2	2.23	0.74
1:A:626:GLN:HE22	1:A:687:ARG:HH22	1.35	0.74
1:A:464:THR:HG22	1:A:465:THR:H	1.52	0.74
1:A:169:SER:HB3	1:A:179:ASP:OD1	1.88	0.73
1:A:170:PHE:O	1:A:177:ILE:HD12	1.88	0.73
1:A:233:VAL:HA	3:A:1240:HOH:O	1.87	0.73
1:A:85:GLN:HA	3:A:1147:HOH:O	1.87	0.73
1:A:613:GLU:HG3	3:A:944:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HB2	1:A:762:MET:HE3	1.71	0.72
1:A:282:ILE:HD11	1:A:345:PRO:CG	2.20	0.72
1:A:355:ARG:NE	1:A:513:GLN:HG3	2.03	0.72
1:A:586:TYR:CE1	1:A:595:GLN:HB2	2.23	0.72
1:A:391:GLY:N	1:A:411:ILE:HD12	2.05	0.72
1:A:114:ASN:HD21	1:A:117:GLN:HG3	1.53	0.71
1:A:689:GLU:HG3	3:A:1517:HOH:O	1.89	0.71
1:A:282:ILE:HD11	1:A:345:PRO:HG2	1.71	0.71
1:A:70:GLY:O	1:A:201:ASP:HA	1.89	0.71
1:A:365:SER:HB2	1:A:481:ALA:O	1.91	0.70
1:A:418:VAL:HG21	3:A:1451:HOH:O	1.90	0.70
1:A:333:SER:HA	3:A:1361:HOH:O	1.92	0.70
1:A:63:MET:HG3	3:A:1091:HOH:O	1.91	0.70
1:A:347:ASP:OD1	1:A:349:THR:HG23	1.90	0.70
1:A:496:LEU:CB	1:A:504:VAL:HG22	2.22	0.70
1:A:281:GLN:HB2	3:A:1253:HOH:O	1.91	0.69
1:A:455:THR:HG23	1:A:464:THR:O	1.93	0.69
1:A:391:GLY:HA2	3:A:854:HOH:O	1.92	0.69
1:A:138:GLN:HA	3:A:1064:HOH:O	1.92	0.68
1:A:586:TYR:CE2	1:A:595:GLN:HG3	2.29	0.68
1:A:453:THR:HG22	1:A:467:ALA:HB2	1.76	0.67
1:A:303:THR:HG23	1:A:335:TYR:O	1.95	0.67
1:A:57:LEU:HD23	1:A:66:TRP:CZ3	2.28	0.67
1:A:271:THR:HB	3:A:1107:HOH:O	1.94	0.67
1:A:421:LEU:HB2	1:A:424:VAL:CG2	2.25	0.67
1:A:722:ASP:HB2	3:A:1384:HOH:O	1.95	0.67
1:A:217:VAL:HG12	3:A:1141:HOH:O	1.93	0.67
1:A:626:GLN:HE21	1:A:687:ARG:NH2	1.91	0.67
1:A:709:THR:HG22	1:A:710:ASN:N	2.09	0.67
1:A:464:THR:HG22	1:A:465:THR:N	2.10	0.66
1:A:117:GLN:NE2	1:A:183:PRO:HB2	2.11	0.66
1:A:640:GLN:HB3	1:A:647:TYR:O	1.94	0.66
1:A:282:ILE:CG1	1:A:345:PRO:HG2	2.25	0.66
1:A:394:ASN:HD21	1:A:487:GLY:HA3	1.58	0.66
1:A:397:GLN:HG3	1:A:406:VAL:HG22	1.77	0.66
1:A:294:ARG:HD3	1:A:570:TYR:HB2	1.78	0.66
1:A:374:LEU:H	1:A:474:ASN:ND2	1.92	0.66
1:A:718:TRP:CE2	1:A:730:PRO:HB3	2.30	0.66
1:A:219:PHE:CB	1:A:762:MET:HE3	2.25	0.66
1:A:709:THR:HG22	1:A:710:ASN:H	1.61	0.66
1:A:47:GLN:NE2	3:A:1494:HOH:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.09	0.66
1:A:52:ASN:HB2	1:A:72:GLY:O	1.97	0.65
1:A:718:TRP:CZ2	1:A:730:PRO:HB3	2.31	0.65
1:A:653:PHE:CE2	1:A:664:LEU:HD12	2.32	0.65
1:A:755:VAL:O	1:A:762:MET:HA	1.96	0.65
1:A:482:ASP:HB3	1:A:485:ILE:HB	1.79	0.65
1:A:652:GLN:HE21	1:A:668:ASN:ND2	1.92	0.65
1:A:676:ILE:HG12	1:A:677:SER:H	1.61	0.65
1:A:411:ILE:HD13	1:A:411:ILE:O	1.95	0.65
1:A:420:ASN:ND2	3:A:868:HOH:O	2.29	0.65
1:A:151:THR:HB	3:A:1030:HOH:O	1.97	0.65
1:A:626:GLN:NE2	1:A:695:HIS:NE2	2.45	0.65
1:A:356:SER:O	1:A:540:GLY:N	2.30	0.65
1:A:727:TRP:O	1:A:728:LYS:HD3	1.97	0.65
1:A:114:ASN:ND2	1:A:117:GLN:HG3	2.12	0.64
1:A:733:LEU:HD22	1:A:767:MET:HE2	1.79	0.64
1:A:667:ALA:HB2	3:A:1388:HOH:O	1.98	0.64
1:A:708:GLY:N	3:A:1192:HOH:O	2.29	0.64
1:A:71:ILE:HD13	1:A:71:ILE:H	1.62	0.64
1:A:216:ASP:HB3	3:A:1142:HOH:O	1.96	0.64
1:A:149:ALA:HA	1:A:152:GLU:HG3	1.79	0.64
1:A:380:TRP:CE2	1:A:447:TYR:HB2	2.32	0.64
1:A:472:GLN:NE2	3:A:1438:HOH:O	2.29	0.64
1:A:625:LEU:HD21	1:A:631:LEU:CB	2.27	0.64
1:A:95:ARG:NH1	3:A:1069:HOH:O	2.30	0.64
1:A:102:VAL:HG12	1:A:125:LEU:HD11	1.78	0.64
1:A:462:GLN:C	1:A:463:ILE:HD13	2.21	0.64
1:A:226:PRO:HA	1:A:241:PHE:O	1.97	0.63
1:A:33:GLY:N	1:A:38:ASP:OD2	2.28	0.63
1:A:188:GLN:NE2	3:A:1010:HOH:O	2.30	0.63
1:A:259:ASP:OD1	1:A:279:THR:HB	1.97	0.63
1:A:106:GLY:HA2	1:A:124:SER:HB2	1.81	0.63
1:A:676:ILE:HG12	1:A:677:SER:N	2.14	0.63
1:A:45:TRP:CE3	1:A:79:TYR:HB2	2.34	0.62
1:A:259:ASP:C	1:A:260:ILE:HD13	2.24	0.62
1:A:284:VAL:HG23	1:A:285:SER:N	2.12	0.62
1:A:446:GLN:O	1:A:454:THR:HG23	1.98	0.62
1:A:506:PHE:CZ	1:A:522:LEU:HD21	2.34	0.62
1:A:579:PHE:HB3	3:A:947:HOH:O	1.98	0.62
1:A:226:PRO:HG3	1:A:762:MET:HG2	1.81	0.62
1:A:625:LEU:HD21	1:A:631:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:O	1:A:64:PRO:HD3	2.00	0.62
1:A:322:ILE:HD12	1:A:323:LYS:H	1.65	0.62
1:A:100:MET:HE1	1:A:110:ASN:ND2	2.15	0.62
1:A:506:PHE:CE1	1:A:522:LEU:HD21	2.35	0.62
1:A:129:GLY:HA3	3:A:1035:HOH:O	1.98	0.62
1:A:279:THR:HG21	1:A:290:PHE:CD1	2.34	0.62
1:A:370:ARG:HB3	1:A:476:ILE:HG23	1.82	0.62
1:A:229:VAL:HG22	1:A:744:TYR:CE2	2.35	0.61
1:A:404:LYS:NZ	1:A:473:GLU:OE1	2.27	0.61
1:A:446:GLN:C	1:A:454:THR:HG23	2.25	0.61
1:A:27:PHE:HZ	1:A:85:GLN:HE22	1.48	0.61
1:A:29:TYR:HA	1:A:43:GLN:OE1	2.00	0.61
1:A:138:GLN:HA	1:A:138:GLN:NE2	2.13	0.61
1:A:295:PRO:HA	1:A:306:VAL:HA	1.82	0.61
1:A:335:TYR:HB2	1:A:342:TRP:CZ3	2.36	0.61
1:A:355:ARG:HG2	1:A:513:GLN:CG	2.31	0.61
1:A:679:GLY:HA3	3:A:973:HOH:O	1.99	0.61
1:A:114:ASN:O	1:A:116:THR:N	2.34	0.61
1:A:35:THR:HG22	1:A:36:GLU:N	2.15	0.60
1:A:381:GLN:HA	1:A:446:GLN:NE2	2.16	0.60
1:A:436:LYS:O	1:A:441:HIS:HE1	1.84	0.60
1:A:137:GLY:N	3:A:1007:HOH:O	2.33	0.60
1:A:489:LEU:HD21	1:A:491:VAL:HG22	1.83	0.60
1:A:246:VAL:HA	3:A:1137:HOH:O	2.01	0.60
1:A:99:GLU:OE1	1:A:207:ARG:HG2	2.02	0.60
1:A:160:PHE:HD1	1:A:168:ALA:HB2	1.65	0.60
1:A:648:SER:HB2	1:A:670:ALA:HB3	1.84	0.60
1:A:764:ILE:HB	3:A:1236:HOH:O	2.02	0.60
1:A:37:PHE:HA	1:A:42:LYS:HG3	1.83	0.60
1:A:478:PHE:CD2	1:A:494:ILE:HD13	2.36	0.60
1:A:133:VAL:HG21	1:A:144:LEU:HD21	1.84	0.59
1:A:449:ALA:O	1:A:450:LEU:C	2.45	0.59
1:A:583:MET:HE1	3:A:1407:HOH:O	2.01	0.59
1:A:725:VAL:HG12	1:A:726:THR:HG23	1.84	0.59
1:A:375:ASN:N	1:A:498:GLN:HE22	2.00	0.59
1:A:282:ILE:CD1	1:A:345:PRO:HG2	2.31	0.59
1:A:567:ARG:NE	1:A:588:ASP:OD1	2.35	0.59
1:A:445:LEU:HD21	1:A:456:LEU:HD13	1.83	0.59
1:A:170:PHE:HD2	1:A:177:ILE:HD13	1.66	0.59
1:A:439:SER:HB2	3:A:889:HOH:O	2.03	0.59
1:A:550:HIS:ND1	3:A:928:HOH:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:PRO:HD2	1:A:709:THR:OG1	2.03	0.59
1:A:621:ASP:HB3	3:A:929:HOH:O	2.02	0.59
1:A:488:ARG:HE	1:A:490:HIS:CE1	2.13	0.58
1:A:648:SER:HB2	1:A:649:PRO:CD	2.33	0.58
1:A:701:ASN:C	1:A:715:LEU:HD12	2.27	0.58
1:A:244:LYS:CB	1:A:261:ILE:HD13	2.31	0.58
1:A:560:ILE:HD11	1:A:628:GLY:C	2.28	0.58
1:A:335:TYR:HB2	1:A:342:TRP:CH2	2.38	0.58
1:A:520:LYS:HA	1:A:525:LEU:HD11	1.84	0.58
1:A:652:GLN:NE2	1:A:668:ASN:HD22	1.98	0.58
1:A:330:ILE:N	1:A:349:THR:HG22	2.17	0.58
1:A:265:SER:HB2	1:A:271:THR:O	2.04	0.58
1:A:351:GLN:OE1	1:A:594:TRP:N	2.33	0.58
1:A:510:TYR:O	1:A:514:GLN:HG2	2.04	0.58
1:A:712:ARG:HB3	3:A:984:HOH:O	2.04	0.57
1:A:632:LEU:O	1:A:652:GLN:HA	2.04	0.57
1:A:96:MET:CE	1:A:191:ILE:HG23	2.34	0.57
1:A:648:SER:HB2	1:A:670:ALA:CB	2.35	0.57
1:A:648:SER:CB	1:A:670:ALA:HB3	2.34	0.57
1:A:404:LYS:O	1:A:468:GLY:HA3	2.03	0.57
1:A:288:PHE:CG	1:A:310:ARG:HD2	2.40	0.57
1:A:753:VAL:HB	1:A:765:LEU:HB2	1.87	0.57
1:A:266:ARG:HB3	3:A:1114:HOH:O	2.04	0.56
1:A:325:TRP:CZ2	1:A:516:PRO:HG3	2.40	0.56
1:A:381:GLN:HA	1:A:446:GLN:HE22	1.71	0.56
1:A:82:SER:HB2	3:A:1208:HOH:O	2.04	0.56
1:A:171:TYR:C	1:A:177:ILE:HD11	2.30	0.56
1:A:226:PRO:HD3	1:A:762:MET:SD	2.45	0.56
1:A:392:ALA:HB2	1:A:410:SER:HB2	1.87	0.56
1:A:377:GLN:O	1:A:449:ALA:HB1	2.05	0.56
1:A:420:ASN:OD1	1:A:427:PRO:HG3	2.05	0.56
1:A:370:ARG:NH1	1:A:504:VAL:HG12	2.21	0.56
1:A:463:ILE:HD13	1:A:463:ILE:N	2.20	0.56
1:A:59:ASN:HA	1:A:63:MET:O	2.05	0.56
1:A:198:SER:HB2	3:A:1023:HOH:O	2.05	0.56
1:A:457:PHE:CE2	1:A:462:GLN:HG3	2.40	0.56
1:A:374:LEU:HD23	1:A:498:GLN:OE1	2.05	0.55
1:A:412:ASP:CB	1:A:416:GLY:H	2.19	0.55
1:A:328:ASN:HD22	1:A:353:LYS:HE3	1.70	0.55
1:A:623:VAL:HG22	1:A:685:ILE:HG23	1.89	0.55
1:A:731:ILE:HD11	1:A:776:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TRP:CD2	1:A:447:TYR:HB2	2.40	0.55
1:A:234:THR:HG22	1:A:237:VAL:HG23	1.89	0.55
1:A:356:SER:N	1:A:540:GLY:HA2	2.08	0.55
1:A:630:LEU:HB2	1:A:655:SER:HB3	1.87	0.55
1:A:648:SER:HB2	1:A:649:PRO:HD2	1.88	0.55
1:A:720:SER:HB2	1:A:727:TRP:CD2	2.42	0.55
1:A:179:ASP:HB3	3:A:1002:HOH:O	2.07	0.54
1:A:138:GLN:HE21	1:A:138:GLN:CA	2.08	0.54
1:A:365:SER:HA	1:A:480:ASN:HD22	1.72	0.54
1:A:381:GLN:CD	1:A:497:THR:HG23	2.33	0.54
1:A:385:LYS:NZ	1:A:492:GLN:OE1	2.40	0.54
1:A:647:TYR:O	1:A:648:SER:O	2.26	0.54
1:A:329:GLY:HA3	1:A:349:THR:CG2	2.38	0.54
1:A:561:SER:HA	3:A:1376:HOH:O	2.07	0.54
1:A:536:MET:HG2	3:A:1298:HOH:O	2.06	0.54
1:A:329:GLY:HA3	1:A:349:THR:HG21	1.90	0.54
1:A:613:GLU:HG2	1:A:642:VAL:HG22	1.90	0.54
1:A:485:ILE:HA	3:A:852:HOH:O	2.07	0.54
1:A:519:GLU:OE1	1:A:524:LYS:HD3	2.07	0.54
1:A:668:ASN:HD22	1:A:668:ASN:C	2.15	0.54
1:A:118:ARG:NH1	1:A:188:GLN:HE22	2.05	0.54
1:A:444:GLU:HB3	1:A:457:PHE:HB2	1.90	0.54
1:A:133:VAL:CG2	1:A:144:LEU:HD21	2.37	0.54
1:A:138:GLN:NE2	3:A:1064:HOH:O	2.38	0.54
1:A:170:PHE:C	1:A:177:ILE:HD12	2.33	0.54
1:A:412:ASP:HB3	1:A:416:GLY:H	1.72	0.54
1:A:160:PHE:CD1	1:A:168:ALA:HB2	2.42	0.53
1:A:728:LYS:O	1:A:729:GLY:O	2.26	0.53
1:A:366:GLU:CG	1:A:531:LYS:HB2	2.38	0.53
1:A:329:GLY:CA	1:A:349:THR:HG22	2.37	0.53
1:A:90:SER:HB2	3:A:1198:HOH:O	2.07	0.53
1:A:31:ALA:HB2	1:A:65:ALA:HA	1.90	0.53
1:A:283:ASN:HB2	1:A:290:PHE:HE1	1.72	0.53
1:A:455:THR:OG1	1:A:465:THR:HG23	2.09	0.53
1:A:458:VAL:HG11	3:A:895:HOH:O	2.08	0.53
1:A:358:GLN:O	1:A:537:SER:HA	2.09	0.53
1:A:476:ILE:HD12	1:A:476:ILE:C	2.32	0.53
1:A:498:GLN:O	1:A:499:GLN:C	2.50	0.53
1:A:215:GLY:HA2	1:A:764:ILE:O	2.09	0.53
1:A:283:ASN:ND2	1:A:286:ASP:HA	2.24	0.53
1:A:157:GLU:OE2	1:A:771:LEU:HD11	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD13	1:A:546:PRO:HG3	1.91	0.53
1:A:225:ILE:HB	1:A:243:GLU:HG3	1.91	0.52
1:A:358:GLN:NE2	1:A:540:GLY:O	2.41	0.52
1:A:705:ASN:CG	1:A:706:PRO:HD3	2.33	0.52
1:A:364:GLY:HA3	1:A:534:ASN:O	2.09	0.52
1:A:623:VAL:HG22	1:A:685:ILE:CG2	2.40	0.52
1:A:741:SER:HB3	1:A:755:VAL:HG13	1.91	0.52
1:A:30:ASN:HB3	1:A:208:ASP:OD1	2.09	0.52
1:A:86:HIS:HD2	1:A:112:TYR:OH	1.93	0.52
1:A:401:GLY:O	1:A:471:SER:O	2.27	0.52
1:A:732:GLN:NE2	1:A:734:VAL:O	2.43	0.52
1:A:611:ILE:O	1:A:611:ILE:HG22	2.09	0.52
1:A:30:ASN:H	1:A:43:GLN:HE22	1.57	0.52
1:A:159:VAL:O	1:A:168:ALA:HA	2.09	0.52
1:A:328:ASN:HD21	1:A:544:VAL:H	1.58	0.52
1:A:492:GLN:HG3	1:A:509:PHE:HB2	1.92	0.51
1:A:576:ASP:OD1	1:A:577:ARG:N	2.43	0.51
1:A:295:PRO:HB3	1:A:306:VAL:HG13	1.92	0.51
1:A:362:TRP:HB3	1:A:604:PHE:CZ	2.45	0.51
1:A:288:PHE:CD1	1:A:310:ARG:HD2	2.46	0.51
1:A:626:GLN:NE2	1:A:695:HIS:CD2	2.78	0.51
1:A:38:ASP:HB2	3:A:1428:HOH:O	2.09	0.51
1:A:406:VAL:HB	1:A:422:ASN:HB3	1.92	0.51
1:A:207:ARG:NH2	3:A:1467:HOH:O	2.31	0.51
1:A:49:ASN:OD1	1:A:75:ALA:HA	2.10	0.51
1:A:51:ASN:C	1:A:53:GLY:H	2.19	0.51
1:A:436:LYS:HE3	3:A:891:HOH:O	2.11	0.51
1:A:399:ALA:O	1:A:475:ASN:N	2.40	0.50
1:A:51:ASN:O	1:A:52:ASN:HB2	2.09	0.50
1:A:457:PHE:CZ	1:A:462:GLN:HG3	2.46	0.50
1:A:322:ILE:HG22	1:A:575:LEU:HD23	1.92	0.50
1:A:392:ALA:CB	1:A:410:SER:HB2	2.42	0.50
1:A:771:LEU:HD21	3:A:1082:HOH:O	2.11	0.50
1:A:103:LEU:N	1:A:203:VAL:O	2.42	0.50
1:A:45:TRP:CZ3	1:A:79:TYR:HB2	2.46	0.50
1:A:166:PRO:O	1:A:167:SER:HB3	2.11	0.50
1:A:322:ILE:HG21	1:A:543:SER:HB3	1.94	0.50
1:A:348:VAL:HG23	1:A:348:VAL:O	2.11	0.50
1:A:623:VAL:HG11	1:A:697:LEU:HD22	1.93	0.50
1:A:680:THR:HA	3:A:976:HOH:O	2.11	0.50
1:A:101:LYS:NZ	1:A:153:TYR:CE2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PHE:CZ	1:A:310:ARG:NH1	2.79	0.50
1:A:454:THR:HG22	1:A:455:THR:N	2.27	0.50
1:A:459:ASP:HB2	3:A:893:HOH:O	2.11	0.50
1:A:606:TRP:CZ2	1:A:612:LEU:HD13	2.47	0.50
1:A:401:GLY:O	1:A:472:GLN:HA	2.11	0.50
1:A:260:ILE:HD13	1:A:260:ILE:N	2.28	0.49
1:A:276:LEU:HA	3:A:1131:HOH:O	2.12	0.49
1:A:309:ALA:HB2	1:A:546:PRO:HD3	1.93	0.49
1:A:625:LEU:HD21	1:A:631:LEU:HB2	1.94	0.49
1:A:675:ASN:HB2	1:A:730:PRO:HG3	1.94	0.49
1:A:625:LEU:N	1:A:625:LEU:HD23	2.27	0.49
1:A:342:TRP:HB3	3:A:1482:HOH:O	2.11	0.49
1:A:619:GLU:OE1	1:A:635:ARG:NH1	2.44	0.49
1:A:303:THR:HG22	1:A:304:VAL:N	2.26	0.49
1:A:527:TRP:CD1	1:A:527:TRP:N	2.80	0.49
1:A:702:PRO:HA	1:A:715:LEU:HA	1.95	0.49
1:A:51:ASN:O	1:A:72:GLY:O	2.31	0.49
1:A:101:LYS:HD2	1:A:151:THR:O	2.12	0.49
1:A:186:SER:HB2	3:A:1010:HOH:O	2.13	0.49
1:A:241:PHE:CE2	1:A:262:THR:CG2	2.92	0.49
1:A:639:ASN:HB3	3:A:945:HOH:O	2.13	0.49
1:A:688:PHE:CE1	1:A:745:GLN:HG3	2.48	0.49
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.66	0.49
1:A:478:PHE:CE2	1:A:494:ILE:HD13	2.48	0.49
1:A:82:SER:OG	1:A:85:GLN:HG3	2.13	0.48
1:A:296:ILE:HG12	1:A:551:GLY:C	2.38	0.48
1:A:401:GLY:N	1:A:473:GLU:O	2.36	0.48
1:A:328:ASN:HD21	1:A:544:VAL:HG22	1.78	0.48
1:A:370:ARG:HB3	1:A:476:ILE:CG2	2.43	0.48
1:A:701:ASN:ND2	1:A:702:PRO:HD2	2.28	0.48
1:A:73:GLY:HA2	3:A:1522:HOH:O	2.12	0.48
1:A:388:ILE:CG2	1:A:411:ILE:HG23	2.44	0.48
1:A:611:ILE:HD13	1:A:611:ILE:HA	1.74	0.48
1:A:683:ALA:HB1	1:A:700:THR:O	2.14	0.47
1:A:182:GLN:NE2	3:A:1519:HOH:O	2.25	0.47
1:A:178:ARG:HD2	1:A:181:ILE:HG12	1.96	0.47
1:A:364:GLY:C	1:A:483:ALA:HA	2.39	0.47
1:A:106:GLY:CA	1:A:124:SER:HB2	2.43	0.47
1:A:276:LEU:HD12	3:A:1131:HOH:O	2.14	0.47
1:A:652:GLN:NE2	1:A:668:ASN:O	2.48	0.47
1:A:115:GLY:HA3	3:A:1480:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HD3	3:A:1089:HOH:O	2.14	0.47
1:A:399:ALA:HB1	1:A:473:GLU:HB2	1.95	0.47
1:A:36:GLU:O	1:A:42:LYS:HG3	2.15	0.47
1:A:102:VAL:HA	1:A:204:ALA:HB2	1.95	0.47
1:A:284:VAL:CG2	1:A:285:SER:N	2.77	0.47
1:A:454:THR:O	1:A:465:THR:HG23	2.15	0.47
1:A:712:ARG:N	3:A:982:HOH:O	2.34	0.47
1:A:190:MET:HG3	1:A:192:VAL:HG23	1.95	0.47
1:A:405:TYR:CE1	1:A:467:ALA:HA	2.50	0.47
1:A:640:GLN:O	1:A:647:TYR:HB2	2.15	0.47
1:A:107:MET:O	1:A:109:THR:HG23	2.14	0.47
1:A:322:ILE:HD12	1:A:323:LYS:N	2.28	0.47
1:A:444:GLU:O	1:A:445:LEU:HD23	2.14	0.47
1:A:49:ASN:HA	1:A:74:ARG:O	2.14	0.47
1:A:320:ASP:OD2	3:A:940:HOH:O	2.20	0.47
1:A:493:LYS:HA	1:A:506:PHE:O	2.15	0.47
1:A:263:ARG:HA	3:A:1129:HOH:O	2.15	0.47
1:A:296:ILE:HG12	1:A:551:GLY:HA3	1.97	0.47
1:A:465:THR:N	3:A:1343:HOH:O	2.48	0.47
1:A:661:THR:HA	3:A:1397:HOH:O	2.15	0.47
1:A:632:LEU:HD12	1:A:633:THR:N	2.31	0.46
1:A:757:THR:OG1	1:A:758:ASP:N	2.48	0.46
1:A:238:VAL:O	1:A:264:THR:HG22	2.15	0.46
1:A:419:ALA:HB2	1:A:430:LEU:HD22	1.97	0.46
1:A:395:GLN:NE2	1:A:481:ALA:HB2	2.30	0.46
1:A:694:SER:HA	3:A:1383:HOH:O	2.15	0.46
1:A:71:ILE:H	1:A:71:ILE:CD1	2.27	0.46
1:A:382:SER:CB	1:A:445:LEU:HB2	2.46	0.46
1:A:395:GLN:NE2	1:A:481:ALA:CB	2.78	0.46
1:A:684:SER:HB2	1:A:741:SER:O	2.15	0.46
1:A:728:LYS:HB3	1:A:776:LEU:HD22	1.98	0.46
1:A:77:TRP:O	1:A:192:VAL:HA	2.16	0.46
1:A:433:GLU:O	1:A:436:LYS:N	2.49	0.46
1:A:626:GLN:HE22	1:A:687:ARG:NH2	2.04	0.46
1:A:59:ASN:HD22	1:A:64:PRO:N	2.13	0.46
1:A:355:ARG:CD	1:A:513:GLN:HG3	2.46	0.46
1:A:366:GLU:HG3	1:A:531:LYS:HB2	1.97	0.46
1:A:679:GLY:HA2	3:A:977:HOH:O	2.15	0.46
1:A:138:GLN:NE2	1:A:138:GLN:CA	2.78	0.46
1:A:237:VAL:HG11	1:A:337:VAL:HG13	1.96	0.46
1:A:335:TYR:HB2	1:A:342:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HG3	3:A:1440:HOH:O	2.15	0.46
1:A:136:GLU:O	1:A:138:GLN:HG2	2.16	0.45
1:A:223:ASP:O	1:A:762:MET:HE2	2.17	0.45
1:A:550:HIS:HE1	3:A:927:HOH:O	1.98	0.45
1:A:165:ASN:N	1:A:165:ASN:OD1	2.49	0.45
1:A:447:TYR:HH	1:A:452:HIS:HD1	1.64	0.45
1:A:478:PHE:CD1	1:A:478:PHE:C	2.94	0.45
1:A:560:ILE:HD11	1:A:628:GLY:HA3	1.96	0.45
1:A:380:TRP:CE2	1:A:447:TYR:CB	2.99	0.45
1:A:380:TRP:CD2	1:A:447:TYR:CB	2.99	0.45
1:A:707:ALA:O	1:A:708:GLY:C	2.59	0.45
1:A:189:ASN:O	1:A:190:MET:HB3	2.15	0.45
1:A:244:LYS:HB2	1:A:261:ILE:CD1	2.38	0.45
1:A:768:PRO:O	1:A:772:LEU:HD12	2.16	0.45
1:A:297:TYR:O	1:A:299:PRO:HD3	2.17	0.45
1:A:369:ARG:HD3	1:A:477:GLN:HE21	1.80	0.45
1:A:380:TRP:CZ2	1:A:447:TYR:HB2	2.52	0.45
1:A:393:ALA:HB3	1:A:485:ILE:HG21	1.99	0.45
1:A:422:ASN:HD21	1:A:469:GLU:H	1.63	0.45
1:A:117:GLN:HE21	1:A:183:PRO:HB2	1.79	0.45
1:A:382:SER:HB2	1:A:445:LEU:HB2	1.98	0.45
1:A:405:TYR:HE1	1:A:467:ALA:HA	1.81	0.45
1:A:741:SER:CB	1:A:755:VAL:HG13	2.46	0.45
1:A:219:PHE:HB3	1:A:762:MET:HE3	1.99	0.45
1:A:506:PHE:HB2	3:A:1281:HOH:O	2.16	0.45
1:A:394:ASN:ND2	1:A:487:GLY:HA3	2.29	0.44
1:A:457:PHE:CE2	1:A:462:GLN:CG	3.00	0.44
1:A:459:ASP:C	1:A:461:GLN:H	2.26	0.44
1:A:100:MET:CE	1:A:110:ASN:ND2	2.80	0.44
1:A:496:LEU:O	1:A:503:LEU:N	2.49	0.44
1:A:732:GLN:C	1:A:733:LEU:HD23	2.42	0.44
1:A:226:PRO:HB2	1:A:754:ILE:HD13	1.98	0.44
1:A:261:ILE:HG22	1:A:277:ASN:HA	1.99	0.44
1:A:329:GLY:CA	1:A:349:THR:CG2	2.94	0.44
1:A:696:PHE:HA	3:A:1380:HOH:O	2.18	0.44
1:A:92:PHE:CZ	1:A:763:ARG:CD	3.00	0.44
1:A:391:GLY:N	1:A:411:ILE:CD1	2.78	0.44
1:A:81:LEU:N	3:A:1479:HOH:O	2.51	0.44
1:A:94:TRP:HA	1:A:212:GLU:O	2.17	0.44
1:A:190:MET:HG3	1:A:192:VAL:CG2	2.48	0.44
1:A:586:TYR:CZ	1:A:595:GLN:CB	2.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ASN:HB3	1:A:732:GLN:NE2	2.32	0.44
1:A:720:SER:HB2	1:A:727:TRP:CE3	2.52	0.44
1:A:102:VAL:HG12	1:A:102:VAL:O	2.17	0.44
1:A:226:PRO:HG3	1:A:762:MET:CG	2.47	0.44
1:A:685:ILE:HD11	1:A:727:TRP:CH2	2.53	0.44
1:A:81:LEU:HD21	1:A:191:ILE:HD11	2.00	0.43
1:A:148:THR:O	1:A:152:GLU:HG3	2.17	0.43
1:A:241:PHE:CE2	1:A:306:VAL:HG21	2.53	0.43
1:A:287:GLU:HG3	3:A:1476:HOH:O	2.18	0.43
1:A:447:TYR:HD1	1:A:454:THR:OG1	2.00	0.43
1:A:454:THR:CG2	1:A:455:THR:N	2.81	0.43
1:A:600:LEU:N	1:A:600:LEU:HD23	2.33	0.43
1:A:709:THR:CG2	1:A:710:ASN:H	2.28	0.43
1:A:719:PHE:CE1	1:A:731:ILE:HD12	2.41	0.43
1:A:29:TYR:HE1	1:A:38:ASP:O	2.01	0.43
1:A:101:LYS:HG3	1:A:151:THR:O	2.18	0.43
1:A:207:ARG:O	1:A:207:ARG:HG3	2.17	0.43
1:A:648:SER:CB	1:A:670:ALA:CB	2.96	0.43
1:A:772:LEU:O	1:A:773:LYS:C	2.59	0.43
1:A:282:ILE:HG22	3:A:1360:HOH:O	2.18	0.43
1:A:464:THR:CG2	1:A:465:THR:H	2.26	0.43
1:A:502:ASN:HD22	1:A:502:ASN:HA	1.67	0.43
1:A:601:PRO:HA	3:A:1398:HOH:O	2.17	0.43
1:A:312:PRO:HB2	3:A:1170:HOH:O	2.18	0.43
1:A:560:ILE:HD11	1:A:628:GLY:CA	2.49	0.43
1:A:648:SER:OG	1:A:650:ARG:O	2.36	0.43
1:A:620:ALA:HB1	1:A:632:LEU:CD1	2.49	0.43
1:A:133:VAL:HG22	1:A:144:LEU:HG	2.01	0.43
1:A:144:LEU:HB3	1:A:172:PHE:CE2	2.53	0.43
1:A:491:VAL:HG11	1:A:494:ILE:CD1	2.49	0.43
1:A:59:ASN:HD22	1:A:64:PRO:CA	2.32	0.43
1:A:515:THR:HB	1:A:516:PRO:HD2	2.01	0.43
1:A:714:ASN:HB3	1:A:732:GLN:HE21	1.84	0.43
1:A:770:THR:HG22	1:A:771:LEU:N	2.34	0.43
1:A:26:LEU:HB3	3:A:1103:HOH:O	2.18	0.42
1:A:30:ASN:H	1:A:43:GLN:NE2	2.17	0.42
1:A:647:TYR:C	1:A:648:SER:O	2.62	0.42
1:A:719:PHE:C	1:A:727:TRP:CE3	2.97	0.42
1:A:92:PHE:CZ	1:A:763:ARG:HD3	2.54	0.42
1:A:399:ALA:HB3	1:A:475:ASN:HB2	2.01	0.42
1:A:478:PHE:CD2	1:A:494:ILE:CD1	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ALA:HB3	3:A:993:HOH:O	2.18	0.42
1:A:224:ARG:C	1:A:225:ILE:HG12	2.44	0.42
1:A:229:VAL:CG1	1:A:230:ALA:N	2.82	0.42
1:A:308:TYR:CD1	1:A:308:TYR:N	2.86	0.42
1:A:355:ARG:HG2	1:A:513:GLN:CD	2.45	0.42
1:A:391:GLY:H	1:A:411:ILE:HD12	1.83	0.42
1:A:631:LEU:HG	3:A:1393:HOH:O	2.19	0.42
1:A:322:ILE:HD12	1:A:326:MET:SD	2.60	0.42
1:A:403:ARG:NH2	1:A:452:HIS:HB3	2.35	0.42
1:A:409:LEU:HD21	1:A:443:TYR:CE2	2.55	0.42
1:A:581:ASN:OD1	1:A:582:VAL:N	2.46	0.42
1:A:728:LYS:HD2	1:A:728:LYS:HA	1.50	0.42
1:A:728:LYS:HG3	3:A:1413:HOH:O	2.19	0.42
1:A:511:LEU:O	1:A:512:ALA:C	2.63	0.42
1:A:521:ASP:O	1:A:522:LEU:C	2.63	0.42
1:A:244:LYS:CA	1:A:261:ILE:HD13	2.48	0.42
1:A:422:ASN:ND2	1:A:469:GLU:H	2.17	0.42
1:A:550:HIS:CE1	1:A:686:THR:HG23	2.55	0.42
1:A:39:SER:O	1:A:42:LYS:HB2	2.19	0.42
1:A:283:ASN:CG	1:A:286:ASP:HA	2.44	0.42
1:A:296:ILE:HG12	1:A:551:GLY:CA	2.49	0.42
1:A:336:ASP:OD2	1:A:339:SER:OG	2.27	0.42
1:A:586:TYR:CD1	1:A:586:TYR:N	2.88	0.42
1:A:609:SER:O	1:A:610:SER:HB2	2.19	0.42
1:A:711:GLY:HA3	3:A:992:HOH:O	2.19	0.42
1:A:775:LYS:NZ	1:A:775:LYS:HB3	2.35	0.42
1:A:141:ARG:NH1	3:A:1044:HOH:O	2.52	0.42
1:A:355:ARG:HD2	3:A:1290:HOH:O	2.19	0.42
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.69	0.42
1:A:391:GLY:H	1:A:411:ILE:CD1	2.32	0.41
1:A:652:GLN:HG3	3:A:1393:HOH:O	2.18	0.41
1:A:27:PHE:HZ	1:A:85:GLN:NE2	2.14	0.41
1:A:197:SER:CB	1:A:200:THR:HB	2.49	0.41
1:A:430:LEU:O	1:A:431:GLN:HG2	2.20	0.41
1:A:445:LEU:CD2	1:A:456:LEU:HD13	2.48	0.41
1:A:457:PHE:HA	1:A:461:GLN:O	2.20	0.41
1:A:71:ILE:O	1:A:71:ILE:HG12	2.20	0.41
1:A:96:MET:CE	1:A:191:ILE:CG2	2.97	0.41
1:A:309:ALA:HB2	1:A:546:PRO:CD	2.50	0.41
1:A:743:ILE:HG12	1:A:744:TYR:N	2.35	0.41
1:A:295:PRO:HA	1:A:305:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:SER:HB2	3:A:869:HOH:O	2.20	0.41
1:A:550:HIS:CE1	3:A:927:HOH:O	2.72	0.41
1:A:565:ASN:ND2	3:A:913:HOH:O	2.53	0.41
1:A:282:ILE:HG23	1:A:282:ILE:HD13	1.73	0.41
1:A:294:ARG:HA	1:A:549:GLY:O	2.21	0.41
1:A:451:ASN:OD1	1:A:453:THR:OG1	2.35	0.41
1:A:491:VAL:HG12	1:A:492:GLN:N	2.35	0.41
1:A:498:GLN:O	1:A:501:HIS:CD2	2.74	0.41
1:A:739:ALA:HB3	1:A:756:GLU:HB2	2.02	0.41
1:A:133:VAL:CG2	1:A:144:LEU:HG	2.51	0.41
1:A:323:LYS:O	1:A:325:TRP:N	2.54	0.41
1:A:46:MET:O	1:A:77:TRP:HE3	2.03	0.41
1:A:131:LEU:HD23	1:A:144:LEU:HB2	2.01	0.41
1:A:355:ARG:HG2	1:A:513:GLN:HG2	2.00	0.41
1:A:632:LEU:HB3	1:A:662:TRP:CZ3	2.56	0.41
1:A:95:ARG:NH2	3:A:1083:HOH:O	2.45	0.41
1:A:133:VAL:HG23	1:A:142:THR:O	2.21	0.41
1:A:233:VAL:HG22	3:A:1240:HOH:O	2.21	0.41
1:A:279:THR:O	1:A:282:ILE:HB	2.20	0.41
1:A:303:THR:HG21	1:A:334:VAL:CG1	2.35	0.41
1:A:335:TYR:HB2	1:A:342:TRP:CZ2	2.55	0.41
1:A:96:MET:HE1	1:A:111:TYR:O	2.21	0.41
1:A:253:ALA:C	1:A:255:SER:N	2.77	0.41
1:A:397:GLN:HB3	1:A:477:GLN:HB3	2.03	0.41
1:A:652:GLN:HE21	1:A:668:ASN:C	2.29	0.41
1:A:39:SER:HB3	1:A:42:LYS:HG2	2.03	0.40
1:A:358:GLN:HB3	1:A:490:HIS:CE1	2.57	0.40
1:A:375:ASN:HD21	1:A:378:GLN:HB3	1.78	0.40
1:A:322:ILE:CG2	1:A:575:LEU:HD23	2.51	0.40
1:A:381:GLN:CA	1:A:446:GLN:HE22	2.34	0.40
1:A:699:PHE:O	1:A:717:LEU:HA	2.22	0.40
1:A:71:ILE:HD13	1:A:71:ILE:N	2.33	0.40
1:A:130:ASN:OD1	1:A:146:THR:HB	2.21	0.40
1:A:520:LYS:HB2	1:A:539:TYR:CE2	2.57	0.40
1:A:107:MET:HE3	1:A:109:THR:CG2	2.52	0.40
1:A:279:THR:CG2	1:A:290:PHE:CD1	3.04	0.40
1:A:347:ASP:OD1	1:A:348:VAL:N	2.55	0.40
1:A:369:ARG:HH11	1:A:477:GLN:NE2	2.19	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	755/757 (100%)	679 (90%)	63 (8%)	13 (2%)	7 7

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	115	GLY
1	A	214	GLN
1	A	648	SER
1	A	729	GLY
1	A	708	GLY
1	A	748	SER
1	A	35	THR
1	A	376	SER
1	A	450	LEU
1	A	706	PRO
1	A	499	GLN
1	A	215	GLY

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	637/637 (100%)	528 (83%)	109 (17%)	2 2

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	38	ASP
1	A	54	SER
1	A	57	LEU
1	A	71	ILE
1	A	76	GLN
1	A	80	SER
1	A	83	THR
1	A	117	GLN
1	A	128	SER
1	A	133	VAL
1	A	138	GLN
1	A	139	THR
1	A	151	THR
1	A	157	GLU
1	A	164	SER
1	A	165	ASN
1	A	177	ILE
1	A	178	ARG
1	A	184	THR
1	A	189	ASN
1	A	200	THR
1	A	218	ILE
1	A	220	ARG
1	A	261	ILE
1	A	262	THR
1	A	264	THR
1	A	265	SER
1	A	270	ILE
1	A	274	THR
1	A	279	THR
1	A	282	ILE
1	A	285	SER
1	A	304	VAL
1	A	305	LEU
1	A	306	VAL
1	A	322	ILE
1	A	348	VAL
1	A	366	GLU
1	A	373	SER
1	A	375	ASN
1	A	378	GLN
1	A	381	GLN

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Mol	Chain	Res	Type
1	A	382	SER
1	A	394	ASN
1	A	398	VAL
1	A	403	ARG
1	A	404	LYS
1	A	408	THR
1	A	411	ILE
1	A	414	SER
1	A	418	VAL
1	A	424	VAL
1	A	428	ILE
1	A	432	SER
1	A	446	GLN
1	A	448	SER
1	A	450	LEU
1	A	451	ASN
1	A	461	GLN
1	A	463	ILE
1	A	466	TRP
1	A	474	ASN
1	A	476	ILE
1	A	486	ASP
1	A	504	VAL
1	A	505	GLU
1	A	515	THR
1	A	517	GLU
1	A	520	LYS
1	A	529	LYS
1	A	531	LYS
1	A	534	ASN
1	A	538	LEU
1	A	544	VAL
1	A	561	SER
1	A	574	VAL
1	A	585	ILE
1	A	592	SER
1	A	595	GLN
1	A	596	THR
1	A	602	ILE
1	A	607	LYS
1	A	611	ILE
1	A	622	MET

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Mol	Chain	Res	Type
1	A	623	VAL
1	A	625	LEU
1	A	632	LEU
1	A	633	THR
1	A	641	ILE
1	A	663	SER
1	A	668	ASN
1	A	672	VAL
1	A	676	ILE
1	A	681	VAL
1	A	686	THR
1	A	689	GLU
1	A	697	LEU
1	A	714	ASN
1	A	723	GLU
1	A	725	VAL
1	A	728	LYS
1	A	743	ILE
1	A	755	VAL
1	A	759	ASN
1	A	766	ARG
1	A	770	THR
1	A	775	LYS
1	A	780	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	47	GLN
1	A	59	ASN
1	A	85	GLN
1	A	86	HIS
1	A	114	ASN
1	A	117	GLN
1	A	138	GLN
1	A	180	ASN
1	A	189	ASN
1	A	195	ASN
1	A	328	ASN
1	A	378	GLN
1	A	383	ASN

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Mol	Chain	Res	Type
1	A	394	ASN
1	A	395	GLN
1	A	397	GLN
1	A	438	HIS
1	A	441	HIS
1	A	446	GLN
1	A	474	ASN
1	A	475	ASN
1	A	480	ASN
1	A	490	HIS
1	A	502	ASN
1	A	550	HIS
1	A	564	GLN
1	A	626	GLN
1	A	639	ASN
1	A	668	ASN
1	A	690	GLN
1	A	710	ASN
1	A	750	ASN
1	A	759	ASN
1	A	774	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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.