Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:29 PM GMT

PDB ID	:	1KIT
Title	:	VIBRIO CHOLERAE 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

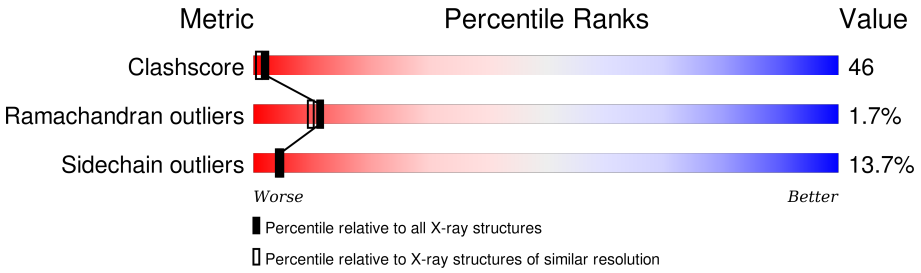
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	757	39% 53% 8%

2 Entry composition (i)

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

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

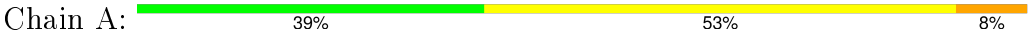
3 Residue-property plots (i)

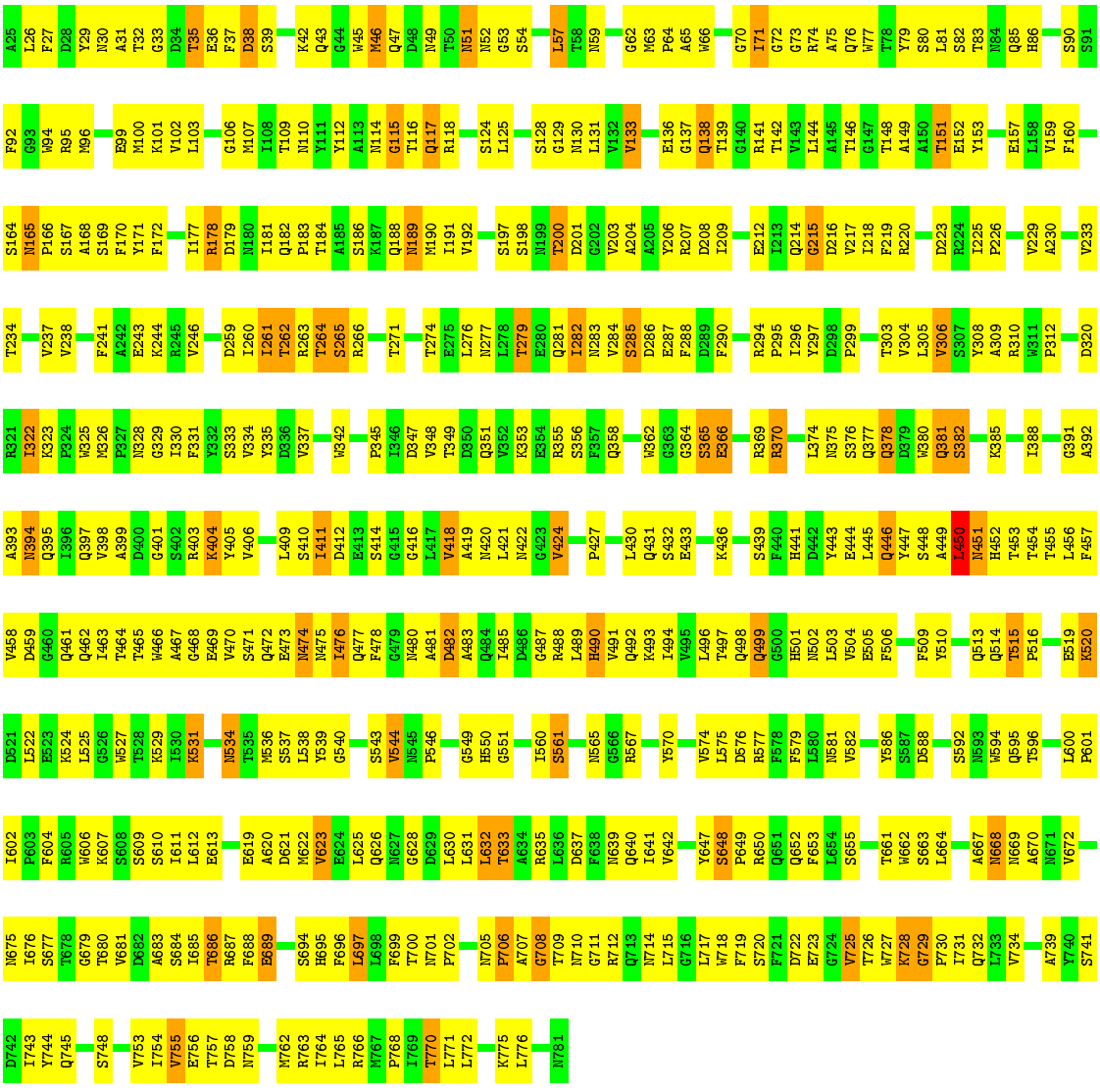
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: SIALIDASE

Chain A:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 V. 5-C	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.77	0/5987	0.87	2/8151 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	637	ASP	N-CA-C	6.64	128.94	111.00
1	A	133	VAL	CB-CA-C	-5.55	100.85	111.40

There are no chirality outliers.

There are no planarity outliers.

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	5859	0	5619	526	0
2	A	2	0	0	0	0
3	A	699	0	0	89	0
All	All	6560	0	5619	526	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 46.

All (526) 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
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:HH11	1:A:178:ARG:HG3	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:421:LEU:HB2	1:A:424:VAL:HG21	1.63	0.81
1:A:330:ILE:H	1:A:349:THR:HG22	1.45	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:NE2	1:A:446:GLN:HA	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:369:ARG:HD3	1:A:477:GLN:NE2	1.99	0.77
1:A:57:LEU:HD23	1:A:66:TRP:HZ3	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:CG1	1:A:297:TYR:HB2	2.16	0.75
1:A:57:LEU:HD22	3:A:1428:HOH:O	1.86	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
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:347:ASP:OD1	1:A:349:THR:HG23	1.90	0.70
1:A:63:MET:HG3	3:A:1091:HOH:O	1.91	0.70
1:A:496:LEU:CB	1:A:504:VAL:HG22	2.22	0.70
1:A:455:THR:HG23	1:A:464:THR:O	1.93	0.69
1:A:281:GLN:HB2	3:A:1253:HOH:O	1.91	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:223:ASP:O	1:A:762:MET:HE2	1.93	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:626:GLN:HE21	1:A:687:ARG:NH2	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:HG12	3:A:1141:HOH:O	1.93	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:397:GLN:HG3	1:A:406:VAL:HG22	1.77	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: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: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
1:A:178:ARG:NH1	1:A:178:ARG:HG3	2.09	0.66
1:A:718:TRP:CZ2	1:A:730:PRO:HB3	2.31	0.65
1:A:52:ASN:HB2	1:A:72:GLY:O	1.97	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:626:GLN:NE2	1:A:695:HIS:NE2	2.45	0.65
1:A:151:THR:HB	3:A:1030:HOH:O	1.97	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: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:H	1:A:71:ILE:HD13	1.62	0.64
1:A:216:ASP:HB3	3:A:1142:HOH:O	1.96	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:149:ALA:HA	1:A:152:GLU:HG3	1.79	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:284:VAL:HG23	1:A:285:SER:N	2.12	0.64
1:A:102:VAL:HG12	1:A:125:LEU:HD11	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:676:ILE:HG12	1:A:677:SER:N	2.14	0.63
1:A:106:GLY:HA2	1:A:124:SER:HB2	1.81	0.63
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:45:TRP:CE3	1:A:79:TYR:HB2	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
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:506:PHE:CE1	1:A:522:LEU:HD21	2.35	0.62
1:A:370:ARG:HB3	1:A:476:ILE:HG23	1.82	0.62
1:A:279:THR:HG21	1:A:290:PHE:CD1	2.34	0.62
1:A:129:GLY:HA3	3:A:1035:HOH:O	1.98	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:29:TYR:HA	1:A:43:GLN:OE1	2.00	0.61
1:A:27:PHE:HZ	1:A:85:GLN:HE22	1.48	0.61
1:A:138:GLN:NE2	1:A:138:GLN:HA	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:381:GLN:HA	1:A:446:GLN:NE2	2.16	0.60
1:A:35:THR:HG22	1:A:36:GLU:N	2.15	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:648:SER:HB2	1:A:670:ALA:HB3	1.84	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:706:PRO:HD2	1:A:709:THR:OG1	2.03	0.59
1:A:462:GLN:C	1:A:463:ILE:HD13	2.21	0.59
1:A:550:HIS:ND1	3:A:928:HOH:O	2.32	0.59
1:A:439:SER:HB2	3:A:889:HOH:O	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:244:LYS:CB	1:A:261:ILE:HD13	2.31	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:259:ASP:C	1:A:260:ILE:HD13	2.24	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:510:TYR:O	1:A:514:GLN:HG2	2.04	0.58
1:A:351:GLN:OE1	1:A:594:TRP:N	2.33	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:648:SER:CB	1:A:670:ALA:HB3	2.34	0.57
1:A:648:SER:HB2	1:A:670:ALA:CB	2.35	0.57
1:A:96:MET:CE	1:A:191:ILE:HG23	2.34	0.57
1:A:404:LYS:O	1:A:468:GLY:HA3	2.03	0.57
1:A:753:VAL:HB	1:A:765:LEU:HB2	1.87	0.57
1:A:288:PHE:CG	1:A:310:ARG:HD2	2.40	0.57
1:A:381:GLN:HA	1:A:446:GLN:HE22	1.71	0.56
1:A:325:TRP:CZ2	1:A:516:PRO:HG3	2.40	0.56
1:A:266:ARG:HB3	3:A:1114:HOH:O	2.04	0.56
1:A:775:LYS:HB3	1:A:775:LYS:HZ2	1.69	0.56
1:A:446:GLN:C	1:A:454:THR:HG23	2.25	0.56
1:A:82:SER:HB2	3:A:1208:HOH:O	2.04	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:420:ASN:OD1	1:A:427:PRO:HG3	2.05	0.56
1:A:377:GLN:O	1:A:449:ALA:HB1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:PHE:CE2	1:A:462:GLN:HG3	2.40	0.56
1:A:198:SER:HB2	3:A:1023:HOH:O	2.05	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:623:VAL:HG22	1:A:685:ILE:HG23	1.89	0.55
1:A:328:ASN:HD22	1:A:353:LYS:HE3	1.70	0.55
1:A:731:ILE:HD11	1:A:776:LEU:HD11	1.89	0.55
1:A:380:TRP:CD2	1:A:447:TYR:HB2	2.40	0.55
1:A:449:ALA:O	1:A:450:LEU:C	2.45	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:720:SER:HB2	1:A:727:TRP:CD2	2.42	0.55
1:A:648:SER:HB2	1:A:649:PRO:HD2	1.88	0.55
1:A:630:LEU:HB2	1:A:655:SER:HB3	1.87	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:647:TYR:O	1:A:648:SER:O	2.26	0.54
1:A:385:LYS:NZ	1:A:492:GLN:OE1	2.40	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:701:ASN:C	1:A:715:LEU:HD12	2.27	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: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:560:ILE:HD11	1:A:628:GLY:C	2.28	0.54
1:A:138:GLN:NE2	3:A:1064:HOH:O	2.38	0.54
1:A:133:VAL:CG2	1:A:144:LEU:HD21	2.37	0.54
1:A:412:ASP:HB3	1:A:416:GLY:H	1.72	0.54
1:A:728:LYS:O	1:A:729:GLY:O	2.26	0.53
1:A:160:PHE:CD1	1:A:168:ALA:HB2	2.42	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:455:THR:OG1	1:A:465:THR:HG23	2.09	0.53
1:A:283:ASN:HB2	1:A:290:PHE:HE1	1.72	0.53
1:A:31:ALA:HB2	1:A:65:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:ASN:ND2	1:A:286:ASP:HA	2.24	0.53
1:A:215:GLY:HA2	1:A:764:ILE:O	2.09	0.53
1:A:330:ILE:HD13	1:A:546:PRO:HG3	1.91	0.53
1:A:157:GLU:OE2	1:A:771:LEU:HD11	2.08	0.53
1:A:358:GLN:NE2	1:A:540:GLY:O	2.41	0.52
1:A:225:ILE:HB	1:A:243:GLU:HG3	1.91	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:364:GLY:HA3	1:A:534:ASN:O	2.09	0.52
1:A:30:ASN:HB3	1:A:208:ASP:OD1	2.09	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:86:HIS:HD2	1:A:112:TYR:OH	1.93	0.52
1:A:611:ILE:O	1:A:611:ILE:HG22	2.09	0.52
1:A:51:ASN:O	1:A:52:ASN:HB2	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:171:TYR:C	1:A:177:ILE:HD11	2.30	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:406:VAL:HB	1:A:422:ASN:HB3	1.92	0.51
1:A:38:ASP:HB2	3:A:1428:HOH:O	2.09	0.51
1:A:207:ARG:NH2	3:A:1467:HOH:O	2.31	0.51
1:A:436:LYS:HE3	3:A:891:HOH:O	2.11	0.51
1:A:49:ASN:OD1	1:A:75:ALA:HA	2.10	0.51
1:A:399:ALA:O	1:A:475:ASN:N	2.40	0.50
1:A:457:PHE:CZ	1:A:462:GLN:HG3	2.46	0.50
1:A:392:ALA:CB	1:A:410:SER:HB2	2.42	0.50
1:A:322:ILE:HG22	1:A:575:LEU:HD23	1.92	0.50
1:A:771:LEU:HD21	3:A:1082:HOH:O	2.11	0.50
1:A:303:THR:HG22	1:A:304:VAL:N	2.26	0.50
1:A:103:LEU:N	1:A:203:VAL:O	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:CZ3	1:A:79:TYR:HB2	2.46	0.50
1:A:322:ILE:HG21	1:A:543:SER:HB3	1.94	0.50
1:A:680:THR:HA	3:A:976:HOH:O	2.11	0.50
1:A:166:PRO:O	1:A:167:SER:HB3	2.11	0.50
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:606:TRP:CZ2	1:A:612:LEU:HD13	2.47	0.50
1:A:459:ASP:HB2	3:A:893:HOH:O	2.11	0.50
1:A:401:GLY:O	1:A:472:GLN:HA	2.11	0.50
1:A:381:GLN:CD	1:A:497:THR:HG23	2.33	0.49
1:A:498:GLN:O	1:A:499:GLN:C	2.50	0.49
1:A:260:ILE:N	1:A:260:ILE:HD13	2.28	0.49
1:A:625:LEU:HD21	1:A:631:LEU:HB2	1.94	0.49
1:A:309:ALA:HB2	1:A:546:PRO:HD3	1.93	0.49
1:A:675:ASN:HB2	1:A:730:PRO:HG3	1.94	0.49
1:A:276:LEU:HA	3:A:1131:HOH:O	2.12	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:668:ASN:C	1:A:668:ASN:HD22	2.15	0.49
1:A:619:GLU:OE1	1:A:635:ARG:NH1	2.44	0.49
1:A:702:PRO:HA	1:A:715:LEU:HA	1.95	0.49
1:A:527:TRP:N	1:A:527:TRP:CD1	2.80	0.49
1:A:170:PHE:C	1:A:177:ILE:HD12	2.33	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:241:PHE:CE2	1:A:262:THR:CG2	2.92	0.49
1:A:186:SER:HB2	3:A:1010:HOH:O	2.13	0.49
1:A:688:PHE:CE1	1:A:745:GLN:HG3	2.48	0.49
1:A:639:ASN:HB3	3:A:945:HOH:O	2.13	0.49
1:A:478:PHE:CE2	1:A:494:ILE:HD13	2.48	0.49
1:A:430:LEU:HA	1:A:430:LEU:HD12	1.66	0.49
1:A:82:SER:OG	1:A:85:GLN:HG3	2.13	0.48
1:A:401:GLY:N	1:A:473:GLU:O	2.36	0.48
1:A:370:ARG:HB3	1:A:476:ILE:CG2	2.43	0.48
1:A:476:ILE:C	1:A:476:ILE:HD12	2.32	0.48
1:A:328:ASN:HD21	1:A:544:VAL:HG22	1.78	0.48
1:A:701:ASN:ND2	1:A:702:PRO:HD2	2.28	0.48
1:A:705:ASN:CG	1:A:706:PRO:HD3	2.33	0.48
1:A:101:LYS:NZ	1:A:153:TYR:CE2	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:652:GLN:NE2	1:A:668:ASN:O	2.48	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:399:ALA:HB1	1:A:473:GLU:HB2	1.95	0.47
1:A:207:ARG:HD3	3:A:1089:HOH:O	2.14	0.47
1:A:115:GLY:HA3	3:A:1480:HOH:O	2.14	0.47
1:A:454:THR:O	1:A:465:THR:HG23	2.15	0.47
1:A:284:VAL:CG2	1:A:285:SER:N	2.77	0.47
1:A:102:VAL:HA	1:A:204:ALA:HB2	1.95	0.47
1:A:36:GLU:O	1:A:42:LYS:HG3	2.15	0.47
1:A:712:ARG:N	3:A:982:HOH:O	2.34	0.47
1:A:640:GLN:O	1:A:647:TYR:HB2	2.15	0.47
1:A:405:TYR:CE1	1:A:467:ALA:HA	2.50	0.47
1:A:190:MET:HG3	1:A:192:VAL:HG23	1.95	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:107:MET:O	1:A:109:THR:HG23	2.14	0.47
1:A:493:LYS:HA	1:A:506:PHE:O	2.15	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:465:THR:N	3:A:1343:HOH:O	2.48	0.47
1:A:296:ILE:HG12	1:A:551:GLY:HA3	1.97	0.47
1:A:661:THR:HA	3:A:1397:HOH:O	2.15	0.47
1:A:263:ARG:HA	3:A:1129: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:419:ALA:HB2	1:A:430:LEU:HD22	1.97	0.46
1:A:238:VAL:O	1:A:264:THR:HG22	2.15	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:728:LYS:HB3	1:A:776:LEU:HD22	1.98	0.46
1:A:684:SER:HB2	1:A:741:SER:O	2.15	0.46
1:A:395:GLN:NE2	1:A:481:ALA:CB	2.78	0.46
1:A:51:ASN:C	1:A:53:GLY:H	2.19	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:626:GLN:HE22	1:A:687:ARG:NH2	2.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:O	1:A:436:LYS:N	2.49	0.46
1:A:77:TRP:O	1:A:192:VAL:HA	2.16	0.46
1:A:355:ARG:CD	1:A:513:GLN:HG3	2.46	0.46
1:A:59:ASN:HD22	1:A:64:PRO:N	2.13	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:335:TYR:HB2	1:A:342:TRP:CE3	2.51	0.46
1:A:138:GLN:NE2	1:A:138:GLN:CA	2.78	0.46
1:A:472:GLN:HG3	3:A:1440:HOH:O	2.15	0.46
1:A:237:VAL:HG11	1:A:337:VAL:HG13	1.96	0.46
1:A:136:GLU:O	1:A:138:GLN:HG2	2.16	0.45
1:A:550:HIS:HE1	3:A:927:HOH:O	1.98	0.45
1:A:560:ILE:HD11	1:A:628:GLY:HA3	1.96	0.45
1:A:165:ASN:N	1:A:165:ASN:OD1	2.49	0.45
1:A:380:TRP:CD2	1:A:447:TYR:CB	2.99	0.45
1:A:380:TRP:CE2	1:A:447:TYR:CB	2.99	0.45
1:A:244:LYS:HB2	1:A:261:ILE:CD1	2.38	0.45
1:A:189:ASN:O	1:A:190:MET:HB3	2.15	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:380:TRP:CZ2	1:A:447:TYR:HB2	2.52	0.45
1:A:369:ARG:HD3	1:A:477:GLN:HE21	1.80	0.45
1:A:422:ASN:HD21	1:A:469:GLU:H	1.63	0.45
1:A:393:ALA:HB3	1:A:485:ILE:HG21	1.99	0.45
1:A:741:SER:CB	1:A:755:VAL:HG13	2.46	0.45
1:A:117:GLN:HE21	1:A:183:PRO:HB2	1.79	0.45
1:A:405:TYR:HE1	1:A:467:ALA:HA	1.81	0.45
1:A:382:SER:HB2	1:A:445:LEU:HB2	1.98	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:496:LEU:O	1:A:503:LEU:N	2.49	0.44
1:A:100:MET:CE	1:A:110:ASN:ND2	2.80	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:226:PRO:HB2	1:A:754:ILE:HD13	1.98	0.44
1:A:696:PHE:HA	3:A:1380:HOH:O	2.18	0.44
1:A:391:GLY:N	1:A:411:ILE:CD1	2.78	0.44
1:A:92:PHE:CZ	1:A:763:ARG:CD	3.00	0.44
1:A:720:SER:HB2	1:A:727:TRP:CE3	2.52	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:81:LEU:N	3:A:1479:HOH:O	2.51	0.44
1:A:714:ASN:HB3	1:A:732:GLN:NE2	2.32	0.44
1:A:190:MET:HG3	1:A:192:VAL:CG2	2.48	0.44
1:A:94:TRP:HA	1:A:212:GLU:O	2.17	0.44
1:A:226:PRO:HG3	1:A:762:MET:CG	2.47	0.44
1:A:102:VAL:HG12	1:A:102:VAL:O	2.17	0.44
1:A:685:ILE:HD11	1:A:727:TRP:CH2	2.53	0.44
1:A:296:ILE:HG12	1:A:551:GLY:C	2.38	0.44
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: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:241:PHE:CE2	1:A:306:VAL:HG21	2.53	0.43
1:A:148:THR:O	1:A:152:GLU:HG3	2.17	0.43
1:A:81:LEU:HD21	1:A:191:ILE:HD11	2.00	0.43
1:A:287:GLU:HG3	3:A:1476:HOH:O	2.18	0.43
1:A:600:LEU:N	1:A:600:LEU:HD23	2.33	0.43
1:A:29:TYR:HE1	1:A:38:ASP:O	2.01	0.43
1:A:648:SER:CB	1:A:670:ALA:CB	2.96	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:464:THR:CG2	1:A:465:THR:H	2.26	0.43
1:A:282:ILE:HG22	3:A:1360:HOH:O	2.18	0.43
1:A:502:ASN:HA	1:A:502:ASN:HD22	1.67	0.43
1:A:601:PRO:HA	3:A:1398:HOH:O	2.17	0.43
1:A:648:SER:OG	1:A:650:ARG:O	2.36	0.43
1:A:560:ILE:HD11	1:A:628:GLY:CA	2.49	0.43
1:A:312:PRO:HB2	3:A:1170:HOH:O	2.18	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:219:PHE:HB2	1:A:762:MET:HE3	2.00	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:770:THR:HG22	1:A:771:LEU:N	2.34	0.43
1:A:364:GLY:C	1:A:483:ALA:HA	2.39	0.43
1:A:714:ASN:HB3	1:A:732:GLN:HE21	1.84	0.43
1:A:30:ASN:H	1:A:43:GLN:NE2	2.17	0.42
1:A:26:LEU:HB3	3:A:1103:HOH:O	2.18	0.42
1:A:707:ALA:HB3	3:A:993:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:92:PHE:CZ	1:A:763:ARG:HD3	2.54	0.42
1:A:229:VAL:CG1	1:A:230:ALA:N	2.82	0.42
1:A:631:LEU:HG	3:A:1393:HOH:O	2.19	0.42
1:A:391:GLY:H	1:A:411:ILE:HD12	1.83	0.42
1:A:308:TYR:CD1	1:A:308:TYR:N	2.86	0.42
1:A:403:ARG:NH2	1:A:452:HIS:HB3	2.35	0.42
1:A:728:LYS:HA	1:A:728:LYS:HD2	1.50	0.42
1:A:728:LYS:HG3	3:A:1413:HOH:O	2.19	0.42
1:A:322:ILE:HD12	1:A:326:MET:SD	2.60	0.42
1:A:581:ASN:OD1	1:A:582:VAL:N	2.46	0.42
1:A:409:LEU:HD21	1:A:443:TYR:CE2	2.55	0.42
1:A:422:ASN:ND2	1:A:469:GLU:H	2.17	0.42
1:A:244:LYS:CA	1:A:261:ILE:HD13	2.48	0.42
1:A:550:HIS:CE1	1:A:686:THR:HG23	2.55	0.42
1:A:586:TYR:CD1	1:A:586:TYR:N	2.88	0.42
1:A:39:SER:O	1:A:42:LYS:HB2	2.19	0.42
1:A:775:LYS:HB3	1:A:775:LYS:NZ	2.35	0.42
1:A:296:ILE:HG12	1:A:551:GLY:CA	2.49	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:259:ASP:O	1:A:260:ILE:HD13	2.20	0.42
1:A:355:ARG:HD2	3:A:1290:HOH:O	2.19	0.42
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.69	0.42
1:A:141:ARG:NH1	3:A:1044:HOH:O	2.52	0.42
1:A:652:GLN:HG3	3:A:1393:HOH:O	2.18	0.41
1:A:391:GLY:H	1:A:411:ILE:CD1	2.32	0.41
1:A:27:PHE:HZ	1:A:85:GLN:NE2	2.14	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:430:LEU:O	1:A:431:GLN:HG2	2.20	0.41
1:A:197:SER:CB	1:A:200:THR:HB	2.49	0.41
1:A:71:ILE:HG12	1:A:71:ILE:O	2.20	0.41
1:A:96:MET:CE	1:A:191:ILE:CG2	2.97	0.41
1:A:743:ILE:HG12	1:A:744:TYR:N	2.35	0.41
1:A:309:ALA:HB2	1:A:546:PRO:CD	2.50	0.41
1:A:295:PRO:HA	1:A:305:LEU:O	2.20	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:O	1:A:501:HIS:CD2	2.74	0.41
1:A:282:ILE:HG23	1:A:282:ILE:HD13	1.73	0.41
1:A:451:ASN:OD1	1:A:453:THR:OG1	2.35	0.41
1:A:294:ARG:HA	1:A:549:GLY:O	2.21	0.41
1:A:491:VAL:HG12	1:A:492:GLN:N	2.35	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: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:46:MET:O	1:A:77:TRP:HE3	2.03	0.41
1:A:335:TYR:HB2	1:A:342:TRP:CZ2	2.55	0.41
1:A:303:THR:HG21	1:A:334:VAL:CG1	2.35	0.41
1:A:279:THR:O	1:A:282:ILE:HB	2.20	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:95:ARG:NH2	3:A:1083:HOH:O	2.45	0.41
1:A:397:GLN:HB3	1:A:477:GLN:HB3	2.03	0.41
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:39:SER:HB3	1:A:42:LYS:HG2	2.03	0.40
1:A:478:PHE:CD1	1:A:478:PHE:C	2.94	0.40
1:A:381:GLN:CA	1:A:446:GLN:HE22	2.34	0.40
1:A:707:ALA:O	1:A:708:GLY:C	2.59	0.40
1:A:322:ILE:CG2	1:A:575:LEU:HD23	2.51	0.40
1:A:699:PHE:O	1:A:717:LEU:HA	2.22	0.40
1:A:71:ILE:N	1:A:71:ILE:HD13	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:369:ARG:HH11	1:A:477:GLN:NE2	2.19	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:107:MET:HE3	1:A:109:THR:CG2	2.52	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	755/757 (100%)	679 (90%)	63 (8%)	13 (2%)	11 10

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

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%)	550 (86%)	87 (14%)	4 4

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	38	ASP
1	A	46	MET
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	138	GLN
1	A	139	THR
1	A	151	THR
1	A	164	SER
1	A	165	ASN
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	274	THR
1	A	279	THR
1	A	282	ILE
1	A	285	SER
1	A	306	VAL
1	A	322	ILE
1	A	365	SER
1	A	366	GLU
1	A	370	ARG
1	A	378	GLN
1	A	381	GLN
1	A	382	SER
1	A	394	ASN
1	A	398	VAL
1	A	404	LYS
1	A	411	ILE
1	A	418	VAL

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Mol	Chain	Res	Type
1	A	424	VAL
1	A	432	SER
1	A	446	GLN
1	A	448	SER
1	A	450	LEU
1	A	451	ASN
1	A	466	TRP
1	A	474	ASN
1	A	476	ILE
1	A	482	ASP
1	A	490	HIS
1	A	505	GLU
1	A	515	THR
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	592	SER
1	A	596	THR
1	A	602	ILE
1	A	607	LYS
1	A	622	MET
1	A	623	VAL
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	681	VAL
1	A	686	THR
1	A	689	GLU
1	A	697	LEU
1	A	723	GLU
1	A	725	VAL
1	A	728	LYS
1	A	755	VAL
1	A	759	ASN

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Mol	Chain	Res	Type
1	A	766	ARG
1	A	770	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
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	189	ASN
1	A	195	ASN
1	A	328	ASN
1	A	383	ASN
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	477	GLN
1	A	480	ASN
1	A	490	HIS
1	A	501	HIS
1	A	502	ASN
1	A	550	HIS
1	A	564	GLN
1	A	626	GLN
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

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 carbohydrates in this entry.

5.6 Ligand geometry

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.