Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:03 PM GMT

PDB ID	:	1ILE
Title	:	ISOLEUCYL-TRNA SYNTHETASE
Authors	:	Nureki, O.; Vassylyev, D.G.; Tateno, M.; Shimada, A.; Nakama, T.; Fukai, S.; Konno, M.; Schimmel, P.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	1998-02-24
Resolution	:	2.50 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:

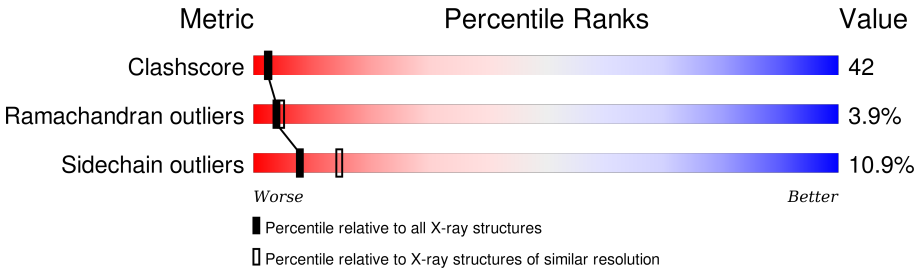
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	821	40% 50% 9% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7022 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 ISOLEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	821	Total	C	N	O	S	0	0	0
			6698	4334	1144	1200	20			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total	O	0	0
			322	322		

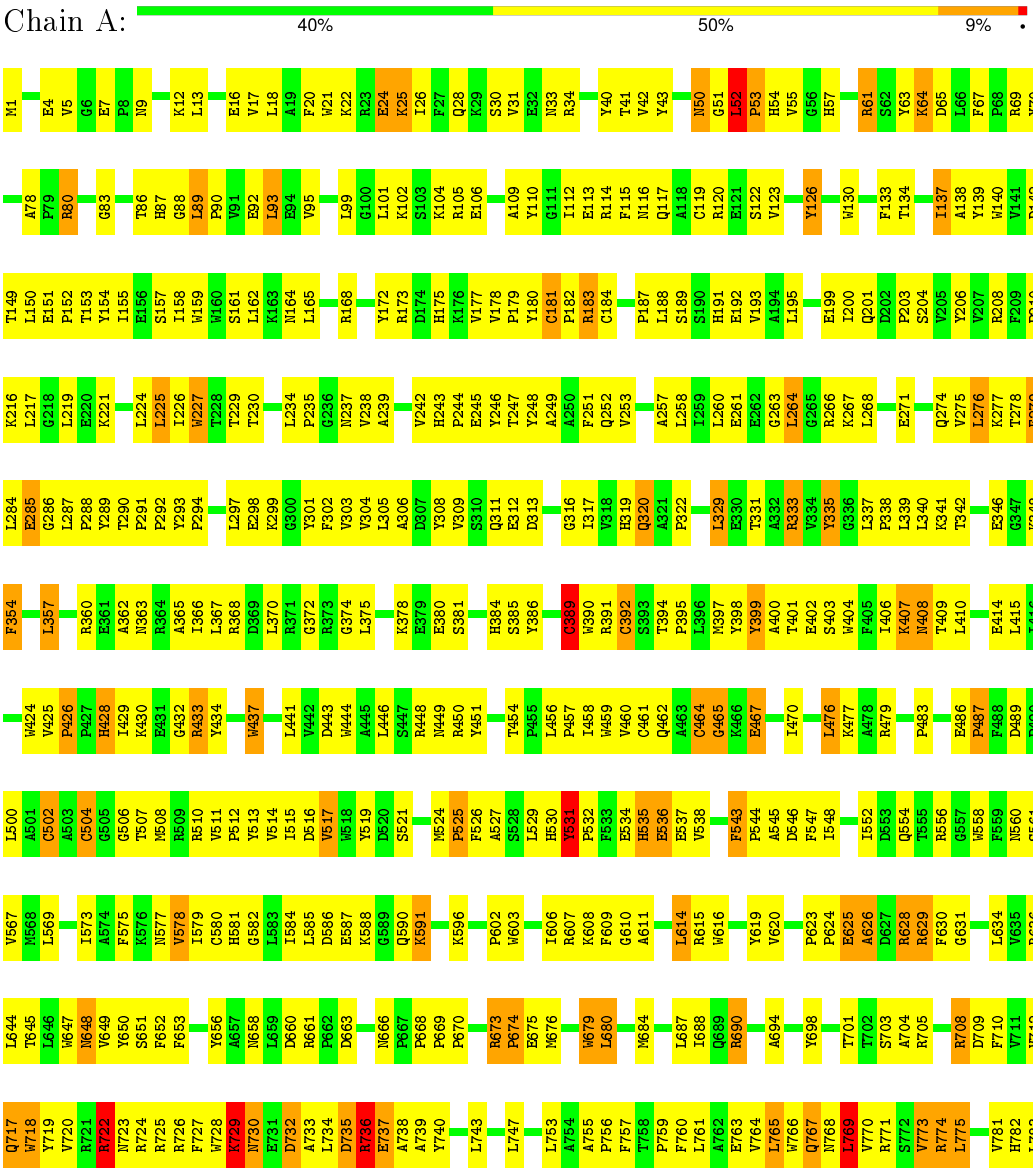
3 Residue-property plots (i)

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: ISOLEUCYL-TRNA SYNTHETASE

Chain A:




E796
A797
L798
V799
A800
Q801
M802
R803
A804
V805
L806
K807
V808
V809
R813
R816
A817
K818
V821

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.10Å 94.80Å 126.50Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.222 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7022	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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: ZN

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	0.61	2/6901 (0.0%)	0.86	16/9386 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	CYS	CB-SG	6.73	1.93	1.82
1	A	24	GLU	CB-CG	5.50	1.62	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	389	CYS	CA-CB-SG	9.37	130.86	114.00
1	A	392	CYS	CA-CB-SG	7.25	127.06	114.00
1	A	502	CYS	CA-CB-SG	7.01	126.61	114.00
1	A	578	VAL	CB-CA-C	-6.51	99.03	111.40
1	A	89	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	714	ASP	N-CA-C	-6.20	94.26	111.00
1	A	467	GLU	N-CA-C	5.92	126.99	111.00
1	A	181	CYS	CA-CB-SG	5.91	124.63	114.00
1	A	504	CYS	CA-CB-SG	5.55	123.98	114.00
1	A	137	ILE	N-CA-C	-5.46	96.27	111.00
1	A	736	ARG	N-CA-C	-5.38	96.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	LEU	CA-CB-CG	-5.21	103.31	115.30
1	A	531	TYR	N-CA-C	5.18	124.98	111.00
1	A	52	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	426	PRO	N-CA-C	-5.12	98.78	112.10
1	A	392	CYS	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	TYR	Sidechain
1	A	399	TYR	Sidechain
1	A	531	TYR	Sidechain

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	6698	0	6574	559	0
2	A	2	0	0	0	0
3	A	322	0	0	115	0
All	All	7022	0	6574	559	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 42.

All (559) 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:464:CYS:SG	1:A:502:CYS:SG	1.15	1.15
1:A:425:VAL:HG21	1:A:579:ILE:HG12	1.34	1.05
1:A:464:CYS:CB	1:A:504:CYS:SG	2.49	1.00
1:A:645:THR:HG23	1:A:715:LEU:HD12	1.45	0.96
1:A:426:PRO:HA	3:A:1200:HOH:O	1.67	0.95
1:A:237:ASN:HB2	3:A:1143:HOH:O	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HA	3:A:1346:HOH:O	1.70	0.91
1:A:461:CYS:SG	1:A:502:CYS:CB	2.58	0.90
1:A:461:CYS:SG	1:A:502:CYS:SG	1.14	0.90
1:A:735:ASP:HB3	1:A:736:ARG:HH21	1.35	0.90
1:A:464:CYS:SG	1:A:504:CYS:SG	1.16	0.90
1:A:234:LEU:HA	3:A:1143:HOH:O	1.72	0.89
1:A:389:CYS:HB3	1:A:392:CYS:O	1.73	0.88
1:A:461:CYS:CB	1:A:464:CYS:SG	2.63	0.87
1:A:351:VAL:HG12	1:A:353:PRO:HD2	1.57	0.86
1:A:502:CYS:CB	1:A:504:CYS:SG	2.63	0.86
1:A:673:ARG:HH11	1:A:674:PRO:HD3	1.41	0.85
1:A:204:SER:HB3	1:A:380:GLU:HB2	1.59	0.84
1:A:408:ASN:H	1:A:408:ASN:HD22	1.24	0.83
1:A:459:TRP:CE2	1:A:510:ARG:HB3	2.15	0.82
1:A:266:ARG:HB3	1:A:271:GLU:HG2	1.63	0.81
1:A:486:GLU:HB2	1:A:487:PRO:HD3	1.63	0.80
1:A:418:ASN:HB3	1:A:573:ILE:HD11	1.64	0.79
1:A:64:LYS:HG3	1:A:139:TYR:HE1	1.44	0.79
1:A:461:CYS:SG	1:A:464:CYS:CB	2.70	0.79
1:A:208:ARG:HH11	1:A:375:LEU:HA	1.46	0.79
1:A:104:LYS:HG2	3:A:1379:HOH:O	1.82	0.79
1:A:418:ASN:HB3	1:A:573:ILE:CD1	2.13	0.78
1:A:239:ALA:HB1	3:A:1417:HOH:O	1.84	0.78
1:A:679:TRP:HA	1:A:798:LEU:HD21	1.65	0.78
1:A:608:LYS:HZ1	1:A:636:ARG:NH2	1.81	0.78
1:A:565:LEU:HG	3:A:1376:HOH:O	1.83	0.77
1:A:561:SER:HB2	3:A:1390:HOH:O	1.83	0.77
1:A:821:VAL:HG23	3:A:1141:HOH:O	1.84	0.77
1:A:679:TRP:CE2	1:A:802:MET:HG2	2.20	0.77
1:A:713:GLU:HA	1:A:717:GLN:HB3	1.66	0.76
1:A:33:ASN:HB3	3:A:1275:HOH:O	1.84	0.76
1:A:404:TRP:HB3	3:A:1374:HOH:O	1.85	0.76
1:A:658:ASN:HA	3:A:1220:HOH:O	1.86	0.76
1:A:55:VAL:HG11	1:A:630:PHE:HE2	1.49	0.75
1:A:235:PRO:HB3	1:A:351:VAL:HG21	1.68	0.75
1:A:464:CYS:HG	1:A:504:CYS:CB	1.96	0.75
1:A:585:LEU:HA	3:A:1190:HOH:O	1.85	0.75
1:A:591:LYS:HA	3:A:1190:HOH:O	1.87	0.75
1:A:424:TRP:HD1	1:A:430:LYS:HE2	1.49	0.74
1:A:157:SER:HB2	3:A:1409:HOH:O	1.87	0.74
1:A:353:PRO:HA	3:A:1156:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:OE2	1:A:538:VAL:HG23	1.89	0.73
1:A:55:VAL:HG11	1:A:630:PHE:CE2	2.23	0.73
1:A:535:HIS:HB3	1:A:538:VAL:HB	1.71	0.73
1:A:649:VAL:HB	1:A:715:LEU:HD23	1.71	0.73
1:A:684:MET:HA	3:A:1288:HOH:O	1.89	0.72
1:A:588:LYS:HA	1:A:629:ARG:HG2	1.70	0.72
1:A:464:CYS:SG	1:A:504:CYS:CB	2.76	0.72
1:A:449:ASN:O	1:A:450:ARG:HD2	1.90	0.72
1:A:153:THR:HB	1:A:530:HIS:CD2	2.24	0.72
1:A:244:PRO:HB3	1:A:305:LEU:HD13	1.72	0.72
1:A:406:ILE:HB	3:A:1389:HOH:O	1.89	0.72
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.54	0.72
1:A:244:PRO:HA	1:A:281:GLY:HA3	1.70	0.72
1:A:673:ARG:HA	1:A:673:ARG:CZ	2.19	0.71
1:A:587:GLU:HG2	1:A:631:GLY:HA3	1.70	0.71
1:A:406:ILE:HD12	3:A:1389:HOH:O	1.90	0.71
1:A:63:TYR:HA	3:A:1386:HOH:O	1.89	0.71
1:A:675:GLU:HA	3:A:1230:HOH:O	1.91	0.71
1:A:408:ASN:HD21	1:A:443:ASP:HA	1.56	0.70
1:A:333:ARG:HG2	3:A:1418:HOH:O	1.91	0.70
1:A:720:VAL:HA	1:A:723:ASN:HB2	1.73	0.70
1:A:280:PRO:O	1:A:283:ALA:HB3	1.92	0.70
1:A:674:PRO:HG2	1:A:726:ARG:HH12	1.55	0.69
1:A:733:ALA:HB3	1:A:736:ARG:HG2	1.72	0.69
1:A:530:HIS:HA	3:A:1399:HOH:O	1.91	0.69
1:A:95:VAL:HG21	1:A:119:CYS:HA	1.73	0.69
1:A:249:ALA:HB3	1:A:251:PHE:CE1	2.27	0.69
1:A:461:CYS:HA	1:A:508:MET:HG2	1.73	0.69
1:A:476:LEU:HB2	3:A:1132:HOH:O	1.91	0.69
1:A:368:ARG:HD3	3:A:1128:HOH:O	1.92	0.69
1:A:415:LEU:HA	3:A:1323:HOH:O	1.90	0.69
1:A:184:CYS:HB3	3:A:1366:HOH:O	1.93	0.68
1:A:280:PRO:HD2	1:A:283:ALA:HB2	1.75	0.68
1:A:101:LEU:HD22	1:A:101:LEU:H	1.59	0.68
1:A:192:GLU:HG2	1:A:390:TRP:NE1	2.10	0.67
1:A:607:ARG:HD2	3:A:1113:HOH:O	1.94	0.67
1:A:425:VAL:HB	1:A:579:ILE:HA	1.77	0.66
1:A:403:SER:HB2	3:A:1361:HOH:O	1.95	0.66
1:A:89:LEU:HB2	3:A:1300:HOH:O	1.95	0.66
1:A:690:ARG:HG2	1:A:690:ARG:HH11	1.61	0.66
1:A:673:ARG:HA	1:A:673:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:PRO:HB3	1:A:726:ARG:HH22	1.61	0.66
1:A:530:HIS:HB3	1:A:534:GLU:HB2	1.76	0.66
1:A:302:PHE:HE2	3:A:1384:HOH:O	1.78	0.65
1:A:710:PHE:HZ	3:A:1226:HOH:O	1.79	0.65
1:A:544:PRO:HB3	3:A:1267:HOH:O	1.94	0.65
1:A:291:PRO:HG2	1:A:294:PRO:HG3	1.78	0.65
1:A:304:VAL:HG22	1:A:335:TYR:CZ	2.32	0.65
1:A:629:ARG:H	1:A:629:ARG:CZ	2.10	0.65
1:A:567:VAL:HG21	3:A:1323:HOH:O	1.96	0.65
1:A:649:VAL:HG23	1:A:720:VAL:HG21	1.78	0.64
1:A:458:ILE:HB	3:A:1161:HOH:O	1.95	0.64
1:A:524:MET:HB3	1:A:525:PRO:HD3	1.79	0.64
1:A:492:ARG:HB3	1:A:493:PRO:HD3	1.80	0.64
1:A:217:LEU:O	1:A:277:LYS:HD2	1.97	0.64
1:A:548:ILE:HG13	1:A:578:VAL:HG13	1.78	0.64
1:A:437:TRP:HE3	3:A:1213:HOH:O	1.78	0.64
1:A:161:SER:O	1:A:164:ASN:HB3	1.98	0.64
1:A:317:ILE:HG23	3:A:1194:HOH:O	1.97	0.64
1:A:717:GLN:O	1:A:718:TRP:HE3	1.80	0.64
1:A:57:HIS:CD2	1:A:130:TRP:CH2	2.86	0.64
1:A:184:CYS:SG	3:A:1366:HOH:O	2.55	0.64
1:A:680:LEU:HD13	1:A:719:TYR:CD2	2.33	0.63
1:A:531:TYR:HB3	1:A:532:PRO:HD3	1.80	0.63
1:A:674:PRO:CB	1:A:726:ARG:HH22	2.11	0.63
1:A:384:HIS:HB2	3:A:1372:HOH:O	1.99	0.63
1:A:247:THR:HG23	3:A:1307:HOH:O	1.98	0.63
1:A:712:VAL:HG23	3:A:1405:HOH:O	1.98	0.63
1:A:451:TYR:HE1	3:A:1379:HOH:O	1.80	0.63
1:A:372:GLY:HA3	3:A:1174:HOH:O	1.99	0.63
1:A:87:HIS:HB2	3:A:1149:HOH:O	1.99	0.63
1:A:628:ARG:HA	1:A:629:ARG:NH2	2.14	0.63
1:A:112:ILE:HG22	1:A:493:PRO:HG3	1.80	0.62
1:A:172:TYR:CE1	1:A:407:LYS:HG3	2.33	0.62
1:A:192:GLU:HG2	1:A:390:TRP:CE2	2.33	0.62
1:A:162:LEU:HD21	3:A:1119:HOH:O	1.97	0.62
1:A:61:ARG:HG2	1:A:61:ARG:NH1	2.14	0.62
1:A:57:HIS:CD2	1:A:130:TRP:HH2	2.17	0.62
1:A:73:MET:HE2	1:A:786:TRP:HE3	1.65	0.62
1:A:408:ASN:ND2	1:A:443:ASP:HA	2.13	0.62
1:A:99:LEU:HB2	1:A:101:LEU:CD2	2.30	0.62
1:A:603:TRP:HA	1:A:606:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:VAL:O	1:A:809:VAL:HG23	1.99	0.61
1:A:515:ILE:HG21	3:A:1286:HOH:O	2.00	0.61
1:A:53:PRO:HA	1:A:57:HIS:CD2	2.35	0.61
1:A:526:PHE:HB2	1:A:531:TYR:CB	2.30	0.61
1:A:764:VAL:HG23	1:A:765:LEU:HD23	1.80	0.61
1:A:767:GLN:HA	1:A:767:GLN:NE2	2.14	0.61
1:A:28:GLN:HB2	3:A:1131:HOH:O	2.00	0.61
1:A:456:LEU:HD12	1:A:457:PRO:HD2	1.81	0.61
1:A:353:PRO:HG2	1:A:354:PHE:CE1	2.35	0.61
1:A:304:VAL:HB	3:A:1417:HOH:O	2.00	0.61
1:A:543:PHE:HB3	3:A:1284:HOH:O	2.00	0.60
1:A:725:ARG:HG2	1:A:725:ARG:HH11	1.66	0.60
1:A:818:LYS:HE2	3:A:1210:HOH:O	2.00	0.60
1:A:179:PRO:O	1:A:187:PRO:HA	2.02	0.60
1:A:456:LEU:HD13	1:A:515:ILE:HD11	1.83	0.60
1:A:718:TRP:HA	1:A:718:TRP:CE3	2.36	0.60
1:A:17:VAL:HG13	1:A:763:GLU:HG2	1.82	0.60
1:A:183:ARG:HB3	1:A:394:THR:HG21	1.84	0.60
1:A:134:THR:HG23	1:A:139:TYR:HD2	1.67	0.59
1:A:116:ASN:O	1:A:119:CYS:HB2	2.02	0.59
1:A:650:TYR:HE1	1:A:769:LEU:HD13	1.67	0.59
1:A:34:ARG:HD3	3:A:1275:HOH:O	2.02	0.59
1:A:774:ARG:HH11	1:A:774:ARG:CG	2.15	0.59
1:A:18:LEU:HD13	3:A:1182:HOH:O	2.02	0.59
1:A:619:TYR:O	1:A:701:THR:HG22	2.03	0.59
1:A:215:LYS:HA	1:A:219:LEU:H	1.67	0.59
1:A:246:TYR:CE2	1:A:311:GLN:HB3	2.36	0.59
1:A:187:PRO:HG3	3:A:1361:HOH:O	2.01	0.59
1:A:43:TYR:CD2	1:A:545:ALA:HB2	2.38	0.59
1:A:213:GLU:HG3	3:A:1123:HOH:O	2.03	0.59
1:A:585:LEU:HD23	3:A:1190:HOH:O	2.03	0.59
1:A:402:GLU:HG2	3:A:1254:HOH:O	2.02	0.59
1:A:645:THR:HG23	1:A:715:LEU:CD1	2.27	0.59
1:A:215:LYS:HZ1	1:A:216:LYS:HB2	1.68	0.59
1:A:88:GLY:HA3	1:A:517:VAL:CG1	2.32	0.59
1:A:652:PHE:HE1	1:A:723:ASN:OD1	1.86	0.58
1:A:426:PRO:HG2	1:A:580:CYS:HB2	1.85	0.58
1:A:720:VAL:HA	1:A:723:ASN:CB	2.34	0.58
1:A:67:PHE:HE1	3:A:1386:HOH:O	1.86	0.58
1:A:515:ILE:HD12	1:A:515:ILE:N	2.18	0.58
1:A:395:PRO:HB3	3:A:1394:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:HA	3:A:1294:HOH:O	2.02	0.58
1:A:653:PHE:HB2	1:A:743:LEU:HD23	1.85	0.58
1:A:774:ARG:HH11	1:A:774:ARG:HG3	1.69	0.58
1:A:172:TYR:HE1	1:A:407:LYS:HG3	1.67	0.58
1:A:653:PHE:HB2	1:A:743:LEU:CD2	2.34	0.58
1:A:515:ILE:HG22	1:A:516:ASP:O	2.03	0.58
1:A:18:LEU:HD22	3:A:1182:HOH:O	2.03	0.58
1:A:486:GLU:HB2	1:A:487:PRO:CD	2.33	0.58
1:A:106:GLU:O	1:A:109:ALA:HB3	2.02	0.58
1:A:177:VAL:HG23	1:A:329:LEU:HD12	1.86	0.57
1:A:264:LEU:O	1:A:267:LYS:HB2	2.03	0.57
1:A:640:ARG:HD3	1:A:644:LEU:HD11	1.84	0.57
1:A:459:TRP:CZ2	1:A:510:ARG:HB3	2.39	0.57
1:A:9:ASN:OD1	1:A:12:LYS:HD3	2.04	0.57
1:A:486:GLU:CB	1:A:487:PRO:HD3	2.34	0.57
1:A:64:LYS:CG	1:A:139:TYR:HE1	2.16	0.57
1:A:43:TYR:CE2	1:A:545:ALA:HB2	2.38	0.57
1:A:679:TRP:HA	1:A:798:LEU:CD2	2.34	0.57
1:A:54:HIS:HB2	3:A:1364:HOH:O	2.05	0.57
1:A:586:ASP:HB2	1:A:590:GLN:O	2.04	0.57
1:A:184:CYS:CB	3:A:1366:HOH:O	2.51	0.57
1:A:88:GLY:HA3	1:A:517:VAL:HG13	1.85	0.57
1:A:148:ALA:O	1:A:151:GLU:HG3	2.04	0.57
1:A:524:MET:HE1	1:A:558:TRP:HZ2	1.70	0.57
1:A:586:ASP:C	1:A:588:LYS:N	2.59	0.57
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.70	0.57
1:A:575:PHE:CD1	1:A:578:VAL:HG22	2.39	0.56
1:A:183:ARG:CB	1:A:394:THR:HG21	2.36	0.56
1:A:524:MET:CE	1:A:558:TRP:HZ2	2.17	0.56
1:A:72:THR:HB	3:A:1316:HOH:O	2.04	0.56
1:A:418:ASN:HB3	1:A:573:ILE:HD13	1.88	0.56
1:A:766:TRP:HB3	1:A:781:VAL:HG22	1.88	0.56
1:A:304:VAL:HG11	1:A:331:THR:HG21	1.88	0.56
1:A:133:PHE:O	1:A:137:ILE:HG12	2.05	0.55
1:A:429:ILE:HD13	1:A:552:ILE:HD11	1.88	0.55
1:A:234:LEU:HB2	1:A:235:PRO:HD3	1.88	0.55
1:A:390:TRP:HA	3:A:1285:HOH:O	2.06	0.55
1:A:329:LEU:HD21	3:A:1283:HOH:O	2.07	0.55
1:A:720:VAL:HG12	1:A:720:VAL:O	2.07	0.55
1:A:391:ARG:HG3	3:A:1300:HOH:O	2.05	0.55
1:A:50:ASN:HD22	1:A:50:ASN:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ARG:HD2	3:A:1169:HOH:O	2.05	0.55
1:A:390:TRP:O	1:A:391:ARG:HD2	2.06	0.55
1:A:215:LYS:NZ	1:A:216:LYS:HB2	2.22	0.55
1:A:649:VAL:CG2	1:A:720:VAL:HG21	2.36	0.55
1:A:684:MET:O	1:A:688:ILE:HG13	2.05	0.55
1:A:733:ALA:CB	1:A:736:ARG:HG2	2.36	0.55
1:A:723:ASN:HD21	1:A:743:LEU:HD22	1.72	0.54
1:A:708:ARG:HD3	1:A:709:ASP:N	2.22	0.54
1:A:715:LEU:HD13	1:A:716:SER:N	2.22	0.54
1:A:201:GLN:HG2	3:A:1318:HOH:O	2.07	0.54
1:A:446:LEU:HD13	3:A:1259:HOH:O	2.06	0.54
1:A:244:PRO:CA	1:A:281:GLY:HA3	2.37	0.54
1:A:661:ARG:H	1:A:661:ARG:HD3	1.72	0.54
1:A:584:ILE:HG23	1:A:630:PHE:HB3	1.89	0.54
1:A:31:VAL:HA	3:A:1407:HOH:O	2.07	0.54
1:A:529:LEU:C	1:A:531:TYR:H	2.11	0.54
1:A:243:HIS:CD2	1:A:245:GLU:H	2.26	0.54
1:A:816:ARG:NH1	1:A:821:VAL:HG12	2.22	0.54
1:A:766:TRP:CB	1:A:781:VAL:HG22	2.38	0.53
1:A:727:PHE:CE1	1:A:739:ALA:HB1	2.43	0.53
1:A:527:ALA:HA	3:A:1409:HOH:O	2.08	0.53
1:A:552:ILE:HD13	1:A:580:CYS:HB3	1.90	0.53
1:A:55:VAL:HG21	1:A:584:ILE:HG21	1.90	0.53
1:A:608:LYS:NZ	1:A:636:ARG:HH21	2.07	0.53
1:A:251:PHE:O	1:A:257:ALA:HA	2.09	0.53
1:A:242:VAL:HG23	1:A:305:LEU:HD23	1.89	0.53
1:A:53:PRO:HD3	1:A:130:TRP:CE2	2.44	0.53
1:A:252:GLN:HB2	1:A:276:LEU:HD21	1.91	0.53
1:A:727:PHE:HE1	1:A:739:ALA:HB1	1.74	0.53
1:A:389:CYS:CA	3:A:1327:HOH:O	2.57	0.53
1:A:200:ILE:HD12	3:A:1394:HOH:O	2.08	0.52
1:A:690:ARG:NH1	1:A:690:ARG:HG2	2.23	0.52
1:A:816:ARG:HH12	1:A:821:VAL:HB	1.75	0.52
1:A:292:PRO:C	1:A:294:PRO:HD3	2.29	0.52
1:A:54:HIS:O	1:A:57:HIS:HB2	2.09	0.52
1:A:547:PHE:CD1	1:A:698:TYR:CE2	2.98	0.52
1:A:234:LEU:HD23	3:A:1143:HOH:O	2.09	0.52
1:A:291:PRO:HG3	1:A:301:TYR:CE1	2.44	0.52
1:A:214:PRO:HG2	3:A:1398:HOH:O	2.09	0.52
1:A:603:TRP:CD2	1:A:606:ILE:HD11	2.44	0.52
1:A:340:LEU:HG	3:A:1242:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:HG2	3:A:1421:HOH:O	2.09	0.52
1:A:302:PHE:HD1	1:A:303:VAL:O	1.93	0.52
1:A:424:TRP:CD1	1:A:430:LYS:HE2	2.38	0.52
1:A:673:ARG:HA	1:A:673:ARG:NE	2.22	0.52
1:A:813:ARG:NH2	3:A:1392:HOH:O	2.41	0.52
1:A:299:LYS:HB3	3:A:1384:HOH:O	2.10	0.51
1:A:616:TRP:O	1:A:620:VAL:HG12	2.09	0.51
1:A:178:VAL:HG21	1:A:187:PRO:HB3	1.92	0.51
1:A:425:VAL:CG2	1:A:579:ILE:HG12	2.25	0.51
1:A:674:PRO:HG2	1:A:726:ARG:NH1	2.24	0.51
1:A:444:TRP:HH2	3:A:1390:HOH:O	1.93	0.51
1:A:390:TRP:CD2	1:A:391:ARG:HD3	2.46	0.51
1:A:42:VAL:HG11	1:A:64:LYS:CD	2.40	0.51
1:A:52:LEU:HB3	1:A:126:TYR:HD2	1.76	0.51
1:A:581:HIS:HE1	3:A:1142:HOH:O	1.93	0.51
1:A:775:LEU:CD2	1:A:775:LEU:H	2.24	0.51
1:A:24:GLU:O	1:A:26:ILE:HD13	2.11	0.51
1:A:408:ASN:N	1:A:408:ASN:HD22	1.98	0.51
1:A:716:SER:OG	1:A:717:GLN:N	2.44	0.51
1:A:235:PRO:O	1:A:342:THR:HG21	2.11	0.51
1:A:217:LEU:HD21	1:A:287:LEU:HD21	1.92	0.51
1:A:53:PRO:HA	1:A:57:HIS:HD2	1.76	0.51
1:A:175:HIS:HD2	3:A:1184:HOH:O	1.94	0.51
1:A:239:ALA:HB2	1:A:337:LEU:HD13	1.92	0.50
1:A:309:VAL:HG11	1:A:316:GLY:O	2.11	0.50
1:A:492:ARG:HB2	3:A:1269:HOH:O	2.12	0.50
1:A:93:LEU:HD22	1:A:391:ARG:HB3	1.93	0.50
1:A:656:TYR:HE2	1:A:728:TRP:HA	1.76	0.50
1:A:304:VAL:HG22	1:A:335:TYR:CE1	2.47	0.50
1:A:764:VAL:CG2	1:A:765:LEU:HD23	2.42	0.50
1:A:306:ALA:HB1	1:A:308:TYR:CE1	2.47	0.50
1:A:558:TRP:CE2	1:A:562:LEU:HD11	2.47	0.50
1:A:282:LYS:HA	1:A:305:LEU:HD11	1.94	0.50
1:A:149:THR:HG22	1:A:154:TYR:CE1	2.46	0.50
1:A:470:ILE:HD11	1:A:500:LEU:CD1	2.42	0.50
1:A:726:ARG:HA	1:A:730:ASN:HB2	1.93	0.50
1:A:42:VAL:HG11	1:A:64:LYS:HD3	1.94	0.50
1:A:210:PRO:HB3	3:A:1144:HOH:O	2.11	0.49
1:A:767:GLN:O	1:A:771:ARG:HB2	2.12	0.49
1:A:304:VAL:HG13	1:A:305:LEU:N	2.27	0.49
1:A:629:ARG:NH1	1:A:629:ARG:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:HD1	3:A:1386:HOH:O	1.93	0.49
1:A:64:LYS:HD2	1:A:64:LYS:O	2.12	0.49
1:A:608:LYS:NZ	1:A:636:ARG:NH2	2.54	0.49
1:A:217:LEU:HD12	1:A:279:PHE:CE2	2.48	0.49
1:A:390:TRP:C	1:A:391:ARG:HD2	2.32	0.49
1:A:437:TRP:HB3	3:A:1213:HOH:O	2.13	0.49
1:A:92:GLU:HG2	1:A:115:PHE:CE2	2.47	0.49
1:A:248:TYR:CD1	1:A:261:GLU:HA	2.48	0.49
1:A:92:GLU:HG2	1:A:115:PHE:HE2	1.78	0.49
1:A:673:ARG:HD2	1:A:738:ALA:HB1	1.95	0.49
1:A:93:LEU:HD22	1:A:391:ARG:CB	2.43	0.49
1:A:155:ILE:O	1:A:158:ILE:HB	2.12	0.49
1:A:801:GLN:O	1:A:805:VAL:HG23	2.13	0.49
1:A:608:LYS:HZ1	1:A:636:ARG:HH22	1.60	0.49
1:A:206:TYR:HA	1:A:226:ILE:O	2.12	0.49
1:A:187:PRO:O	1:A:188:LEU:HD23	2.12	0.49
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.28	0.49
1:A:302:PHE:CD1	1:A:303:VAL:O	2.66	0.48
1:A:161:SER:HB2	3:A:1278:HOH:O	2.13	0.48
1:A:12:LYS:O	1:A:16:GLU:HG3	2.13	0.48
1:A:116:ASN:HD22	1:A:493:PRO:HD3	1.78	0.48
1:A:9:ASN:HD21	1:A:12:LYS:HE2	1.78	0.48
1:A:753:LEU:O	1:A:756:PRO:HD2	2.12	0.48
1:A:719:TYR:HA	1:A:722:ARG:NH1	2.28	0.48
1:A:285:GLU:O	1:A:287:LEU:N	2.46	0.48
1:A:603:TRP:CE3	1:A:606:ILE:HD11	2.48	0.48
1:A:288:PRO:HA	1:A:302:PHE:HA	1.96	0.48
1:A:816:ARG:HH12	1:A:821:VAL:CG1	2.27	0.48
1:A:173:ARG:HD2	1:A:402:GLU:OE2	2.12	0.48
1:A:489:ASP:HA	3:A:1362:HOH:O	2.13	0.48
1:A:694:ALA:HB3	1:A:703:SER:HB3	1.96	0.48
1:A:208:ARG:NH1	1:A:375:LEU:HA	2.22	0.48
1:A:333:ARG:HA	1:A:333:ARG:NE	2.28	0.48
1:A:101:LEU:HD22	1:A:101:LEU:N	2.29	0.48
1:A:464:CYS:CB	1:A:504:CYS:CB	2.91	0.48
1:A:719:TYR:HA	1:A:722:ARG:HH12	1.78	0.48
1:A:724:ARG:HD2	3:A:1339:HOH:O	2.12	0.48
1:A:43:TYR:HB3	1:A:524:MET:HE1	1.96	0.48
1:A:189:SER:O	1:A:193:VAL:HG23	2.13	0.48
1:A:114:ARG:HG2	3:A:1368:HOH:O	2.13	0.48
1:A:729:LYS:HD3	1:A:729:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:CD1	1:A:515:ILE:N	2.76	0.48
1:A:547:PHE:CE1	1:A:579:ILE:HG13	2.48	0.48
1:A:353:PRO:HG2	1:A:354:PHE:CD1	2.49	0.48
1:A:365:ALA:O	1:A:368:ARG:HB3	2.14	0.48
1:A:581:HIS:HA	1:A:624:PRO:O	2.14	0.48
1:A:138:ALA:HB3	1:A:759:PRO:HG3	1.96	0.48
1:A:544:PRO:HD3	3:A:1284:HOH:O	2.13	0.48
1:A:816:ARG:HH12	1:A:821:VAL:CB	2.27	0.47
1:A:640:ARG:HD3	1:A:644:LEU:CD1	2.44	0.47
1:A:656:TYR:CE2	1:A:728:TRP:HA	2.49	0.47
1:A:459:TRP:HA	1:A:510:ARG:HA	1.96	0.47
1:A:99:LEU:HD13	1:A:110:TYR:CE2	2.50	0.47
1:A:673:ARG:HD3	1:A:674:PRO:HD3	1.96	0.47
1:A:425:VAL:HB	1:A:426:PRO:HD3	1.96	0.47
1:A:244:PRO:HB2	3:A:1404:HOH:O	2.14	0.47
1:A:582:GLY:HA3	1:A:626:ALA:O	2.14	0.47
1:A:547:PHE:HE1	1:A:579:ILE:HG13	1.80	0.47
1:A:716:SER:O	1:A:718:TRP:N	2.48	0.47
1:A:816:ARG:HH12	1:A:821:VAL:HG12	1.79	0.47
1:A:708:ARG:C	1:A:708:ARG:HD3	2.35	0.47
1:A:723:ASN:ND2	1:A:743:LEU:HD13	2.30	0.47
1:A:676:MET:HB3	1:A:722:ARG:NH2	2.28	0.47
1:A:652:PHE:CE1	1:A:723:ASN:OD1	2.66	0.47
1:A:64:LYS:HG3	1:A:139:TYR:CE1	2.36	0.47
1:A:95:VAL:HG12	1:A:95:VAL:O	2.14	0.47
1:A:224:LEU:HB3	1:A:317:ILE:HD13	1.96	0.47
1:A:526:PHE:HB2	1:A:531:TYR:HB2	1.96	0.47
1:A:407:LYS:O	1:A:410:LEU:HB2	2.14	0.47
1:A:339:LEU:HD22	3:A:1283:HOH:O	2.15	0.47
1:A:113:GLU:HA	1:A:493:PRO:HG2	1.97	0.47
1:A:534:GLU:O	1:A:536:GLU:N	2.48	0.47
1:A:158:ILE:HG21	1:A:454:THR:HG21	1.96	0.47
1:A:764:VAL:CG2	1:A:765:LEU:N	2.77	0.47
1:A:143:LEU:HD11	3:A:1121:HOH:O	2.15	0.47
1:A:204:SER:OG	1:A:227:TRP:CZ3	2.66	0.46
1:A:408:ASN:H	1:A:408:ASN:ND2	2.01	0.46
1:A:243:HIS:HD2	1:A:245:GLU:H	1.61	0.46
1:A:704:ALA:HB2	1:A:757:PHE:CE2	2.50	0.46
1:A:729:LYS:HZ2	1:A:730:ASN:ND2	2.12	0.46
1:A:797:ALA:O	1:A:800:ALA:HB3	2.15	0.46
1:A:50:ASN:HD22	1:A:51:GLY:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:CD1	3:A:1259:HOH:O	2.62	0.46
1:A:712:VAL:O	1:A:712:VAL:HG12	2.15	0.46
1:A:730:ASN:HB3	1:A:736:ARG:CB	2.45	0.46
1:A:42:VAL:HG12	1:A:43:TYR:N	2.30	0.46
1:A:661:ARG:HD3	1:A:661:ARG:N	2.30	0.46
1:A:248:TYR:HD1	1:A:261:GLU:N	2.14	0.46
1:A:203:PRO:O	1:A:229:THR:HA	2.15	0.46
1:A:614:LEU:HB2	3:A:1420:HOH:O	2.14	0.46
1:A:375:LEU:HD12	1:A:375:LEU:O	2.16	0.46
1:A:284:LEU:O	1:A:285:GLU:O	2.33	0.46
1:A:575:PHE:CE1	1:A:578:VAL:HG21	2.51	0.46
1:A:606:ILE:O	1:A:610:GLY:HA2	2.16	0.46
1:A:386:TYR:HD1	3:A:1394:HOH:O	1.98	0.46
1:A:30:SER:HB2	3:A:1316:HOH:O	2.14	0.46
1:A:341:LYS:NZ	1:A:400:ALA:O	2.47	0.46
1:A:253:VAL:HG11	1:A:258:LEU:HD12	1.97	0.46
1:A:802:MET:O	1:A:805:VAL:HB	2.16	0.46
1:A:479:ARG:CB	1:A:500:LEU:HD22	2.46	0.46
1:A:42:VAL:CG1	1:A:43:TYR:N	2.79	0.46
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.69	0.46
1:A:647:TRP:O	1:A:650:TYR:HB3	2.16	0.45
1:A:52:LEU:HD23	1:A:126:TYR:CD2	2.50	0.45
1:A:21:TRP:HA	1:A:26:ILE:HG12	1.98	0.45
1:A:648:ASN:C	1:A:648:ASN:OD1	2.54	0.45
1:A:673:ARG:NH1	1:A:674:PRO:HD3	2.20	0.45
1:A:297:LEU:HD12	1:A:301:TYR:CE2	2.51	0.45
1:A:322:PRO:O	1:A:329:LEU:HG	2.16	0.45
1:A:729:LYS:NZ	1:A:730:ASN:ND2	2.64	0.45
1:A:249:ALA:HB1	1:A:275:VAL:HG13	1.99	0.45
1:A:390:TRP:CE2	1:A:391:ARG:HD3	2.52	0.45
1:A:191:HIS:HE1	1:A:516:ASP:OD2	2.00	0.45
1:A:775:LEU:HD23	1:A:775:LEU:H	1.81	0.45
1:A:719:TYR:CE2	1:A:722:ARG:NH2	2.84	0.45
1:A:1:MET:CB	3:A:1220:HOH:O	2.64	0.45
1:A:199:GLU:HA	1:A:385:SER:HA	1.97	0.45
1:A:40:TYR:CE1	1:A:71:LYS:HE2	2.52	0.45
1:A:715:LEU:O	1:A:716:SER:HB3	2.16	0.45
1:A:451:TYR:N	1:A:451:TYR:CD1	2.84	0.45
1:A:587:GLU:O	1:A:588:LYS:HG2	2.16	0.45
1:A:492:ARG:HD2	1:A:492:ARG:HA	1.84	0.45
1:A:90:PRO:HG3	3:A:1300:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:O	1:A:267:LYS:HG3	2.17	0.45
1:A:620:VAL:HG23	1:A:705:ARG:HG2	1.97	0.45
1:A:83:GLY:HA3	1:A:147:TYR:CZ	2.52	0.45
1:A:730:ASN:C	1:A:732:ASP:H	2.20	0.45
1:A:64:LYS:HZ3	1:A:65:ASP:HA	1.82	0.45
1:A:502:CYS:N	1:A:506:GLY:O	2.50	0.45
1:A:670:PRO:O	1:A:673:ARG:HB2	2.16	0.45
1:A:737:GLU:O	1:A:740:TYR:HB2	2.17	0.45
1:A:434:TYR:HE1	1:A:560:ASN:HD22	1.64	0.45
1:A:735:ASP:C	1:A:737:GLU:H	2.20	0.45
1:A:1:MET:HB2	3:A:1220:HOH:O	2.17	0.45
1:A:429:ILE:CD1	1:A:552:ILE:HD11	2.47	0.44
1:A:86:THR:HB	1:A:150:LEU:HD23	1.99	0.44
1:A:804:ALA:O	1:A:807:LYS:HB3	2.18	0.44
1:A:668:PRO:HG3	1:A:738:ALA:CB	2.47	0.44
1:A:64:LYS:CG	1:A:139:TYR:CE1	3.00	0.44
1:A:55:VAL:HG12	1:A:602:PRO:HB3	1.99	0.44
1:A:575:PHE:HE1	1:A:578:VAL:HG21	1.82	0.44
1:A:13:LEU:O	1:A:16:GLU:HB2	2.18	0.44
1:A:266:ARG:NH1	1:A:271:GLU:HB3	2.32	0.44
1:A:543:PHE:O	1:A:544:PRO:C	2.54	0.44
1:A:575:PHE:CE1	1:A:578:VAL:CG2	3.00	0.44
1:A:456:LEU:CD1	1:A:515:ILE:HD11	2.48	0.44
1:A:546:ASP:O	1:A:577:ASN:HB2	2.16	0.44
1:A:479:ARG:NH2	1:A:508:MET:CE	2.81	0.44
1:A:670:PRO:HA	1:A:673:ARG:HG2	2.00	0.44
1:A:238:VAL:HG11	3:A:1242:HOH:O	2.17	0.44
1:A:628:ARG:HG2	1:A:628:ARG:O	2.18	0.44
1:A:407:LYS:HE3	3:A:1396:HOH:O	2.18	0.44
1:A:80:ARG:O	1:A:142:ASP:HB2	2.17	0.44
1:A:89:LEU:N	1:A:90:PRO:CD	2.81	0.44
1:A:718:TRP:HB3	1:A:719:TYR:H	1.65	0.44
1:A:266:ARG:HH12	1:A:271:GLU:HB3	1.83	0.43
1:A:303:VAL:CG1	1:A:304:VAL:N	2.81	0.43
1:A:425:VAL:HA	3:A:1153:HOH:O	2.16	0.43
1:A:289:TYR:CZ	1:A:301:TYR:HA	2.53	0.43
1:A:687:LEU:HD21	1:A:753:LEU:HD12	2.00	0.43
1:A:165:LEU:HA	1:A:165:LEU:HD23	1.74	0.43
1:A:722:ARG:HB3	1:A:722:ARG:HH11	1.83	0.43
1:A:668:PRO:HG3	1:A:738:ALA:HB2	2.01	0.43
1:A:302:PHE:CD1	1:A:302:PHE:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:CG2	1:A:584:ILE:HG21	2.48	0.43
1:A:17:VAL:O	1:A:20:PHE:HB3	2.18	0.43
1:A:338:PRO:HG2	3:A:1242:HOH:O	2.17	0.43
1:A:460:VAL:O	1:A:508:MET:HA	2.18	0.43
1:A:588:LYS:HD3	1:A:588:LYS:HA	1.78	0.43
1:A:458:ILE:O	1:A:511:VAL:HG13	2.18	0.43
1:A:464:CYS:CB	1:A:504:CYS:HB2	2.48	0.43
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.75	0.43
1:A:173:ARG:HD2	1:A:402:GLU:CD	2.39	0.43
1:A:278:THR:HG21	3:A:1146:HOH:O	2.19	0.43
1:A:304:VAL:HG22	1:A:335:TYR:CE2	2.53	0.43
1:A:99:LEU:HB2	1:A:101:LEU:HD21	1.97	0.43
1:A:783:LEU:HD23	1:A:783:LEU:HA	1.85	0.43
1:A:164:ASN:ND2	1:A:168:ARG:HH11	2.17	0.43
1:A:656:TYR:HE2	1:A:728:TRP:CD1	2.36	0.43
1:A:768:ASN:O	1:A:770:VAL:N	2.52	0.43
1:A:623:PRO:HA	1:A:701:THR:HG21	2.01	0.43
1:A:456:LEU:HA	1:A:515:ILE:HD11	2.00	0.43
1:A:477:LYS:HZ2	1:A:483:PRO:HA	1.84	0.43
1:A:417:ARG:O	1:A:420:GLN:HB2	2.19	0.43
1:A:795:ASP:O	1:A:798:LEU:HB3	2.19	0.43
1:A:159:TRP:HZ3	3:A:1132:HOH:O	2.02	0.43
1:A:755:ALA:HB3	1:A:756:PRO:HD3	2.01	0.43
1:A:479:ARG:HB2	1:A:500:LEU:HD22	1.99	0.42
1:A:433:ARG:O	1:A:556:ARG:NH2	2.52	0.42
1:A:418:ASN:O	1:A:573:ILE:HD11	2.19	0.42
1:A:645:THR:HG21	1:A:712:VAL:HG22	2.01	0.42
1:A:249:ALA:HB3	1:A:251:PHE:HE1	1.82	0.42
1:A:57:HIS:HD2	1:A:130:TRP:CH2	2.37	0.42
1:A:138:ALA:HB3	1:A:615:ARG:NH2	2.33	0.42
1:A:587:GLU:OE2	1:A:634:LEU:HD13	2.20	0.42
1:A:83:GLY:HA2	1:A:147:TYR:O	2.20	0.42
1:A:426:PRO:HG3	1:A:625:GLU:CG	2.50	0.42
1:A:370:LEU:HD22	1:A:375:LEU:HD11	2.02	0.42
1:A:529:LEU:C	1:A:531:TYR:N	2.73	0.42
1:A:208:ARG:HD3	3:A:1144:HOH:O	2.19	0.42
1:A:726:ARG:O	1:A:730:ASN:HB2	2.19	0.42
1:A:83:GLY:HA3	1:A:147:TYR:CE2	2.54	0.42
1:A:663:ASP:OD2	1:A:666:ASN:HB2	2.19	0.42
1:A:609:PHE:HD2	1:A:639:VAL:HG21	1.84	0.42
1:A:519:TYR:HA	3:A:1390:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:VAL:HA	3:A:1297:HOH:O	2.20	0.42
1:A:761:LEU:O	1:A:764:VAL:HG22	2.20	0.42
1:A:181:CYS:HB3	1:A:184:CYS:HB2	1.89	0.42
1:A:320:GLN:NE2	3:A:1301:HOH:O	2.52	0.42
1:A:204:SER:OG	1:A:227:TRP:HZ3	2.02	0.42
1:A:55:VAL:HG13	1:A:602:PRO:HD3	2.02	0.42
1:A:694:ALA:CB	1:A:703:SER:HB3	2.50	0.42
1:A:363:ASN:O	1:A:367:LEU:HD13	2.20	0.42
1:A:743:LEU:O	1:A:747:LEU:HD12	2.20	0.41
1:A:281:GLY:C	1:A:283:ALA:N	2.72	0.41
1:A:430:LYS:HB2	1:A:430:LYS:HE3	1.67	0.41
1:A:289:TYR:C	1:A:289:TYR:CD1	2.93	0.41
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.80	0.41
1:A:348:LYS:HA	1:A:357:LEU:O	2.19	0.41
1:A:652:PHE:HZ	1:A:724:ARG:HA	1.84	0.41
1:A:569:LEU:HD21	3:A:1278:HOH:O	2.20	0.41
1:A:5:VAL:HG11	1:A:651:SER:HA	2.02	0.41
1:A:464:CYS:SG	1:A:502:CYS:HG	1.00	0.41
1:A:243:HIS:HA	1:A:244:PRO:HD2	1.78	0.41
1:A:773:VAL:HG12	1:A:774:ARG:HD2	2.01	0.41
1:A:69:ARG:NH2	1:A:140:TRP:CD2	2.87	0.41
1:A:105:ARG:NE	1:A:346:GLU:OE2	2.53	0.41
1:A:461:CYS:HB3	1:A:465:GLY:O	2.20	0.41
1:A:304:VAL:CG1	1:A:305:LEU:N	2.83	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.85	0.41
1:A:293:TYR:N	1:A:294:PRO:HD3	2.35	0.41
1:A:399:TYR:HE2	3:A:1135:HOH:O	2.03	0.41
1:A:552:ILE:C	1:A:554:GLN:H	2.24	0.41
1:A:429:ILE:HG12	1:A:433:ARG:HB3	2.02	0.41
1:A:113:GLU:O	1:A:117:GLN:HG3	2.21	0.41
1:A:249:ALA:HB1	1:A:275:VAL:CG1	2.51	0.41
1:A:206:TYR:HD2	1:A:378:LYS:HB3	1.86	0.41
1:A:419:ASN:ND2	1:A:434:TYR:HD2	2.17	0.41
1:A:78:ALA:O	1:A:80:ARG:HD2	2.20	0.41
1:A:362:ALA:O	1:A:363:ASN:C	2.57	0.41
1:A:389:CYS:CB	3:A:1327:HOH:O	2.69	0.41
1:A:177:VAL:CG1	1:A:398:TYR:HB3	2.50	0.41
1:A:70:TYR:CZ	1:A:74:ARG:HD2	2.54	0.41
1:A:803:ARG:HA	1:A:806:LEU:HD12	2.02	0.41
1:A:736:ARG:N	1:A:736:ARG:HE	2.19	0.41
1:A:586:ASP:C	1:A:588:LYS:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HA	1:A:279:PHE:O	2.20	0.41
1:A:775:LEU:N	1:A:775:LEU:HD23	2.35	0.41
1:A:120:ARG:O	1:A:123:VAL:HG22	2.21	0.41
1:A:727:PHE:CE1	1:A:739:ALA:CB	3.04	0.41
1:A:502:CYS:C	1:A:504:CYS:N	2.73	0.40
1:A:244:PRO:HA	1:A:281:GLY:CA	2.45	0.40
1:A:221:LYS:HD2	1:A:221:LYS:HA	1.89	0.40
1:A:22:LYS:HB2	1:A:22:LYS:HE3	1.88	0.40
1:A:366:ILE:O	1:A:370:LEU:HG	2.22	0.40
1:A:102:LYS:HB2	1:A:106:GLU:OE2	2.22	0.40
1:A:581:HIS:CE1	3:A:1142:HOH:O	2.70	0.40
1:A:656:TYR:CE2	1:A:728:TRP:CD1	3.09	0.40
1:A:180:TYR:CE1	1:A:182:PRO:HA	2.56	0.40
1:A:239:ALA:HB2	1:A:337:LEU:CD1	2.52	0.40
1:A:588:LYS:HD3	1:A:629:ARG:HG2	2.02	0.40
1:A:759:PRO:O	1:A:782:HIS:HE1	2.04	0.40
1:A:611:ALA:HB3	1:A:760:PHE:HE2	1.86	0.40
1:A:668:PRO:HA	1:A:669:PRO:HD3	1.95	0.40
1:A:208:ARG:NH1	1:A:374:GLY:O	2.54	0.40
1:A:797:ALA:O	1:A:801:GLN:HG3	2.21	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	819/821 (100%)	687 (84%)	100 (12%)	32 (4%)	4 5

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LYS

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Mol	Chain	Res	Type
1	A	285	GLU
1	A	467	GLU
1	A	513	TYR
1	A	531	TYR
1	A	535	HIS
1	A	543	PHE
1	A	674	PRO
1	A	717	GLN
1	A	734	LEU
1	A	286	GLY
1	A	428	HIS
1	A	432	GLY
1	A	464	CYS
1	A	465	GLY
1	A	591	LYS
1	A	713	GLU
1	A	722	ARG
1	A	729	LYS
1	A	769	LEU
1	A	122	SER
1	A	276	LEU
1	A	730	ASN
1	A	433	ARG
1	A	462	GLN
1	A	487	PRO
1	A	512	PRO
1	A	626	ALA
1	A	407	LYS
1	A	492	ARG
1	A	773	VAL
1	A	53	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	698/698 (100%)	622 (89%)	76 (11%)	8 15

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	7	GLU
1	A	25	LYS
1	A	41	THR
1	A	50	ASN
1	A	52	LEU
1	A	61	ARG
1	A	64	LYS
1	A	80	ARG
1	A	126	TYR
1	A	143	LEU
1	A	152	PRO
1	A	183	ARG
1	A	195	LEU
1	A	215	LYS
1	A	225	LEU
1	A	227	TRP
1	A	230	THR
1	A	260	LEU
1	A	264	LEU
1	A	268	LEU
1	A	279	PHE
1	A	290	THR
1	A	298	GLU
1	A	312	GLU
1	A	313	ASP
1	A	319	HIS
1	A	320	GLN
1	A	329	LEU
1	A	333	ARG
1	A	354	PHE
1	A	357	LEU
1	A	360	ARG
1	A	381	SER
1	A	389	CYS

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Mol	Chain	Res	Type
1	A	397	MET
1	A	401	THR
1	A	408	ASN
1	A	409	THR
1	A	414	GLU
1	A	428	HIS
1	A	437	TRP
1	A	441	LEU
1	A	476	LEU
1	A	491	HIS
1	A	507	THR
1	A	514	VAL
1	A	517	VAL
1	A	521	SER
1	A	525	PRO
1	A	536	GLU
1	A	596	LYS
1	A	614	LEU
1	A	625	GLU
1	A	628	ARG
1	A	629	ARG
1	A	648	ASN
1	A	660	ASP
1	A	673	ARG
1	A	679	TRP
1	A	680	LEU
1	A	690	ARG
1	A	708	ARG
1	A	713	GLU
1	A	718	TRP
1	A	722	ARG
1	A	729	LYS
1	A	732	ASP
1	A	735	ASP
1	A	736	ARG
1	A	737	GLU
1	A	765	LEU
1	A	767	GLN
1	A	769	LEU
1	A	774	ARG
1	A	775	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	50	ASN
1	A	57	HIS
1	A	164	ASN
1	A	191	HIS
1	A	237	ASN
1	A	243	HIS
1	A	295	GLN
1	A	319	HIS
1	A	320	GLN
1	A	408	ASN
1	A	419	ASN
1	A	440	ASN
1	A	449	ASN
1	A	560	ASN
1	A	563	HIS
1	A	581	HIS
1	A	730	ASN
1	A	782	HIS

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 carbohydrates 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 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.