Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:29 pm BST

PDB ID	:	1MUK
Title	:	reovirus lambda3 native structure
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Deposited on	:	2002-09-24
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

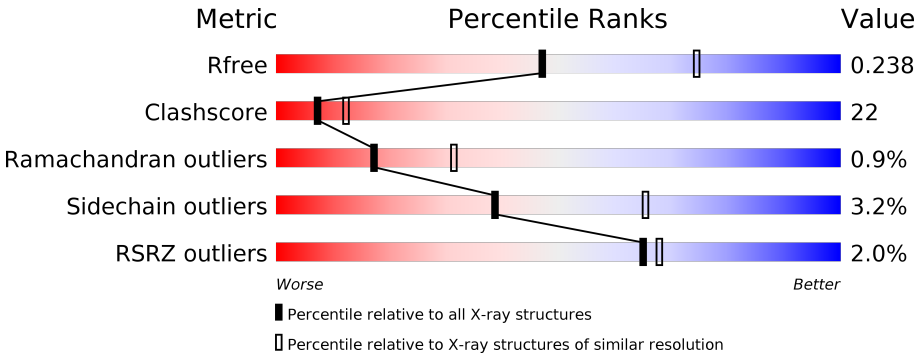
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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.

Mol	Chain	Length	Quality of chain
1	A	1267	2% 66% 31%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10478 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 MINOR CORE PROTEIN LAMBDA 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1256	9929	6337	1697	1831	64	27	0	0

- Molecule 2 is water.

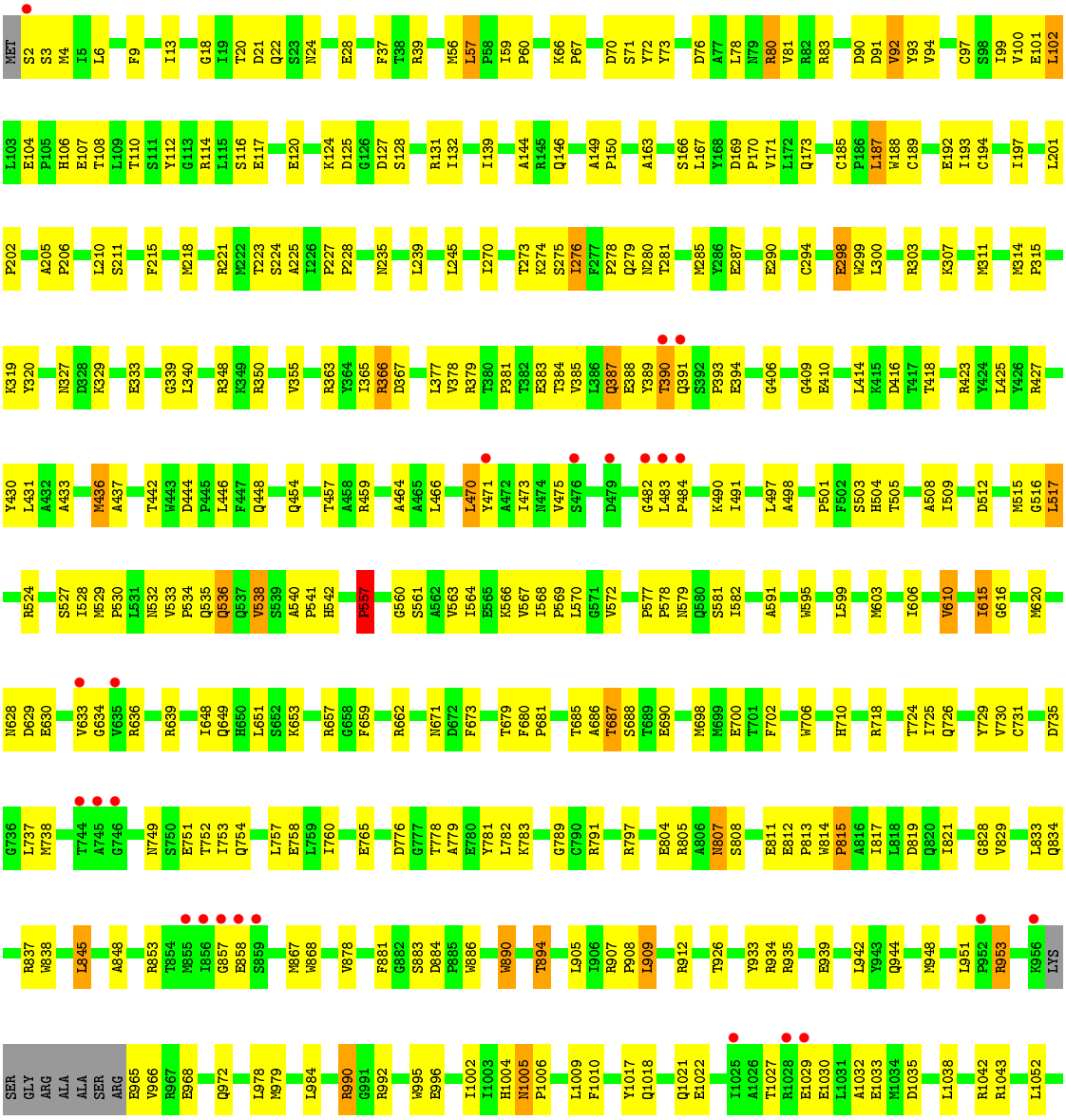
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	549	549	549	0	0

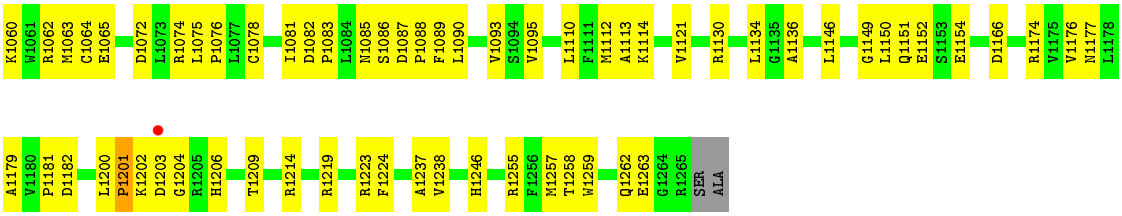
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Molecule 1: MINOR CORE PROTEIN LAMBDA 3

Chain A: 2% 66% 31%




K1060 W1061 R1062 M1063 C1064 E1065
D1072 L1073 R1074 L1075 P1076 L1077 C1078
I1081 D1082 P1083 L1084 N1085 S1086 D1087 P1088 F1089 L1090
V1093 S1094 V1095
L1110 F1111 M1112 A1113 K1114
V1121
R1130
L1134 G1135 A1136
L1146
G1149 L1150 Q1151 E1152 S1153 E1154
D1166
R1174 V1175 V1176 N1177 L1178
A1179 V1180 P1181 D1182
L1200 P1201 K1202 D1203 G1204 R1205 H1206
T1209
R1214
R1219
R1223 F1224
A1237 V1238
H1246
R1255 F1256 M1257 T1258 W1259
Q1262 E1263 G1264 R1265 SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.87Å 85.16Å 248.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.94 – 2.50 42.94 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (42.94-2.50) 97.8 (42.94-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.239 0.207 , 0.238	Depositor DCC
R_{free} test set	2767 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10478	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/10181	0.64	0/13828

There are no bond length outliers.

There are no bond angle outliers.

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	9929	0	9840	442	0
2	A	549	0	0	169	0
All	All	10478	0	9840	442	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 22.

All (442) 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:1060:LYS:HD3	2:A:1401:HOH:O	1.47	1.12
1:A:726:GLN:HG2	2:A:1374:HOH:O	1.48	1.11
1:A:529:MET:HG2	2:A:1576:HOH:O	1.53	1.07
1:A:274:LYS:HE2	2:A:1795:HOH:O	1.54	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG22	1:A:225:ALA:H	1.21	1.04
1:A:350:ARG:HD2	2:A:1803:HOH:O	1.57	1.02
1:A:1202:LYS:HB3	2:A:1809:HOH:O	1.61	0.99
1:A:634:GLY:HA2	2:A:1791:HOH:O	1.61	0.97
1:A:393:PRO:HA	2:A:1527:HOH:O	1.66	0.96
1:A:724:THR:HG22	1:A:726:GLN:H	1.31	0.95
1:A:1112:MET:HE2	2:A:1355:HOH:O	1.66	0.93
1:A:749:ASN:HD21	1:A:751:GLU:HB3	1.35	0.92
1:A:22:GLN:NE2	1:A:878:VAL:H	1.68	0.90
1:A:125:ASP:HB3	2:A:1743:HOH:O	1.71	0.89
1:A:615:ILE:HG23	1:A:616:GLY:H	1.39	0.88
1:A:270:ILE:HA	2:A:1433:HOH:O	1.74	0.87
1:A:688:SER:HB3	2:A:1793:HOH:O	1.74	0.85
1:A:2:SER:N	1:A:6:LEU:HB2	1.91	0.85
1:A:749:ASN:HD22	1:A:752:THR:H	1.19	0.85
1:A:319:LYS:NZ	2:A:1774:HOH:O	2.10	0.84
1:A:633:VAL:HA	2:A:1656:HOH:O	1.77	0.83
1:A:1112:MET:CE	2:A:1355:HOH:O	2.25	0.82
1:A:39:ARG:NH2	2:A:1731:HOH:O	2.10	0.82
1:A:114:ARG:HB2	1:A:215:PHE:CE1	2.16	0.81
1:A:1114:LYS:NZ	2:A:1752:HOH:O	2.12	0.81
1:A:104:GLU:HG3	1:A:116:SER:HA	1.63	0.81
1:A:557:PRO:HD2	1:A:731:CYS:O	1.81	0.80
1:A:388:GLU:HB2	2:A:1620:HOH:O	1.81	0.80
1:A:965:GLU:N	2:A:1382:HOH:O	2.14	0.79
1:A:18:GLY:HA2	2:A:1550:HOH:O	1.84	0.78
1:A:807:ASN:ND2	2:A:1491:HOH:O	2.16	0.78
1:A:114:ARG:HB2	1:A:215:PHE:HE1	1.47	0.77
1:A:1004:HIS:C	1:A:1006:PRO:HD3	2.05	0.77
1:A:1072:ASP:OD1	1:A:1074:ARG:HD3	1.85	0.76
1:A:280:ASN:HA	2:A:1638:HOH:O	1.84	0.76
1:A:808:SER:HB2	2:A:1767:HOH:O	1.85	0.76
1:A:146:GLN:HE22	1:A:805:ARG:H	1.32	0.76
1:A:81:VAL:H	1:A:671:ASN:HD21	1.31	0.76
1:A:348:ARG:NE	2:A:1638:HOH:O	2.19	0.75
1:A:76:ASP:OD2	1:A:80:ARG:NH1	2.20	0.75
1:A:951:LEU:O	2:A:1564:HOH:O	2.05	0.75
1:A:114:ARG:HG3	2:A:1554:HOH:O	1.86	0.75
1:A:120:GLU:O	1:A:124:LYS:HG3	1.87	0.74
1:A:797:ARG:NH1	2:A:1716:HOH:O	2.20	0.74
1:A:926:THR:HG21	1:A:1246:HIS:CG	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:HH22	1:A:834:GLN:HE22	1.35	0.74
1:A:615:ILE:HG23	1:A:616:GLY:N	2.01	0.73
1:A:388:GLU:CB	2:A:1620:HOH:O	2.36	0.73
1:A:821:ILE:HG23	1:A:845:LEU:HD13	1.71	0.73
1:A:1004:HIS:CD2	2:A:1585:HOH:O	2.41	0.72
1:A:101:GLU:HG2	1:A:102:LEU:HD13	1.71	0.72
1:A:536:GLN:HE22	1:A:685:THR:H	1.35	0.72
1:A:529:MET:N	2:A:1576:HOH:O	2.23	0.72
1:A:1179:ALA:O	2:A:1679:HOH:O	2.07	0.71
1:A:907:ARG:NH2	2:A:1401:HOH:O	2.22	0.71
1:A:22:GLN:HE21	1:A:878:VAL:H	1.35	0.71
1:A:423:ARG:CD	2:A:1497:HOH:O	2.39	0.71
1:A:423:ARG:HD2	2:A:1497:HOH:O	1.89	0.70
1:A:1113:ALA:O	2:A:1412:HOH:O	2.08	0.70
1:A:749:ASN:ND2	1:A:751:GLU:HB3	2.06	0.70
1:A:1005:ASN:OD1	2:A:1711:HOH:O	2.09	0.70
1:A:483:LEU:HG	1:A:966:VAL:HG13	1.71	0.70
1:A:290:GLU:HB3	1:A:355:VAL:HG12	1.73	0.70
1:A:541:PRO:HB2	1:A:648:ILE:HD11	1.72	0.70
1:A:996:GLU:OE1	2:A:1784:HOH:O	2.09	0.69
1:A:1005:ASN:N	1:A:1006:PRO:HD3	2.08	0.69
1:A:628:ASN:HD21	1:A:636:ARG:HE	1.40	0.69
1:A:173:GLN:OE1	2:A:1344:HOH:O	2.10	0.69
1:A:905:LEU:HD23	1:A:1063:MET:HE1	1.73	0.68
1:A:348:ARG:CZ	2:A:1638:HOH:O	2.40	0.68
1:A:423:ARG:HE	1:A:427:ARG:NH2	1.90	0.68
1:A:414:LEU:HD11	1:A:418:THR:HG21	1.74	0.68
1:A:564:ILE:HG23	2:A:1551:HOH:O	1.93	0.67
1:A:503:SER:HB3	2:A:1766:HOH:O	1.93	0.67
1:A:410:GLU:N	1:A:649:GLN:OE1	2.22	0.67
1:A:886:TRP:HA	2:A:1285:HOH:O	1.94	0.67
1:A:953:ARG:NE	2:A:1564:HOH:O	2.20	0.67
1:A:536:GLN:HA	1:A:536:GLN:HE21	1.59	0.66
1:A:1181:PRO:HD3	2:A:1679:HOH:O	1.95	0.66
1:A:636:ARG:NH2	2:A:1744:HOH:O	2.28	0.66
1:A:729:TYR:O	2:A:1464:HOH:O	2.12	0.66
1:A:1114:LYS:HA	2:A:1412:HOH:O	1.95	0.66
1:A:221:ARG:NE	2:A:1483:HOH:O	2.26	0.66
1:A:1043:ARG:CZ	2:A:1427:HOH:O	2.43	0.66
1:A:578:PRO:CD	2:A:1583:HOH:O	2.43	0.66
1:A:781:TYR:O	2:A:1724:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:NH2	2:A:1638:HOH:O	2.28	0.65
1:A:718:ARG:HD2	2:A:1728:HOH:O	1.96	0.65
1:A:56:MET:HG2	1:A:188:TRP:CE2	2.31	0.65
1:A:560:GLY:C	2:A:1442:HOH:O	2.35	0.65
1:A:70:ASP:OD2	2:A:1792:HOH:O	2.15	0.65
1:A:791:ARG:NH1	2:A:1403:HOH:O	2.30	0.65
1:A:1004:HIS:HD2	2:A:1585:HOH:O	1.77	0.65
1:A:1151:GLN:HG2	2:A:1339:HOH:O	1.97	0.65
1:A:144:ALA:O	2:A:1353:HOH:O	2.14	0.65
1:A:18:GLY:CA	2:A:1550:HOH:O	2.42	0.65
1:A:566:LYS:HE3	2:A:1442:HOH:O	1.97	0.65
1:A:570:LEU:HD21	1:A:730:VAL:HG21	1.79	0.65
1:A:894:THR:OG1	2:A:1781:HOH:O	2.15	0.64
1:A:1082:ASP:HB2	1:A:1083:PRO:CD	2.27	0.64
1:A:1154:GLU:OE2	2:A:1597:HOH:O	2.15	0.64
1:A:783:LYS:CD	2:A:1522:HOH:O	2.44	0.64
1:A:688:SER:N	2:A:1793:HOH:O	2.30	0.64
1:A:287:GLU:OE2	2:A:1683:HOH:O	2.14	0.64
1:A:718:ARG:CZ	2:A:1414:HOH:O	2.44	0.64
1:A:501:PRO:HD2	1:A:504:HIS:CD2	2.33	0.63
1:A:776:ASP:OD1	1:A:778:THR:HB	1.98	0.63
1:A:718:ARG:NH2	2:A:1414:HOH:O	2.31	0.63
1:A:749:ASN:HD22	1:A:752:THR:N	1.95	0.63
1:A:1027:THR:HG23	1:A:1030:GLU:H	1.62	0.63
1:A:320:TYR:O	2:A:1428:HOH:O	2.15	0.63
1:A:378:VAL:N	2:A:1359:HOH:O	2.26	0.63
1:A:529:MET:HA	1:A:529:MET:HE3	1.81	0.63
1:A:20:THR:HG22	1:A:21:ASP:O	1.99	0.63
1:A:464:ALA:HB3	2:A:1696:HOH:O	1.99	0.62
1:A:444:ASP:CG	2:A:1507:HOH:O	2.37	0.62
1:A:221:ARG:NH2	2:A:1483:HOH:O	2.31	0.62
1:A:385:VAL:HG22	1:A:515:MET:HE3	1.79	0.62
1:A:83:ARG:HG2	1:A:92:VAL:HA	1.81	0.62
1:A:188:TRP:CZ2	1:A:192:GLU:HG3	2.35	0.62
1:A:848:ALA:O	2:A:1469:HOH:O	2.16	0.62
1:A:926:THR:CG2	1:A:1246:HIS:CG	2.83	0.62
1:A:528:ILE:O	1:A:530:PRO:HD3	2.00	0.62
1:A:735:ASP:OD1	2:A:1603:HOH:O	2.16	0.61
1:A:636:ARG:CZ	2:A:1744:HOH:O	2.47	0.61
1:A:1087:ASP:HB3	1:A:1088:PRO:HD3	1.82	0.61
1:A:1151:GLN:CG	2:A:1339:HOH:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:THR:HG22	1:A:726:GLN:N	2.10	0.61
1:A:303:ARG:HH11	1:A:303:ARG:HG3	1.64	0.61
1:A:1002:ILE:HD13	1:A:1136:ALA:HB2	1.82	0.61
1:A:1201:PRO:HB2	1:A:1204:GLY:O	2.01	0.61
1:A:1082:ASP:HB2	1:A:1083:PRO:HD2	1.82	0.60
1:A:1005:ASN:ND2	1:A:1263:GLU:HB3	2.16	0.60
1:A:837:ARG:HG2	2:A:1625:HOH:O	1.99	0.60
1:A:1005:ASN:HD21	1:A:1263:GLU:HB3	1.65	0.60
1:A:965:GLU:OE2	2:A:1682:HOH:O	2.16	0.60
1:A:366:ARG:NH2	2:A:1270:HOH:O	2.31	0.60
1:A:579:ASN:N	2:A:1583:HOH:O	2.34	0.60
1:A:532:ASN:OD1	1:A:535:GLN:HG3	2.01	0.60
1:A:894:THR:CB	2:A:1781:HOH:O	2.49	0.60
1:A:657:ARG:HG2	1:A:657:ARG:HH11	1.66	0.60
1:A:990:ARG:NE	2:A:1459:HOH:O	2.34	0.60
1:A:319:LYS:NZ	2:A:1722:HOH:O	2.34	0.59
1:A:634:GLY:CA	2:A:1791:HOH:O	2.35	0.59
1:A:566:LYS:HD3	1:A:782:LEU:O	2.02	0.59
1:A:1032:ALA:O	2:A:1690:HOH:O	2.16	0.59
1:A:482:GLY:N	2:A:1672:HOH:O	2.18	0.59
1:A:470:LEU:HD13	1:A:508:ALA:HB2	1.84	0.59
1:A:409:GLY:HA3	1:A:649:GLN:OE1	2.01	0.59
1:A:146:GLN:NE2	1:A:805:ARG:H	1.99	0.59
1:A:1043:ARG:NH2	2:A:1427:HOH:O	2.35	0.59
1:A:894:THR:HB	2:A:1781:HOH:O	2.03	0.59
1:A:385:VAL:HG22	1:A:515:MET:CE	2.32	0.59
1:A:210:LEU:HD11	1:A:215:PHE:CD2	2.38	0.58
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.67	0.58
1:A:992:ARG:HH11	1:A:1010:PHE:HD2	1.51	0.58
1:A:189:CYS:O	1:A:193:ILE:HG12	2.03	0.58
1:A:1018:GLN:O	1:A:1022:GLU:HG3	2.04	0.58
1:A:557:PRO:CD	1:A:731:CYS:O	2.51	0.58
1:A:394:GLU:N	2:A:1527:HOH:O	2.23	0.57
1:A:512:ASP:HB3	1:A:662:ARG:HG3	1.86	0.57
1:A:758:GLU:OE1	2:A:1783:HOH:O	2.18	0.57
1:A:128:SER:HB2	2:A:1477:HOH:O	2.03	0.57
1:A:542:HIS:NE2	1:A:690:GLU:CG	2.67	0.57
1:A:884:ASP:OD2	2:A:1399:HOH:O	2.17	0.57
1:A:227:PRO:HB2	1:A:228:PRO:HD3	1.87	0.57
1:A:926:THR:HG23	1:A:1246:HIS:CD2	2.39	0.57
1:A:907:ARG:HB3	1:A:908:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:CG1	1:A:383:GLU:HB3	2.35	0.57
1:A:578:PRO:N	2:A:1583:HOH:O	2.37	0.57
1:A:718:ARG:NH1	2:A:1728:HOH:O	2.16	0.57
1:A:1152:GLU:CD	2:A:1459:HOH:O	2.43	0.56
1:A:128:SER:CB	2:A:1477:HOH:O	2.53	0.56
1:A:595:TRP:HA	1:A:599:LEU:HB2	1.86	0.56
1:A:171:VAL:HG11	1:A:1090:LEU:HD11	1.87	0.56
1:A:804:GLU:OE1	2:A:1648:HOH:O	2.18	0.56
1:A:454:GLN:OE1	2:A:1337:HOH:O	2.18	0.56
1:A:1206:HIS:HB2	1:A:1209:THR:HG23	1.87	0.56
1:A:817:ILE:O	1:A:821:ILE:HG12	2.05	0.56
1:A:24:ASN:O	1:A:28:GLU:HG3	2.05	0.56
1:A:557:PRO:HG3	1:A:781:TYR:OH	2.05	0.56
1:A:384:THR:HG23	2:A:1293:HOH:O	2.04	0.56
1:A:436:MET:HE2	1:A:442:THR:OG1	2.05	0.55
1:A:649:GLN:HG3	2:A:1698:HOH:O	2.05	0.55
1:A:457:THR:O	1:A:491:ILE:HG13	2.06	0.55
1:A:542:HIS:NE2	1:A:690:GLU:HG2	2.21	0.55
1:A:797:ARG:CZ	2:A:1716:HOH:O	2.54	0.55
1:A:953:ARG:NH2	2:A:1564:HOH:O	2.37	0.55
1:A:279:GLN:HG3	1:A:327:ASN:HD22	1.71	0.55
1:A:425:LEU:HB2	1:A:698:MET:HE1	1.87	0.55
1:A:965:GLU:CA	2:A:1382:HOH:O	2.54	0.55
1:A:1062:ARG:NH1	2:A:1809:HOH:O	2.40	0.55
1:A:905:LEU:CD2	1:A:1063:MET:HE1	2.37	0.55
1:A:279:GLN:HG3	1:A:327:ASN:ND2	2.22	0.55
1:A:446:LEU:HD13	1:A:1149:GLY:HA3	1.87	0.55
1:A:563:VAL:HG12	1:A:568:ILE:HD11	1.88	0.55
1:A:688:SER:CB	2:A:1793:HOH:O	2.44	0.55
1:A:393:PRO:HD3	1:A:591:ALA:O	2.07	0.54
1:A:578:PRO:CG	2:A:1583:HOH:O	2.55	0.54
1:A:783:LYS:HD2	2:A:1522:HOH:O	2.07	0.54
1:A:686:ALA:O	1:A:690:GLU:HB2	2.07	0.54
1:A:94:VAL:HG22	1:A:139:ILE:HG23	1.90	0.54
1:A:414:LEU:CD1	1:A:418:THR:HG21	2.38	0.54
1:A:385:VAL:HG22	1:A:515:MET:SD	2.48	0.54
1:A:57:LEU:HD22	1:A:185:CYS:SG	2.47	0.54
1:A:223:THR:HG22	1:A:224:SER:N	2.22	0.53
1:A:71:SER:OG	2:A:1370:HOH:O	2.18	0.53
1:A:106:HIS:CE1	1:A:108:THR:H	2.27	0.53
1:A:149:ALA:HB1	1:A:150:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:CYS:SG	1:A:577:PRO:HD2	2.49	0.53
1:A:536:GLN:NE2	1:A:685:THR:HG23	2.24	0.53
1:A:894:THR:HB	2:A:1549:HOH:O	2.07	0.53
1:A:783:LYS:HE3	2:A:1716:HOH:O	2.09	0.53
1:A:1224:PHE:HE2	2:A:1679:HOH:O	1.89	0.53
1:A:194:CYS:SG	1:A:206:PRO:HG2	2.49	0.53
1:A:459:ARG:NE	2:A:1802:HOH:O	2.42	0.53
1:A:299:TRP:CD2	1:A:303:ARG:HG2	2.44	0.52
1:A:235:ASN:O	1:A:239:LEU:HG	2.09	0.52
1:A:470:LEU:HD11	1:A:505:THR:HA	1.91	0.52
1:A:281:THR:O	1:A:285:MET:HG2	2.09	0.52
1:A:533:VAL:HB	1:A:534:PRO:HD3	1.90	0.52
1:A:603:MET:HE1	1:A:651:LEU:HD23	1.91	0.52
1:A:1095:VAL:HG23	1:A:1237:ALA:HB2	1.91	0.52
1:A:290:GLU:CB	1:A:355:VAL:HG12	2.38	0.52
1:A:104:GLU:CD	1:A:117:GLU:H	2.13	0.52
1:A:298:GLU:HB2	1:A:311:MET:CE	2.40	0.52
1:A:968:GLU:OE2	2:A:1755:HOH:O	2.19	0.52
1:A:884:ASP:HB3	2:A:1535:HOH:O	2.10	0.52
1:A:881:PHE:O	1:A:909:LEU:HD12	2.10	0.52
1:A:807:ASN:H	1:A:807:ASN:HD22	1.58	0.51
1:A:965:GLU:HA	2:A:1382:HOH:O	2.10	0.51
1:A:1209:THR:OG1	2:A:1308:HOH:O	2.17	0.51
1:A:807:ASN:HD22	1:A:807:ASN:N	2.08	0.51
1:A:1065:GLU:CD	1:A:1065:GLU:H	2.13	0.51
1:A:497:LEU:HD22	1:A:505:THR:HG21	1.93	0.51
1:A:319:LYS:HB2	2:A:1521:HOH:O	2.10	0.51
1:A:406:GLY:HA3	1:A:630:GLU:O	2.10	0.51
1:A:81:VAL:HG13	1:A:132:ILE:HD13	1.92	0.51
1:A:92:VAL:HG11	1:A:383:GLU:HB3	1.92	0.51
1:A:942:LEU:O	1:A:942:LEU:HD23	2.10	0.51
1:A:299:TRP:CE2	1:A:303:ARG:HG2	2.46	0.51
1:A:765:GLU:OE2	2:A:1452:HOH:O	2.19	0.51
1:A:223:THR:CG2	1:A:224:SER:N	2.74	0.51
1:A:541:PRO:HB2	1:A:648:ILE:CD1	2.40	0.51
1:A:778:THR:CG2	1:A:779:ALA:N	2.72	0.51
1:A:78:LEU:HD12	1:A:80:ARG:NH2	2.25	0.51
1:A:430:TYR:OH	2:A:1589:HOH:O	2.14	0.51
1:A:754:GLN:O	1:A:758:GLU:HG3	2.11	0.51
1:A:783:LYS:NZ	2:A:1770:HOH:O	2.44	0.50
1:A:1005:ASN:N	1:A:1006:PRO:CD	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HB2	1:A:221:ARG:NH1	2.26	0.50
1:A:285:MET:HG3	1:A:365:ILE:HD11	1.93	0.50
1:A:490:LYS:NZ	2:A:1416:HOH:O	2.44	0.50
1:A:379:ARG:HH12	1:A:387:GLN:NE2	2.07	0.50
1:A:628:ASN:HD21	1:A:636:ARG:NE	2.08	0.50
1:A:107:GLU:HB2	2:A:1451:HOH:O	2.11	0.50
1:A:110:THR:OG1	2:A:1764:HOH:O	2.19	0.50
1:A:505:THR:OG1	2:A:1794:HOH:O	2.19	0.50
1:A:538:VAL:HG13	1:A:651:LEU:HB2	1.94	0.50
1:A:724:THR:CG2	1:A:726:GLN:H	2.15	0.50
1:A:819:ASP:OD1	1:A:953:ARG:NH1	2.43	0.50
1:A:389:TYR:OH	1:A:527:SER:HB2	2.10	0.50
1:A:942:LEU:HD23	1:A:942:LEU:C	2.32	0.50
1:A:9:PHE:O	1:A:13:ILE:HG13	2.12	0.50
1:A:629:ASP:OD2	1:A:639:ARG:CZ	2.60	0.49
1:A:529:MET:CE	1:A:529:MET:HA	2.42	0.49
1:A:275:SER:O	1:A:278:PRO:HD2	2.12	0.49
1:A:127:ASP:O	1:A:131:ARG:HG3	2.12	0.49
1:A:73:TYR:HB2	1:A:132:ILE:HG23	1.93	0.49
1:A:149:ALA:HB1	1:A:150:PRO:HD2	1.95	0.49
1:A:166:SER:OG	2:A:1592:HOH:O	2.17	0.49
1:A:221:ARG:CZ	2:A:1483:HOH:O	2.59	0.49
1:A:1134:LEU:HA	1:A:1257:MET:CE	2.43	0.49
1:A:653:LYS:NZ	2:A:1773:HOH:O	2.45	0.49
1:A:934:ARG:HB2	2:A:1381:HOH:O	2.12	0.49
1:A:995:TRP:CZ2	1:A:1006:PRO:HG3	2.48	0.49
1:A:1200:LEU:C	1:A:1200:LEU:HD23	2.33	0.49
1:A:883:SER:HB2	2:A:1357:HOH:O	2.13	0.49
1:A:1086:SER:O	1:A:1090:LEU:HG	2.13	0.48
1:A:39:ARG:NH1	1:A:39:ARG:HG3	2.28	0.48
1:A:1065:GLU:OE1	2:A:1429:HOH:O	2.20	0.48
1:A:197:ILE:O	1:A:221:ARG:NH1	2.31	0.48
1:A:482:GLY:CA	2:A:1672:HOH:O	2.59	0.48
1:A:853:ARG:NH1	2:A:1806:HOH:O	2.46	0.48
1:A:1203:ASP:N	2:A:1809:HOH:O	2.45	0.48
1:A:606:ILE:O	1:A:610:VAL:HB	2.13	0.48
1:A:829:VAL:HG13	1:A:890:TRP:CD1	2.48	0.48
1:A:114:ARG:HG2	2:A:1602:HOH:O	2.12	0.48
1:A:649:GLN:CG	2:A:1698:HOH:O	2.61	0.48
1:A:857:GLY:O	1:A:858:GLU:HB3	2.13	0.48
1:A:582:ILE:HG21	1:A:757:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:ARG:NH1	2:A:1298:HOH:O	2.41	0.48
1:A:944:GLN:HB3	1:A:948:MET:CE	2.44	0.48
1:A:363:ARG:HH22	1:A:834:GLN:NE2	2.09	0.48
1:A:582:ILE:HG21	1:A:757:LEU:HD21	1.95	0.48
1:A:944:GLN:HB3	1:A:948:MET:HE2	1.95	0.48
1:A:700:GLU:HB2	1:A:725:ILE:HD13	1.96	0.48
1:A:516:GLY:O	1:A:517:LEU:HD12	2.14	0.47
1:A:437:ALA:HB2	1:A:610:VAL:HG22	1.96	0.47
1:A:1085:ASN:O	1:A:1088:PRO:HD2	2.14	0.47
1:A:1258:THR:HG23	1:A:1262:GLN:NE2	2.29	0.47
1:A:688:SER:CA	2:A:1793:HOH:O	2.62	0.47
1:A:211:SER:HA	1:A:811:GLU:OE2	2.14	0.47
1:A:1075:LEU:HA	1:A:1076:PRO:HD3	1.82	0.47
1:A:377:LEU:N	1:A:377:LEU:HD12	2.30	0.47
1:A:935:ARG:O	1:A:939:GLU:HG3	2.15	0.47
1:A:1110:LEU:HD22	1:A:1121:VAL:HG12	1.96	0.47
1:A:448:GLN:NE2	1:A:620:MET:H	2.12	0.47
1:A:100:VAL:HG13	1:A:101:GLU:N	2.29	0.47
1:A:829:VAL:HG13	1:A:890:TRP:CE2	2.50	0.47
1:A:578:PRO:HG2	2:A:1583:HOH:O	2.15	0.46
1:A:582:ILE:HB	1:A:738:MET:HB3	1.98	0.46
1:A:628:ASN:ND2	1:A:636:ARG:HE	2.11	0.46
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.79	0.46
1:A:515:MET:HA	1:A:529:MET:CE	2.45	0.46
1:A:314:MET:CE	1:A:315:PRO:HD2	2.45	0.46
1:A:388:GLU:CG	2:A:1620:HOH:O	2.64	0.46
1:A:1002:ILE:HD13	1:A:1136:ALA:CB	2.44	0.46
1:A:355:VAL:O	1:A:355:VAL:HG12	2.15	0.46
1:A:503:SER:CB	2:A:1718:HOH:O	2.63	0.46
1:A:814:TRP:CD2	1:A:815:PRO:HB3	2.50	0.46
1:A:542:HIS:HE2	1:A:690:GLU:CG	2.28	0.46
1:A:724:THR:HB	2:A:1733:HOH:O	2.16	0.46
1:A:390:THR:HG22	1:A:391:GLN:HG3	1.97	0.46
1:A:540:ALA:HB3	1:A:541:PRO:HD3	1.98	0.46
1:A:67:PRO:O	1:A:97:CYS:HB3	2.15	0.46
1:A:568:ILE:HB	1:A:569:PRO:HD3	1.98	0.45
1:A:1078:CYS:HB3	1:A:1081:ILE:HD12	1.98	0.45
1:A:595:TRP:HZ2	2:A:1761:HOH:O	1.99	0.45
1:A:783:LYS:HD2	2:A:1716:HOH:O	2.16	0.45
1:A:414:LEU:HD12	2:A:1450:HOH:O	2.16	0.45
1:A:1064:CYS:HB3	1:A:1065:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:VAL:HG13	1:A:789:GLY:O	2.17	0.45
1:A:381:PRO:O	1:A:385:VAL:HG23	2.17	0.45
1:A:972:GLN:HG2	2:A:1755:HOH:O	2.16	0.45
1:A:197:ILE:C	1:A:221:ARG:HH12	2.17	0.45
1:A:416:ASP:O	2:A:1497:HOH:O	2.20	0.45
1:A:433:ALA:HB1	1:A:610:VAL:HG23	1.98	0.45
1:A:532:ASN:OD1	1:A:534:PRO:HD2	2.17	0.45
1:A:22:GLN:HE22	1:A:878:VAL:H	1.58	0.45
1:A:581:SER:HB2	1:A:737:LEU:HD11	1.99	0.44
1:A:542:HIS:HE2	1:A:690:GLU:HG2	1.80	0.44
1:A:1255:ARG:HG2	2:A:1496:HOH:O	2.16	0.44
1:A:80:ARG:HD3	1:A:673:PHE:CD2	2.52	0.44
1:A:828:GLY:HA3	1:A:838:TRP:NE1	2.32	0.44
1:A:706:TRP:O	1:A:710:HIS:HD2	2.00	0.44
1:A:791:ARG:NH1	1:A:1078:CYS:SG	2.90	0.44
1:A:905:LEU:HD23	1:A:1063:MET:CE	2.43	0.44
1:A:1224:PHE:CE2	2:A:1679:HOH:O	2.57	0.44
1:A:13:ILE:HD13	1:A:163:ALA:HB3	1.98	0.44
1:A:57:LEU:HD21	1:A:189:CYS:SG	2.58	0.44
1:A:509:ILE:HD13	1:A:538:VAL:HG21	1.99	0.44
1:A:1029:GLU:CD	1:A:1029:GLU:H	2.20	0.44
1:A:1177:ASN:ND2	1:A:1259:TRP:HH2	2.16	0.44
1:A:1214:ARG:HG3	1:A:1214:ARG:NH1	2.32	0.44
1:A:81:VAL:HG13	1:A:132:ILE:CD1	2.48	0.44
1:A:388:GLU:HG3	2:A:1620:HOH:O	2.17	0.44
1:A:389:TYR:HD1	1:A:679:THR:HB	1.83	0.44
1:A:1112:MET:CE	1:A:1150:LEU:HD11	2.47	0.44
1:A:131:ARG:HD3	2:A:1338:HOH:O	2.18	0.44
1:A:657:ARG:HG2	1:A:657:ARG:NH1	2.30	0.44
1:A:978:LEU:HG	1:A:979:MET:HE2	1.98	0.44
1:A:1089:PHE:O	1:A:1093:VAL:HG23	2.18	0.44
1:A:782:LEU:HB2	2:A:1724:HOH:O	2.17	0.44
1:A:1200:LEU:HD23	1:A:1201:PRO:O	2.17	0.43
1:A:20:THR:HG21	2:A:1568:HOH:O	2.17	0.43
1:A:223:THR:HG22	1:A:225:ALA:N	2.06	0.43
1:A:90:ASP:O	1:A:92:VAL:N	2.45	0.43
1:A:1027:THR:HG22	1:A:1030:GLU:CD	2.39	0.43
1:A:390:THR:CG2	1:A:391:GLN:HG3	2.48	0.43
1:A:926:THR:CG2	1:A:1246:HIS:CD2	3.01	0.43
1:A:1174:ARG:HG3	2:A:1281:HOH:O	2.18	0.43
1:A:603:MET:CE	1:A:651:LEU:HD23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:O	1:A:83:ARG:HD2	2.19	0.43
1:A:933:TYR:CE1	1:A:934:ARG:HG3	2.53	0.43
1:A:990:ARG:CD	2:A:1459:HOH:O	2.66	0.43
1:A:201:LEU:HA	1:A:202:PRO:HD3	1.84	0.43
1:A:423:ARG:NE	2:A:1497:HOH:O	2.49	0.43
1:A:169:ASP:HA	1:A:170:PRO:HD3	1.91	0.43
1:A:329:LYS:O	1:A:333:GLU:HG3	2.19	0.43
1:A:484:PRO:HB2	1:A:1021:GLN:HE21	1.84	0.43
1:A:473:ILE:HG13	1:A:475:VAL:HG23	2.01	0.43
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.84	0.43
1:A:245:LEU:HD22	1:A:367:ASP:HA	2.01	0.43
1:A:671:ASN:N	1:A:671:ASN:HD22	2.16	0.43
1:A:783:LYS:HD3	2:A:1522:HOH:O	2.12	0.43
1:A:680:PHE:CD2	1:A:681:PRO:HD2	2.54	0.43
1:A:814:TRP:CE2	1:A:815:PRO:HB3	2.54	0.43
1:A:197:ILE:HA	1:A:221:ARG:HH11	1.83	0.42
1:A:457:THR:C	1:A:491:ILE:HG13	2.40	0.42
1:A:636:ARG:NE	2:A:1744:HOH:O	2.52	0.42
1:A:990:ARG:HG3	2:A:1459:HOH:O	2.18	0.42
1:A:1176:VAL:O	1:A:1176:VAL:HG13	2.19	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.88	0.42
1:A:221:ARG:HB2	1:A:221:ARG:HH11	1.83	0.42
1:A:393:PRO:CA	2:A:1527:HOH:O	2.42	0.42
1:A:581:SER:HA	1:A:738:MET:O	2.19	0.42
1:A:812:GLU:HA	1:A:813:PRO:HD3	1.80	0.42
1:A:225:ALA:O	1:A:228:PRO:HD2	2.19	0.42
1:A:471:TYR:CD1	1:A:471:TYR:C	2.93	0.42
1:A:1146:LEU:HD21	1:A:1152:GLU:HG3	2.02	0.42
1:A:1035:ASP:HB2	2:A:1690:HOH:O	2.19	0.42
1:A:515:MET:HA	1:A:529:MET:HE3	2.01	0.42
1:A:702:PHE:CZ	1:A:760:ILE:HG13	2.55	0.42
1:A:948:MET:HE2	1:A:1042:ARG:HA	2.02	0.42
1:A:339:GLY:O	1:A:340:LEU:HD23	2.19	0.42
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.89	0.41
1:A:563:VAL:HB	2:A:1551:HOH:O	2.20	0.41
1:A:603:MET:CE	1:A:648:ILE:HG23	2.50	0.41
1:A:1005:ASN:ND2	1:A:1263:GLU:CB	2.81	0.41
1:A:567:VAL:HG12	1:A:567:VAL:O	2.20	0.41
1:A:811:GLU:OE1	2:A:1347:HOH:O	2.22	0.41
1:A:205:ALA:HA	1:A:206:PRO:HD3	1.89	0.41
1:A:112:TYR:HB3	1:A:215:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HB2	1:A:307:LYS:O	2.20	0.41
1:A:483:LEU:HA	1:A:484:PRO:HD3	1.85	0.41
1:A:984:LEU:HD11	1:A:1009:LEU:CD1	2.50	0.41
1:A:100:VAL:CG1	1:A:101:GLU:N	2.83	0.41
1:A:659:PHE:CE2	1:A:681:PRO:HD3	2.56	0.41
1:A:1223:ARG:HD3	2:A:1804:HOH:O	2.20	0.41
1:A:389:TYR:OH	1:A:527:SER:CB	2.69	0.41
1:A:603:MET:HE3	1:A:648:ILE:HG23	2.02	0.41
1:A:273:THR:O	1:A:276:ILE:HG12	2.20	0.41
1:A:561:SER:N	2:A:1442:HOH:O	2.52	0.41
1:A:59:ILE:HA	1:A:60:PRO:HD3	1.92	0.41
1:A:867:MET:HG3	1:A:868:TRP:N	2.35	0.41
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.34	0.41
1:A:1110:LEU:HD13	1:A:1121:VAL:HG11	2.01	0.41
1:A:18:GLY:N	2:A:1550:HOH:O	2.47	0.41
1:A:912:ARG:NH2	2:A:1468:HOH:O	2.37	0.41
1:A:2:SER:O	1:A:4:MET:N	2.54	0.41
1:A:833:LEU:HD12	1:A:838:TRP:CD2	2.56	0.41
1:A:1017:TYR:C	1:A:1017:TYR:CD1	2.94	0.41
1:A:197:ILE:HA	1:A:221:ARG:NH1	2.35	0.40
1:A:542:HIS:NE2	1:A:690:GLU:HG3	2.35	0.40
1:A:90:ASP:HB2	2:A:1340:HOH:O	2.20	0.40
1:A:659:PHE:CZ	1:A:681:PRO:HD3	2.56	0.40
1:A:93:TYR:HB3	2:A:1273:HOH:O	2.22	0.40
1:A:686:ALA:O	1:A:687:THR:C	2.60	0.40
1:A:66:LYS:HB3	1:A:97:CYS:HA	2.04	0.40
1:A:1005:ASN:HB2	1:A:1130:ARG:HH22	1.86	0.40
1:A:582:ILE:HD11	1:A:753:ILE:HG21	2.03	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	1252/1267 (99%)	1187 (95%)	54 (4%)	11 (1%)	17 31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	615	ILE
1	A	3	SER
1	A	91	ASP
1	A	498	ALA
1	A	557	PRO
1	A	687	THR
1	A	1201	PRO
1	A	218	MET
1	A	1005	ASN
1	A	99	ILE
1	A	276	ILE

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	1076/1083 (99%)	1042 (97%)	34 (3%)	39 65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	57	LEU
1	A	80	ARG
1	A	92	VAL
1	A	102	LEU
1	A	167	LEU
1	A	187	LEU
1	A	298	GLU
1	A	366	ARG
1	A	387	GLN

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Mol	Chain	Res	Type
1	A	390	THR
1	A	431	LEU
1	A	436	MET
1	A	466	LEU
1	A	470	LEU
1	A	517	LEU
1	A	536	GLN
1	A	538	VAL
1	A	557	PRO
1	A	610	VAL
1	A	807	ASN
1	A	815	PRO
1	A	845	LEU
1	A	890	TRP
1	A	894	THR
1	A	909	LEU
1	A	953	ARG
1	A	990	ARG
1	A	1033	GLU
1	A	1038	LEU
1	A	1052	LEU
1	A	1166	ASP
1	A	1182	ASP
1	A	1238	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	121	ASN
1	A	146	GLN
1	A	173	GLN
1	A	255	GLN
1	A	387	GLN
1	A	448	GLN
1	A	499	ASN
1	A	504	HIS
1	A	536	GLN
1	A	628	ASN
1	A	664	ASN
1	A	671	ASN
1	A	710	HIS

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Mol	Chain	Res	Type
1	A	728	ASN
1	A	749	ASN
1	A	807	ASN
1	A	834	GLN
1	A	852	GLN
1	A	930	ASN
1	A	980	GLN
1	A	1005	ASN
1	A	1165	GLN
1	A	1246	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1253/1267 (98%)	-0.15	25 (1%) 65 68	7, 21, 44, 63	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	6.3
1	A	857	GLY	5.1
1	A	471	TYR	4.4
1	A	744	THR	4.3
1	A	855	MET	4.2
1	A	856	ILE	4.1
1	A	956	LYS	3.8
1	A	482	GLY	3.8
1	A	484	PRO	3.8
1	A	1025	ILE	3.4
1	A	483	LEU	3.1
1	A	391	GLN	2.8
1	A	859	SER	2.7
1	A	1028	ARG	2.7
1	A	952	PRO	2.6
1	A	858	GLU	2.5
1	A	746	GLY	2.4
1	A	1029	GLU	2.4
1	A	745	ALA	2.2
1	A	633	VAL	2.2
1	A	476	SER	2.2
1	A	479	ASP	2.1
1	A	635	VAL	2.1
1	A	1203	ASP	2.1
1	A	390	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.