



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:53 AM GMT

PDB ID : 2P3N
Title : Thermotoga maritima IMPase TM1415
Authors : Stieglitz, K.A.; Roberts, M.F.; Li, W.; Stec, B.
Deposited on : 2007-03-09
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

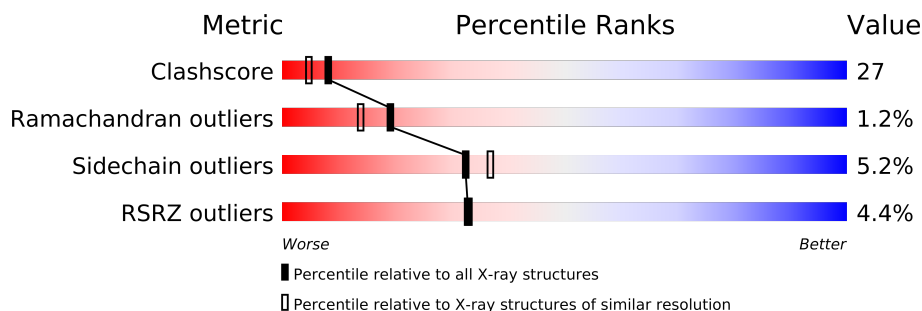
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	
1	C	256	
1	D	256	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8390 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Inositol-1-monophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total 2021	C 1289	N 348	O 377	S 7	0	0	0
1	B	256	Total 2021	C 1289	N 348	O 377	S 7	0	0	0
1	C	256	Total 2021	C 1289	N 348	O 377	S 7	0	0	0
1	D	256	Total 2021	C 1289	N 348	O 377	S 7	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

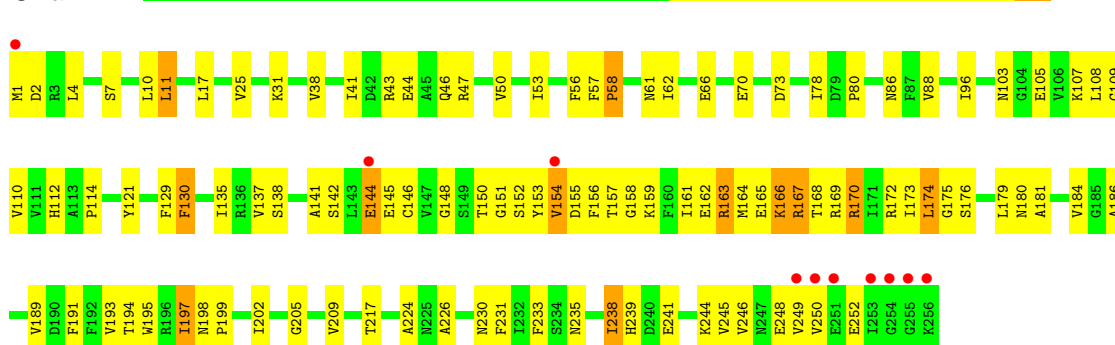
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total 64	O 64	0	0
3	B	61	Total 61	O 61	0	0
3	C	85	Total 85	O 85	0	0
3	D	92	Total 92	O 92	0	0

3 Residue-property plots

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.

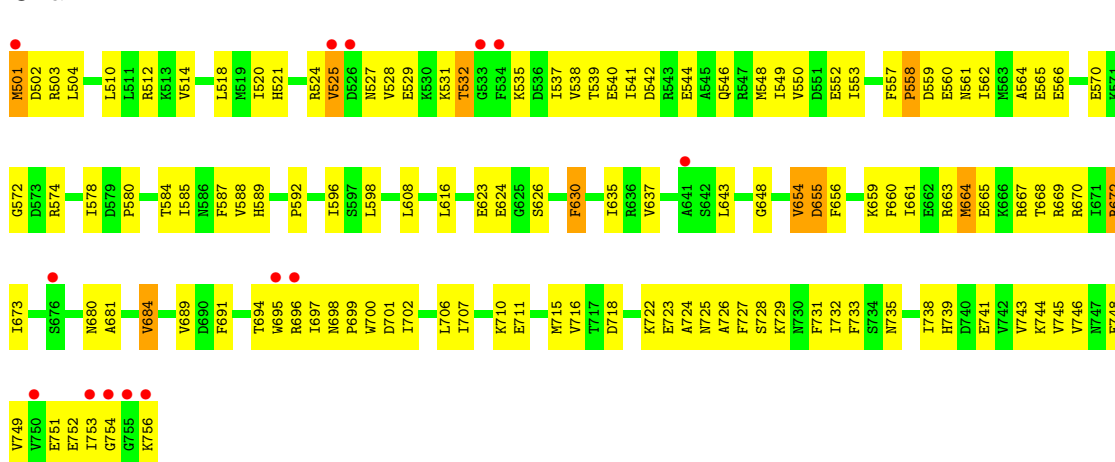
• Molecule 1: Inositol-1-monophosphatase

Chain A:



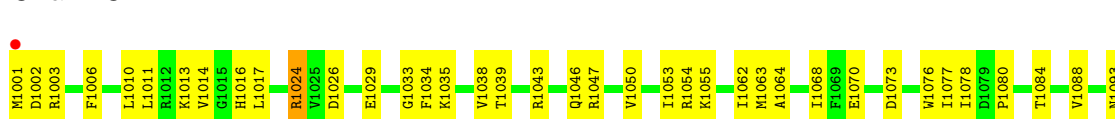
• Molecule 1: Inositol-1-monophosphatase

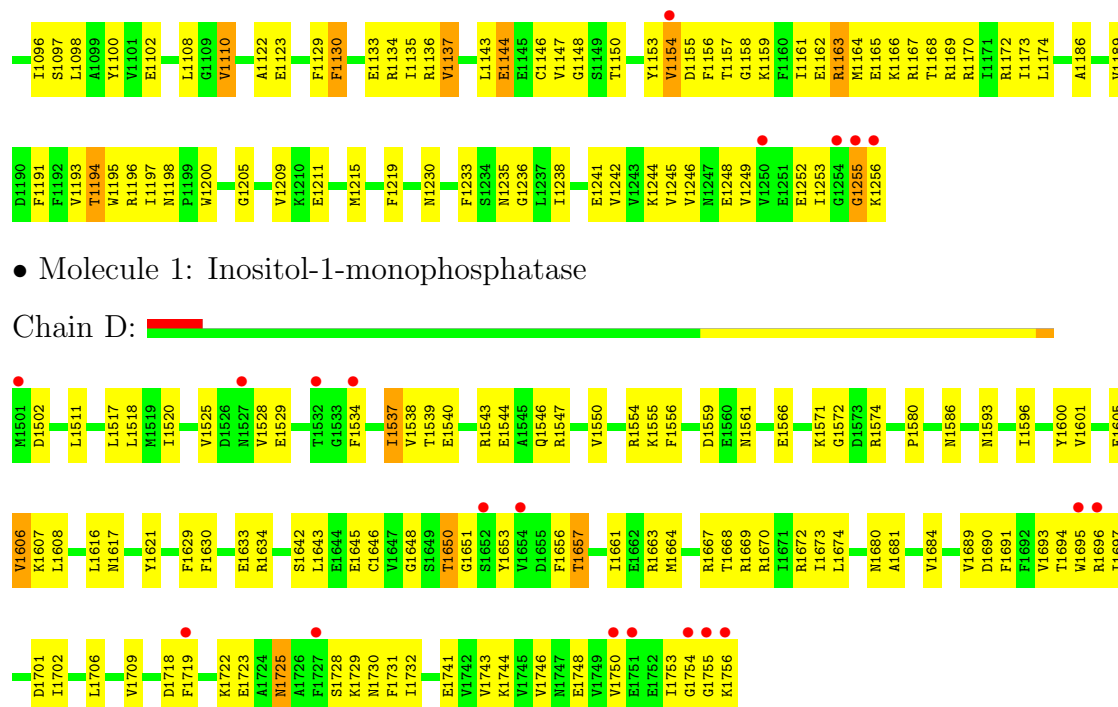
Chain B:



• Molecule 1: Inositol-1-monophosphatase

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.02Å 103.87Å 80.51Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	42.00 – 2.20 31.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (42.00-2.20) 85.5 (31.38-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.279 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 64570 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8390	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/2059	0.64	0/2773
1	B	0.38	0/2059	0.64	0/2773
1	C	0.40	0/2059	0.67	0/2773
1	D	0.42	0/2059	0.69	2/2773 (0.1%)
All	All	0.40	0/8236	0.66	2/11092 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1608	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	1502	ASP	N-CA-C	-5.39	96.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2021	0	2009	117	0
1	B	2021	0	2006	135	0
1	C	2021	0	2006	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2021	0	2006	86	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	64	0	0	1	0
3	B	61	0	0	3	0
3	C	85	0	0	6	0
3	D	92	0	0	3	0
All	All	8390	0	8027	429	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (429) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:ARG:HB2	1:A:167:ARG:HH11	1.12	1.14
1:C:1001:MET:HG3	1:C:1003:ARG:H	1.23	1.02
1:C:1154:VAL:HG13	1:C:1155:ASP:H	1.24	1.01
1:B:654:VAL:HG13	1:B:655:ASP:H	1.28	0.97
1:A:154:VAL:HG13	1:A:155:ASP:H	1.28	0.96
1:C:1001:MET:HE2	1:C:1002:ASP:H	1.33	0.92
1:C:1205:GLY:O	1:C:1209:VAL:HG12	1.73	0.88
1:C:1196:ARG:H	1:C:1230:ASN:ND2	1.71	0.87
1:A:163:ARG:HG3	1:A:249:VAL:HG22	1.56	0.87
1:B:706:LEU:HD12	1:B:716:VAL:HG11	1.56	0.86
1:B:637:VAL:HG21	1:B:735:ASN:HA	1.57	0.86
1:B:514:VAL:HG22	1:B:548:MET:HE3	1.55	0.86
1:B:722:LYS:HZ2	1:B:723:GLU:H	1.24	0.85
1:B:501:MET:HE2	1:B:503:ARG:H	1.44	0.83
1:B:722:LYS:NZ	1:B:723:GLU:H	1.75	0.83
1:A:167:ARG:CB	1:A:167:ARG:HH11	1.91	0.83
1:B:501:MET:HG3	1:B:502:ASP:H	1.45	0.82
1:A:163:ARG:HG3	1:A:249:VAL:CG2	2.09	0.81
1:D:1670:ARG:HG3	1:D:1670:ARG:HH11	1.44	0.81
1:C:1170:ARG:HH11	1:C:1170:ARG:HG3	1.46	0.81
1:C:1209:VAL:HG11	1:C:1233:PHE:HD2	1.47	0.80
1:D:1694:THR:HG22	1:D:1731:PHE:HB2	1.64	0.79
1:C:1001:MET:HG3	1:C:1003:ARG:N	1.97	0.79
1:B:745:VAL:O	1:B:749:VAL:HG23	1.84	0.77
1:A:174:LEU:H	1:A:174:LEU:HD12	1.48	0.77
1:A:146:CYS:O	1:A:169:ARG:HB3	1.84	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1169:ARG:O	1:C:1170:ARG:HG3	1.86	0.76
1:A:197:ILE:H	1:A:197:ILE:HD13	1.51	0.76
1:A:184:VAL:HG12	1:A:189:VAL:HG23	1.68	0.75
1:B:525:VAL:HG11	1:B:539:THR:HG21	1.68	0.75
1:B:654:VAL:HG13	1:B:655:ASP:N	2.02	0.74
1:B:643:LEU:O	1:B:668:THR:HA	1.87	0.74
1:C:1150:THR:HG22	1:C:1193:VAL:HB	1.69	0.74
1:C:1154:VAL:HG13	1:C:1155:ASP:N	2.00	0.74
1:A:167:ARG:HB2	1:A:167:ARG:NH1	1.98	0.73
1:A:154:VAL:HG22	1:A:155:ASP:OD1	1.87	0.73
1:A:41:ILE:HD12	1:A:41:ILE:N	2.03	0.73
1:D:1546:GLN:HE22	1:D:1566:GLU:H	1.34	0.73
1:B:698:ASN:HB3	1:B:699:PRO:HD2	1.70	0.73
1:A:31:LYS:HD2	1:A:38:VAL:HB	1.70	0.73
1:A:154:VAL:HG13	1:A:155:ASP:N	2.01	0.73
1:B:643:LEU:HD13	1:B:667:ARG:HG3	1.69	0.72
1:C:1001:MET:HG2	1:C:1003:ARG:HB2	1.72	0.72
1:D:1561:ASN:ND2	1:D:1572:GLY:HA3	2.05	0.72
1:A:246:VAL:O	1:A:250:VAL:HG23	1.89	0.72
1:D:1670:ARG:HD3	1:D:1672:ARG:HH22	1.55	0.71
1:A:174:LEU:N	1:A:174:LEU:HD12	2.04	0.71
1:B:696:ARG:HA	1:B:729:LYS:HD2	1.73	0.71
1:B:643:LEU:HG	1:B:738:ILE:HD11	1.71	0.71
1:A:105:GLU:HB2	1:A:107:LYS:HE2	1.74	0.70
1:D:1681:ALA:O	1:D:1684:VAL:HG22	1.91	0.70
1:A:238:ILE:HD13	1:A:238:ILE:H	1.54	0.70
1:B:654:VAL:HG22	1:B:655:ASP:OD1	1.91	0.70
1:C:1161:ILE:HD12	1:D:1661:ILE:HG13	1.74	0.69
1:A:156:PHE:HB2	1:A:195:TRP:CZ3	2.27	0.69
1:D:1697:ILE:H	1:D:1729:LYS:HG2	1.58	0.69
1:C:1196:ARG:H	1:C:1230:ASN:HD21	1.41	0.69
1:C:1137:VAL:HG21	1:C:1235:ASN:HA	1.75	0.68
1:A:205:GLY:O	1:A:209:VAL:HG23	1.94	0.68
1:B:722:LYS:HZ2	1:B:723:GLU:N	1.92	0.68
1:A:142:SER:OG	1:A:144:GLU:HG3	1.94	0.68
1:A:73:ASP:HB2	1:A:103:ASN:ND2	2.09	0.67
1:A:137:VAL:HG23	1:A:184:VAL:O	1.95	0.66
1:B:741:GLU:O	1:B:745:VAL:HG23	1.95	0.66
1:C:1157:THR:HG22	1:D:1661:ILE:HG21	1.78	0.66
1:D:1574:ARG:HG2	1:D:1600:TYR:OH	1.95	0.66
1:C:1046:GLN:HB2	1:C:1080:PRO:HB3	1.78	0.66
1:D:1648:GLY:HA3	1:D:1691:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:THR:HG22	1:A:151:GLY:N	2.10	0.66
1:B:531:LYS:O	1:B:532:THR:HG23	1.95	0.66
1:C:1255:GLY:O	1:C:1256:LYS:HG3	1.96	0.65
1:C:1197:ILE:HG13	1:C:1198:ASN:H	1.62	0.65
1:A:137:VAL:HG22	1:A:235:ASN:HB3	1.79	0.65
1:D:1546:GLN:HE22	1:D:1566:GLU:N	1.95	0.65
1:D:1753:ILE:HG13	1:D:1754:GLY:H	1.61	0.65
1:B:710:LYS:HE3	1:B:716:VAL:HB	1.79	0.64
1:D:1741:GLU:O	1:D:1744:LYS:HB3	1.98	0.64
1:A:135:ILE:HB	1:A:186:ALA:HA	1.80	0.64
1:B:561:ASN:ND2	1:B:572:GLY:HA3	2.12	0.64
1:D:1669:ARG:O	1:D:1670:ARG:HG3	1.97	0.63
1:B:637:VAL:HG23	1:B:684:VAL:O	1.99	0.63
1:B:503:ARG:NH1	1:B:574:ARG:HH11	1.97	0.63
1:D:1621:TYR:CE1	1:D:1629:PHE:HB2	2.34	0.63
1:A:197:ILE:HD11	1:A:231:PHE:HD2	1.63	0.62
1:D:1546:GLN:NE2	1:D:1566:GLU:H	1.97	0.62
1:A:86:ASN:HD21	1:B:672:ARG:HH21	1.47	0.62
1:B:518:LEU:HD22	1:B:596:ILE:HD11	1.81	0.62
1:B:643:LEU:HD13	1:B:667:ARG:CG	2.29	0.62
1:C:1137:VAL:CG2	1:C:1235:ASN:HA	2.29	0.62
1:B:557:PHE:HB3	1:B:560:GLU:HG3	1.81	0.62
1:A:166:LYS:HB2	1:A:166:LYS:NZ	2.14	0.62
1:C:1062:ILE:O	1:C:1070:GLU:HB2	1.99	0.62
1:D:1670:ARG:HG3	1:D:1670:ARG:NH1	2.15	0.62
1:B:565:GLU:HG2	1:B:566:GLU:HG3	1.81	0.61
1:C:1001:MET:CG	1:C:1003:ARG:HB2	2.29	0.61
1:B:592:PRO:HB2	1:B:616:LEU:HD21	1.82	0.61
1:A:7:SER:HB3	1:A:110:VAL:HG11	1.81	0.61
1:A:61:ASN:HD22	1:A:70:GLU:HB3	1.65	0.61
1:A:86:ASN:ND2	1:B:672:ARG:HH21	1.99	0.61
1:B:520:ILE:HG12	1:C:1016:HIS:HB2	1.82	0.61
1:A:245:VAL:O	1:A:249:VAL:HG23	1.99	0.61
1:C:1047:ARG:HG3	1:C:1047:ARG:HH11	1.65	0.61
1:B:637:VAL:HG22	1:B:735:ASN:HB3	1.82	0.60
1:C:1163:ARG:HB3	1:C:1163:ARG:HH11	1.65	0.60
1:C:1154:VAL:CG1	1:C:1155:ASP:H	2.07	0.60
1:A:238:ILE:H	1:A:238:ILE:CD1	2.14	0.60
1:B:585:ILE:H	1:B:585:ILE:HD12	1.65	0.60
1:A:142:SER:HB3	1:A:145:GLU:HG2	1.83	0.60
1:A:56:PHE:C	1:A:58:PRO:HD3	2.22	0.60
1:B:585:ILE:N	1:B:585:ILE:HD12	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:ALA:O	1:A:184:VAL:HG22	2.02	0.59
1:A:73:ASP:HB2	1:A:103:ASN:HD22	1.68	0.59
1:D:1746:VAL:O	1:D:1750:VAL:HG23	2.03	0.59
1:D:1684:VAL:HG12	1:D:1689:VAL:HG12	1.85	0.59
1:C:1137:VAL:HG13	1:C:1235:ASN:HB2	1.85	0.58
1:D:1670:ARG:HD3	1:D:1672:ARG:NH2	2.18	0.58
1:B:745:VAL:HA	1:B:748:GLU:HG2	1.84	0.58
1:B:664:MET:HG3	1:B:667:ARG:HB3	1.84	0.58
1:B:549:ILE:O	1:B:553:ILE:HG12	2.03	0.58
1:B:664:MET:HE3	1:B:745:VAL:HG21	1.86	0.58
1:A:112:HIS:O	1:A:114:PRO:HD3	2.04	0.58
1:D:1663:ARG:NH2	1:D:1748:GLU:HB3	2.18	0.58
1:B:546:GLN:HB2	1:B:580:PRO:HB3	1.86	0.57
1:A:152:SER:HB2	1:B:670:ARG:HD3	1.84	0.57
1:A:141:ALA:O	1:A:238:ILE:HG22	2.05	0.57
1:C:1136:ARG:HG3	1:C:1136:ARG:HH11	1.70	0.57
1:A:150:THR:HG22	1:A:151:GLY:H	1.69	0.57
1:A:209:VAL:HG21	1:A:233:PHE:HD2	1.69	0.57
1:C:1154:VAL:HG12	1:C:1195:TRP:HZ3	1.69	0.56
1:B:501:MET:CG	1:B:502:ASP:H	2.17	0.56
1:B:539:THR:HG22	1:B:540:GLU:H	1.70	0.56
1:C:1252:GLU:HB3	3:C:2283:HOH:O	2.05	0.56
1:D:1528:VAL:HG13	1:D:1537:ILE:HG13	1.86	0.56
1:A:163:ARG:CG	1:A:249:VAL:HG22	2.31	0.56
1:A:108:LEU:HD23	1:A:109:GLY:N	2.21	0.56
1:D:1555:LYS:HE3	1:D:1556:PHE:CE2	2.41	0.56
1:A:217:THR:CG2	1:A:239:HIS:NE2	2.69	0.56
1:B:525:VAL:CG1	1:B:539:THR:HG21	2.36	0.56
1:C:1170:ARG:HG3	1:C:1170:ARG:NH1	2.17	0.56
1:D:1664:MET:O	1:D:1668:THR:HG22	2.04	0.56
1:A:152:SER:CB	1:B:670:ARG:HD3	2.36	0.55
1:A:148:GLY:HA3	1:A:191:PHE:CE1	2.41	0.55
1:C:1033:GLY:HA3	3:C:2165:HOH:O	2.07	0.55
1:B:608:LEU:HA	1:B:707:ILE:HD13	1.87	0.55
1:C:1242:VAL:O	1:C:1246:VAL:HG23	2.07	0.55
1:D:1697:ILE:HG13	1:D:1701:ASP:HB2	1.89	0.55
1:C:1143:LEU:HG	1:C:1238:ILE:HD11	1.89	0.55
1:C:1055:LYS:HD2	3:C:2049:HOH:O	2.06	0.55
1:A:86:ASN:HD21	1:B:672:ARG:HD2	1.70	0.55
1:A:25:VAL:CG1	1:A:88:VAL:HG22	2.37	0.55
1:A:137:VAL:HG21	1:A:235:ASN:HA	1.89	0.54
1:B:725:ASN:CG	1:B:726:ALA:N	2.60	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:ILE:HD11	1:A:231:PHE:CD2	2.41	0.54
1:B:550:VAL:HG13	1:B:562:ILE:HD13	1.89	0.54
1:B:580:PRO:HG2	3:B:2188:HOH:O	2.07	0.54
1:A:57:PHE:N	1:A:58:PRO:HD3	2.23	0.54
1:B:656:PHE:O	1:B:660:PHE:HB2	2.07	0.54
1:D:1719:PHE:O	1:D:1743:VAL:HG13	2.07	0.54
1:D:1694:THR:CG2	1:D:1731:PHE:HB2	2.35	0.54
1:A:209:VAL:HG21	1:A:233:PHE:CD2	2.42	0.54
1:B:584:THR:O	1:B:588:VAL:HG23	2.07	0.54
1:B:630:PHE:HB2	1:B:635:ILE:HG21	1.89	0.54
1:C:1100:TYR:HB3	1:C:1108:LEU:HG	1.89	0.54
1:A:41:ILE:N	1:A:41:ILE:CD1	2.71	0.53
1:C:1244:LYS:O	1:C:1248:GLU:HG3	2.09	0.53
1:A:217:THR:HG22	1:A:239:HIS:NE2	2.23	0.53
1:C:1173:ILE:CD1	1:D:1673:ILE:HD12	2.39	0.53
1:B:748:GLU:HA	1:B:751:GLU:HG2	1.90	0.53
1:C:1054:ARG:NH1	1:C:1070:GLU:OE2	2.42	0.53
1:B:637:VAL:CG2	1:B:735:ASN:HA	2.34	0.53
1:B:696:ARG:HA	1:B:729:LYS:CD	2.38	0.53
1:C:1245:VAL:HA	1:C:1248:GLU:OE1	2.09	0.53
1:D:1646:CYS:HA	1:D:1690:ASP:OD2	2.08	0.53
1:A:194:THR:HB	1:A:197:ILE:HG21	1.91	0.53
1:C:1161:ILE:HD11	1:C:1173:ILE:HD11	1.90	0.53
1:C:1164:MET:CE	1:C:1245:VAL:HG21	2.39	0.53
1:B:578:ILE:HG12	1:B:598:LEU:HD13	1.91	0.53
1:A:154:VAL:HG22	1:A:155:ASP:N	2.24	0.52
1:B:669:ARG:O	1:B:670:ARG:HG2	2.09	0.52
1:C:1076:TRP:HE3	1:C:1098:LEU:HD11	1.75	0.52
1:B:728:SER:HB2	1:B:731:PHE:CZ	2.44	0.52
1:C:1150:THR:CG2	1:C:1193:VAL:HB	2.37	0.52
1:B:550:VAL:HG13	1:B:562:ILE:CD1	2.40	0.52
1:C:1159:LYS:HG3	1:C:1253:ILE:HD11	1.90	0.52
1:C:1084:THR:O	1:C:1088:VAL:HG23	2.09	0.52
1:D:1702:ILE:HA	3:D:2077:HOH:O	2.08	0.52
1:C:1219:PHE:CE2	1:C:1230:ASN:HB3	2.45	0.52
1:C:1046:GLN:O	1:C:1050:VAL:HG23	2.09	0.52
1:C:1215:MET:HE2	1:C:1236:GLY:HA2	1.90	0.52
1:B:667:ARG:HH22	1:B:744:LYS:NZ	2.07	0.52
1:B:539:THR:HG22	1:B:540:GLU:N	2.25	0.52
1:C:1164:MET:HE1	1:C:1245:VAL:HG21	1.90	0.52
1:B:578:ILE:HG12	1:B:598:LEU:CD1	2.40	0.52
1:D:1684:VAL:CG2	1:D:1709:VAL:HG22	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1170:ARG:HD3	1:C:1172:ARG:HH22	1.74	0.52
1:D:1732:ILE:HD11	1:D:1746:VAL:HG21	1.92	0.52
1:B:558:PRO:HG2	1:B:559:ASP:H	1.74	0.52
1:D:1544:GLU:HG3	1:D:1547:ARG:NH2	2.24	0.51
1:A:176:SER:HB3	1:A:179:LEU:HB3	1.93	0.51
1:B:565:GLU:HG3	1:B:700:TRP:CZ2	2.45	0.51
1:D:1544:GLU:HG3	1:D:1547:ARG:HH22	1.75	0.51
1:B:697:ILE:HG21	1:B:702:ILE:HD13	1.91	0.51
1:D:1657:THR:O	1:D:1661:ILE:HG12	2.11	0.51
1:C:1164:MET:O	1:C:1168:THR:HG22	2.11	0.51
1:D:1511:LEU:HD22	1:D:1596:ILE:HG21	1.92	0.51
1:B:654:VAL:CG1	1:B:655:ASP:H	2.11	0.51
1:D:1744:LYS:HB3	1:D:1744:LYS:HZ3	1.76	0.51
1:A:199:PRO:HB3	1:A:226:ALA:O	2.11	0.51
1:A:217:THR:HA	1:A:224:ALA:H	1.75	0.51
1:A:25:VAL:HG11	1:A:88:VAL:HG22	1.92	0.50
1:C:1024:ARG:HG3	3:C:2149:HOH:O	2.11	0.50
1:B:681:ALA:O	1:B:684:VAL:HG13	2.11	0.50
1:B:701:ASP:C	1:B:702:ILE:HD12	2.31	0.50
1:A:156:PHE:HB2	1:A:195:TRP:CE3	2.46	0.50
1:D:1528:VAL:CG1	1:D:1537:ILE:HG13	2.42	0.50
1:A:161:ILE:HG13	1:B:661:ILE:HD12	1.93	0.50
1:A:170:ARG:HD2	1:A:172:ARG:NH1	2.27	0.50
1:C:1011:LEU:HD12	1:C:1110:VAL:CG2	2.41	0.50
1:A:174:LEU:HD13	1:A:180:ASN:ND2	2.26	0.50
1:A:137:VAL:HG11	1:A:235:ASN:HA	1.93	0.50
1:B:694:THR:HG23	1:B:694:THR:O	2.11	0.50
1:C:1147:VAL:HG12	1:C:1189:VAL:HG23	1.94	0.50
1:C:1158:GLY:O	1:C:1162:GLU:HG3	2.12	0.50
1:B:510:LEU:HD13	1:B:552:GLU:HG2	1.94	0.49
1:D:1653:TYR:HB2	1:D:1656:PHE:HB3	1.94	0.49
1:B:659:LYS:O	1:B:663:ARG:HB2	2.11	0.49
1:D:1571:LYS:HG3	3:D:2172:HOH:O	2.11	0.49
1:A:194:THR:OG1	1:A:231:PHE:HB2	2.12	0.49
1:C:1249:VAL:O	1:C:1253:ILE:HD13	2.12	0.49
1:B:643:LEU:CG	1:B:738:ILE:HD11	2.40	0.49
1:A:17:LEU:HD21	1:A:44:GLU:HG2	1.94	0.49
1:C:1209:VAL:HG11	1:C:1233:PHE:CD2	2.37	0.49
1:C:1050:VAL:HG13	1:C:1062:ILE:HD13	1.93	0.49
1:D:1728:SER:O	1:D:1731:PHE:HE2	1.96	0.49
1:C:1011:LEU:HD22	1:C:1096:ILE:HG21	1.93	0.49
1:A:184:VAL:HG12	1:A:189:VAL:CG2	2.39	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1093:ASN:ND2	1:C:1174:LEU:HB3	2.28	0.49
1:B:520:ILE:HD11	1:C:1017:LEU:HA	1.94	0.49
1:B:739:HIS:O	1:B:743:VAL:HG23	2.13	0.49
1:D:1634:ARG:HG3	1:D:1634:ARG:HH11	1.77	0.49
1:C:1148:GLY:HA3	1:C:1191:PHE:CZ	2.47	0.48
1:A:154:VAL:CG1	1:A:155:ASP:N	2.71	0.48
1:A:197:ILE:H	1:A:197:ILE:CD1	2.23	0.48
1:B:514:VAL:CG2	1:B:548:MET:HE3	2.35	0.48
1:D:1616:LEU:O	1:D:1617:ASN:HB2	2.12	0.48
1:A:11:LEU:HD13	1:A:96:ILE:HB	1.94	0.48
1:B:529:GLU:HB2	1:B:538:VAL:HG12	1.96	0.48
1:D:1732:ILE:CD1	1:D:1746:VAL:HG21	2.44	0.48
1:B:529:GLU:HB2	1:B:538:VAL:CG1	2.44	0.48
1:B:585:ILE:CD1	1:B:585:ILE:H	2.25	0.48
1:B:624:GLU:HA	1:B:711:GLU:OE1	2.13	0.48
1:B:654:VAL:CG1	1:B:695:TRP:HZ3	2.26	0.48
1:C:1256:LYS:NZ	1:C:1256:LYS:HB2	2.28	0.48
1:C:1136:ARG:HG3	1:C:1136:ARG:NH1	2.28	0.48
1:B:524:ARG:HH11	1:C:1013:LYS:HZ3	1.61	0.48
1:A:159:LYS:O	1:A:163:ARG:HG2	2.14	0.48
1:A:137:VAL:CG2	1:A:235:ASN:HB3	2.44	0.48
1:B:546:GLN:O	1:B:550:VAL:HG23	2.14	0.48
1:D:1650:THR:HG23	1:D:1693:VAL:CG2	2.44	0.48
1:C:1248:GLU:O	1:C:1252:GLU:HG3	2.14	0.48
1:B:694:THR:HG22	1:B:731:PHE:HB2	1.96	0.47
1:B:667:ARG:HH22	1:B:744:LYS:HZ3	1.62	0.47
1:C:1143:LEU:HD11	1:C:1241:GLU:HB3	1.96	0.47
1:D:1601:VAL:HG22	1:D:1606:VAL:HB	1.96	0.47
1:A:167:ARG:CG	1:A:167:ARG:HH11	2.28	0.47
1:C:1001:MET:HB2	1:C:1123:GLU:OE1	2.14	0.47
1:C:1146:CYS:O	1:C:1169:ARG:HB2	2.14	0.47
1:C:1196:ARG:H	1:C:1230:ASN:HD22	1.57	0.47
1:D:1674:LEU:HD22	3:D:2141:HOH:O	2.13	0.47
1:C:1144:GLU:HG2	1:C:1144:GLU:O	2.13	0.47
1:B:684:VAL:HA	1:B:689:VAL:O	2.13	0.47
1:A:175:GLY:HA2	1:B:672:ARG:NH1	2.30	0.47
1:D:1650:THR:HG22	1:D:1651:GLY:H	1.79	0.47
1:A:202:ILE:HG12	1:A:231:PHE:CE2	2.49	0.47
1:D:1728:SER:HB2	1:D:1731:PHE:CZ	2.50	0.47
1:B:702:ILE:O	1:B:702:ILE:CG2	2.63	0.47
1:D:1605:GLU:HB2	1:D:1607:LYS:NZ	2.29	0.47
1:B:608:LEU:C	1:B:608:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:ASN:HB3	1:A:199:PRO:HD2	1.97	0.47
1:C:1219:PHE:CD2	1:C:1230:ASN:HB3	2.49	0.47
1:D:1546:GLN:HG3	1:D:1580:PRO:HG3	1.97	0.47
1:B:697:ILE:HG13	1:B:701:ASP:HB2	1.95	0.47
1:C:1195:TRP:HA	1:C:1230:ASN:HD22	1.80	0.47
1:B:748:GLU:HA	1:B:751:GLU:CG	2.44	0.47
1:D:1642:SER:O	1:D:1645:GLU:HB2	2.14	0.47
1:B:514:VAL:HA	1:B:548:MET:HE3	1.96	0.46
1:B:691:PHE:HA	1:B:733:PHE:O	2.15	0.46
1:A:159:LYS:HD2	1:A:252:GLU:OE1	2.14	0.46
1:D:1718:ASP:HA	1:D:1730:ASN:O	2.15	0.46
1:D:1643:LEU:HD12	1:D:1667:ARG:CZ	2.45	0.46
1:A:150:THR:CG2	1:A:151:GLY:N	2.78	0.46
1:A:80:PRO:HG2	3:A:2189:HOH:O	2.16	0.46
1:A:244:LYS:NZ	1:A:248:GLU:OE2	2.44	0.46
1:C:1245:VAL:O	1:C:1249:VAL:HG23	2.16	0.46
1:A:46:GLN:HE22	1:A:66:GLU:N	2.13	0.46
1:A:43:ARG:O	1:A:47:ARG:HG3	2.15	0.46
1:B:524:ARG:HE	1:C:1013:LYS:HZ2	1.63	0.46
1:B:501:MET:HG3	1:B:502:ASP:N	2.23	0.46
1:A:174:LEU:CD1	1:A:174:LEU:N	2.76	0.46
1:D:1601:VAL:HA	1:D:1606:VAL:HA	1.97	0.46
1:C:1153:TYR:HB2	1:C:1156:PHE:HB3	1.97	0.46
1:D:1511:LEU:HD22	1:D:1596:ILE:CG2	2.46	0.45
1:A:44:GLU:HA	1:A:47:ARG:HH11	1.81	0.45
1:D:1744:LYS:NZ	1:D:1744:LYS:HB3	2.30	0.45
1:B:501:MET:HE2	1:B:503:ARG:N	2.23	0.45
1:A:46:GLN:NE2	1:A:66:GLU:HB2	2.32	0.45
1:A:193:VAL:HA	1:A:231:PHE:O	2.16	0.45
1:C:1035:LYS:HE2	1:D:1668:THR:O	2.17	0.45
1:C:1011:LEU:HD22	1:C:1096:ILE:CG2	2.46	0.45
1:B:756:LYS:HG2	1:B:756:LYS:OXT	2.17	0.45
1:A:46:GLN:HE22	1:A:66:GLU:H	1.64	0.45
1:A:174:LEU:CD1	1:A:174:LEU:H	2.21	0.45
1:D:1697:ILE:HG22	1:D:1729:LYS:HA	1.98	0.45
1:B:663:ARG:NH2	1:B:752:GLU:OE1	2.50	0.45
1:C:1063:MET:HA	1:C:1068:ILE:O	2.16	0.45
1:A:53:ILE:HD12	1:A:78:ILE:HD11	1.99	0.45
1:B:525:VAL:HG21	1:B:587:PHE:HE1	1.81	0.44
1:D:1566:GLU:HG2	1:D:1580:PRO:HG2	1.99	0.44
1:B:521:HIS:CD2	1:B:541:ILE:HD12	2.53	0.44
1:D:1550:VAL:O	1:D:1554:ARG:HG2	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1173:ILE:HD12	1:D:1673:ILE:HD12	2.00	0.44
1:C:1135:ILE:HD12	1:C:1186:ALA:HA	1.99	0.44
1:A:173:ILE:HD12	1:B:673:ILE:HD12	1.99	0.44
1:C:1153:TYR:OH	1:C:1194:THR:HG22	2.18	0.44
1:B:535:LYS:HD2	1:B:535:LYS:C	2.37	0.44
1:C:1002:ASP:O	1:C:1006:PHE:HB2	2.17	0.44
1:A:153:TYR:OH	1:A:194:THR:HA	2.18	0.44
1:B:661:ILE:O	1:B:665:GLU:N	2.49	0.44
1:C:1215:MET:CE	1:C:1236:GLY:HA2	2.47	0.44
1:B:702:ILE:HG23	1:B:733:PHE:HZ	1.82	0.44
1:C:1191:PHE:HA	1:C:1233:PHE:O	2.18	0.44
1:A:175:GLY:HA2	1:B:672:ARG:CZ	2.47	0.44
1:D:1648:GLY:HA3	1:D:1691:PHE:CE2	2.53	0.44
1:A:25:VAL:O	1:A:25:VAL:HG13	2.17	0.44
1:C:1165:GLU:HG3	1:C:1166:LYS:N	2.32	0.44
1:A:137:VAL:HG22	1:A:138:SER:N	2.32	0.44
1:C:1050:VAL:HG13	1:C:1062:ILE:CD1	2.48	0.43
1:C:1010:LEU:O	1:C:1014:VAL:HG23	2.18	0.43
1:A:158:GLY:O	1:A:162:GLU:HG3	2.17	0.43
1:A:130:PHE:HB2	1:A:135:ILE:HG21	1.99	0.43
1:A:217:THR:HG21	1:A:239:HIS:NE2	2.32	0.43
1:D:1605:GLU:O	1:D:1607:LYS:HE3	2.18	0.43
1:D:1725:ASN:HD22	1:D:1725:ASN:H	1.65	0.43
1:B:589:HIS:ND1	3:B:2245:HOH:O	2.37	0.43
1:B:722:LYS:HZ2	1:B:723:GLU:CB	2.32	0.43
1:B:722:LYS:HZ3	1:B:723:GLU:H	1.64	0.43
1:A:50:VAL:HG13	1:A:62:ILE:HD12	2.00	0.43
1:C:1001:MET:HG3	1:C:1002:ASP:N	2.33	0.43
1:B:654:VAL:HG12	1:B:695:TRP:HZ3	1.83	0.43
1:B:715:MET:HB3	1:B:739:HIS:CE1	2.53	0.43
1:D:1529:GLU:O	1:D:1537:ILE:HB	2.19	0.43
1:B:697:ILE:HG12	1:B:702:ILE:CD1	2.48	0.43
1:B:725:ASN:ND2	1:B:727:PHE:H	2.17	0.43
1:D:1538:VAL:HG22	1:D:1539:THR:N	2.34	0.42
1:C:1195:TRP:O	1:C:1196:ARG:C	2.57	0.42
1:C:1148:GLY:HA3	1:C:1191:PHE:CE1	2.54	0.42
1:B:540:GLU:O	1:B:544:GLU:N	2.38	0.42
1:A:184:VAL:HG22	1:A:209:VAL:HG22	2.01	0.42
1:C:1080:PRO:HG2	3:C:2105:HOH:O	2.18	0.42
1:D:1741:GLU:N	1:D:1741:GLU:OE2	2.40	0.42
1:C:1053:ILE:HD12	1:C:1078:ILE:HD11	1.99	0.42
1:C:1078:ILE:HG12	1:C:1098:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:ARG:HD2	1:A:172:ARG:HH12	1.84	0.42
1:A:153:TYR:O	1:A:154:VAL:O	2.37	0.42
1:B:564:ALA:HA	1:B:578:ILE:O	2.20	0.42
1:C:1129:PHE:CE2	1:C:1134:ARG:HD2	2.54	0.42
1:B:592:PRO:HB2	1:B:616:LEU:CD2	2.48	0.42
1:D:1719:PHE:CD2	1:D:1730:ASN:HB3	2.54	0.42
1:C:1073:ASP:O	1:C:1102:GLU:HA	2.19	0.42
1:A:191:PHE:HA	1:A:233:PHE:O	2.20	0.42
1:C:1047:ARG:HH11	1:C:1047:ARG:CG	2.32	0.42
1:A:57:PHE:N	1:A:58:PRO:CD	2.83	0.42
1:A:174:LEU:HD13	1:A:180:ASN:HD21	1.85	0.42
1:C:1150:THR:HG22	1:C:1193:VAL:O	2.20	0.42
1:C:1143:LEU:HD23	1:C:1238:ILE:HG12	2.02	0.42
1:D:1653:TYR:HB3	1:D:1695:TRP:CE3	2.55	0.42
1:B:539:THR:N	1:B:542:ASP:OD2	2.53	0.41
1:A:159:LYS:HD3	1:A:162:GLU:OE2	2.20	0.41
1:B:697:ILE:CG1	1:B:701:ASP:HB2	2.50	0.41
1:B:702:ILE:HG22	1:B:702:ILE:O	2.19	0.41
1:A:161:ILE:O	1:A:165:GLU:HG2	2.20	0.41
1:B:501:MET:N	1:B:504:LEU:HB3	2.35	0.41
1:B:531:LYS:HD2	1:B:538:VAL:HB	2.02	0.41
1:C:1011:LEU:HD12	1:C:1110:VAL:HG23	2.02	0.41
1:D:1695:TRP:O	1:D:1696:ARG:HB2	2.20	0.41
1:C:1064:ALA:N	1:C:1068:ILE:O	2.51	0.41
1:D:1540:GLU:OE2	1:D:1543:ARG:NH1	2.53	0.41
1:C:1077:ILE:CG2	1:C:1200:TRP:HA	2.50	0.41
1:C:1144:GLU:HG2	1:D:1534:PHE:CG	2.55	0.41
1:D:1517:LEU:HD11	1:D:1544:GLU:OE2	2.21	0.41
1:C:1144:GLU:HB3	3:C:2126:HOH:O	2.20	0.41
1:C:1029:GLU:OE2	1:C:1043:ARG:NH2	2.54	0.41
1:A:162:GLU:O	1:A:165:GLU:HG2	2.20	0.41
1:A:166:LYS:HB2	1:A:166:LYS:HZ2	1.86	0.41
1:A:154:VAL:CG1	1:A:155:ASP:H	2.05	0.41
1:B:716:VAL:HG12	1:B:724:ALA:HB3	2.03	0.41
1:D:1670:ARG:CG	1:D:1670:ARG:NH1	2.82	0.41
1:D:1719:PHE:CG	1:D:1730:ASN:HB3	2.56	0.41
1:A:17:LEU:HA	1:D:1520:ILE:HD11	2.02	0.41
1:A:161:ILE:HG13	1:B:661:ILE:CD1	2.50	0.41
1:B:670:ARG:HD2	1:B:672:ARG:NH1	2.36	0.41
1:C:1143:LEU:HB3	1:C:1167:ARG:O	2.21	0.41
1:D:1756:LYS:HG3	1:D:1756:LYS:OXT	2.20	0.41
1:A:121:TYR:CE2	1:A:129:PHE:HB2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:514:VAL:HA	1:B:548:MET:CE	2.50	0.41
1:B:643:LEU:HD22	1:B:664:MET:HE2	2.03	0.41
1:B:672:ARG:NH1	3:B:2299:HOH:O	2.48	0.41
1:B:702:ILE:HG23	1:B:733:PHE:CZ	2.56	0.41
1:D:1651:GLY:HA3	1:D:1653:TYR:CZ	2.56	0.41
1:C:1122:ALA:HB1	1:C:1211:GLU:HG3	2.03	0.41
1:B:623:GLU:HB3	1:B:626:SER:HB2	2.03	0.41
1:C:1108:LEU:C	1:C:1108:LEU:HD12	2.42	0.41
1:D:1525:VAL:HG11	1:D:1539:THR:HG21	2.02	0.40
1:B:753:ILE:HG23	1:B:754:GLY:N	2.35	0.40
1:C:1038:VAL:HG22	1:C:1039:THR:N	2.35	0.40
1:D:1725:ASN:ND2	1:D:1725:ASN:C	2.74	0.40
1:B:512:ARG:NH1	1:D:1633:GLU:HG3	2.35	0.40
1:B:741:GLU:O	1:B:744:LYS:HB3	2.21	0.40
1:B:648:GLY:HA3	1:B:691:PHE:CZ	2.57	0.40
1:A:1:MET:HB3	1:A:2:ASP:H	1.51	0.40
1:C:1130:PHE:O	1:C:1133:GLU:HG2	2.22	0.40
1:B:528:VAL:CG1	1:B:537:ILE:HD12	2.51	0.40
1:D:1684:VAL:CG2	1:D:1709:VAL:CG2	2.99	0.40
1:A:4:LEU:HA	1:A:108:LEU:HD11	2.04	0.40
1:C:1135:ILE:HB	1:C:1186:ALA:HA	2.04	0.40
1:C:1034:PHE:O	1:D:1669:ARG:HG2	2.22	0.40
1:C:1170:ARG:CG	1:C:1170:ARG:NH1	2.81	0.40
1:B:732:ILE:HD11	1:B:746:VAL:HG11	2.03	0.40
1:D:1586:ASN:ND2	1:D:1593:ASN:HB2	2.37	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	254/256 (99%)	232 (91%)	19 (8%)	3 (1%)	19	14
1	B	254/256 (99%)	220 (87%)	30 (12%)	4 (2%)	14	9
1	C	254/256 (99%)	230 (91%)	22 (9%)	2 (1%)	27	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	254/256 (99%)	230 (91%)	21 (8%)	3 (1%)	19	14
All	All	1016/1024 (99%)	912 (90%)	92 (9%)	12 (1%)	19	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	B	570	GLU
1	B	654	VAL
1	C	1154	VAL
1	D	1723	GLU
1	A	157	THR
1	B	532	THR
1	C	1255	GLY
1	D	1657	THR
1	A	58	PRO
1	B	558	PRO
1	D	1755	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	213/213 (100%)	198 (93%)	15 (7%)	21	22
1	B	213/213 (100%)	203 (95%)	10 (5%)	36	42
1	C	213/213 (100%)	204 (96%)	9 (4%)	40	48
1	D	213/213 (100%)	203 (95%)	10 (5%)	36	42
All	All	852/852 (100%)	808 (95%)	44 (5%)	32	37

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	11	LEU
1	A	130	PHE

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Mol	Chain	Res	Type
1	A	144	GLU
1	A	163	ARG
1	A	164	MET
1	A	166	LYS
1	A	167	ARG
1	A	168	THR
1	A	170	ARG
1	A	174	LEU
1	A	197	ILE
1	A	230	ASN
1	A	238	ILE
1	A	241	GLU
1	B	501	MET
1	B	525	VAL
1	B	527	ASN
1	B	630	PHE
1	B	655	ASP
1	B	664	MET
1	B	672	ARG
1	B	680	ASN
1	B	684	VAL
1	B	718	ASP
1	C	1024	ARG
1	C	1026	ASP
1	C	1097	SER
1	C	1110	VAL
1	C	1130	PHE
1	C	1137	VAL
1	C	1144	GLU
1	C	1163	ARG
1	C	1194	THR
1	D	1518	LEU
1	D	1537	ILE
1	D	1559	ASP
1	D	1606	VAL
1	D	1630	PHE
1	D	1650	THR
1	D	1680	ASN
1	D	1706	LEU
1	D	1722	LYS
1	D	1725	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	ASN
1	A	86	ASN
1	A	103	ASN
1	A	140	ASN
1	A	180	ASN
1	A	247	ASN
1	B	521	HIS
1	B	561	ASN
1	C	1027	ASN
1	C	1230	ASN
1	C	1247	ASN
1	D	1546	GLN
1	D	1561	ASN
1	D	1680	ASN
1	D	1725	ASN
1	D	1730	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 4 ligands modelled in this entry, 4 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.

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, 95th 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	256/256 (100%)	0.07	10 (3%) 37 38	20, 45, 84, 139	0
1	B	256/256 (100%)	0.29	14 (5%) 24 24	23, 51, 95, 154	0
1	C	256/256 (100%)	-0.26	6 (2%) 57 58	19, 38, 65, 109	0
1	D	256/256 (100%)	-0.08	15 (5%) 22 21	18, 38, 83, 157	0
All	All	1024/1024 (100%)	0.01	45 (4%) 33 33	18, 42, 84, 157	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1755	GLY	11.9
1	A	256	LYS	6.4
1	D	1756	LYS	6.2
1	B	756	LYS	5.7
1	B	501	MET	5.3
1	B	753	ILE	5.2
1	A	255	GLY	5.1
1	A	249	VAL	5.0
1	B	755	GLY	5.0
1	B	695	TRP	4.9
1	C	1256	LYS	4.7
1	C	1255	GLY	4.7
1	B	526	ASP	4.5
1	C	1001	MET	4.2
1	D	1534	PHE	4.2
1	A	254	GLY	4.1
1	B	750	VAL	3.7
1	A	250	VAL	3.6
1	A	253	ILE	3.3
1	D	1696	ARG	3.2
1	A	144	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	1652	SER	3.0
1	D	1532	THR	2.9
1	B	525	VAL	2.9
1	B	754	GLY	2.7
1	B	534	PHE	2.7
1	B	696	ARG	2.7
1	A	154	VAL	2.6
1	B	533	GLY	2.6
1	D	1727	PHE	2.6
1	C	1254	GLY	2.5
1	A	1	MET	2.4
1	D	1654	VAL	2.4
1	D	1695	TRP	2.4
1	B	641	ALA	2.3
1	C	1250	VAL	2.2
1	D	1754	GLY	2.2
1	D	1719	PHE	2.2
1	D	1751	GLU	2.2
1	D	1527	ASN	2.2
1	B	676	SER	2.1
1	D	1750	VAL	2.1
1	D	1501	MET	2.0
1	C	1154	VAL	2.0
1	A	251	GLU	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	C	1761	1/1	0.09	-0.54	27,27,27,27	0
2	MG	B	1759	1/1	0.08	-2.21	40,40,40,40	0
2	MG	D	1763	1/1	0.06	-2.50	20,20,20,20	0
2	MG	A	1758	1/1	0.05	-2.68	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.