Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:19 pm BST

PDB ID	:	5C6N
Title	:	protein A
Authors	:	Lu, M.
Deposited on	:	2015-06-23
Resolution	:	3.00 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:

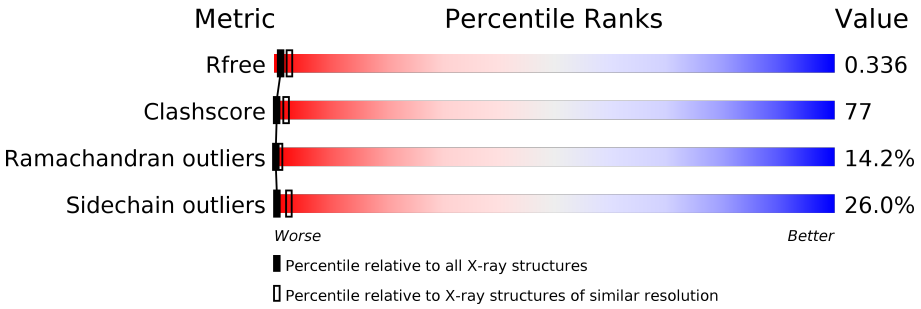
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	463	20% 51% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3413 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 BH2163 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3413	2263	549	573	28	0	0	0

There is a discrepancy between the modelled and reference sequences:

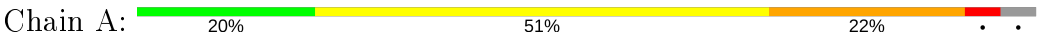
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ASP	conflict	UNP Q9KAX3

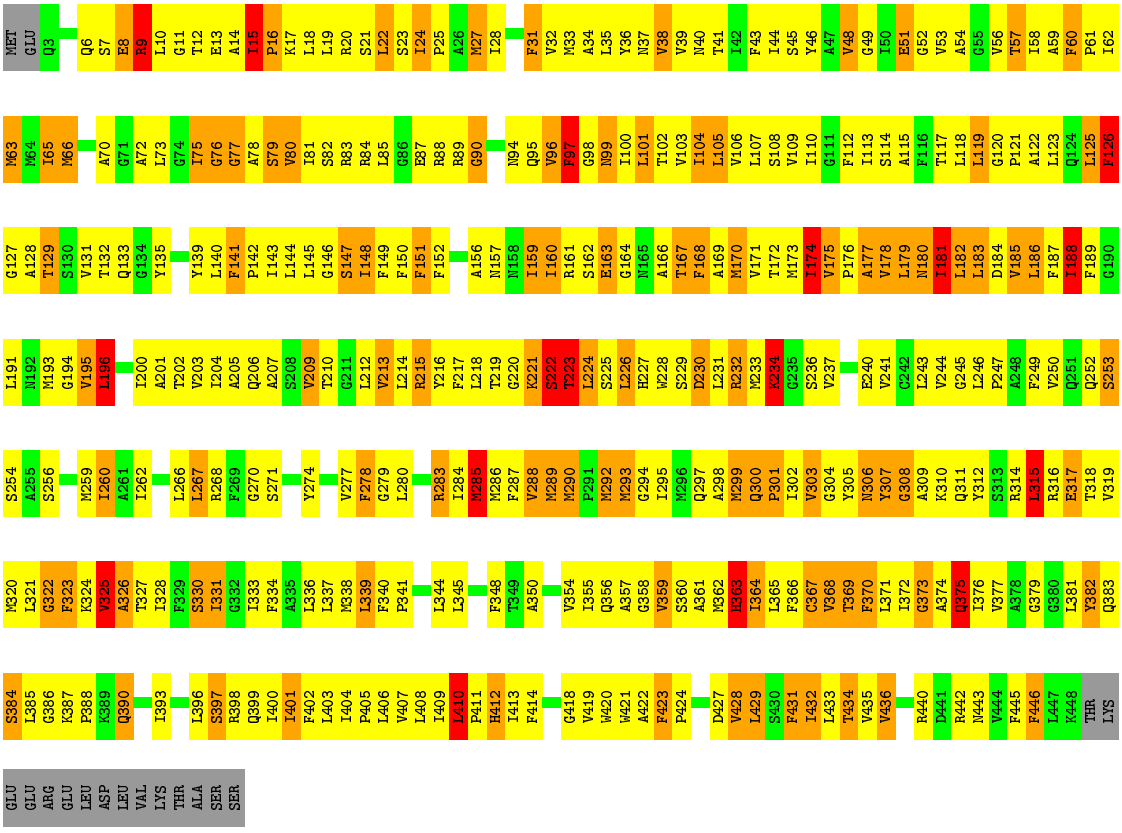
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: BH2163 protein

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.68Å 93.42Å 101.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-3.00) 87.6 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.280 , 0.300 0.339 , 0.336	Depositor DCC
R_{free} test set	772 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , -9.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.145 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3413	wwPDB-VP
Average B, all atoms (Å^2)	202.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.22% 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	0.60	0/3481	0.93	2/4714 (0.0%)

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	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	GLY	N-CA-C	-6.09	97.87	113.10
1	A	315	LEU	CB-CG-CD1	6.05	121.28	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	LEU	Peptide
1	A	15	ILE	Peptide
1	A	195	VAL	Peptide
1	A	306	ASN	Peptide
1	A	307	TYR	Peptide

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	3413	0	3610	544	0
All	All	3413	0	3610	544	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 77.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:O	1:A:176:PRO:HD2	1.33	1.27
1:A:224:LEU:O	1:A:226:LEU:HG	1.44	1.14
1:A:404:ILE:HG13	1:A:405:PRO:CD	1.75	1.14
1:A:289:MET:HA	1:A:289:MET:CE	1.77	1.13
1:A:404:ILE:CG1	1:A:405:PRO:HD3	1.78	1.12
1:A:78:ALA:HA	1:A:162:SER:HB2	1.20	1.11
1:A:289:MET:HA	1:A:289:MET:HE2	1.31	1.11
1:A:364:ILE:HG23	1:A:367:CYS:SG	1.94	1.07
1:A:78:ALA:HA	1:A:162:SER:CB	1.84	1.07
1:A:59:ALA:HB1	1:A:140:LEU:HD13	1.30	1.07
1:A:247:PRO:HG3	1:A:388:PRO:HB2	1.34	1.06
1:A:407:VAL:O	1:A:411:PRO:HD2	1.54	1.05
1:A:15:ILE:HD13	1:A:15:ILE:O	1.56	1.04
1:A:222:SER:O	1:A:226:LEU:HD11	1.58	1.02
1:A:149:PHE:HD2	1:A:207:ALA:HA	1.21	1.01
1:A:420:TRP:O	1:A:424:PRO:HD2	1.59	1.00
1:A:173:MET:O	1:A:175:VAL:N	1.95	0.99
1:A:364:ILE:HG22	1:A:420:TRP:HZ2	1.27	0.98
1:A:156:ALA:O	1:A:160:ILE:HG23	1.64	0.96
1:A:298:ALA:O	1:A:301:PRO:HD2	1.66	0.96
1:A:300:GLN:HB3	1:A:301:PRO:HD3	1.48	0.95
1:A:187:PHE:HA	1:A:191:LEU:HD12	1.50	0.93
1:A:361:ALA:O	1:A:365:LEU:HB2	1.69	0.93
1:A:149:PHE:CD2	1:A:207:ALA:HA	2.03	0.93
1:A:24:ILE:HG13	1:A:25:PRO:HD3	1.52	0.92
1:A:59:ALA:HB1	1:A:140:LEU:CD1	1.99	0.92
1:A:183:LEU:HD13	1:A:187:PHE:HE1	1.32	0.91
1:A:19:LEU:HD12	1:A:321:LEU:HD23	1.54	0.89
1:A:115:ALA:HB2	1:A:144:LEU:HB3	1.55	0.89
1:A:87:GLU:HB2	1:A:308:GLY:HA2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLY:HA3	1:A:241:VAL:HG13	1.53	0.87
1:A:106:VAL:O	1:A:110:ILE:HD12	1.74	0.87
1:A:7:SER:HB2	1:A:223:THR:O	1.74	0.86
1:A:148:ILE:HG13	1:A:149:PHE:N	1.91	0.85
1:A:13:GLU:OE2	1:A:306:ASN:ND2	2.09	0.85
1:A:35:LEU:O	1:A:38:VAL:HB	1.75	0.85
1:A:411:PRO:HD3	1:A:418:GLY:HA3	1.58	0.84
1:A:51:GLU:CD	1:A:52:GLY:H	1.79	0.84
1:A:60:PHE:HB3	1:A:61:PRO:HD3	1.59	0.84
1:A:402:PHE:CD1	1:A:429:LEU:HD21	2.13	0.83
1:A:240:GLU:HA	1:A:243:LEU:HD12	1.59	0.83
1:A:299:MET:CE	1:A:322:GLY:HA2	2.08	0.83
1:A:364:ILE:CG2	1:A:367:CYS:SG	2.67	0.83
1:A:78:ALA:CA	1:A:162:SER:HB2	2.07	0.82
1:A:36:TYR:HD1	1:A:181:ILE:CD1	1.91	0.82
1:A:308:GLY:O	1:A:310:LYS:N	2.13	0.81
1:A:314:ARG:O	1:A:317:GLU:HB3	1.78	0.81
1:A:406:LEU:HD22	1:A:422:ALA:HA	1.62	0.81
1:A:315:LEU:HD12	1:A:316:ARG:N	1.95	0.81
1:A:20:ARG:O	1:A:24:ILE:HG23	1.80	0.81
1:A:361:ALA:O	1:A:365:LEU:CB	2.28	0.80
1:A:128:ALA:HB1	1:A:133:GLN:OE1	1.79	0.80
1:A:94:ASN:O	1:A:231:LEU:HD21	1.79	0.80
1:A:299:MET:HE1	1:A:322:GLY:HA2	1.61	0.80
1:A:396:LEU:O	1:A:401:ILE:HG12	1.82	0.79
1:A:323:PHE:CD1	1:A:377:VAL:HG11	2.18	0.78
1:A:108:SER:OG	1:A:148:ILE:HA	1.83	0.78
1:A:224:LEU:O	1:A:226:LEU:CG	2.30	0.78
1:A:195:VAL:N	1:A:196:LEU:HD12	1.99	0.77
1:A:310:LYS:O	1:A:312:TYR:HD1	1.68	0.77
1:A:180:ASN:OD1	1:A:202:THR:HG23	1.84	0.77
1:A:364:ILE:HG22	1:A:420:TRP:CZ2	2.15	0.77
1:A:173:MET:O	1:A:176:PRO:CD	2.26	0.77
1:A:16:PRO:HD2	1:A:17:LYS:H	1.49	0.77
1:A:163:GLU:HG3	1:A:164:GLY:H	1.50	0.76
1:A:31:PHE:HB2	1:A:290:MET:SD	2.26	0.76
1:A:17:LYS:HA	1:A:20:ARG:HB2	1.66	0.76
1:A:325:VAL:O	1:A:328:ILE:HG22	1.86	0.75
1:A:407:VAL:O	1:A:411:PRO:CD	2.32	0.74
1:A:325:VAL:HG13	1:A:326:ALA:H	1.52	0.74
1:A:15:ILE:O	1:A:15:ILE:CD1	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HG22	1:A:182:LEU:HD23	1.68	0.74
1:A:184:ASP:OD1	1:A:201:ALA:HB1	1.88	0.73
1:A:390:GLN:HA	1:A:393:ILE:HD12	1.68	0.73
1:A:299:MET:HE1	1:A:322:GLY:CA	2.20	0.72
1:A:397:SER:OG	1:A:398:ARG:N	2.20	0.72
1:A:183:LEU:HD13	1:A:187:PHE:CE1	2.22	0.71
1:A:350:ALA:HB3	1:A:354:VAL:HG21	1.71	0.71
1:A:139:TYR:O	1:A:142:PRO:HG2	1.91	0.71
1:A:334:PHE:HE1	1:A:367:CYS:HA	1.55	0.70
1:A:184:ASP:OD1	1:A:201:ALA:CB	2.38	0.70
1:A:382:TYR:CE1	1:A:390:GLN:HB2	2.26	0.70
1:A:125:LEU:O	1:A:126:PHE:HB2	1.92	0.70
1:A:420:TRP:HZ3	1:A:421:TRP:CE3	2.09	0.70
1:A:110:ILE:HA	1:A:113:ILE:HD12	1.74	0.70
1:A:224:LEU:C	1:A:226:LEU:HG	2.12	0.70
1:A:247:PRO:HG2	1:A:383:GLN:NE2	2.07	0.70
1:A:365:LEU:HD23	1:A:366:PHE:CE1	2.26	0.70
1:A:279:GLY:O	1:A:283:ARG:HD2	1.92	0.69
1:A:365:LEU:HD23	1:A:366:PHE:CZ	2.26	0.69
1:A:218:LEU:HA	1:A:221:LYS:HD3	1.75	0.69
1:A:410:LEU:HB3	1:A:418:GLY:HA2	1.74	0.69
1:A:88:ARG:O	1:A:90:GLY:N	2.22	0.69
1:A:410:LEU:O	1:A:414:PHE:N	2.26	0.68
1:A:129:THR:HB	1:A:132:THR:HG22	1.76	0.68
1:A:78:ALA:CA	1:A:162:SER:CB	2.69	0.68
1:A:397:SER:HB2	1:A:402:PHE:CD1	2.29	0.68
1:A:364:ILE:CG2	1:A:420:TRP:HZ2	2.03	0.67
1:A:179:LEU:CD1	1:A:205:ALA:HA	2.23	0.67
1:A:423:PHE:O	1:A:424:PRO:C	2.32	0.67
1:A:187:PHE:HB3	1:A:193:MET:HB2	1.76	0.67
1:A:320:MET:HG3	1:A:445:PHE:CE1	2.30	0.66
1:A:170:MET:O	1:A:174:ILE:HG23	1.94	0.66
1:A:249:PHE:O	1:A:253:SER:OG	2.08	0.66
1:A:222:SER:O	1:A:226:LEU:CD1	2.39	0.66
1:A:334:PHE:HB2	1:A:369:THR:HB	1.76	0.66
1:A:149:PHE:H	1:A:149:PHE:HD1	1.38	0.66
1:A:420:TRP:O	1:A:424:PRO:CD	2.40	0.66
1:A:227:HIS:CD2	1:A:231:LEU:HB2	2.31	0.65
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.26	0.65
1:A:144:LEU:O	1:A:147:SER:OG	2.13	0.65
1:A:19:LEU:HD22	1:A:298:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:O	1:A:402:PHE:N	2.29	0.65
1:A:100:ILE:HG22	1:A:104:ILE:HD11	1.78	0.65
1:A:148:ILE:HG13	1:A:149:PHE:H	1.62	0.65
1:A:181:ILE:H	1:A:181:ILE:HD13	1.60	0.65
1:A:323:PHE:HD1	1:A:377:VAL:HG11	1.59	0.65
1:A:112:PHE:HD1	1:A:145:LEU:O	1.80	0.65
1:A:299:MET:CE	1:A:322:GLY:CA	2.73	0.65
1:A:11:GLY:HA2	1:A:305:TYR:CE1	2.32	0.65
1:A:66:MET:HB2	1:A:151:PHE:CE2	2.32	0.65
1:A:141:PHE:O	1:A:145:LEU:HG	1.97	0.64
1:A:19:LEU:HD23	1:A:298:ALA:HB1	1.80	0.64
1:A:288:VAL:O	1:A:288:VAL:HG13	1.96	0.64
1:A:87:GLU:H	1:A:308:GLY:CA	2.11	0.64
1:A:320:MET:HB2	1:A:445:PHE:HE1	1.63	0.64
1:A:364:ILE:C	1:A:420:TRP:HE1	2.01	0.64
1:A:167:THR:O	1:A:170:MET:HB3	1.97	0.64
1:A:53:VAL:O	1:A:57:THR:OG1	2.15	0.64
1:A:289:MET:CA	1:A:289:MET:CE	2.66	0.63
1:A:82:SER:HB2	1:A:304:GLY:HA3	1.79	0.63
1:A:297:GLN:HA	1:A:300:GLN:HB2	1.81	0.63
1:A:304:GLY:O	1:A:307:TYR:O	2.15	0.63
1:A:409:ILE:O	1:A:409:ILE:CG2	2.47	0.63
1:A:36:TYR:HA	1:A:181:ILE:HD11	1.81	0.63
1:A:31:PHE:HD2	1:A:32:VAL:HG23	1.64	0.63
1:A:410:LEU:HB3	1:A:418:GLY:CA	2.29	0.63
1:A:159:ILE:HD11	1:A:217:PHE:CZ	2.33	0.62
1:A:108:SER:O	1:A:148:ILE:HG22	1.99	0.62
1:A:331:ILE:C	1:A:331:ILE:HD12	2.20	0.62
1:A:46:TYR:N	1:A:48:VAL:O	2.32	0.62
1:A:58:ILE:O	1:A:61:PRO:HD2	1.98	0.62
1:A:195:VAL:H	1:A:196:LEU:HD12	1.64	0.62
1:A:299:MET:HE3	1:A:322:GLY:HA2	1.81	0.62
1:A:87:GLU:H	1:A:308:GLY:HA3	1.63	0.62
1:A:106:VAL:O	1:A:110:ILE:CD1	2.46	0.62
1:A:84:ARG:HA	1:A:87:GLU:O	1.99	0.62
1:A:16:PRO:CD	1:A:17:LYS:H	2.09	0.62
1:A:97:PHE:HE1	1:A:101:LEU:HD11	1.65	0.62
1:A:167:THR:O	1:A:170:MET:CB	2.47	0.62
1:A:65:ILE:HG22	1:A:66:MET:N	2.14	0.62
1:A:10:LEU:HD23	1:A:12:THR:HB	1.81	0.62
1:A:299:MET:HA	1:A:302:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:CD1	1:A:181:ILE:CD1	2.78	0.61
1:A:322:GLY:O	1:A:325:VAL:CG1	2.48	0.61
1:A:370:PHE:CD2	1:A:370:PHE:N	2.68	0.61
1:A:222:SER:O	1:A:224:LEU:N	2.34	0.61
1:A:363:HIS:O	1:A:365:LEU:N	2.32	0.61
1:A:373:GLY:O	1:A:377:VAL:HG23	1.99	0.61
1:A:223:THR:HG22	1:A:224:LEU:HD12	1.82	0.61
1:A:407:VAL:HG12	1:A:411:PRO:HG2	1.83	0.61
1:A:65:ILE:CG2	1:A:66:MET:N	2.63	0.61
1:A:152:PHE:HE2	1:A:213:VAL:HB	1.66	0.61
1:A:62:ILE:HD12	1:A:62:ILE:N	2.15	0.61
1:A:385:LEU:O	1:A:387:LYS:N	2.32	0.61
1:A:46:TYR:HB3	1:A:189:PHE:CZ	2.35	0.61
1:A:24:ILE:HG13	1:A:25:PRO:CD	2.29	0.61
1:A:303:VAL:HG12	1:A:303:VAL:O	2.01	0.61
1:A:364:ILE:O	1:A:367:CYS:SG	2.56	0.60
1:A:408:LEU:N	1:A:408:LEU:HD23	2.15	0.60
1:A:247:PRO:HG3	1:A:388:PRO:CB	2.22	0.60
1:A:140:LEU:HA	1:A:143:ILE:HD12	1.82	0.60
1:A:173:MET:C	1:A:175:VAL:H	2.03	0.60
1:A:18:LEU:O	1:A:22:LEU:HB2	2.02	0.60
1:A:19:LEU:CD2	1:A:298:ALA:CB	2.80	0.60
1:A:227:HIS:HB3	1:A:231:LEU:HB2	1.84	0.60
1:A:41:THR:O	1:A:44:ILE:N	2.34	0.60
1:A:25:PRO:HB3	1:A:166:ALA:O	2.02	0.60
1:A:374:ALA:O	1:A:376:ILE:N	2.35	0.60
1:A:70:ALA:HA	1:A:73:LEU:HD12	1.83	0.59
1:A:97:PHE:O	1:A:101:LEU:HD23	2.01	0.59
1:A:370:PHE:HD2	1:A:370:PHE:H	1.48	0.59
1:A:66:MET:HB2	1:A:151:PHE:HE2	1.66	0.59
1:A:254:SER:HB3	1:A:399:GLN:HG2	1.85	0.59
1:A:254:SER:CB	1:A:399:GLN:HG2	2.33	0.59
1:A:46:TYR:HB3	1:A:189:PHE:HZ	1.68	0.59
1:A:94:ASN:HD21	1:A:227:HIS:HB2	1.66	0.59
1:A:156:ALA:HB1	1:A:213:VAL:HG11	1.85	0.59
1:A:88:ARG:C	1:A:90:GLY:H	2.07	0.59
1:A:323:PHE:CE1	1:A:377:VAL:CG1	2.86	0.58
1:A:303:VAL:HG12	1:A:385:LEU:HD21	1.85	0.58
1:A:177:ALA:O	1:A:178:VAL:C	2.42	0.58
1:A:420:TRP:HZ3	1:A:421:TRP:CD2	2.21	0.58
1:A:169:ALA:O	1:A:171:VAL:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:CB	1:A:418:GLY:HA2	2.33	0.58
1:A:322:GLY:O	1:A:325:VAL:HG13	2.03	0.58
1:A:79:SER:HB2	1:A:383:GLN:O	2.03	0.58
1:A:402:PHE:CG	1:A:429:LEU:HD21	2.38	0.58
1:A:103:VAL:O	1:A:106:VAL:HB	2.04	0.58
1:A:62:ILE:HD12	1:A:62:ILE:H	1.69	0.57
1:A:25:PRO:HA	1:A:170:MET:HE1	1.86	0.57
1:A:24:ILE:C	1:A:24:ILE:HD12	2.25	0.57
1:A:72:ALA:CB	1:A:249:PHE:HD2	2.17	0.57
1:A:149:PHE:N	1:A:149:PHE:CD1	2.69	0.57
1:A:310:LYS:O	1:A:312:TYR:CD1	2.55	0.57
1:A:404:ILE:C	1:A:406:LEU:H	2.08	0.57
1:A:409:ILE:O	1:A:409:ILE:HG22	2.04	0.57
1:A:149:PHE:CD2	1:A:207:ALA:CA	2.83	0.57
1:A:38:VAL:HG12	1:A:39:VAL:N	2.19	0.57
1:A:390:GLN:O	1:A:393:ILE:HB	2.05	0.57
1:A:51:GLU:CD	1:A:52:GLY:N	2.55	0.57
1:A:96:VAL:HA	1:A:99:ASN:OD1	2.04	0.57
1:A:315:LEU:CD1	1:A:316:ARG:N	2.67	0.57
1:A:169:ALA:O	1:A:170:MET:C	2.42	0.56
1:A:10:LEU:HD23	1:A:12:THR:CB	2.35	0.56
1:A:80:VAL:HG12	1:A:81:ILE:N	2.19	0.56
1:A:188:ILE:HG23	1:A:189:PHE:N	2.20	0.56
1:A:43:PHE:O	1:A:46:TYR:HB2	2.06	0.56
1:A:410:LEU:HD21	1:A:421:TRP:HB2	1.86	0.56
1:A:115:ALA:HB2	1:A:144:LEU:CB	2.32	0.56
1:A:330:SER:HB3	1:A:370:PHE:HA	1.86	0.56
1:A:397:SER:HB2	1:A:402:PHE:CE1	2.41	0.56
1:A:43:PHE:HB3	1:A:188:ILE:HD12	1.86	0.56
1:A:23:SER:OG	1:A:24:ILE:N	2.37	0.56
1:A:19:LEU:HD11	1:A:299:MET:HE1	1.87	0.55
1:A:114:SER:HA	1:A:117:THR:HB	1.88	0.55
1:A:96:VAL:HG12	1:A:97:PHE:N	2.21	0.55
1:A:179:LEU:O	1:A:183:LEU:N	2.39	0.55
1:A:420:TRP:CZ3	1:A:421:TRP:CD2	2.94	0.55
1:A:383:GLN:C	1:A:385:LEU:H	2.09	0.55
1:A:370:PHE:HD2	1:A:370:PHE:N	2.03	0.55
1:A:423:PHE:HB2	1:A:424:PRO:CD	2.36	0.55
1:A:176:PRO:O	1:A:179:LEU:HB3	2.06	0.55
1:A:24:ILE:HA	1:A:27:MET:HB2	1.88	0.55
1:A:302:ILE:C	1:A:304:GLY:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:HD21	1:A:202:THR:HA	1.72	0.55
1:A:443:ASN:O	1:A:446:PHE:CD2	2.59	0.55
1:A:96:VAL:O	1:A:97:PHE:C	2.44	0.55
1:A:100:ILE:HG22	1:A:104:ILE:CD1	2.37	0.55
1:A:330:SER:HB3	1:A:370:PHE:O	2.05	0.54
1:A:187:PHE:O	1:A:191:LEU:HB2	2.07	0.54
1:A:102:THR:HG21	1:A:233:MET:O	2.08	0.54
1:A:233:MET:HG3	1:A:234:LYS:HG3	1.88	0.54
1:A:289:MET:HA	1:A:289:MET:HE3	1.82	0.54
1:A:13:GLU:OE2	1:A:314:ARG:HB2	2.07	0.54
1:A:19:LEU:CD2	1:A:298:ALA:HB1	2.37	0.54
1:A:367:CYS:SG	1:A:367:CYS:O	2.65	0.54
1:A:184:ASP:O	1:A:187:PHE:N	2.41	0.54
1:A:19:LEU:HD22	1:A:298:ALA:CB	2.36	0.54
1:A:320:MET:HB2	1:A:445:PHE:CE1	2.43	0.54
1:A:59:ALA:CB	1:A:140:LEU:HD13	2.21	0.54
1:A:183:LEU:O	1:A:186:LEU:HB2	2.08	0.54
1:A:181:ILE:N	1:A:181:ILE:CD1	2.71	0.54
1:A:404:ILE:HG13	1:A:405:PRO:HD3	0.82	0.54
1:A:233:MET:HG3	1:A:234:LYS:CG	2.38	0.54
1:A:98:GLY:HA2	1:A:101:LEU:HG	1.90	0.54
1:A:160:ILE:HD13	1:A:168:PHE:CE1	2.43	0.53
1:A:63:MET:O	1:A:66:MET:HG3	2.07	0.53
1:A:97:PHE:C	1:A:97:PHE:CD1	2.82	0.53
1:A:174:ILE:O	1:A:178:VAL:HG22	2.08	0.53
1:A:292:MET:HE1	1:A:330:SER:HA	1.90	0.53
1:A:25:PRO:HA	1:A:170:MET:CE	2.38	0.53
1:A:76:GLY:HA2	1:A:244:VAL:HB	1.90	0.53
1:A:323:PHE:HE1	1:A:377:VAL:HG12	1.74	0.53
1:A:118:LEU:HA	1:A:121:PRO:HG2	1.89	0.53
1:A:180:ASN:ND2	1:A:201:ALA:O	2.41	0.53
1:A:181:ILE:H	1:A:181:ILE:CD1	2.22	0.53
1:A:18:LEU:HB3	1:A:302:ILE:HD13	1.90	0.53
1:A:215:ARG:O	1:A:217:PHE:N	2.42	0.53
1:A:404:ILE:O	1:A:406:LEU:N	2.41	0.53
1:A:36:TYR:HD1	1:A:181:ILE:HD13	1.71	0.53
1:A:15:ILE:HA	1:A:18:LEU:HB2	1.91	0.52
1:A:293:MET:CE	1:A:376:ILE:HD11	2.39	0.52
1:A:383:GLN:C	1:A:385:LEU:N	2.62	0.52
1:A:75:ILE:HG22	1:A:76:GLY:N	2.24	0.52
1:A:254:SER:HB3	1:A:399:GLN:CG	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HA	1:A:104:ILE:HD12	1.91	0.52
1:A:318:THR:O	1:A:322:GLY:N	2.39	0.52
1:A:60:PHE:HB3	1:A:61:PRO:CD	2.35	0.52
1:A:96:VAL:O	1:A:100:ILE:HG12	2.10	0.52
1:A:396:LEU:O	1:A:401:ILE:CG1	2.55	0.52
1:A:145:LEU:N	1:A:146:GLY:HA3	2.24	0.52
1:A:188:ILE:HG23	1:A:189:PHE:H	1.74	0.52
1:A:40:ASN:ND2	1:A:184:ASP:OD2	2.42	0.52
1:A:178:VAL:O	1:A:181:ILE:HB	2.09	0.52
1:A:250:VAL:O	1:A:254:SER:N	2.42	0.52
1:A:220:GLY:O	1:A:222:SER:N	2.42	0.52
1:A:340:PHE:N	1:A:341:PRO:HD3	2.25	0.52
1:A:365:LEU:N	1:A:420:TRP:HE1	2.08	0.52
1:A:383:GLN:O	1:A:385:LEU:N	2.42	0.52
1:A:149:PHE:HB3	1:A:206:GLN:O	2.09	0.52
1:A:72:ALA:HB2	1:A:249:PHE:HD2	1.75	0.52
1:A:94:ASN:ND2	1:A:231:LEU:HD13	2.25	0.52
1:A:8:GLU:O	1:A:9:ARG:C	2.47	0.52
1:A:303:VAL:HG23	1:A:318:THR:HG21	1.92	0.51
1:A:112:PHE:CD1	1:A:145:LEU:O	2.61	0.51
1:A:160:ILE:CD1	1:A:168:PHE:CD1	2.94	0.51
1:A:295:ILE:O	1:A:298:ALA:HB3	2.09	0.51
1:A:400:ILE:HG13	1:A:401:ILE:H	1.76	0.51
1:A:411:PRO:O	1:A:412:HIS:C	2.46	0.51
1:A:166:ALA:O	1:A:169:ALA:HB3	2.11	0.51
1:A:170:MET:O	1:A:174:ILE:N	2.39	0.51
1:A:188:ILE:CG2	1:A:189:PHE:H	2.24	0.51
1:A:442:ARG:O	1:A:446:PHE:HB3	2.11	0.51
1:A:141:PHE:N	1:A:142:PRO:HD2	2.26	0.51
1:A:227:HIS:HB3	1:A:231:LEU:HD13	1.93	0.51
1:A:25:PRO:HA	1:A:170:MET:SD	2.50	0.51
1:A:247:PRO:CG	1:A:388:PRO:HB2	2.23	0.51
1:A:397:SER:HB2	1:A:402:PHE:HD1	1.75	0.51
1:A:411:PRO:O	1:A:412:HIS:O	2.29	0.51
1:A:35:LEU:O	1:A:36:TYR:C	2.48	0.50
1:A:105:LEU:HA	1:A:108:SER:HB2	1.93	0.50
1:A:163:GLU:HG3	1:A:164:GLY:N	2.21	0.50
1:A:315:LEU:HD12	1:A:316:ARG:H	1.76	0.50
1:A:369:THR:O	1:A:372:ILE:N	2.36	0.50
1:A:54:ALA:O	1:A:57:THR:N	2.44	0.50
1:A:131:VAL:HG23	1:A:132:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HD23	1:A:298:ALA:CB	2.40	0.50
1:A:237:VAL:HA	1:A:240:GLU:HG3	1.93	0.50
1:A:357:ALA:HA	1:A:360:SER:HB2	1.92	0.50
1:A:46:TYR:CB	1:A:189:PHE:HZ	2.24	0.50
1:A:65:ILE:HG22	1:A:66:MET:H	1.77	0.50
1:A:78:ALA:HA	1:A:162:SER:HB3	1.82	0.50
1:A:410:LEU:CD2	1:A:421:TRP:HB2	2.41	0.50
1:A:10:LEU:HB3	1:A:12:THR:H	1.76	0.49
1:A:148:ILE:CG1	1:A:149:PHE:CD1	2.95	0.49
1:A:209:VAL:O	1:A:212:LEU:N	2.45	0.49
1:A:210:THR:HA	1:A:213:VAL:HG23	1.94	0.49
1:A:107:LEU:HA	1:A:110:ILE:HD13	1.95	0.49
1:A:306:ASN:HB3	1:A:315:LEU:HB3	1.93	0.49
1:A:337:LEU:HD21	1:A:366:PHE:CB	2.41	0.49
1:A:148:ILE:CG1	1:A:149:PHE:N	2.71	0.49
1:A:297:GLN:O	1:A:301:PRO:HD3	2.12	0.49
1:A:325:VAL:HG22	1:A:326:ALA:N	2.28	0.49
1:A:7:SER:CB	1:A:223:THR:O	2.56	0.49
1:A:184:ASP:O	1:A:185:VAL:C	2.51	0.49
1:A:129:THR:OG1	1:A:267:LEU:HD11	2.13	0.49
1:A:169:ALA:HA	1:A:172:THR:OG1	2.12	0.49
1:A:24:ILE:N	1:A:25:PRO:CD	2.75	0.49
1:A:323:PHE:CE1	1:A:377:VAL:HG11	2.48	0.49
1:A:45:SER:HA	1:A:49:GLY:O	2.13	0.49
1:A:97:PHE:C	1:A:97:PHE:HD1	2.16	0.49
1:A:100:ILE:C	1:A:104:ILE:HD12	2.33	0.49
1:A:120:GLY:N	1:A:121:PRO:HD2	2.28	0.49
1:A:157:ASN:ND2	1:A:172:THR:OG1	2.45	0.49
1:A:31:PHE:CB	1:A:290:MET:SD	2.99	0.49
1:A:331:ILE:O	1:A:331:ILE:HD12	2.13	0.49
1:A:215:ARG:C	1:A:217:PHE:H	2.16	0.49
1:A:28:ILE:HB	1:A:170:MET:SD	2.53	0.48
1:A:163:GLU:CD	1:A:223:THR:HB	2.33	0.48
1:A:333:ILE:O	1:A:337:LEU:N	2.41	0.48
1:A:161:ARG:O	1:A:163:GLU:O	2.32	0.48
1:A:292:MET:CE	1:A:330:SER:HA	2.44	0.48
1:A:337:LEU:HD21	1:A:366:PHE:CG	2.49	0.48
1:A:303:VAL:CG1	1:A:303:VAL:O	2.60	0.48
1:A:358:GLY:O	1:A:362:MET:HG2	2.13	0.48
1:A:375:GLN:HG3	1:A:431:PHE:HA	1.96	0.48
1:A:433:LEU:O	1:A:436:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:OD1	1:A:201:ALA:HB3	2.12	0.48
1:A:18:LEU:HB3	1:A:302:ILE:CD1	2.44	0.48
1:A:283:ARG:O	1:A:287:PHE:HB2	2.14	0.48
1:A:302:ILE:HG22	1:A:303:VAL:N	2.27	0.48
1:A:436:VAL:O	1:A:440:ARG:HB2	2.14	0.48
1:A:178:VAL:O	1:A:182:LEU:HG	2.13	0.48
1:A:330:SER:OG	1:A:373:GLY:N	2.45	0.48
1:A:410:LEU:O	1:A:414:PHE:HB2	2.13	0.48
1:A:19:LEU:CD2	1:A:298:ALA:HB3	2.40	0.48
1:A:36:TYR:O	1:A:37:ASN:C	2.52	0.48
1:A:320:MET:HG3	1:A:445:PHE:CZ	2.49	0.48
1:A:152:PHE:CD2	1:A:210:THR:HG23	2.49	0.47
1:A:302:ILE:C	1:A:304:GLY:N	2.67	0.47
1:A:98:GLY:C	1:A:232:ARG:HB3	2.34	0.47
1:A:16:PRO:CD	1:A:17:LYS:N	2.75	0.47
1:A:115:ALA:HA	1:A:144:LEU:HD22	1.95	0.47
1:A:227:HIS:CB	1:A:231:LEU:HB2	2.44	0.47
1:A:362:MET:C	1:A:363:HIS:O	2.53	0.47
1:A:187:PHE:HA	1:A:191:LEU:CD1	2.35	0.47
1:A:401:ILE:O	1:A:402:PHE:CD2	2.68	0.47
1:A:148:ILE:HG13	1:A:149:PHE:CD1	2.50	0.47
1:A:262:ILE:HB	1:A:278:PHE:CZ	2.50	0.47
1:A:221:LYS:HB3	1:A:226:LEU:HD12	1.97	0.47
1:A:31:PHE:CA	1:A:290:MET:SD	3.03	0.47
1:A:322:GLY:O	1:A:325:VAL:HG12	2.14	0.47
1:A:365:LEU:HA	1:A:424:PRO:HG3	1.97	0.47
1:A:151:PHE:O	1:A:152:PHE:C	2.53	0.46
1:A:300:GLN:CB	1:A:301:PRO:HD3	2.31	0.46
1:A:371:LEU:HD13	1:A:428:VAL:HG23	1.97	0.46
1:A:34:ALA:O	1:A:38:VAL:HG23	2.15	0.46
1:A:183:LEU:O	1:A:187:PHE:CD1	2.69	0.46
1:A:125:LEU:O	1:A:126:PHE:CB	2.62	0.46
1:A:160:ILE:HD13	1:A:168:PHE:CD1	2.50	0.46
1:A:195:VAL:HG12	1:A:196:LEU:N	2.30	0.46
1:A:184:ASP:O	1:A:186:LEU:N	2.48	0.46
1:A:224:LEU:HB3	1:A:225:SER:H	1.55	0.46
1:A:31:PHE:C	1:A:31:PHE:CD2	2.89	0.46
1:A:139:TYR:O	1:A:143:ILE:HD12	2.16	0.46
1:A:173:MET:O	1:A:174:ILE:C	2.52	0.46
1:A:286:MET:O	1:A:289:MET:HB2	2.16	0.46
1:A:340:PHE:N	1:A:341:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:MET:HA	1:A:341:PRO:HG3	1.98	0.46
1:A:15:ILE:HD13	1:A:15:ILE:C	2.31	0.46
1:A:188:ILE:CG2	1:A:189:PHE:N	2.79	0.46
1:A:122:ALA:O	1:A:125:LEU:HB2	2.16	0.46
1:A:179:LEU:HD22	1:A:183:LEU:HB2	1.97	0.46
1:A:160:ILE:HG22	1:A:217:PHE:CZ	2.50	0.46
1:A:156:ALA:CB	1:A:213:VAL:HG11	2.46	0.46
1:A:362:MET:SD	1:A:362:MET:N	2.89	0.45
1:A:101:LEU:HD23	1:A:101:LEU:H	1.81	0.45
1:A:157:ASN:ND2	1:A:169:ALA:HA	2.31	0.45
1:A:396:LEU:C	1:A:401:ILE:HG12	2.35	0.45
1:A:434:THR:CG2	1:A:435:VAL:N	2.79	0.45
1:A:148:ILE:HG12	1:A:149:PHE:CD1	2.52	0.45
1:A:36:TYR:CE1	1:A:180:ASN:OD1	2.69	0.45
1:A:277:VAL:HA	1:A:280:LEU:HD12	1.99	0.45
1:A:187:PHE:CD1	1:A:201:ALA:HB2	2.51	0.45
1:A:94:ASN:HD21	1:A:227:HIS:CB	2.29	0.45
1:A:110:ILE:O	1:A:113:ILE:HB	2.15	0.45
1:A:245:GLY:O	1:A:246:LEU:C	2.55	0.45
1:A:252:GLN:O	1:A:256:SER:N	2.37	0.45
1:A:302:ILE:CG2	1:A:318:THR:HG21	2.47	0.45
1:A:368:VAL:HG11	1:A:427:ASP:CB	2.47	0.45
1:A:7:SER:O	1:A:8:GLU:C	2.56	0.45
1:A:260:ILE:HG13	1:A:260:ILE:H	1.63	0.44
1:A:365:LEU:HD11	1:A:423:PHE:CD1	2.52	0.44
1:A:48:VAL:HG11	1:A:135:TYR:CE2	2.53	0.44
1:A:420:TRP:CZ3	1:A:421:TRP:CE3	2.97	0.44
1:A:160:ILE:HD11	1:A:169:ALA:N	2.32	0.44
1:A:227:HIS:HD2	1:A:231:LEU:HB2	1.81	0.44
1:A:339:LEU:C	1:A:341:PRO:HD3	2.38	0.44
1:A:177:ALA:O	1:A:180:ASN:N	2.51	0.44
1:A:300:GLN:O	1:A:384:SER:HB3	2.18	0.44
1:A:356:GLN:O	1:A:360:SER:N	2.50	0.44
1:A:219:THR:O	1:A:220:GLY:C	2.56	0.44
1:A:270:GLY:HA3	1:A:274:TYR:CD1	2.53	0.44
1:A:406:LEU:O	1:A:406:LEU:HD23	2.18	0.44
1:A:107:LEU:C	1:A:109:VAL:N	2.71	0.44
1:A:23:SER:C	1:A:25:PRO:HD2	2.37	0.44
1:A:87:GLU:N	1:A:308:GLY:CA	2.80	0.44
1:A:157:ASN:HD21	1:A:169:ALA:HA	1.83	0.44
1:A:237:VAL:O	1:A:240:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:MET:O	1:A:289:MET:N	2.51	0.44
1:A:292:MET:HE3	1:A:330:SER:N	2.33	0.44
1:A:15:ILE:HG21	1:A:314:ARG:HB3	1.99	0.44
1:A:377:VAL:O	1:A:381:LEU:HG	2.18	0.44
1:A:75:ILE:O	1:A:76:GLY:C	2.56	0.44
1:A:104:ILE:O	1:A:107:LEU:N	2.51	0.43
1:A:333:ILE:HG22	1:A:369:THR:HG21	2.00	0.43
1:A:120:GLY:O	1:A:121:PRO:C	2.55	0.43
1:A:283:ARG:O	1:A:287:PHE:CB	2.67	0.43
1:A:288:VAL:O	1:A:288:VAL:CG1	2.65	0.43
1:A:357:ALA:HA	1:A:360:SER:CB	2.47	0.43
1:A:365:LEU:O	1:A:365:LEU:HG	2.17	0.43
1:A:368:VAL:CG2	1:A:424:PRO:HA	2.48	0.43
1:A:180:ASN:OD1	1:A:202:THR:CG2	2.63	0.43
1:A:57:THR:H	1:A:57:THR:HG1	1.51	0.43
1:A:227:HIS:CG	1:A:231:LEU:HB2	2.53	0.43
1:A:292:MET:CE	1:A:330:SER:CA	2.97	0.43
1:A:339:LEU:N	1:A:341:PRO:HD3	2.33	0.43
1:A:303:VAL:O	1:A:385:LEU:HD21	2.18	0.43
1:A:95:GLN:HA	1:A:95:GLN:HE21	1.84	0.43
1:A:127:GLY:HA3	1:A:267:LEU:HG	2.00	0.43
1:A:254:SER:HB2	1:A:399:GLN:HG2	2.01	0.43
1:A:169:ALA:C	1:A:171:VAL:N	2.72	0.43
1:A:230:ASP:O	1:A:231:LEU:C	2.57	0.43
1:A:279:GLY:O	1:A:283:ARG:CD	2.65	0.43
1:A:32:VAL:O	1:A:35:LEU:N	2.52	0.43
1:A:374:ALA:C	1:A:376:ILE:H	2.23	0.43
1:A:400:ILE:O	1:A:403:LEU:N	2.51	0.43
1:A:25:PRO:HB2	1:A:166:ALA:HB1	2.00	0.42
1:A:287:PHE:C	1:A:287:PHE:CD2	2.92	0.42
1:A:428:VAL:O	1:A:432:ILE:HD12	2.19	0.42
1:A:12:THR:O	1:A:305:TYR:OH	2.29	0.42
1:A:173:MET:C	1:A:175:VAL:N	2.60	0.42
1:A:183:LEU:HD22	1:A:183:LEU:HA	1.50	0.42
1:A:446:PHE:HD2	1:A:446:PHE:H	1.67	0.42
1:A:301:PRO:HD2	1:A:302:ILE:H	1.84	0.42
1:A:76:GLY:O	1:A:77:GLY:C	2.57	0.42
1:A:78:ALA:CA	1:A:162:SER:HB3	2.44	0.42
1:A:12:THR:HG22	1:A:14:ALA:H	1.84	0.42
1:A:176:PRO:HD3	1:A:209:VAL:CG1	2.50	0.42
1:A:252:GLN:O	1:A:254:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:O	1:A:181:ILE:C	2.58	0.42
1:A:246:LEU:N	1:A:247:PRO:HD2	2.35	0.42
1:A:292:MET:CE	1:A:330:SER:N	2.83	0.42
1:A:340:PHE:O	1:A:344:LEU:HD12	2.20	0.42
1:A:174:ILE:O	1:A:177:ALA:HB3	2.20	0.42
1:A:184:ASP:C	1:A:186:LEU:N	2.73	0.42
1:A:363:HIS:HB3	1:A:364:ILE:H	1.75	0.42
1:A:119:LEU:O	1:A:123:LEU:HB2	2.20	0.42
1:A:178:VAL:HG23	1:A:179:LEU:H	1.85	0.42
1:A:237:VAL:HA	1:A:240:GLU:CG	2.49	0.42
1:A:180:ASN:HD21	1:A:202:THR:CA	2.31	0.42
1:A:19:LEU:HD21	1:A:299:MET:HG2	2.01	0.42
1:A:27:MET:SD	1:A:294:GLY:HA3	2.60	0.41
1:A:157:ASN:HD21	1:A:169:ALA:CB	2.33	0.41
1:A:173:MET:CE	1:A:173:MET:HA	2.50	0.41
1:A:13:GLU:CD	1:A:306:ASN:HD21	2.18	0.41
1:A:374:ALA:C	1:A:376:ILE:N	2.74	0.41
1:A:244:VAL:HA	1:A:388:PRO:CG	2.51	0.41
1:A:180:ASN:HA	1:A:180:ASN:HD22	1.58	0.41
1:A:321:LEU:O	1:A:322:GLY:C	2.58	0.41
1:A:331:ILE:HG22	1:A:370:PHE:HB2	2.02	0.41
1:A:12:THR:HG22	1:A:13:GLU:N	2.36	0.41
1:A:183:LEU:O	1:A:186:LEU:CB	2.68	0.41
1:A:187:PHE:CA	1:A:191:LEU:HD12	2.34	0.41
1:A:292:MET:O	1:A:293:MET:C	2.59	0.41
1:A:354:VAL:O	1:A:358:GLY:HA3	2.21	0.41
1:A:20:ARG:HD3	1:A:20:ARG:HA	1.72	0.41
1:A:247:PRO:HG2	1:A:383:GLN:HE22	1.83	0.41
1:A:404:ILE:C	1:A:406:LEU:N	2.72	0.41
1:A:301:PRO:CD	1:A:302:ILE:H	2.34	0.41
1:A:312:TYR:O	1:A:316:ARG:HG3	2.21	0.41
1:A:320:MET:HG3	1:A:445:PHE:HE1	1.81	0.41
1:A:323:PHE:HE1	1:A:377:VAL:CG1	2.29	0.41
1:A:148:ILE:HG12	1:A:149:PHE:CE1	2.55	0.41
1:A:95:GLN:HE22	1:A:232:ARG:HA	1.86	0.41
1:A:379:GLY:O	1:A:383:GLN:HG3	2.21	0.41
1:A:390:GLN:HG2	1:A:390:GLN:H	1.61	0.41
1:A:18:LEU:HD23	1:A:302:ILE:HG12	2.03	0.41
1:A:183:LEU:HD12	1:A:201:ALA:HA	2.03	0.41
1:A:232:ARG:H	1:A:232:ARG:HG3	1.57	0.41
1:A:160:ILE:HA	1:A:163:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:N	1:A:181:ILE:HD13	2.30	0.41
1:A:301:PRO:C	1:A:304:GLY:H	2.24	0.41
1:A:325:VAL:O	1:A:328:ILE:N	2.54	0.41
1:A:331:ILE:CD1	1:A:331:ILE:C	2.83	0.41
1:A:428:VAL:CG1	1:A:429:LEU:N	2.82	0.41
1:A:83:ARG:O	1:A:87:GLU:HB3	2.21	0.41
1:A:160:ILE:HD12	1:A:168:PHE:CD1	2.55	0.40
1:A:214:LEU:N	1:A:214:LEU:HD23	2.35	0.40
1:A:35:LEU:O	1:A:39:VAL:HG22	2.21	0.40
1:A:413:ILE:O	1:A:414:PHE:CD1	2.74	0.40
1:A:78:ALA:O	1:A:82:SER:OG	2.36	0.40
1:A:36:TYR:CD2	1:A:37:ASN:N	2.89	0.40
1:A:96:VAL:O	1:A:99:ASN:N	2.54	0.40
1:A:320:MET:CB	1:A:445:PHE:HE1	2.30	0.40
1:A:6:GLN:HG3	1:A:6:GLN:O	2.22	0.40
1:A:100:ILE:O	1:A:104:ILE:HD12	2.21	0.40
1:A:266:LEU:HD22	1:A:278:PHE:CE1	2.56	0.40
1:A:341:PRO:HB2	1:A:359:VAL:CG2	2.52	0.40
1:A:96:VAL:HG22	1:A:237:VAL:HG11	2.04	0.40
1:A:252:GLN:C	1:A:254:SER:H	2.24	0.40
1:A:302:ILE:HG22	1:A:318:THR:HG21	2.03	0.40
1:A:434:THR:O	1:A:435:VAL:C	2.60	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	444/463 (96%)	252 (57%)	129 (29%)	63 (14%)	0 1

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ARG
1	A	15	ILE
1	A	16	PRO
1	A	38	VAL
1	A	89	ARG
1	A	170	MET
1	A	174	ILE
1	A	177	ALA
1	A	181	ILE
1	A	185	VAL
1	A	196	LEU
1	A	216	TYR
1	A	221	LYS
1	A	223	THR
1	A	290	MET
1	A	300	GLN
1	A	309	ALA
1	A	311	GLN
1	A	323	PHE
1	A	324	LYS
1	A	363	HIS
1	A	369	THR
1	A	375	GLN
1	A	386	GLY
1	A	401	ILE
1	A	77	GLY
1	A	85	LEU
1	A	90	GLY
1	A	96	VAL
1	A	97	PHE
1	A	151	PHE
1	A	163	GLU
1	A	194	GLY
1	A	222	SER
1	A	234	LYS
1	A	253	SER
1	A	322	GLY
1	A	326	ALA
1	A	364	ILE
1	A	368	VAL
1	A	373	GLY
1	A	126	PHE

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Mol	Chain	Res	Type
1	A	215	ARG
1	A	293	MET
1	A	301	PRO
1	A	325	VAL
1	A	367	CYS
1	A	384	SER
1	A	412	HIS
1	A	60	PHE
1	A	76	GLY
1	A	229	SER
1	A	355	ILE
1	A	285	MET
1	A	327	THR
1	A	423	PHE
1	A	56	VAL
1	A	188	ILE
1	A	303	VAL
1	A	80	VAL
1	A	410	LEU
1	A	104	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	366/382 (96%)	271 (74%)	95 (26%)	0 2

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	15	ILE
1	A	21	SER
1	A	22	LEU
1	A	24	ILE
1	A	27	MET

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Mol	Chain	Res	Type
1	A	31	PHE
1	A	33	MET
1	A	48	VAL
1	A	51	GLU
1	A	57	THR
1	A	63	MET
1	A	65	ILE
1	A	66	MET
1	A	75	ILE
1	A	79	SER
1	A	97	PHE
1	A	99	ASN
1	A	101	LEU
1	A	105	LEU
1	A	119	LEU
1	A	126	PHE
1	A	129	THR
1	A	141	PHE
1	A	147	SER
1	A	148	ILE
1	A	150	PHE
1	A	159	ILE
1	A	160	ILE
1	A	167	THR
1	A	168	PHE
1	A	174	ILE
1	A	175	VAL
1	A	178	VAL
1	A	179	LEU
1	A	180	ASN
1	A	181	ILE
1	A	182	LEU
1	A	183	LEU
1	A	186	LEU
1	A	188	ILE
1	A	196	LEU
1	A	200	ILE
1	A	203	VAL
1	A	204	ILE
1	A	209	VAL
1	A	213	VAL
1	A	222	SER

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Mol	Chain	Res	Type
1	A	223	THR
1	A	224	LEU
1	A	226	LEU
1	A	228	TRP
1	A	230	ASP
1	A	232	ARG
1	A	234	LYS
1	A	236	SER
1	A	259	MET
1	A	260	ILE
1	A	267	LEU
1	A	268	ARG
1	A	271	SER
1	A	278	PHE
1	A	283	ARG
1	A	284	ILE
1	A	285	MET
1	A	288	VAL
1	A	289	MET
1	A	292	MET
1	A	299	MET
1	A	315	LEU
1	A	317	GLU
1	A	319	VAL
1	A	325	VAL
1	A	330	SER
1	A	331	ILE
1	A	336	LEU
1	A	339	LEU
1	A	345	LEU
1	A	348	PHE
1	A	359	VAL
1	A	363	HIS
1	A	370	PHE
1	A	375	GLN
1	A	382	TYR
1	A	390	GLN
1	A	397	SER
1	A	410	LEU
1	A	419	VAL
1	A	428	VAL
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	431	PHE
1	A	432	ILE
1	A	434	THR
1	A	436	VAL
1	A	446	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	95	GLN
1	A	157	ASN
1	A	180	ASN
1	A	227	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.