Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:27 PM EDT

PDB ID	:	4LZ6
Title	:	Structure of MATE multidrug transporter DinF-BH
Authors	:	Lu, M.; Radchenko, M.; Symersky, J.; Nie, R.; Guo, Y.
Deposited on	:	2013-07-31
Resolution	:	3.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

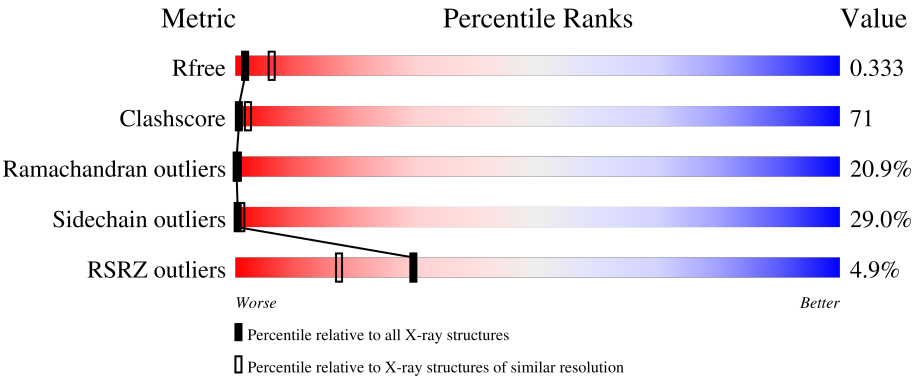
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of 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	446	5% 17% 49% 29% 5%

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.

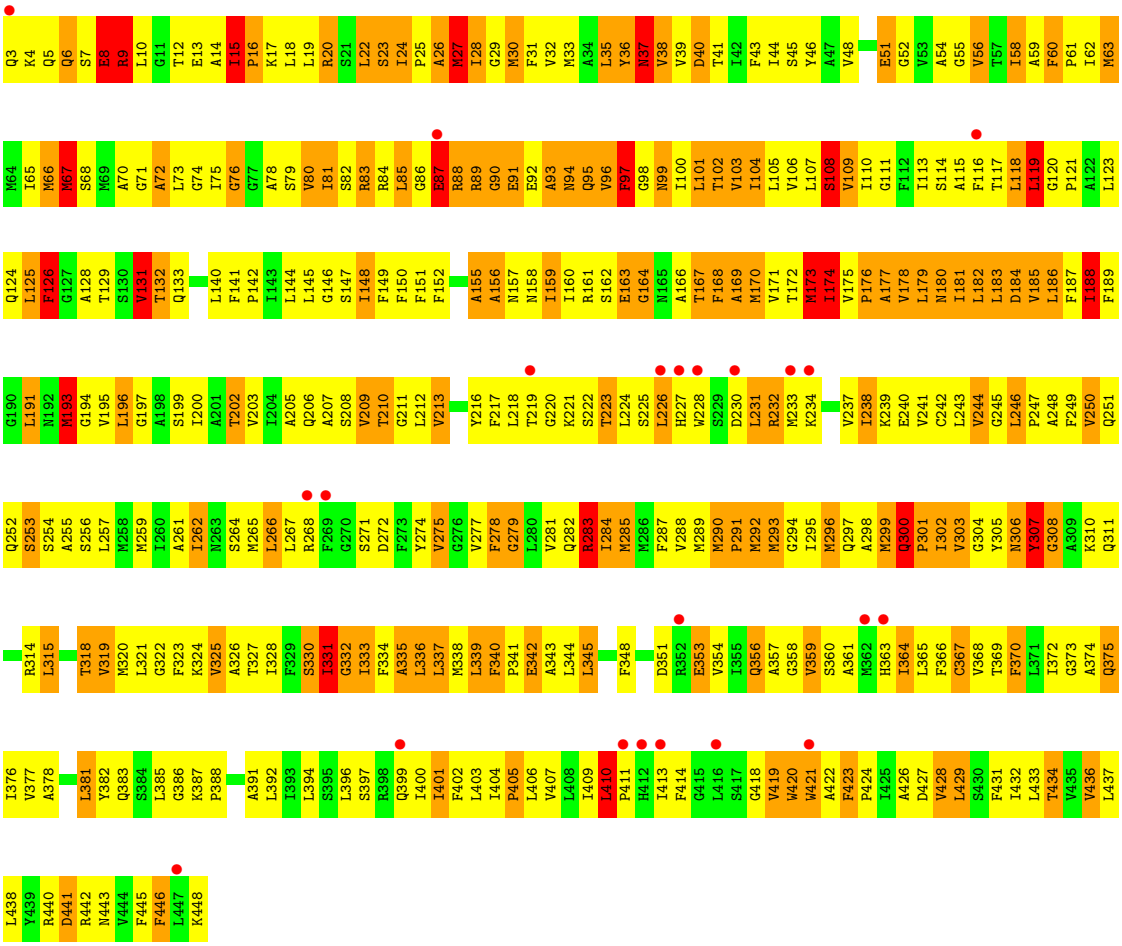
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3413	2263	548	574	28	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 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	90.76Å 95.07Å 101.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 14.96 – 3.18	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.20) 97.9 (14.96-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.290 , 0.310 0.296 , 0.333	Depositor DCC
R_{free} test set	745 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	154.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 83.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.086 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3413	wwPDB-VP
Average B, all atoms (Å^2)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.79% 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	0.57	0/3481	0.95	7/4714 (0.1%)

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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	ILE	C-N-CD	-10.88	96.67	120.60
1	A	308	GLY	N-CA-C	-9.09	90.39	113.10
1	A	315	LEU	CA-CB-CG	7.22	131.90	115.30
1	A	315	LEU	CB-CG-CD1	5.91	121.05	111.00
1	A	307	TYR	N-CA-C	-5.52	96.09	111.00
1	A	15	ILE	N-CA-C	5.14	124.87	111.00
1	A	86	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ILE	Peptide
1	A	306	ASN	Peptide
1	A	307	TYR	Peptide
1	A	8	GLU	Peptide
1	A	87	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3413	0	3608	496	0
All	All	3413	0	3608	496	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 71.

All (496) 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:224:LEU:O	1:A:226:LEU:HG	1.47	1.14
1:A:404:ILE:HG13	1:A:405:PRO:HD3	1.20	1.14
1:A:254:SER:HB3	1:A:399:GLN:HG2	1.25	1.12
1:A:78:ALA:HA	1:A:162:SER:HB2	1.20	1.10
1:A:404:ILE:HG13	1:A:405:PRO:CD	1.82	1.09
1:A:173:MET:O	1:A:175:VAL:N	1.85	1.09
1:A:24:ILE:HG13	1:A:25:PRO:HD3	1.35	1.07
1:A:402:PHE:CD1	1:A:429:LEU:HD21	1.92	1.05
1:A:78:ALA:HA	1:A:162:SER:CB	1.89	1.03
1:A:173:MET:O	1:A:176:PRO:HD2	1.59	1.01
1:A:407:VAL:O	1:A:411:PRO:HD2	1.58	1.01
1:A:19:LEU:HD12	1:A:321:LEU:HD23	1.42	1.00
1:A:88:ARG:O	1:A:90:GLY:N	1.93	1.00
1:A:369:THR:HA	1:A:372:ILE:HD12	1.41	0.97
1:A:96:VAL:HG22	1:A:237:VAL:HG11	1.47	0.97
1:A:320:MET:HB2	1:A:445:PHE:HE1	1.29	0.96
1:A:7:SER:HB2	1:A:223:THR:O	1.65	0.96
1:A:148:ILE:HG13	1:A:149:PHE:N	1.76	0.96
1:A:32:VAL:O	1:A:35:LEU:HB2	1.67	0.95
1:A:209:VAL:O	1:A:212:LEU:N	2.01	0.94
1:A:244:VAL:O	1:A:247:PRO:HD2	1.68	0.94
1:A:60:PHE:HB3	1:A:61:PRO:HD3	1.47	0.94
1:A:179:LEU:CD1	1:A:205:ALA:HA	1.98	0.93
1:A:373:GLY:O	1:A:377:VAL:HG23	1.68	0.92
1:A:96:VAL:HA	1:A:99:ASN:OD1	1.70	0.92
1:A:320:MET:HB2	1:A:445:PHE:CE1	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG23	1:A:189:PHE:H	1.33	0.90
1:A:402:PHE:CG	1:A:429:LEU:HD21	2.07	0.90
1:A:411:PRO:HD3	1:A:418:GLY:HA3	1.53	0.89
1:A:142:PRO:HG2	1:A:199:SER:HB2	1.54	0.89
1:A:364:ILE:HG22	1:A:420:TRP:HZ2	1.40	0.86
1:A:353:GLU:HA	1:A:356:GLN:HB2	1.57	0.86
1:A:227:HIS:HB3	1:A:231:LEU:HD22	1.57	0.85
1:A:289:MET:HA	1:A:289:MET:HE2	1.56	0.85
1:A:365:LEU:HD23	1:A:366:PHE:CE1	2.12	0.84
1:A:187:PHE:HA	1:A:191:LEU:HD12	1.60	0.84
1:A:184:ASP:O	1:A:186:LEU:N	2.11	0.83
1:A:87:GLU:HB2	1:A:308:GLY:HA2	1.59	0.83
1:A:78:ALA:CA	1:A:162:SER:HB2	2.04	0.83
1:A:29:GLY:HA2	1:A:32:VAL:HG23	1.61	0.82
1:A:394:LEU:HD13	1:A:437:LEU:HD12	1.60	0.82
1:A:237:VAL:O	1:A:240:GLU:N	2.11	0.81
1:A:357:ALA:HA	1:A:360:SER:HB2	1.62	0.81
1:A:224:LEU:O	1:A:226:LEU:CG	2.29	0.81
1:A:289:MET:HA	1:A:289:MET:CE	2.10	0.81
1:A:302:ILE:C	1:A:304:GLY:H	1.83	0.80
1:A:97:PHE:HE2	1:A:217:PHE:CE2	1.99	0.80
1:A:368:VAL:HG11	1:A:427:ASP:HB2	1.63	0.80
1:A:156:ALA:HB1	1:A:213:VAL:HG11	1.65	0.79
1:A:342:GLU:O	1:A:345:LEU:N	2.16	0.79
1:A:15:ILE:O	1:A:15:ILE:HD13	1.82	0.79
1:A:28:ILE:O	1:A:31:PHE:HB3	1.83	0.79
1:A:29:GLY:HA2	1:A:32:VAL:CG2	2.13	0.78
1:A:174:ILE:O	1:A:178:VAL:HG22	1.82	0.78
1:A:290:MET:HB3	1:A:291:PRO:HD2	1.66	0.78
1:A:385:LEU:O	1:A:387:LYS:N	2.17	0.78
1:A:407:VAL:O	1:A:411:PRO:CD	2.32	0.78
1:A:169:ALA:O	1:A:172:THR:N	2.16	0.77
1:A:372:ILE:O	1:A:376:ILE:HG22	1.84	0.77
1:A:18:LEU:HB3	1:A:302:ILE:HD11	1.66	0.77
1:A:170:MET:O	1:A:174:ILE:HG23	1.85	0.77
1:A:148:ILE:HG13	1:A:149:PHE:H	1.50	0.77
1:A:178:VAL:O	1:A:182:LEU:HG	1.85	0.77
1:A:279:GLY:O	1:A:283:ARG:HD2	1.86	0.75
1:A:281:VAL:HA	1:A:284:ILE:HD11	1.67	0.75
1:A:88:ARG:C	1:A:90:GLY:H	1.91	0.74
1:A:374:ALA:O	1:A:376:ILE:N	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:288:VAL:HG13	1.86	0.74
1:A:299:MET:CE	1:A:322:GLY:CA	2.66	0.74
1:A:368:VAL:HG21	1:A:424:PRO:HA	1.69	0.73
1:A:89:ARG:O	1:A:91:GLU:N	2.21	0.73
1:A:300:GLN:CB	1:A:301:PRO:HD3	2.19	0.73
1:A:370:PHE:H	1:A:370:PHE:HD2	1.34	0.73
1:A:59:ALA:HB1	1:A:140:LEU:HD13	1.69	0.73
1:A:63:MET:O	1:A:66:MET:HG3	1.89	0.73
1:A:254:SER:HB3	1:A:399:GLN:CG	2.13	0.73
1:A:281:VAL:HG12	1:A:281:VAL:O	1.89	0.72
1:A:179:LEU:HD13	1:A:205:ALA:HA	1.70	0.72
1:A:184:ASP:O	1:A:185:VAL:C	2.28	0.72
1:A:83:ARG:O	1:A:84:ARG:HG3	1.90	0.71
1:A:227:HIS:CD2	1:A:231:LEU:HB2	2.24	0.71
1:A:299:MET:CE	1:A:322:GLY:HA3	2.21	0.71
1:A:17:LYS:HA	1:A:20:ARG:HB2	1.72	0.71
1:A:404:ILE:CG1	1:A:405:PRO:HD3	2.11	0.71
1:A:118:LEU:HA	1:A:121:PRO:HG2	1.71	0.71
1:A:298:ALA:O	1:A:301:PRO:HD2	1.91	0.71
1:A:31:PHE:N	1:A:290:MET:SD	2.64	0.70
1:A:365:LEU:HA	1:A:424:PRO:HG3	1.73	0.70
1:A:259:MET:HA	1:A:262:ILE:HG13	1.71	0.70
1:A:288:VAL:O	1:A:288:VAL:CG1	2.38	0.70
1:A:368:VAL:HG11	1:A:427:ASP:CB	2.21	0.70
1:A:382:TYR:OH	1:A:437:LEU:O	2.09	0.70
1:A:410:LEU:HD21	1:A:421:TRP:HB2	1.73	0.70
1:A:36:TYR:O	1:A:40:ASP:HB3	1.92	0.70
1:A:156:ALA:CB	1:A:213:VAL:HG11	2.21	0.70
1:A:40:ASP:O	1:A:43:PHE:HB2	1.92	0.70
1:A:142:PRO:HG3	1:A:199:SER:OG	1.90	0.70
1:A:179:LEU:O	1:A:183:LEU:HB2	1.92	0.69
1:A:290:MET:HA	1:A:293:MET:HB2	1.74	0.69
1:A:367:CYS:O	1:A:367:CYS:SG	2.49	0.69
1:A:24:ILE:HG13	1:A:25:PRO:CD	2.17	0.69
1:A:142:PRO:CG	1:A:199:SER:HB2	2.22	0.69
1:A:36:TYR:HA	1:A:181:ILE:HD11	1.74	0.69
1:A:304:GLY:O	1:A:307:TYR:O	2.10	0.69
1:A:103:VAL:O	1:A:106:VAL:HB	1.93	0.69
1:A:111:GLY:HA2	1:A:114:SER:OG	1.93	0.69
1:A:147:SER:HB3	1:A:151:PHE:HE1	1.58	0.69
1:A:30:MET:HB3	1:A:290:MET:SD	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:N	1:A:341:PRO:HD3	2.08	0.69
1:A:202:THR:HG22	1:A:202:THR:O	1.91	0.68
1:A:293:MET:CE	1:A:376:ILE:HD11	2.24	0.68
1:A:364:ILE:C	1:A:420:TRP:HE1	1.97	0.68
1:A:147:SER:HB3	1:A:151:PHE:CE1	2.29	0.68
1:A:188:ILE:HG23	1:A:189:PHE:N	2.08	0.67
1:A:163:GLU:HG3	1:A:164:GLY:H	1.60	0.67
1:A:43:PHE:HB3	1:A:188:ILE:HD12	1.77	0.66
1:A:149:PHE:CD2	1:A:207:ALA:HA	2.30	0.66
1:A:410:LEU:O	1:A:414:PHE:HB2	1.96	0.66
1:A:255:ALA:HB2	1:A:399:GLN:HE22	1.61	0.66
1:A:107:LEU:O	1:A:109:VAL:N	2.28	0.66
1:A:299:MET:HE3	1:A:322:GLY:CA	2.24	0.66
1:A:41:THR:HA	1:A:44:ILE:HD12	1.78	0.66
1:A:149:PHE:HD2	1:A:207:ALA:HA	1.60	0.66
1:A:166:ALA:O	1:A:169:ALA:HB3	1.95	0.66
1:A:299:MET:CE	1:A:322:GLY:HA2	2.25	0.66
1:A:60:PHE:O	1:A:63:MET:N	2.30	0.65
1:A:334:PHE:CE1	1:A:367:CYS:HA	2.31	0.65
1:A:357:ALA:HA	1:A:360:SER:CB	2.25	0.65
1:A:369:THR:HA	1:A:372:ILE:CD1	2.21	0.65
1:A:169:ALA:O	1:A:171:VAL:N	2.30	0.65
1:A:80:VAL:HG11	1:A:96:VAL:HG21	1.80	0.64
1:A:96:VAL:CG2	1:A:237:VAL:HG11	2.25	0.64
1:A:188:ILE:CG2	1:A:189:PHE:H	2.09	0.64
1:A:299:MET:HE1	1:A:322:GLY:CA	2.28	0.64
1:A:94:ASN:O	1:A:231:LEU:HD21	1.98	0.64
1:A:368:VAL:CG2	1:A:424:PRO:HA	2.27	0.63
1:A:16:PRO:O	1:A:20:ARG:HG2	1.99	0.63
1:A:97:PHE:CE2	1:A:217:PHE:CE2	2.83	0.63
1:A:128:ALA:HB1	1:A:133:GLN:OE1	1.98	0.63
1:A:281:VAL:O	1:A:281:VAL:CG1	2.47	0.63
1:A:300:GLN:HB2	1:A:301:PRO:HD3	1.80	0.63
1:A:283:ARG:O	1:A:287:PHE:HB2	1.98	0.63
1:A:369:THR:CA	1:A:372:ILE:HD12	2.25	0.63
1:A:32:VAL:O	1:A:35:LEU:CB	2.46	0.62
1:A:339:LEU:C	1:A:341:PRO:CD	2.67	0.62
1:A:7:SER:O	1:A:9:ARG:N	2.33	0.62
1:A:59:ALA:O	1:A:62:ILE:HD12	2.00	0.62
1:A:81:ILE:CG2	1:A:81:ILE:O	2.47	0.62
1:A:306:ASN:ND2	1:A:311:GLN:HB2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:ND2	1:A:172:THR:OG1	2.33	0.61
1:A:173:MET:O	1:A:176:PRO:CD	2.42	0.61
1:A:410:LEU:HB3	1:A:418:GLY:CA	2.31	0.61
1:A:16:PRO:HD2	1:A:17:LYS:N	2.15	0.61
1:A:255:ALA:HB2	1:A:399:GLN:NE2	2.14	0.61
1:A:407:VAL:HG12	1:A:411:PRO:HG2	1.81	0.61
1:A:148:ILE:CG1	1:A:149:PHE:N	2.58	0.60
1:A:293:MET:O	1:A:296:MET:HB3	2.01	0.60
1:A:6:GLN:HG2	1:A:88:ARG:NH2	2.17	0.60
1:A:97:PHE:O	1:A:101:LEU:HD23	2.01	0.60
1:A:323:PHE:HD1	1:A:377:VAL:HG11	1.67	0.60
1:A:76:GLY:HA2	1:A:244:VAL:HB	1.84	0.60
1:A:225:SER:O	1:A:226:LEU:HD23	2.02	0.60
1:A:142:PRO:HG2	1:A:199:SER:CB	2.31	0.59
1:A:442:ARG:O	1:A:446:PHE:HB3	2.02	0.59
1:A:16:PRO:HD2	1:A:17:LYS:H	1.67	0.59
1:A:27:MET:HE1	1:A:295:ILE:HG12	1.82	0.59
1:A:9:ARG:HB2	1:A:223:THR:CG2	2.32	0.59
1:A:96:VAL:HG13	1:A:100:ILE:HD11	1.84	0.59
1:A:217:PHE:O	1:A:221:LYS:HD3	2.03	0.59
1:A:303:VAL:HG12	1:A:385:LEU:HD21	1.82	0.59
1:A:323:PHE:CD1	1:A:377:VAL:HG11	2.38	0.59
1:A:364:ILE:HG22	1:A:420:TRP:CZ2	2.31	0.59
1:A:334:PHE:HE1	1:A:367:CYS:HA	1.66	0.59
1:A:59:ALA:HB1	1:A:140:LEU:CD1	2.32	0.59
1:A:96:VAL:HG12	1:A:97:PHE:N	2.18	0.58
1:A:16:PRO:CD	1:A:17:LYS:N	2.65	0.58
1:A:247:PRO:O	1:A:251:GLN:HG3	2.03	0.58
1:A:299:MET:HE1	1:A:322:GLY:HA2	1.84	0.58
1:A:335:ALA:O	1:A:338:MET:N	2.29	0.58
1:A:423:PHE:HB2	1:A:424:PRO:CD	2.33	0.58
1:A:370:PHE:N	1:A:370:PHE:CD2	2.68	0.58
1:A:374:ALA:C	1:A:376:ILE:H	2.06	0.57
1:A:93:ALA:O	1:A:94:ASN:C	2.41	0.57
1:A:27:MET:SD	1:A:294:GLY:HA3	2.44	0.57
1:A:108:SER:OG	1:A:148:ILE:HA	2.05	0.57
1:A:221:LYS:HB3	1:A:226:LEU:HD12	1.86	0.57
1:A:339:LEU:C	1:A:341:PRO:HD3	2.25	0.57
1:A:152:PHE:O	1:A:155:ALA:HB3	2.05	0.57
1:A:410:LEU:HD23	1:A:418:GLY:HA2	1.86	0.57
1:A:325:VAL:HG22	1:A:326:ALA:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HD3	1:A:5:GLN:H	1.70	0.57
1:A:15:ILE:HA	1:A:18:LEU:HB2	1.86	0.57
1:A:54:ALA:O	1:A:58:ILE:HG13	2.05	0.56
1:A:302:ILE:C	1:A:304:GLY:N	2.54	0.56
1:A:331:ILE:HG13	1:A:332:GLY:N	2.18	0.56
1:A:142:PRO:CG	1:A:199:SER:CB	2.83	0.56
1:A:157:ASN:HD22	1:A:160:ILE:HD11	1.69	0.56
1:A:375:GLN:HA	1:A:434:THR:HG21	1.88	0.56
1:A:96:VAL:O	1:A:97:PHE:C	2.44	0.56
1:A:152:PHE:CD2	1:A:210:THR:HG23	2.40	0.56
1:A:288:VAL:O	1:A:289:MET:CE	2.53	0.56
1:A:353:GLU:CA	1:A:356:GLN:HB2	2.34	0.56
1:A:31:PHE:HA	1:A:290:MET:HE1	1.87	0.56
1:A:345:LEU:HG	1:A:359:VAL:HG23	1.87	0.56
1:A:94:ASN:N	1:A:225:SER:OG	2.38	0.56
1:A:337:LEU:HD21	1:A:366:PHE:CG	2.41	0.56
1:A:302:ILE:HG22	1:A:303:VAL:N	2.20	0.56
1:A:125:LEU:O	1:A:126:PHE:HB2	2.05	0.55
1:A:420:TRP:O	1:A:424:PRO:HD2	2.06	0.55
1:A:155:ALA:O	1:A:156:ALA:C	2.45	0.55
1:A:60:PHE:HB3	1:A:61:PRO:CD	2.31	0.55
1:A:423:PHE:HB2	1:A:424:PRO:HD3	1.88	0.55
1:A:6:GLN:HG2	1:A:88:ARG:HH21	1.70	0.55
1:A:97:PHE:HE2	1:A:217:PHE:CD2	2.23	0.55
1:A:85:LEU:HD13	1:A:224:LEU:HD13	1.88	0.55
1:A:148:ILE:CG1	1:A:149:PHE:H	2.17	0.55
1:A:88:ARG:O	1:A:88:ARG:HG2	2.06	0.55
1:A:97:PHE:C	1:A:97:PHE:CD1	2.80	0.55
1:A:18:LEU:HD21	1:A:305:TYR:OH	2.07	0.55
1:A:13:GLU:O	1:A:13:GLU:HG3	2.06	0.54
1:A:25:PRO:HB2	1:A:166:ALA:HB1	1.88	0.54
1:A:159:ILE:HG13	1:A:160:ILE:N	2.22	0.54
1:A:184:ASP:O	1:A:187:PHE:N	2.40	0.54
1:A:237:VAL:HG22	1:A:240:GLU:HG3	1.89	0.54
1:A:107:LEU:C	1:A:109:VAL:N	2.61	0.54
1:A:239:LYS:O	1:A:243:LEU:HG	2.07	0.54
1:A:97:PHE:C	1:A:97:PHE:HD1	2.10	0.54
1:A:247:PRO:HG2	1:A:383:GLN:NE2	2.21	0.54
1:A:290:MET:CB	1:A:291:PRO:HD2	2.35	0.54
1:A:159:ILE:O	1:A:162:SER:N	2.39	0.54
1:A:266:LEU:HD13	1:A:278:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:O	1:A:202:THR:CG2	2.55	0.54
1:A:18:LEU:O	1:A:22:LEU:HB2	2.08	0.54
1:A:301:PRO:HD2	1:A:302:ILE:H	1.73	0.54
1:A:361:ALA:O	1:A:365:LEU:HB2	2.08	0.53
1:A:292:MET:O	1:A:293:MET:C	2.46	0.53
1:A:19:LEU:HD12	1:A:321:LEU:CD2	2.28	0.53
1:A:111:GLY:O	1:A:144:LEU:HD23	2.08	0.53
1:A:173:MET:C	1:A:175:VAL:H	2.07	0.53
1:A:247:PRO:HG3	1:A:388:PRO:HB2	1.90	0.53
1:A:262:ILE:HA	1:A:265:MET:HG2	1.90	0.53
1:A:169:ALA:O	1:A:170:MET:C	2.47	0.53
1:A:410:LEU:HB3	1:A:418:GLY:HA3	1.90	0.53
1:A:29:GLY:CA	1:A:32:VAL:HG23	2.33	0.53
1:A:38:VAL:HG12	1:A:39:VAL:HG13	1.89	0.53
1:A:13:GLU:OE2	1:A:314:ARG:HB2	2.09	0.53
1:A:252:GLN:O	1:A:254:SER:N	2.41	0.53
1:A:330:SER:OG	1:A:373:GLY:N	2.42	0.53
1:A:410:LEU:HB3	1:A:418:GLY:HA2	1.91	0.53
1:A:290:MET:O	1:A:291:PRO:C	2.47	0.53
1:A:337:LEU:CD2	1:A:366:PHE:CG	2.92	0.53
1:A:176:PRO:O	1:A:177:ALA:C	2.47	0.52
1:A:10:LEU:HD22	1:A:18:LEU:HD12	1.91	0.52
1:A:66:MET:HB2	1:A:151:PHE:CE2	2.43	0.52
1:A:174:ILE:O	1:A:177:ALA:HB3	2.10	0.52
1:A:38:VAL:HG12	1:A:39:VAL:N	2.25	0.52
1:A:72:ALA:HB2	1:A:249:PHE:HB3	1.92	0.52
1:A:288:VAL:HG13	1:A:333:ILE:HG12	1.90	0.52
1:A:303:VAL:HG12	1:A:303:VAL:O	2.09	0.52
1:A:374:ALA:O	1:A:377:VAL:N	2.37	0.52
1:A:96:VAL:O	1:A:99:ASN:N	2.43	0.52
1:A:184:ASP:C	1:A:186:LEU:N	2.63	0.52
1:A:325:VAL:O	1:A:326:ALA:C	2.46	0.52
1:A:145:LEU:N	1:A:146:GLY:HA3	2.25	0.52
1:A:250:VAL:HG12	1:A:251:GLN:N	2.24	0.52
1:A:161:ARG:NH1	1:A:297:GLN:NE2	2.57	0.52
1:A:15:ILE:O	1:A:15:ILE:CD1	2.57	0.51
1:A:46:TYR:HB3	1:A:189:PHE:CZ	2.45	0.51
1:A:105:LEU:HA	1:A:108:SER:HB2	1.91	0.51
1:A:24:ILE:HA	1:A:27:MET:HB2	1.90	0.51
1:A:31:PHE:CE2	1:A:35:LEU:HD13	2.45	0.51
1:A:220:GLY:O	1:A:221:LYS:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PHE:O	1:A:253:SER:OG	2.27	0.51
1:A:120:GLY:O	1:A:121:PRO:C	2.48	0.51
1:A:397:SER:HB2	1:A:402:PHE:CE1	2.45	0.51
1:A:163:GLU:CG	1:A:164:GLY:H	2.23	0.51
1:A:195:VAL:O	1:A:197:GLY:N	2.43	0.51
1:A:237:VAL:HA	1:A:240:GLU:CG	2.41	0.51
1:A:410:LEU:CD2	1:A:421:TRP:HB2	2.40	0.51
1:A:441:ASP:C	1:A:443:ASN:H	2.13	0.51
1:A:245:GLY:O	1:A:246:LEU:C	2.47	0.51
1:A:23:SER:OG	1:A:24:ILE:N	2.43	0.51
1:A:85:LEU:CD1	1:A:224:LEU:HD13	2.41	0.51
1:A:78:ALA:CA	1:A:162:SER:CB	2.77	0.51
1:A:107:LEU:C	1:A:109:VAL:H	2.14	0.51
1:A:82:SER:HB2	1:A:304:GLY:HA3	1.93	0.51
1:A:84:ARG:O	1:A:85:LEU:HG	2.11	0.50
1:A:174:ILE:HG13	1:A:175:VAL:N	2.25	0.50
1:A:232:ARG:O	1:A:232:ARG:NE	2.44	0.50
1:A:274:TYR:O	1:A:277:VAL:HG22	2.11	0.50
1:A:170:MET:O	1:A:174:ILE:N	2.45	0.50
1:A:318:THR:O	1:A:319:VAL:C	2.50	0.50
1:A:428:VAL:CG1	1:A:429:LEU:N	2.74	0.50
1:A:302:ILE:O	1:A:304:GLY:N	2.44	0.50
1:A:330:SER:OG	1:A:373:GLY:CA	2.60	0.50
1:A:334:PHE:HB2	1:A:369:THR:HB	1.92	0.50
1:A:28:ILE:O	1:A:32:VAL:HG23	2.11	0.50
1:A:209:VAL:O	1:A:210:THR:C	2.49	0.50
1:A:6:GLN:O	1:A:6:GLN:HG3	2.12	0.50
1:A:37:ASN:O	1:A:38:VAL:C	2.50	0.50
1:A:282:GLN:O	1:A:285:MET:N	2.45	0.49
1:A:359:VAL:O	1:A:359:VAL:HG13	2.11	0.49
1:A:8:GLU:O	1:A:9:ARG:C	2.51	0.49
1:A:321:LEU:O	1:A:324:LYS:HB3	2.12	0.49
1:A:107:LEU:O	1:A:110:ILE:N	2.44	0.49
1:A:419:VAL:O	1:A:423:PHE:CD1	2.65	0.49
1:A:25:PRO:HA	1:A:170:MET:SD	2.52	0.49
1:A:75:ILE:O	1:A:76:GLY:C	2.50	0.49
1:A:36:TYR:O	1:A:37:ASN:O	2.31	0.49
1:A:252:GLN:C	1:A:254:SER:N	2.65	0.49
1:A:354:VAL:O	1:A:358:GLY:HA3	2.13	0.49
1:A:93:ALA:O	1:A:95:GLN:N	2.45	0.49
1:A:161:ARG:HH12	1:A:297:GLN:NE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PHE:CE1	1:A:101:LEU:HD21	2.48	0.49
1:A:227:HIS:HD2	1:A:231:LEU:HB2	1.78	0.49
1:A:241:VAL:HG12	1:A:242:CYS:N	2.28	0.49
1:A:300:GLN:CB	1:A:301:PRO:CD	2.89	0.49
1:A:99:ASN:O	1:A:99:ASN:ND2	2.46	0.48
1:A:173:MET:O	1:A:174:ILE:C	2.49	0.48
1:A:66:MET:HB2	1:A:151:PHE:HE2	1.78	0.48
1:A:94:ASN:HB2	1:A:225:SER:HB2	1.95	0.48
1:A:245:GLY:O	1:A:248:ALA:N	2.46	0.48
1:A:31:PHE:C	1:A:31:PHE:CD2	2.86	0.48
1:A:288:VAL:O	1:A:289:MET:HE2	2.13	0.48
1:A:67:MET:O	1:A:67:MET:HG3	2.14	0.48
1:A:219:THR:O	1:A:220:GLY:C	2.50	0.48
1:A:16:PRO:CD	1:A:17:LYS:H	2.22	0.48
1:A:365:LEU:HD23	1:A:366:PHE:CD1	2.49	0.48
1:A:394:LEU:HD13	1:A:437:LEU:CD1	2.38	0.48
1:A:19:LEU:HD23	1:A:302:ILE:HD12	1.95	0.48
1:A:97:PHE:CE2	1:A:217:PHE:CD2	3.02	0.48
1:A:30:MET:HE3	1:A:293:MET:HB3	1.95	0.48
1:A:104:ILE:O	1:A:107:LEU:N	2.46	0.47
1:A:397:SER:HB2	1:A:402:PHE:HE1	1.79	0.47
1:A:335:ALA:O	1:A:337:LEU:N	2.46	0.47
1:A:441:ASP:C	1:A:443:ASN:N	2.67	0.47
1:A:35:LEU:O	1:A:38:VAL:HB	2.15	0.47
1:A:436:VAL:O	1:A:440:ARG:HB2	2.14	0.47
1:A:18:LEU:HB3	1:A:302:ILE:CD1	2.41	0.47
1:A:9:ARG:O	1:A:10:LEU:HG	2.14	0.47
1:A:10:LEU:C	1:A:12:THR:H	2.18	0.47
1:A:26:ALA:O	1:A:27:MET:C	2.51	0.47
1:A:76:GLY:HA2	1:A:244:VAL:CB	2.44	0.47
1:A:92:GLU:O	1:A:95:GLN:HB3	2.13	0.47
1:A:120:GLY:N	1:A:121:PRO:HD2	2.30	0.47
1:A:237:VAL:HA	1:A:240:GLU:HG3	1.95	0.47
1:A:318:THR:O	1:A:321:LEU:N	2.48	0.47
1:A:365:LEU:CD2	1:A:366:PHE:CE1	2.91	0.47
1:A:13:GLU:OE2	1:A:314:ARG:CB	2.63	0.46
1:A:32:VAL:O	1:A:35:LEU:N	2.48	0.46
1:A:423:PHE:O	1:A:424:PRO:C	2.53	0.46
1:A:131:VAL:HG23	1:A:132:THR:H	1.80	0.46
1:A:333:ILE:O	1:A:337:LEU:HB2	2.15	0.46
1:A:98:GLY:O	1:A:101:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:MET:HA	1:A:262:ILE:CG1	2.41	0.46
1:A:30:MET:CE	1:A:293:MET:CB	2.94	0.46
1:A:46:TYR:CB	1:A:189:PHE:HZ	2.29	0.46
1:A:10:LEU:HD22	1:A:18:LEU:CD1	2.45	0.46
1:A:129:THR:HB	1:A:132:THR:HG22	1.97	0.46
1:A:400:ILE:O	1:A:402:PHE:N	2.49	0.46
1:A:288:VAL:O	1:A:289:MET:HE3	2.16	0.46
1:A:340:PHE:O	1:A:344:LEU:HD12	2.16	0.46
1:A:6:GLN:CG	1:A:88:ARG:NH2	2.78	0.46
1:A:37:ASN:HB3	1:A:38:VAL:H	1.35	0.46
1:A:87:GLU:HB2	1:A:308:GLY:CA	2.36	0.46
1:A:124:GLN:HB3	1:A:133:GLN:HE22	1.80	0.46
1:A:339:LEU:CA	1:A:341:PRO:HD3	2.46	0.46
1:A:51:GLU:CD	1:A:52:GLY:N	2.70	0.45
1:A:81:ILE:O	1:A:81:ILE:HG23	2.15	0.45
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.64	0.45
1:A:149:PHE:HB3	1:A:206:GLN:O	2.16	0.45
1:A:206:GLN:HA	1:A:209:VAL:CG2	2.46	0.45
1:A:366:PHE:C	1:A:368:VAL:H	2.19	0.45
1:A:56:VAL:O	1:A:59:ALA:HB3	2.16	0.45
1:A:124:GLN:HA	1:A:128:ALA:HB2	1.98	0.45
1:A:124:GLN:O	1:A:126:PHE:N	2.40	0.45
1:A:278:PHE:O	1:A:279:GLY:C	2.55	0.45
1:A:428:VAL:O	1:A:432:ILE:HD12	2.17	0.45
1:A:436:VAL:HG12	1:A:437:LEU:N	2.30	0.45
1:A:38:VAL:O	1:A:40:ASP:N	2.50	0.45
1:A:396:LEU:O	1:A:401:ILE:HG23	2.16	0.45
1:A:115:ALA:C	1:A:117:THR:H	2.20	0.45
1:A:244:VAL:HA	1:A:388:PRO:HG3	1.99	0.45
1:A:289:MET:O	1:A:292:MET:N	2.50	0.45
1:A:195:VAL:C	1:A:197:GLY:N	2.70	0.45
1:A:431:PHE:O	1:A:434:THR:HG22	2.17	0.45
1:A:4:LYS:HG3	1:A:225:SER:HB3	1.98	0.45
1:A:41:THR:HA	1:A:44:ILE:CD1	2.44	0.45
1:A:73:LEU:HD23	1:A:241:VAL:CG1	2.47	0.45
1:A:188:ILE:CG2	1:A:189:PHE:N	2.76	0.45
1:A:237:VAL:HG13	1:A:240:GLU:HB2	1.98	0.45
1:A:431:PHE:HA	1:A:434:THR:HG22	1.99	0.45
1:A:13:GLU:HG3	1:A:15:ILE:HG22	1.99	0.44
1:A:252:GLN:C	1:A:254:SER:H	2.20	0.44
1:A:361:ALA:O	1:A:365:LEU:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:THR:O	1:A:330:SER:HB2	2.18	0.44
1:A:24:ILE:O	1:A:28:ILE:HG13	2.17	0.44
1:A:169:ALA:C	1:A:171:VAL:N	2.71	0.44
1:A:187:PHE:HA	1:A:191:LEU:CD1	2.39	0.44
1:A:407:VAL:HG22	1:A:422:ALA:HB1	2.00	0.44
1:A:126:PHE:HB3	1:A:264:SER:CB	2.47	0.44
1:A:237:VAL:O	1:A:238:ILE:C	2.55	0.44
1:A:319:VAL:HB	1:A:381:LEU:HD13	2.00	0.44
1:A:337:LEU:HD21	1:A:366:PHE:CD1	2.52	0.44
1:A:365:LEU:CA	1:A:424:PRO:HG3	2.45	0.44
1:A:124:GLN:C	1:A:126:PHE:H	2.21	0.44
1:A:172:THR:O	1:A:176:PRO:CD	2.66	0.44
1:A:290:MET:CB	1:A:291:PRO:CD	2.96	0.44
1:A:428:VAL:HG12	1:A:429:LEU:N	2.33	0.43
1:A:292:MET:HE1	1:A:330:SER:HA	2.00	0.43
1:A:299:MET:HE3	1:A:322:GLY:HA2	1.91	0.43
1:A:404:ILE:HG13	1:A:405:PRO:HD2	1.88	0.43
1:A:431:PHE:CD2	1:A:432:ILE:N	2.86	0.43
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.87	0.43
1:A:207:ALA:O	1:A:209:VAL:N	2.51	0.43
1:A:297:GLN:HG2	1:A:300:GLN:HE21	1.83	0.43
1:A:20:ARG:HA	1:A:20:ARG:HD3	1.84	0.43
1:A:79:SER:OG	1:A:244:VAL:HG11	2.18	0.43
1:A:107:LEU:HA	1:A:110:ILE:HD13	2.01	0.43
1:A:180:ASN:HD22	1:A:180:ASN:HA	1.56	0.43
1:A:299:MET:HE1	1:A:322:GLY:HA3	1.95	0.43
1:A:410:LEU:O	1:A:414:PHE:N	2.52	0.43
1:A:60:PHE:O	1:A:62:ILE:N	2.52	0.43
1:A:128:ALA:CB	1:A:133:GLN:OE1	2.65	0.43
1:A:102:THR:OG1	1:A:103:VAL:N	2.51	0.43
1:A:168:PHE:HZ	1:A:213:VAL:HG13	1.84	0.43
1:A:68:SER:HB2	1:A:252:GLN:HB2	2.00	0.43
1:A:80:VAL:HG12	1:A:81:ILE:N	2.34	0.43
1:A:289:MET:CE	1:A:289:MET:CA	2.90	0.43
1:A:142:PRO:HG3	1:A:199:SER:CB	2.48	0.42
1:A:240:GLU:HA	1:A:243:LEU:HD12	2.01	0.42
1:A:409:ILE:O	1:A:409:ILE:CG2	2.67	0.42
1:A:168:PHE:CZ	1:A:216:TYR:HB2	2.54	0.42
1:A:255:ALA:O	1:A:256:SER:C	2.58	0.42
1:A:364:ILE:CG2	1:A:420:TRP:HZ2	2.21	0.42
1:A:100:ILE:C	1:A:102:THR:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:HA2	1:A:248:ALA:HB3	2.01	0.42
1:A:419:VAL:O	1:A:423:PHE:HD1	2.01	0.42
1:A:233:MET:HG2	1:A:234:LYS:HG2	2.01	0.42
1:A:25:PRO:HB3	1:A:166:ALA:O	2.20	0.42
1:A:230:ASP:O	1:A:231:LEU:C	2.58	0.42
1:A:356:GLN:O	1:A:360:SER:HB2	2.20	0.42
1:A:363:HIS:O	1:A:365:LEU:N	2.52	0.42
1:A:423:PHE:O	1:A:426:ALA:N	2.53	0.42
1:A:299:MET:HE3	1:A:322:GLY:HA3	1.92	0.42
1:A:299:MET:O	1:A:300:GLN:C	2.57	0.42
1:A:342:GLU:O	1:A:344:LEU:N	2.53	0.42
1:A:35:LEU:O	1:A:36:TYR:C	2.56	0.42
1:A:72:ALA:CB	1:A:249:PHE:HD2	2.33	0.42
1:A:82:SER:C	1:A:84:ARG:H	2.23	0.42
1:A:382:TYR:HB2	1:A:391:ALA:HB2	2.01	0.42
1:A:38:VAL:C	1:A:40:ASP:H	2.23	0.42
1:A:80:VAL:O	1:A:82:SER:N	2.53	0.42
1:A:441:ASP:HB3	1:A:443:ASN:HD22	1.85	0.42
1:A:310:LYS:HB3	1:A:311:GLN:OE1	2.20	0.42
1:A:37:ASN:OD1	1:A:283:ARG:HG2	2.19	0.41
1:A:175:VAL:HA	1:A:178:VAL:CG2	2.50	0.41
1:A:325:VAL:O	1:A:328:ILE:N	2.52	0.41
1:A:330:SER:HB3	1:A:370:PHE:O	2.20	0.41
1:A:142:PRO:O	1:A:145:LEU:N	2.48	0.41
1:A:438:LEU:C	1:A:440:ARG:N	2.73	0.41
1:A:30:MET:CE	1:A:293:MET:HB3	2.50	0.41
1:A:72:ALA:HB2	1:A:249:PHE:HD2	1.85	0.41
1:A:119:LEU:HB3	1:A:120:GLY:H	1.68	0.41
1:A:210:THR:O	1:A:211:GLY:C	2.59	0.41
1:A:115:ALA:HA	1:A:119:LEU:HD23	2.02	0.41
1:A:218:LEU:O	1:A:221:LYS:HG2	2.20	0.41
1:A:299:MET:HA	1:A:302:ILE:HB	2.01	0.41
1:A:338:MET:C	1:A:341:PRO:HD3	2.41	0.41
1:A:372:ILE:O	1:A:372:ILE:CG2	2.68	0.41
1:A:374:ALA:C	1:A:376:ILE:N	2.70	0.41
1:A:224:LEU:HB3	1:A:225:SER:H	1.56	0.41
1:A:294:GLY:HA2	1:A:297:GLN:OE1	2.20	0.41
1:A:420:TRP:HZ3	1:A:421:TRP:CE3	2.38	0.41
1:A:52:GLY:C	1:A:54:ALA:N	2.71	0.41
1:A:156:ALA:O	1:A:160:ILE:HG23	2.21	0.41
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HE3	1:A:311:GLN:OE1	2.21	0.41
1:A:148:ILE:O	1:A:149:PHE:C	2.59	0.41
1:A:253:SER:O	1:A:257:LEU:HB2	2.21	0.41
1:A:339:LEU:C	1:A:341:PRO:HD2	2.41	0.41
1:A:372:ILE:O	1:A:373:GLY:C	2.59	0.41
1:A:403:LEU:O	1:A:407:VAL:HG23	2.21	0.41
1:A:420:TRP:O	1:A:422:ALA:N	2.53	0.41
1:A:39:VAL:HG23	1:A:181:ILE:CD1	2.51	0.41
1:A:83:ARG:C	1:A:84:ARG:HG3	2.41	0.41
1:A:151:PHE:O	1:A:152:PHE:C	2.58	0.41
1:A:448:LYS:HD2	1:A:448:LYS:HA	1.88	0.41
1:A:167:THR:O	1:A:171:VAL:HG23	2.21	0.40
1:A:70:ALA:O	1:A:74:GLY:N	2.54	0.40
1:A:193:MET:HB2	1:A:197:GLY:HA3	2.03	0.40
1:A:272:ASP:HA	1:A:275:VAL:HG23	2.03	0.40
1:A:71:GLY:O	1:A:75:ILE:HG12	2.22	0.40
1:A:302:ILE:HG21	1:A:318:THR:HG21	2.02	0.40
1:A:388:PRO:O	1:A:392:LEU:HB2	2.21	0.40
1:A:410:LEU:CB	1:A:418:GLY:HA2	2.51	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	444/446 (100%)	228 (51%)	123 (28%)	93 (21%)	0 0

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ARG

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Mol	Chain	Res	Type
1	A	16	PRO
1	A	27	MET
1	A	37	ASN
1	A	38	VAL
1	A	56	VAL
1	A	60	PHE
1	A	81	ILE
1	A	89	ARG
1	A	90	GLY
1	A	93	ALA
1	A	94	ASN
1	A	97	PHE
1	A	108	SER
1	A	116	PHE
1	A	126	PHE
1	A	170	MET
1	A	174	ILE
1	A	177	ALA
1	A	185	VAL
1	A	188	ILE
1	A	196	LEU
1	A	291	PRO
1	A	303	VAL
1	A	335	ALA
1	A	343	ALA
1	A	375	GLN
1	A	386	GLY
1	A	413	ILE
1	A	14	ALA
1	A	23	SER
1	A	26	ALA
1	A	28	ILE
1	A	96	VAL
1	A	104	ILE
1	A	119	LEU
1	A	125	LEU
1	A	155	ALA
1	A	169	ALA
1	A	208	SER
1	A	231	LEU
1	A	253	SER
1	A	261	ALA

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Mol	Chain	Res	Type
1	A	279	GLY
1	A	301	PRO
1	A	331	ILE
1	A	342	GLU
1	A	420	TRP
1	A	6	GLN
1	A	83	ARG
1	A	85	LEU
1	A	87	GLU
1	A	163	GLU
1	A	184	ASP
1	A	283	ARG
1	A	293	MET
1	A	340	PHE
1	A	421	TRP
1	A	15	ILE
1	A	88	ARG
1	A	101	LEU
1	A	102	THR
1	A	156	ALA
1	A	176	PRO
1	A	290	MET
1	A	332	GLY
1	A	378	ALA
1	A	423	PHE
1	A	36	TYR
1	A	67	MET
1	A	72	ALA
1	A	164	GLY
1	A	191	LEU
1	A	193	MET
1	A	222	SER
1	A	336	LEU
1	A	173	MET
1	A	194	GLY
1	A	202	THR
1	A	76	GLY
1	A	113	ILE
1	A	364	ILE
1	A	410	LEU
1	A	238	ILE
1	A	55	GLY

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Mol	Chain	Res	Type
1	A	80	VAL
1	A	131	VAL
1	A	244	VAL
1	A	333	ILE
1	A	300	GLN
1	A	405	PRO
1	A	436	VAL

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	366/366 (100%)	260 (71%)	106 (29%)	0 1

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	ARG
1	A	15	ILE
1	A	20	ARG
1	A	22	LEU
1	A	24	ILE
1	A	27	MET
1	A	30	MET
1	A	33	MET
1	A	35	LEU
1	A	37	ASN
1	A	40	ASP
1	A	45	SER
1	A	48	VAL
1	A	51	GLU
1	A	58	ILE
1	A	63	MET
1	A	65	ILE
1	A	66	MET

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Mol	Chain	Res	Type
1	A	67	MET
1	A	91	GLU
1	A	95	GLN
1	A	97	PHE
1	A	99	ASN
1	A	103	VAL
1	A	108	SER
1	A	109	VAL
1	A	118	LEU
1	A	119	LEU
1	A	123	LEU
1	A	126	PHE
1	A	131	VAL
1	A	132	THR
1	A	141	PHE
1	A	148	ILE
1	A	150	PHE
1	A	158	ASN
1	A	159	ILE
1	A	167	THR
1	A	168	PHE
1	A	173	MET
1	A	174	ILE
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	193	MET
1	A	196	LEU
1	A	200	ILE
1	A	203	VAL
1	A	209	VAL
1	A	210	THR
1	A	213	VAL
1	A	223	THR
1	A	226	LEU
1	A	228	TRP
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	250	VAL
1	A	262	ILE
1	A	266	LEU
1	A	267	LEU
1	A	268	ARG
1	A	271	SER
1	A	275	VAL
1	A	278	PHE
1	A	283	ARG
1	A	284	ILE
1	A	285	MET
1	A	292	MET
1	A	296	MET
1	A	299	MET
1	A	300	GLN
1	A	302	ILE
1	A	315	LEU
1	A	318	THR
1	A	319	VAL
1	A	325	VAL
1	A	330	SER
1	A	331	ILE
1	A	336	LEU
1	A	337	LEU
1	A	339	LEU
1	A	345	LEU
1	A	348	PHE
1	A	351	ASP
1	A	353	GLU
1	A	356	GLN
1	A	359	VAL
1	A	367	CYS
1	A	370	PHE
1	A	381	LEU
1	A	401	ILE
1	A	406	LEU
1	A	410	LEU
1	A	419	VAL
1	A	428	VAL
1	A	429	LEU
1	A	433	LEU

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Mol	Chain	Res	Type
1	A	434	THR
1	A	441	ASP
1	A	446	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	180	ASN
1	A	227	HIS
1	A	300	GLN
1	A	306	ASN
1	A	399	GLN
1	A	412	HIS
1	A	443	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	446/446 (100%)	-0.22	22 (4%) 29 17	121, 182, 250, 337	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	PHE	5.2
1	A	416	LEU	5.1
1	A	412	HIS	4.9
1	A	413	ILE	4.6
1	A	233	MET	4.2
1	A	447	LEU	4.1
1	A	219	THR	4.1
1	A	362	MET	3.6
1	A	411	PRO	3.5
1	A	87	GLU	3.2
1	A	268	ARG	3.2
1	A	234	LYS	3.2
1	A	363	HIS	2.8
1	A	3	GLN	2.7
1	A	226	LEU	2.5
1	A	227	HIS	2.4
1	A	399	GLN	2.4
1	A	228	TRP	2.3
1	A	116	PHE	2.3
1	A	230	ASP	2.2
1	A	352	ARG	2.1
1	A	421	TRP	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.