Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 08:20 PM EST

PDB ID	:	4HUL
Title	:	MATE transporter NorM-NG in complex with Cs+ and monobody
Authors	:	Lu, M.
Deposited on	:	2012-11-02
Resolution	:	3.81 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 (i) 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 (i)) were used in the production of this report:

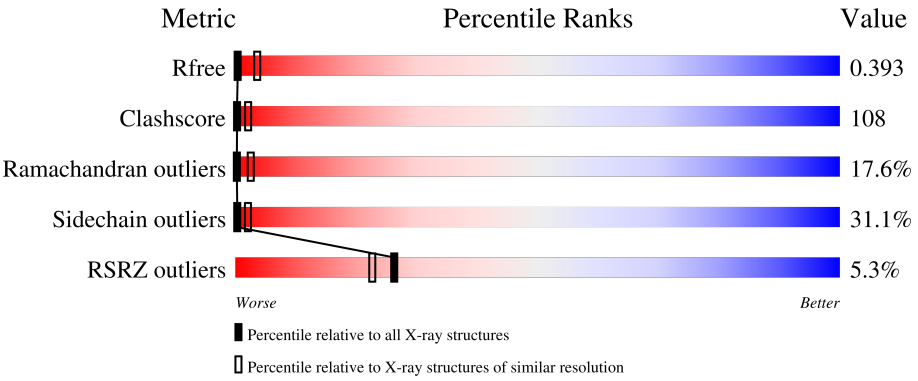
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.81 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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	459	5% 12% 53% 29% 6%
2	B	99	5% 8% 43% 35% 5% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4216 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 Multidrug efflux protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3508	2338	558	589	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	SER	-	expression tag	UNP E8SM44
A	461	SER	-	expression tag	UNP E8SM44
A	462	GLY	-	expression tag	UNP E8SM44
A	463	LEU	-	expression tag	UNP E8SM44

- Molecule 2 is a protein called Protein B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	0	0	0
			707	457	110	140			

- Molecule 3 is CESIUM ION (three-letter code: CS) (formula: Cs).

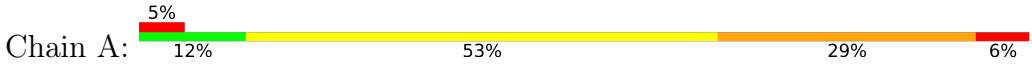
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cs	0	0
			1	1		

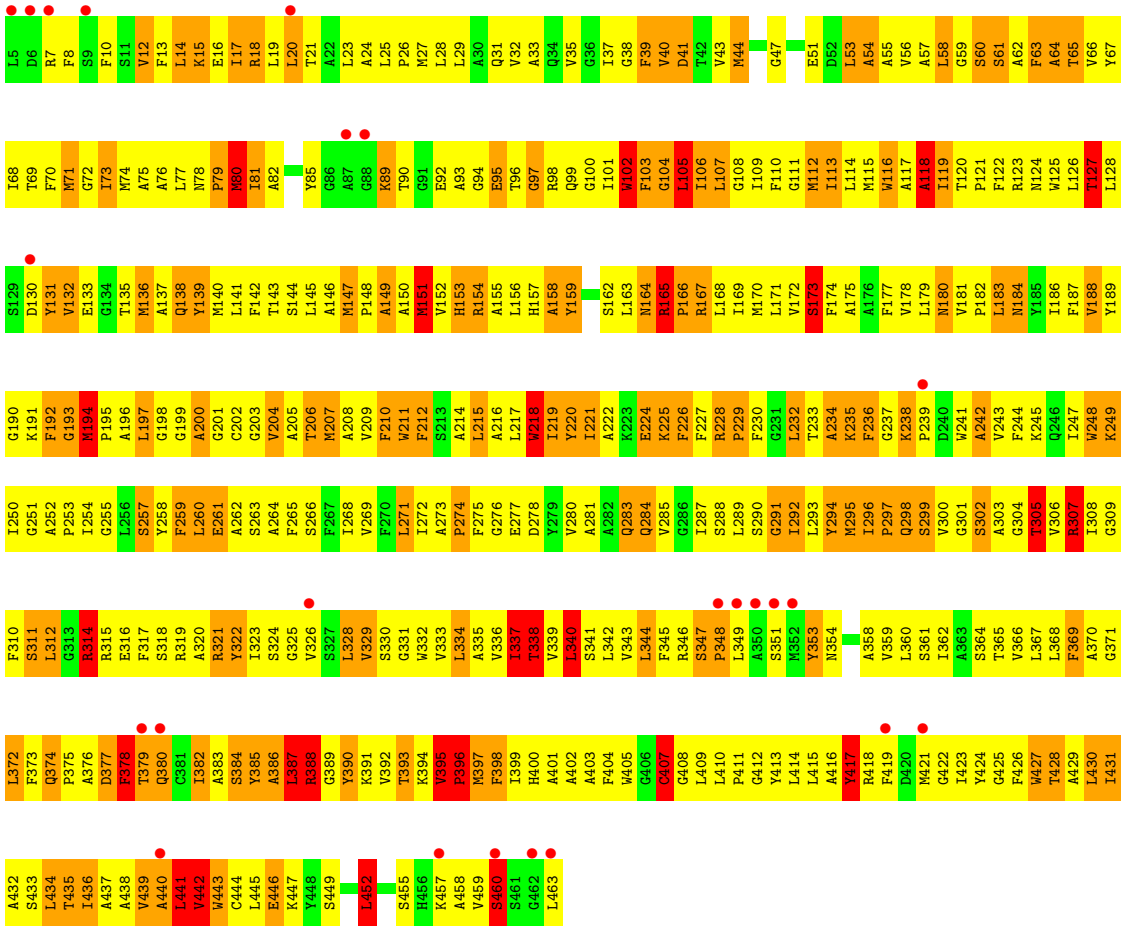
3 Residue-property plots (i)

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: Multidrug efflux protein

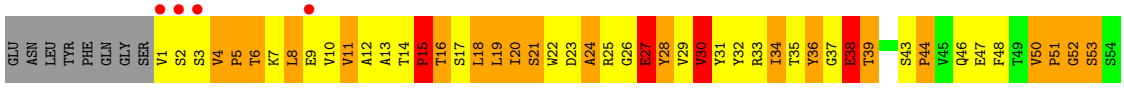
Chain A:





• Molecule 2: Protein B

Chain B:




S55
T56
A57
T58
I59
S60
G61
L62
S63
P64
G65
V66
D67
Y68
T69
I70
T71
V72
Y73
A74
R75
S76
Y77
Y78
W79
G80
W81
Y82
S83
P84
I85
S86
I87
N88
Y89
R90
T91

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.33Å 118.33Å 227.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.81 52.48 – 3.81	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.81) 98.3 (52.48-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.311 , 0.376 0.318 , 0.393	Depositor DCC
R_{free} test set	933 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	119.9	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 135.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	0.197 for -h,-k,l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	4216	wwPDB-VP
Average B, all atoms (Å^2)	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

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

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	0.92	5/3605 (0.1%)	1.08	10/4898 (0.2%)
2	B	0.95	0/729	1.19	2/1004 (0.2%)
All	All	0.92	5/4334 (0.1%)	1.10	12/5902 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	24
2	B	0	4
All	All	0	28

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	TRP	CD2-CE2	5.48	1.48	1.41
1	A	211	TRP	CD2-CE2	5.37	1.47	1.41
1	A	102	TRP	CD2-CE2	5.32	1.47	1.41
1	A	218	TRP	CD2-CE2	5.25	1.47	1.41
1	A	443	TRP	CD2-CE2	5.22	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	30	VAL	CB-CA-C	-8.80	94.68	111.40
1	A	340	LEU	CA-CB-CG	6.67	130.64	115.30
1	A	221	ILE	N-CA-C	-6.12	94.49	111.00
1	A	441	LEU	CA-CB-CG	6.07	129.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	312	LEU	CA-CB-CG	5.86	128.77	115.30
2	B	27	GLU	C-N-CA	-5.65	107.57	121.70
1	A	407	CYS	CA-CB-SG	5.51	123.92	114.00
1	A	105	LEU	CA-CB-CG	-5.33	103.03	115.30
1	A	340	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	218	TRP	CA-CB-CG	-5.01	104.18	113.70
1	A	388	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ALA	Peptide
1	A	131	TYR	Peptide
1	A	138	GLN	Peptide
1	A	165	ARG	Peptide
1	A	188	VAL	Peptide
1	A	194	MET	Peptide
1	A	220	TYR	Peptide
1	A	226	PHE	Peptide
1	A	249	LYS	Peptide
1	A	273	ALA	Peptide
1	A	314	ARG	Peptide
1	A	322	TYR	Peptide
1	A	337	ILE	Peptide
1	A	338	THR	Peptide
1	A	387	LEU	Peptide
1	A	393	THR	Peptide
1	A	395	VAL	Peptide
1	A	396	PRO	Peptide
1	A	40	VAL	Peptide
1	A	430	LEU	Peptide
1	A	442	VAL	Peptide
1	A	446	GLU	Peptide
1	A	452	LEU	Peptide
1	A	54	ALA	Peptide
2	B	15	PRO	Peptide
2	B	27	GLU	Peptide
2	B	4	VAL	Peptide
2	B	82	TYR	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	3508	0	3586	744	0
2	B	707	0	681	189	0
3	A	1	0	0	0	0
All	All	4216	0	4267	918	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 108.

All (918) 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:158:ALA:HB2	1:A:217:LEU:CD1	1.28	1.62
1:A:158:ALA:CB	1:A:217:LEU:HD11	1.47	1.43
1:A:144:SER:CB	1:A:204:VAL:HG12	1.58	1.31
1:A:78:ASN:HA	1:A:163:LEU:CD1	1.65	1.24
1:A:343:VAL:HG13	1:A:367:LEU:O	1.35	1.23
1:A:268:ILE:HD13	1:A:287:ILE:CD1	1.72	1.20
2:B:4:VAL:HG22	2:B:6:THR:HG23	1.19	1.17
1:A:78:ASN:HA	1:A:163:LEU:HD11	1.27	1.16
2:B:19:LEU:HD11	2:B:21:SER:OG	1.46	1.13
1:A:387:LEU:HD12	1:A:393:THR:CG2	1.78	1.11
1:A:65:THR:O	1:A:69:THR:HG22	1.50	1.11
1:A:149:ALA:HA	1:A:152:VAL:HG21	1.32	1.10
2:B:30:VAL:HG13	2:B:30:VAL:O	1.40	1.09
1:A:268:ILE:CD1	1:A:287:ILE:HD11	1.81	1.09
1:A:149:ALA:HA	1:A:152:VAL:CG2	1.82	1.09
1:A:73:ILE:O	1:A:76:ALA:HB3	1.51	1.08
1:A:183:LEU:HA	1:A:186:ILE:HD12	1.36	1.08
1:A:288:SER:O	1:A:292:ILE:HG23	1.50	1.08
1:A:369:PHE:HB3	1:A:372:LEU:HD12	1.34	1.08
1:A:372:LEU:HB3	1:A:431:ILE:HG21	1.36	1.07
2:B:12:ALA:O	2:B:18:LEU:HD23	1.54	1.06
2:B:4:VAL:CG2	2:B:6:THR:HG23	1.87	1.05
2:B:19:LEU:HA	2:B:58:THR:HG22	1.38	1.05
1:A:418:ARG:HG2	1:A:422:GLY:HA3	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:SER:HB3	1:A:204:VAL:CG1	1.88	1.04
1:A:339:VAL:HG21	1:A:375:PRO:HD3	1.40	1.04
1:A:411:PRO:CB	1:A:428:THR:HG23	1.87	1.03
1:A:395:VAL:HG13	1:A:396:PRO:HD3	1.37	1.01
1:A:387:LEU:HD12	1:A:393:THR:HG22	1.40	1.01
1:A:105:LEU:O	1:A:109:ILE:HG23	1.60	1.00
1:A:158:ALA:CB	1:A:217:LEU:CD1	2.17	1.00
1:A:394:LYS:HA	1:A:397:MET:HB2	1.41	1.00
1:A:145:LEU:HD13	1:A:203:GLY:O	1.62	0.99
1:A:289:LEU:HD13	1:A:292:ILE:HG12	1.43	0.99
1:A:411:PRO:HB3	1:A:428:THR:CG2	1.92	0.99
1:A:339:VAL:HA	1:A:342:LEU:CD1	1.94	0.98
1:A:308:ILE:CD1	1:A:386:ALA:HA	1.94	0.98
1:A:141:LEU:CD1	1:A:145:LEU:HD23	1.93	0.98
1:A:218:TRP:HA	1:A:218:TRP:CE3	1.94	0.97
1:A:411:PRO:HB3	1:A:428:THR:HG23	0.98	0.97
1:A:268:ILE:HD13	1:A:287:ILE:HD11	0.97	0.96
2:B:65:GLY:HA2	2:B:91:THR:CB	1.96	0.96
1:A:214:ALA:C	1:A:215:LEU:HD23	1.86	0.95
2:B:30:VAL:O	2:B:30:VAL:CG1	2.12	0.95
1:A:144:SER:HB3	1:A:204:VAL:HG12	0.97	0.95
1:A:333:VAL:HG12	1:A:334:LEU:HD13	1.44	0.95
1:A:107:LEU:HD23	1:A:108:GLY:N	1.82	0.95
1:A:158:ALA:HB2	1:A:217:LEU:HD12	1.46	0.94
1:A:168:LEU:HA	1:A:171:LEU:HD13	1.47	0.94
1:A:78:ASN:HA	1:A:163:LEU:HD13	1.48	0.94
1:A:372:LEU:CD1	1:A:427:TRP:HB2	1.99	0.93
1:A:260:LEU:HD21	1:A:404:PHE:O	1.69	0.92
1:A:460:SER:O	2:B:8:LEU:CD1	2.17	0.92
1:A:260:LEU:HD11	1:A:404:PHE:HB2	1.52	0.92
1:A:115:MET:O	1:A:118:ALA:HB3	1.70	0.91
1:A:290:SER:O	1:A:294:TYR:HB3	1.71	0.91
1:A:164:ASN:O	1:A:166:PRO:HD3	1.71	0.91
1:A:254:ILE:HB	1:A:394:LYS:NZ	1.85	0.91
1:A:460:SER:O	2:B:8:LEU:HD12	1.69	0.91
1:A:261:GLU:HA	1:A:264:ALA:HB3	1.53	0.90
1:A:306:VAL:O	1:A:308:ILE:N	2.04	0.90
1:A:251:GLY:O	1:A:254:ILE:HG22	1.71	0.90
1:A:410:LEU:O	1:A:414:LEU:HD13	1.72	0.90
1:A:339:VAL:HG23	1:A:342:LEU:HD12	1.53	0.90
1:A:349:LEU:HD21	1:A:360:LEU:HD11	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HG22	1:A:280:VAL:O	1.71	0.90
1:A:351:SER:O	1:A:359:VAL:HG11	1.72	0.90
1:A:372:LEU:HD13	1:A:427:TRP:HB2	1.53	0.90
1:A:372:LEU:HD13	1:A:427:TRP:CB	2.01	0.89
2:B:67:ASP:HA	2:B:90:ARG:HG2	1.51	0.89
1:A:107:LEU:HD23	1:A:108:GLY:H	1.37	0.89
2:B:4:VAL:HG22	2:B:6:THR:CG2	2.01	0.89
2:B:67:ASP:HA	2:B:90:ARG:CG	2.02	0.88
1:A:254:ILE:HD11	1:A:388:ARG:HH11	1.37	0.88
2:B:36:TYR:HA	2:B:70:ILE:HD11	1.55	0.88
1:A:145:LEU:HD12	1:A:207:MET:HB3	1.52	0.88
2:B:24:ALA:O	2:B:53:SER:OG	1.92	0.87
1:A:254:ILE:HD11	1:A:388:ARG:NH1	1.89	0.87
1:A:158:ALA:CA	1:A:217:LEU:HD11	2.04	0.87
1:A:113:ILE:HG22	1:A:114:LEU:HD23	1.57	0.87
1:A:44:MET:SD	1:A:206:THR:HG23	2.15	0.86
1:A:218:TRP:HA	1:A:218:TRP:HE3	1.36	0.86
1:A:368:LEU:HD12	1:A:423:ILE:CG2	2.05	0.86
1:A:73:ILE:O	1:A:76:ALA:CB	2.23	0.86
1:A:159:TYR:HB3	1:A:169:ILE:HD13	1.56	0.86
1:A:339:VAL:HA	1:A:342:LEU:HD12	1.56	0.86
1:A:168:LEU:HD23	1:A:171:LEU:HD22	1.58	0.86
2:B:19:LEU:C	2:B:20:ILE:HD13	1.96	0.86
1:A:337:ILE:HD12	1:A:337:ILE:O	1.73	0.86
1:A:387:LEU:HD12	1:A:393:THR:HG21	1.57	0.86
1:A:425:GLY:O	1:A:428:THR:CG2	2.23	0.86
1:A:188:VAL:HA	1:A:198:GLY:HA2	1.58	0.85
1:A:141:LEU:HD11	1:A:145:LEU:HD23	1.57	0.85
1:A:346:ARG:CD	1:A:367:LEU:HD11	2.07	0.84
2:B:65:GLY:HA2	2:B:91:THR:HB	1.59	0.83
1:A:259:PHE:HA	1:A:262:ALA:HB3	1.60	0.83
1:A:425:GLY:O	1:A:428:THR:HG22	1.78	0.83
1:A:63:PHE:O	1:A:65:THR:N	2.12	0.82
2:B:19:LEU:C	2:B:19:LEU:HD13	1.99	0.82
1:A:395:VAL:CG1	1:A:396:PRO:HD3	2.07	0.82
1:A:58:LEU:HD12	1:A:138:GLN:CD	2.00	0.82
1:A:301:GLY:O	1:A:305:THR:HG22	1.79	0.82
2:B:12:ALA:O	2:B:18:LEU:CD2	2.27	0.81
2:B:20:ILE:HD11	2:B:59:ILE:HG23	1.60	0.81
2:B:87:ILE:HG22	2:B:88:ASN:H	1.45	0.81
1:A:53:LEU:HD22	1:A:135:THR:HG21	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD12	1:A:341:SER:H	1.44	0.81
1:A:172:VAL:HG21	1:A:216:ALA:CB	2.10	0.81
1:A:394:LYS:HA	1:A:397:MET:CB	2.10	0.81
1:A:137:ALA:O	1:A:199:GLY:O	1.98	0.80
1:A:44:MET:CE	1:A:180:ASN:HD21	1.94	0.80
1:A:215:LEU:HD23	1:A:215:LEU:N	1.92	0.80
1:A:63:PHE:C	1:A:65:THR:H	1.81	0.80
1:A:397:MET:O	1:A:400:HIS:N	2.15	0.80
1:A:115:MET:O	1:A:118:ALA:CB	2.30	0.80
1:A:441:LEU:O	1:A:444:CYS:N	2.15	0.79
1:A:329:VAL:HA	1:A:332:TRP:HB3	1.64	0.79
2:B:35:THR:HG23	2:B:73:TYR:HE1	1.48	0.78
1:A:415:LEU:HD11	1:A:423:ILE:HD12	1.64	0.78
1:A:442:VAL:HG23	1:A:445:LEU:HD22	1.64	0.78
2:B:38:GLU:HA	2:B:68:TYR:HA	1.64	0.78
1:A:132:VAL:HG13	1:A:133:GLU:H	1.49	0.78
1:A:141:LEU:HD13	1:A:145:LEU:HD23	1.64	0.78
1:A:31:GLN:NE2	1:A:296:ILE:O	2.17	0.78
1:A:55:ALA:O	1:A:58:LEU:HD11	1.83	0.78
1:A:429:ALA:O	1:A:433:SER:CB	2.32	0.78
1:A:149:ALA:HA	1:A:152:VAL:HG22	1.65	0.78
2:B:86:SER:O	2:B:87:ILE:HD13	1.84	0.77
1:A:40:VAL:HG12	1:A:44:MET:HE3	1.66	0.77
2:B:76:SER:HB3	2:B:82:TYR:CD2	2.19	0.77
1:A:411:PRO:HG3	1:A:429:ALA:HB3	1.64	0.77
1:A:463:LEU:O	2:B:3:SER:OG	2.02	0.77
2:B:31:TYR:HB3	2:B:75:ARG:HB3	1.67	0.77
1:A:297:PRO:O	1:A:299:SER:N	2.18	0.76
1:A:305:THR:HB	1:A:385:TYR:O	1.86	0.76
1:A:172:VAL:HG21	1:A:216:ALA:HB1	1.66	0.76
1:A:148:PRO:O	1:A:150:ALA:N	2.19	0.76
1:A:151:MET:HB2	1:A:211:TRP:CE2	2.20	0.76
1:A:78:ASN:CA	1:A:163:LEU:CD1	2.58	0.76
1:A:77:LEU:HD11	1:A:247:ILE:HG12	1.67	0.76
1:A:180:ASN:O	1:A:184:ASN:N	2.19	0.75
2:B:39:THR:HG1	2:B:69:THR:HG1	1.32	0.75
1:A:55:ALA:HB1	1:A:58:LEU:HD21	1.69	0.75
1:A:404:PHE:HA	1:A:433:SER:OG	1.86	0.75
1:A:144:SER:CB	1:A:204:VAL:CG1	2.53	0.75
1:A:148:PRO:HB2	1:A:152:VAL:HG11	1.67	0.75
1:A:334:LEU:HD12	1:A:337:ILE:HD11	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:HB1	1:A:310:PHE:HB2	1.68	0.74
1:A:184:ASN:HA	1:A:205:ALA:HB1	1.67	0.74
2:B:35:THR:O	2:B:70:ILE:HG12	1.86	0.74
1:A:399:ILE:HG23	1:A:402:ALA:HB3	1.70	0.74
1:A:359:VAL:HG12	1:A:360:LEU:HD22	1.70	0.74
1:A:168:LEU:HD23	1:A:171:LEU:CD2	2.17	0.74
2:B:36:TYR:HA	2:B:70:ILE:CD1	2.18	0.73
2:B:87:ILE:HG22	2:B:88:ASN:N	2.03	0.73
1:A:78:ASN:CA	1:A:163:LEU:HD13	2.18	0.73
2:B:30:VAL:CG2	2:B:51:PRO:O	2.36	0.73
1:A:102:TRP:CD1	1:A:233:THR:OG1	2.41	0.73
1:A:259:PHE:HA	1:A:262:ALA:CB	2.18	0.73
1:A:339:VAL:CG2	1:A:375:PRO:HD3	2.17	0.73
1:A:230:PHE:CE1	1:A:233:THR:HG21	2.23	0.73
1:A:260:LEU:O	1:A:262:ALA:N	2.22	0.73
1:A:12:VAL:HG23	1:A:13:PHE:H	1.54	0.73
1:A:247:ILE:HG23	1:A:250:ILE:CD1	2.18	0.73
1:A:332:TRP:HA	1:A:335:ALA:CB	2.19	0.73
1:A:395:VAL:CG1	1:A:396:PRO:CD	2.67	0.72
1:A:168:LEU:CD2	1:A:171:LEU:HD22	2.20	0.72
1:A:61:SER:O	1:A:265:PHE:HZ	1.71	0.72
1:A:188:VAL:HA	1:A:198:GLY:CA	2.20	0.72
1:A:344:LEU:HD22	1:A:345:PHE:CD2	2.24	0.72
1:A:79:PRO:O	1:A:80:MET:C	2.27	0.72
1:A:58:LEU:HD12	1:A:138:GLN:NE2	2.04	0.72
1:A:334:LEU:HA	1:A:337:ILE:HG13	1.72	0.72
1:A:300:VAL:O	1:A:304:GLY:N	2.23	0.71
1:A:365:THR:HA	1:A:368:LEU:HD11	1.72	0.71
1:A:247:ILE:HG23	1:A:250:ILE:HD11	1.69	0.71
2:B:31:TYR:CD1	2:B:75:ARG:NH1	2.58	0.71
1:A:255:GLY:O	1:A:258:TYR:N	2.24	0.71
1:A:458:ALA:HB3	2:B:8:LEU:C	2.10	0.71
1:A:61:SER:O	1:A:265:PHE:CZ	2.44	0.71
1:A:296:ILE:HG22	1:A:297:PRO:HD3	1.73	0.71
2:B:16:THR:O	2:B:61:GLY:O	2.08	0.71
1:A:337:ILE:O	1:A:338:THR:OG1	2.08	0.71
1:A:44:MET:HE1	1:A:180:ASN:HD21	1.55	0.71
1:A:408:GLY:HA2	1:A:411:PRO:HG2	1.72	0.71
1:A:432:ALA:O	1:A:436:ILE:HG23	1.91	0.71
1:A:439:VAL:CG2	1:A:440:ALA:N	2.54	0.71
1:A:151:MET:SD	1:A:211:TRP:CE3	2.84	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ALA:O	1:A:433:SER:HB2	1.89	0.70
1:A:365:THR:HB	1:A:423:ILE:HG21	1.72	0.70
1:A:306:VAL:C	1:A:308:ILE:H	1.95	0.70
1:A:333:VAL:HG12	1:A:334:LEU:CD1	2.20	0.70
1:A:51:GLU:O	1:A:54:ALA:HB3	1.91	0.70
1:A:159:TYR:CB	1:A:169:ILE:HD13	2.21	0.70
1:A:250:ILE:HA	1:A:394:LYS:HD2	1.72	0.70
1:A:308:ILE:HD13	1:A:386:ALA:HA	1.71	0.70
1:A:349:LEU:CD2	1:A:360:LEU:HD11	2.20	0.70
1:A:343:VAL:HG22	1:A:370:ALA:C	2.12	0.70
1:A:340:LEU:HD13	1:A:341:SER:OG	1.92	0.70
1:A:387:LEU:CD1	1:A:393:THR:CG2	2.66	0.70
1:A:400:HIS:CE1	1:A:401:ALA:HB2	2.26	0.70
1:A:442:VAL:HG23	1:A:445:LEU:CD2	2.20	0.70
1:A:297:PRO:O	1:A:298:GLN:C	2.30	0.70
1:A:435:THR:HG22	1:A:438:ALA:HB2	1.74	0.70
1:A:318:SER:HA	1:A:321:ARG:H	1.56	0.70
1:A:346:ARG:HD3	1:A:367:LEU:HD11	1.73	0.70
2:B:78:TYR:O	2:B:80:GLY:N	2.25	0.70
1:A:116:TRP:HH2	1:A:147:MET:HA	1.57	0.69
1:A:372:LEU:HD11	1:A:427:TRP:HB2	1.74	0.69
1:A:158:ALA:HB2	1:A:217:LEU:HD11	0.70	0.69
1:A:339:VAL:CG2	1:A:342:LEU:HD12	2.21	0.69
1:A:393:THR:HG22	1:A:393:THR:O	1.91	0.69
1:A:268:ILE:CD1	1:A:269:VAL:HG23	2.23	0.69
1:A:424:TYR:HA	1:A:427:TRP:CD1	2.28	0.69
2:B:20:ILE:CD1	2:B:59:ILE:HG23	2.22	0.69
1:A:59:GLY:O	1:A:63:PHE:N	2.26	0.69
1:A:302:SER:HA	1:A:305:THR:CG2	2.22	0.69
2:B:50:VAL:HG12	2:B:51:PRO:HD3	1.75	0.69
1:A:141:LEU:HD22	1:A:203:GLY:HA3	1.74	0.69
1:A:260:LEU:CD2	1:A:404:PHE:O	2.40	0.69
1:A:103:PHE:O	1:A:105:LEU:N	2.24	0.68
2:B:72:VAL:HG22	2:B:73:TYR:H	1.57	0.68
1:A:144:SER:HB2	1:A:204:VAL:HG12	1.69	0.68
1:A:53:LEU:HD22	1:A:135:THR:CG2	2.23	0.68
2:B:57:ALA:O	2:B:58:THR:HG23	1.92	0.68
1:A:7:ARG:NH1	1:A:12:VAL:HG21	2.08	0.68
1:A:178:VAL:O	1:A:182:PRO:HD2	1.94	0.68
1:A:321:ARG:HH22	1:A:391:LYS:HB2	1.59	0.68
1:A:103:PHE:HA	1:A:106:ILE:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:HA	1:A:19:LEU:HD12	1.76	0.68
1:A:141:LEU:O	1:A:145:LEU:HB3	1.94	0.68
1:A:148:PRO:O	1:A:152:VAL:HG13	1.94	0.68
1:A:23:LEU:HD23	1:A:23:LEU:O	1.95	0.67
1:A:103:PHE:O	1:A:107:LEU:HD22	1.93	0.67
2:B:10:VAL:HG12	2:B:18:LEU:CD2	2.25	0.67
1:A:329:VAL:HA	1:A:332:TRP:CB	2.25	0.67
1:A:372:LEU:HD11	1:A:424:TYR:HB2	1.77	0.67
1:A:328:LEU:O	1:A:332:TRP:HB2	1.95	0.66
1:A:235:LYS:HB2	1:A:241:TRP:HB3	1.75	0.66
2:B:31:TYR:C	2:B:32:TYR:CD2	2.68	0.66
1:A:27:MET:HG3	1:A:303:ALA:O	1.95	0.66
1:A:340:LEU:HD12	1:A:341:SER:N	2.11	0.66
1:A:118:ALA:HB3	1:A:119:ILE:HG13	1.78	0.66
1:A:177:PHE:O	1:A:181:VAL:HG23	1.95	0.66
1:A:216:ALA:HA	1:A:219:ILE:HG12	1.77	0.66
1:A:33:ALA:HB2	1:A:170:MET:HA	1.78	0.66
2:B:75:ARG:NE	2:B:79:TRP:O	2.28	0.66
1:A:308:ILE:HD11	1:A:386:ALA:HA	1.78	0.66
1:A:372:LEU:HD22	1:A:431:ILE:HG12	1.76	0.66
1:A:387:LEU:CD1	1:A:393:THR:HG21	2.24	0.66
1:A:372:LEU:HD13	1:A:427:TRP:HB3	1.76	0.66
1:A:193:GLY:O	1:A:195:PRO:CD	2.45	0.65
1:A:346:ARG:CG	1:A:367:LEU:HD11	2.26	0.65
1:A:458:ALA:HB1	2:B:8:LEU:HB2	1.77	0.65
2:B:63:SER:HB2	2:B:68:TYR:OH	1.97	0.65
1:A:145:LEU:CD1	1:A:207:MET:HB3	2.27	0.65
1:A:254:ILE:HB	1:A:394:LYS:CE	2.27	0.65
2:B:38:GLU:H	2:B:38:GLU:CD	2.00	0.65
2:B:69:THR:HA	2:B:88:ASN:HA	1.77	0.65
1:A:302:SER:HA	1:A:305:THR:HG22	1.77	0.65
1:A:132:VAL:O	1:A:133:GLU:HG2	1.96	0.65
1:A:290:SER:O	1:A:291:GLY:C	2.34	0.65
2:B:19:LEU:HD13	2:B:20:ILE:N	2.12	0.65
2:B:51:PRO:O	2:B:52:GLY:O	2.15	0.65
1:A:147:MET:HE1	1:A:207:MET:SD	2.37	0.65
1:A:158:ALA:CB	1:A:217:LEU:HD12	2.13	0.65
1:A:340:LEU:CD1	1:A:341:SER:OG	2.45	0.64
2:B:27:GLU:HG2	2:B:30:VAL:HG23	1.77	0.64
2:B:71:THR:OG1	2:B:86:SER:HB2	1.97	0.64
1:A:180:ASN:C	1:A:180:ASN:ND2	2.49	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:CE2	1:A:298:GLN:HB2	2.31	0.64
1:A:318:SER:HA	1:A:321:ARG:N	2.11	0.64
1:A:294:TYR:C	1:A:294:TYR:CD2	2.71	0.64
2:B:87:ILE:CG2	2:B:88:ASN:H	2.09	0.64
1:A:268:ILE:CD1	1:A:287:ILE:CD1	2.55	0.64
2:B:17:SER:HA	2:B:61:GLY:HA3	1.80	0.64
2:B:27:GLU:O	2:B:28:TYR:CD2	2.50	0.64
2:B:59:ILE:HD12	2:B:61:GLY:CA	2.27	0.64
1:A:144:SER:O	1:A:207:MET:HG2	1.97	0.64
1:A:290:SER:O	1:A:294:TYR:CB	2.46	0.64
1:A:411:PRO:HA	1:A:414:LEU:HB2	1.78	0.64
1:A:332:TRP:HA	1:A:335:ALA:HB2	1.77	0.64
1:A:372:LEU:CB	1:A:431:ILE:HG21	2.22	0.64
1:A:417:TYR:CG	1:A:417:TYR:O	2.50	0.64
1:A:458:ALA:HB3	2:B:8:LEU:O	1.97	0.64
1:A:149:ALA:CA	1:A:152:VAL:HG22	2.27	0.64
1:A:141:LEU:CD2	1:A:203:GLY:HA3	2.29	0.63
1:A:372:LEU:CD1	1:A:427:TRP:CB	2.69	0.63
2:B:78:TYR:C	2:B:80:GLY:H	2.01	0.63
2:B:67:ASP:CA	2:B:90:ARG:HG2	2.28	0.63
1:A:65:THR:HG23	1:A:66:VAL:HG13	1.79	0.63
1:A:97:GLY:HA3	1:A:227:PHE:CZ	2.34	0.63
1:A:44:MET:SD	1:A:206:THR:CG2	2.87	0.63
1:A:147:MET:SD	1:A:148:PRO:HD3	2.38	0.63
1:A:460:SER:O	2:B:8:LEU:CG	2.45	0.63
1:A:65:THR:CG2	1:A:66:VAL:HG13	2.29	0.63
2:B:50:VAL:HG12	2:B:51:PRO:CD	2.28	0.63
1:A:40:VAL:O	1:A:43:VAL:HG12	1.99	0.63
1:A:439:VAL:HG23	1:A:440:ALA:N	2.12	0.62
1:A:441:LEU:O	1:A:443:TRP:N	2.32	0.62
2:B:19:LEU:HD22	2:B:20:ILE:H	1.64	0.62
1:A:297:PRO:HB3	1:A:378:PHE:CE2	2.34	0.62
1:A:68:ILE:HA	1:A:71:MET:HB2	1.79	0.62
1:A:33:ALA:CB	1:A:170:MET:HA	2.30	0.62
1:A:73:ILE:HG13	1:A:251:GLY:CA	2.30	0.62
1:A:78:ASN:O	1:A:163:LEU:HD13	1.99	0.62
1:A:346:ARG:HG2	1:A:367:LEU:HD11	1.81	0.62
1:A:368:LEU:HD12	1:A:423:ILE:HG22	1.79	0.62
2:B:13:ALA:HA	2:B:18:LEU:HA	1.80	0.62
1:A:455:SER:O	2:B:11:VAL:HA	1.99	0.62
2:B:65:GLY:HA2	2:B:91:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ASP:HA	2:B:90:ARG:CB	2.29	0.62
1:A:98:ARG:O	1:A:101:ILE:N	2.32	0.62
1:A:194:MET:O	1:A:196:ALA:N	2.33	0.62
1:A:408:GLY:HA3	1:A:430:LEU:HG	1.80	0.62
1:A:149:ALA:C	1:A:152:VAL:HG22	2.20	0.62
1:A:187:PHE:HD1	1:A:205:ALA:HB2	1.65	0.62
1:A:379:THR:O	1:A:382:ILE:N	2.33	0.61
1:A:149:ALA:CA	1:A:152:VAL:CG2	2.70	0.61
1:A:184:ASN:HA	1:A:205:ALA:CB	2.31	0.61
1:A:369:PHE:CB	1:A:372:LEU:HD12	2.23	0.61
1:A:429:ALA:HA	1:A:432:ALA:HB3	1.83	0.61
1:A:254:ILE:HG23	1:A:255:GLY:H	1.64	0.61
1:A:368:LEU:HD12	1:A:423:ILE:HG21	1.81	0.61
2:B:19:LEU:HD11	2:B:21:SER:CB	2.30	0.61
1:A:414:LEU:O	1:A:418:ARG:NH1	2.32	0.61
1:A:369:PHE:HD2	1:A:424:TYR:CB	2.14	0.61
1:A:382:ILE:HA	1:A:385:TYR:CD2	2.35	0.61
1:A:435:THR:HG22	1:A:438:ALA:CB	2.31	0.61
1:A:33:ALA:HB2	1:A:170:MET:CA	2.30	0.61
1:A:413:TYR:O	1:A:414:LEU:HD12	2.01	0.61
2:B:10:VAL:HG12	2:B:18:LEU:HD22	1.82	0.61
1:A:103:PHE:O	1:A:107:LEU:CD2	2.48	0.60
1:A:344:LEU:HD22	1:A:345:PHE:CG	2.36	0.60
1:A:375:PRO:HA	1:A:378:PHE:HB2	1.83	0.60
1:A:340:LEU:CD1	1:A:341:SER:N	2.64	0.60
1:A:294:TYR:O	1:A:297:PRO:HB2	2.01	0.60
2:B:8:LEU:HD13	2:B:87:ILE:HD11	1.83	0.60
1:A:388:ARG:N	1:A:393:THR:O	2.35	0.60
2:B:1:VAL:O	2:B:1:VAL:HG13	2.01	0.60
2:B:33:ARG:NE	2:B:47:GLU:OE2	2.35	0.60
1:A:98:ARG:CD	1:A:229:PRO:O	2.49	0.60
1:A:98:ARG:HD2	1:A:229:PRO:O	2.02	0.60
2:B:19:LEU:HD22	2:B:20:ILE:N	2.16	0.60
1:A:183:LEU:HD21	1:A:209:VAL:HG23	1.82	0.60
1:A:53:LEU:CD2	1:A:135:THR:CG2	2.80	0.59
1:A:308:ILE:HD13	1:A:386:ALA:CB	2.32	0.59
1:A:218:TRP:CE3	1:A:218:TRP:CA	2.79	0.59
1:A:441:LEU:C	1:A:443:TRP:N	2.56	0.59
1:A:81:ILE:HD12	1:A:81:ILE:O	2.02	0.59
2:B:19:LEU:HD11	2:B:21:SER:HG	1.63	0.59
1:A:248:TRP:CZ3	1:A:252:ALA:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:CA	1:A:397:MET:HB2	2.24	0.59
1:A:458:ALA:CB	2:B:8:LEU:HB2	2.32	0.59
1:A:159:TYR:HA	1:A:162:SER:OG	2.03	0.59
1:A:260:LEU:HD21	1:A:404:PHE:C	2.22	0.59
1:A:242:ALA:O	1:A:243:VAL:HG22	2.03	0.59
2:B:4:VAL:HG12	2:B:83:SER:OG	2.02	0.59
1:A:218:TRP:CZ3	1:A:221:ILE:HD11	2.38	0.59
1:A:305:THR:HA	1:A:308:ILE:HD11	1.85	0.59
1:A:31:GLN:HG3	1:A:296:ILE:HA	1.84	0.59
1:A:172:VAL:HG21	1:A:216:ALA:HB2	1.82	0.59
1:A:332:TRP:HD1	1:A:379:THR:HG21	1.67	0.59
1:A:339:VAL:HG11	1:A:375:PRO:HG3	1.85	0.59
1:A:71:MET:HG2	1:A:156:LEU:HD22	1.84	0.59
1:A:338:THR:HG23	1:A:340:LEU:HD12	1.84	0.58
1:A:212:PHE:C	1:A:212:PHE:CD2	2.76	0.58
1:A:339:VAL:HA	1:A:342:LEU:CG	2.32	0.58
1:A:122:PHE:HA	1:A:133:GLU:OE2	2.02	0.58
1:A:193:GLY:O	1:A:195:PRO:N	2.37	0.58
1:A:127:THR:HG22	1:A:128:LEU:H	1.68	0.58
1:A:102:TRP:O	1:A:106:ILE:N	2.36	0.58
1:A:374:GLN:HB3	1:A:375:PRO:HD3	1.86	0.58
2:B:14:THR:O	2:B:16:THR:N	2.34	0.58
1:A:119:ILE:HG12	1:A:142:PHE:CD2	2.39	0.58
2:B:4:VAL:CG2	2:B:6:THR:CG2	2.71	0.58
1:A:100:GLY:O	1:A:104:GLY:N	2.29	0.58
1:A:332:TRP:HA	1:A:335:ALA:HB3	1.86	0.58
2:B:4:VAL:HG11	2:B:84:PRO:O	2.03	0.58
1:A:308:ILE:HD13	1:A:386:ALA:CA	2.34	0.58
1:A:379:THR:HG22	1:A:382:ILE:HG12	1.85	0.58
1:A:55:ALA:O	1:A:58:LEU:CD1	2.51	0.57
1:A:193:GLY:O	1:A:195:PRO:HD3	2.04	0.57
1:A:66:VAL:O	1:A:66:VAL:HG23	2.03	0.57
1:A:373:PHE:HB2	1:A:434:LEU:CD1	2.33	0.57
1:A:387:LEU:HD21	1:A:444:CYS:O	2.04	0.57
2:B:67:ASP:HA	2:B:90:ARG:HB3	1.84	0.57
1:A:102:TRP:O	1:A:106:ILE:HB	2.03	0.57
1:A:460:SER:O	2:B:8:LEU:HG	2.04	0.57
1:A:38:GLY:O	1:A:41:ASP:OD2	2.22	0.57
1:A:250:ILE:HA	1:A:394:LYS:CD	2.35	0.57
1:A:429:ALA:O	1:A:433:SER:HB3	2.03	0.57
1:A:112:MET:CG	1:A:147:MET:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ALA:O	1:A:407:CYS:HB2	2.05	0.57
1:A:411:PRO:HG3	1:A:429:ALA:CB	2.34	0.57
1:A:411:PRO:HB2	1:A:426:PHE:O	2.05	0.57
1:A:377:ASP:O	1:A:378:PHE:C	2.43	0.57
1:A:395:VAL:HG12	1:A:396:PRO:CD	2.34	0.57
2:B:29:VAL:O	2:B:30:VAL:HG12	2.05	0.57
2:B:43:SER:O	2:B:44:PRO:O	2.22	0.57
1:A:318:SER:C	1:A:320:ALA:N	2.58	0.57
2:B:10:VAL:HG12	2:B:10:VAL:O	2.04	0.57
1:A:260:LEU:C	1:A:262:ALA:H	2.08	0.57
1:A:415:LEU:CD1	1:A:423:ILE:HA	2.35	0.57
1:A:439:VAL:CG2	1:A:440:ALA:H	2.17	0.57
1:A:289:LEU:HD13	1:A:292:ILE:CG1	2.28	0.56
1:A:274:PRO:C	1:A:276:GLY:H	2.09	0.56
2:B:5:PRO:CD	2:B:74:ALA:HB2	2.35	0.56
1:A:156:LEU:CD1	1:A:159:TYR:CE1	2.88	0.56
1:A:191:LYS:O	1:A:192:PHE:C	2.41	0.56
1:A:346:ARG:O	1:A:348:PRO:HD3	2.05	0.56
2:B:19:LEU:CD1	2:B:21:SER:OG	2.38	0.56
2:B:63:SER:HB3	2:B:64:PRO:HD2	1.87	0.56
1:A:302:SER:CA	1:A:305:THR:HG22	2.36	0.56
2:B:9:GLU:O	2:B:22:TRP:NE1	2.38	0.56
2:B:78:TYR:C	2:B:80:GLY:N	2.59	0.56
1:A:33:ALA:HB2	1:A:170:MET:CB	2.35	0.56
1:A:116:TRP:CH2	1:A:147:MET:HA	2.40	0.56
1:A:148:PRO:HG3	1:A:207:MET:HB2	1.88	0.56
1:A:268:ILE:HD12	1:A:269:VAL:HG23	1.87	0.56
1:A:322:TYR:HE1	1:A:449:SER:HB2	1.71	0.56
2:B:32:TYR:HB2	2:B:50:VAL:HG23	1.87	0.56
1:A:57:ALA:O	1:A:60:SER:N	2.39	0.56
2:B:27:GLU:O	2:B:28:TYR:HD2	1.88	0.56
1:A:43:VAL:HG13	1:A:44:MET:HE3	1.88	0.56
1:A:292:ILE:HD12	1:A:293:LEU:HG	1.87	0.56
1:A:321:ARG:NH2	1:A:391:LYS:HB2	2.20	0.56
1:A:384:SER:C	1:A:386:ALA:H	2.08	0.56
1:A:99:GLN:NE2	1:A:234:ALA:O	2.38	0.56
1:A:430:LEU:HA	1:A:433:SER:HB3	1.87	0.56
1:A:27:MET:O	1:A:303:ALA:HB3	2.06	0.56
1:A:90:THR:O	1:A:94:GLY:N	2.39	0.56
1:A:304:GLY:O	1:A:306:VAL:N	2.39	0.56
2:B:87:ILE:CG2	2:B:88:ASN:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:SER:HA	1:A:366:VAL:HG22	1.87	0.55
1:A:415:LEU:HD12	1:A:423:ILE:HA	1.88	0.55
1:A:108:GLY:O	1:A:112:MET:HB2	2.05	0.55
1:A:205:ALA:O	1:A:208:ALA:HB3	2.06	0.55
1:A:292:ILE:HG13	1:A:293:LEU:H	1.71	0.55
2:B:7:LYS:O	2:B:8:LEU:HD23	2.06	0.55
1:A:365:THR:O	1:A:423:ILE:HG21	2.07	0.55
2:B:19:LEU:C	2:B:19:LEU:CD1	2.70	0.55
2:B:22:TRP:HZ3	2:B:85:ILE:HG23	1.72	0.55
1:A:109:ILE:HA	1:A:112:MET:HB2	1.88	0.55
1:A:217:LEU:O	1:A:218:TRP:C	2.43	0.55
1:A:40:VAL:HG22	1:A:177:PHE:HB2	1.88	0.55
1:A:155:ALA:HB2	1:A:214:ALA:HA	1.89	0.55
1:A:372:LEU:CD1	1:A:424:TYR:HB2	2.37	0.55
1:A:457:LYS:HB3	2:B:10:VAL:HB	1.89	0.55
2:B:65:GLY:HA2	2:B:91:THR:HG21	1.89	0.55
1:A:292:ILE:HD12	1:A:293:LEU:CG	2.37	0.54
1:A:411:PRO:CG	1:A:429:ALA:HB3	2.37	0.54
1:A:459:VAL:O	1:A:460:SER:OG	2.24	0.54
1:A:15:LYS:HG2	1:A:322:TYR:HA	1.88	0.54
1:A:315:ARG:HH21	2:B:11:VAL:HG11	1.73	0.54
1:A:63:PHE:C	1:A:65:THR:N	2.54	0.54
1:A:145:LEU:HD22	1:A:203:GLY:HA3	1.87	0.54
1:A:218:TRP:CE3	1:A:221:ILE:HD11	2.42	0.54
2:B:4:VAL:HG21	2:B:85:ILE:HB	1.88	0.54
1:A:427:TRP:CD1	1:A:427:TRP:N	2.76	0.54
1:A:65:THR:O	1:A:69:THR:CG2	2.40	0.54
1:A:112:MET:SD	1:A:147:MET:HA	2.48	0.54
1:A:335:ALA:O	1:A:375:PRO:HB3	2.07	0.54
1:A:76:ALA:O	1:A:250:ILE:HD13	2.08	0.54
1:A:103:PHE:O	1:A:106:ILE:N	2.41	0.54
1:A:109:ILE:HD11	1:A:110:PHE:CE2	2.43	0.54
2:B:68:TYR:O	2:B:88:ASN:O	2.26	0.54
2:B:37:GLY:N	2:B:70:ILE:HD11	2.23	0.54
1:A:74:MET:C	1:A:76:ALA:H	2.12	0.54
1:A:97:GLY:HA3	1:A:227:PHE:CE2	2.42	0.54
1:A:97:GLY:HA2	1:A:157:HIS:HE1	1.73	0.54
1:A:109:ILE:O	1:A:113:ILE:HB	2.08	0.54
1:A:156:LEU:HD12	1:A:159:TYR:CE1	2.43	0.54
2:B:38:GLU:CD	2:B:38:GLU:N	2.61	0.54
2:B:5:PRO:HD3	2:B:74:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:THR:C	2:B:61:GLY:O	2.47	0.53
1:A:31:GLN:OE1	1:A:299:SER:O	2.27	0.53
1:A:203:GLY:HA2	1:A:206:THR:OG1	2.08	0.53
1:A:263:SER:C	1:A:265:PHE:H	2.10	0.53
1:A:325:GLY:O	1:A:328:LEU:N	2.42	0.53
1:A:269:VAL:HG12	1:A:269:VAL:O	2.08	0.53
2:B:20:ILE:HD13	2:B:20:ILE:N	2.23	0.53
1:A:369:PHE:HA	1:A:372:LEU:HB2	1.89	0.53
1:A:316:GLU:HB3	1:A:319:ARG:HB2	1.91	0.53
1:A:369:PHE:HD2	1:A:424:TYR:HB3	1.73	0.53
2:B:71:THR:HG23	2:B:85:ILE:C	2.29	0.53
1:A:44:MET:CE	1:A:180:ASN:ND2	2.70	0.53
2:B:20:ILE:HG12	2:B:58:THR:HA	1.91	0.53
2:B:65:GLY:CA	2:B:91:THR:HB	2.36	0.53
1:A:106:ILE:CG2	1:A:107:LEU:N	2.72	0.53
1:A:151:MET:HB2	1:A:211:TRP:CZ2	2.43	0.53
2:B:27:GLU:HG2	2:B:30:VAL:CG2	2.38	0.53
1:A:141:LEU:HB2	1:A:200:ALA:HA	1.91	0.53
1:A:154:ARG:HH21	1:A:215:LEU:HD22	1.74	0.53
1:A:89:LYS:O	1:A:89:LYS:HG2	2.09	0.52
1:A:384:SER:HA	1:A:387:LEU:HB2	1.91	0.52
1:A:434:LEU:HD23	1:A:434:LEU:O	2.08	0.52
1:A:442:VAL:HA	1:A:445:LEU:HB3	1.92	0.52
1:A:12:VAL:HG23	1:A:13:PHE:N	2.23	0.52
1:A:27:MET:O	1:A:303:ALA:CB	2.57	0.52
1:A:78:ASN:CA	1:A:163:LEU:HD11	2.19	0.52
1:A:103:PHE:HD2	1:A:106:ILE:CG2	2.22	0.52
1:A:318:SER:C	1:A:320:ALA:H	2.10	0.52
1:A:339:VAL:HG23	1:A:374:GLN:HB3	1.91	0.52
1:A:364:SER:C	1:A:366:VAL:H	2.11	0.52
1:A:425:GLY:O	1:A:428:THR:HG21	2.09	0.52
1:A:439:VAL:HG22	1:A:440:ALA:H	1.74	0.52
2:B:26:GLY:O	2:B:53:SER:OG	2.27	0.52
1:A:294:TYR:CZ	1:A:298:GLN:HB2	2.45	0.52
1:A:373:PHE:HB2	1:A:434:LEU:HD11	1.90	0.52
1:A:15:LYS:NZ	1:A:446:GLU:OE1	2.42	0.52
1:A:127:THR:HG22	1:A:128:LEU:N	2.24	0.52
1:A:268:ILE:HD11	1:A:269:VAL:HG23	1.91	0.52
2:B:4:VAL:HG12	2:B:83:SER:CB	2.40	0.52
2:B:27:GLU:HG3	2:B:52:GLY:C	2.30	0.52
1:A:38:GLY:O	1:A:41:ASP:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:N	1:A:215:LEU:CD2	2.65	0.52
1:A:251:GLY:O	1:A:254:ILE:CG2	2.53	0.52
1:A:302:SER:HA	1:A:305:THR:HG21	1.92	0.52
2:B:31:TYR:CB	2:B:75:ARG:HB3	2.37	0.52
1:A:143:THR:HA	1:A:146:ALA:HB3	1.91	0.52
1:A:156:LEU:HD13	1:A:159:TYR:CZ	2.44	0.52
1:A:28:LEU:O	1:A:32:VAL:HG23	2.10	0.52
1:A:112:MET:SD	1:A:147:MET:O	2.68	0.52
1:A:415:LEU:O	1:A:418:ARG:HB2	2.10	0.52
1:A:77:LEU:HD12	1:A:250:ILE:CD1	2.39	0.52
1:A:261:GLU:HA	1:A:264:ALA:CB	2.34	0.52
1:A:151:MET:SD	1:A:211:TRP:HA	2.50	0.51
1:A:365:THR:HA	1:A:368:LEU:CD1	2.40	0.51
1:A:132:VAL:HG13	1:A:133:GLU:N	2.20	0.51
1:A:383:ALA:HB3	1:A:441:LEU:HD12	1.92	0.51
2:B:13:ALA:HA	2:B:18:LEU:HD23	1.92	0.51
1:A:29:LEU:N	1:A:29:LEU:HD23	2.25	0.51
1:A:40:VAL:CG1	1:A:180:ASN:ND2	2.73	0.51
1:A:44:MET:HE1	1:A:180:ASN:ND2	2.24	0.51
1:A:418:ARG:HG2	1:A:422:GLY:CA	2.25	0.51
1:A:247:ILE:HG23	1:A:250:ILE:HD12	1.93	0.51
1:A:254:ILE:HG23	1:A:255:GLY:N	2.25	0.51
1:A:329:VAL:CA	1:A:332:TRP:HB3	2.35	0.51
1:A:388:ARG:O	1:A:390:TYR:N	2.44	0.51
1:A:73:ILE:HA	1:A:254:ILE:HG21	1.93	0.51
1:A:151:MET:HB2	1:A:211:TRP:CD2	2.46	0.51
1:A:151:MET:O	1:A:214:ALA:HB2	2.09	0.51
1:A:221:ILE:HD13	1:A:228:ARG:HG3	1.93	0.51
1:A:119:ILE:HG23	1:A:142:PHE:CG	2.46	0.50
1:A:191:LYS:C	1:A:193:GLY:N	2.64	0.50
1:A:202:CYS:O	1:A:205:ALA:HB3	2.11	0.50
1:A:40:VAL:HG22	1:A:177:PHE:HD1	1.76	0.50
1:A:150:ALA:C	1:A:152:VAL:H	2.14	0.50
1:A:191:LYS:O	1:A:193:GLY:N	2.43	0.50
1:A:321:ARG:HA	1:A:324:SER:HB3	1.94	0.50
1:A:366:VAL:HA	1:A:369:PHE:CZ	2.46	0.50
2:B:24:ALA:HB1	2:B:53:SER:HA	1.94	0.50
1:A:103:PHE:HD2	1:A:106:ILE:HG22	1.77	0.50
1:A:253:PRO:O	1:A:257:SER:HB2	2.11	0.50
1:A:337:ILE:O	1:A:337:ILE:CD1	2.52	0.50
1:A:376:ALA:HB1	1:A:435:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLU:O	2:B:22:TRP:CD1	2.65	0.50
1:A:221:ILE:HD13	1:A:228:ARG:HB2	1.92	0.50
1:A:207:MET:SD	1:A:207:MET:C	2.90	0.50
1:A:344:LEU:HD13	1:A:345:PHE:CE2	2.46	0.50
2:B:10:VAL:HG12	2:B:18:LEU:HD21	1.93	0.50
1:A:119:ILE:HG23	1:A:142:PHE:CD2	2.47	0.50
1:A:136:MET:O	1:A:136:MET:HG2	2.11	0.50
1:A:18:ARG:O	1:A:18:ARG:HD3	2.11	0.50
1:A:19:LEU:HB3	1:A:326:VAL:HG21	1.94	0.50
1:A:101:ILE:HD11	1:A:217:LEU:CD2	2.42	0.50
1:A:397:MET:O	1:A:400:HIS:CB	2.60	0.50
2:B:35:THR:HG23	2:B:73:TYR:CE1	2.38	0.50
1:A:197:LEU:O	1:A:201:GLY:HA3	2.12	0.50
2:B:13:ALA:HB1	2:B:17:SER:O	2.12	0.50
2:B:85:ILE:HG23	2:B:85:ILE:O	2.12	0.50
1:A:68:ILE:HA	1:A:71:MET:CB	2.42	0.50
1:A:147:MET:CE	1:A:207:MET:CE	2.90	0.50
1:A:331:GLY:O	1:A:335:ALA:N	2.45	0.50
1:A:411:PRO:HG3	1:A:429:ALA:C	2.32	0.49
2:B:82:TYR:O	2:B:83:SER:HB2	2.12	0.49
1:A:141:LEU:CD2	1:A:145:LEU:HD22	2.42	0.49
1:A:151:MET:CG	1:A:211:TRP:CE3	2.95	0.49
1:A:242:ALA:HA	1:A:245:LYS:H	1.77	0.49
1:A:301:GLY:O	1:A:305:THR:N	2.31	0.49
2:B:30:VAL:O	2:B:31:TYR:HB2	2.11	0.49
2:B:29:VAL:O	2:B:30:VAL:CB	2.60	0.49
1:A:79:PRO:O	1:A:81:ILE:N	2.44	0.49
1:A:180:ASN:CA	1:A:209:VAL:HG21	2.42	0.49
1:A:374:GLN:OE1	1:A:378:PHE:CE1	2.66	0.49
1:A:377:ASP:O	1:A:379:THR:N	2.45	0.49
1:A:393:THR:CG2	1:A:393:THR:O	2.60	0.49
1:A:441:LEU:C	1:A:443:TRP:H	2.14	0.49
1:A:73:ILE:HA	1:A:251:GLY:HA2	1.93	0.49
1:A:172:VAL:HG11	1:A:216:ALA:HB1	1.94	0.49
2:B:22:TRP:O	2:B:56:THR:CG2	2.61	0.49
2:B:29:VAL:HG23	2:B:77:TYR:N	2.28	0.49
1:A:115:MET:HB3	1:A:146:ALA:HB1	1.94	0.49
1:A:224:GLU:HG2	1:A:225:LYS:N	2.28	0.49
2:B:29:VAL:H	2:B:76:SER:HA	1.78	0.49
2:B:30:VAL:HG22	2:B:51:PRO:O	2.11	0.49
1:A:179:LEU:O	1:A:183:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HA	1:A:280:VAL:HG12	1.94	0.49
1:A:289:LEU:HA	1:A:292:ILE:HG12	1.94	0.49
2:B:24:ALA:HB3	2:B:53:SER:O	2.12	0.49
1:A:89:LYS:CG	1:A:92:GLU:HB3	2.43	0.49
1:A:156:LEU:CD1	1:A:159:TYR:CZ	2.96	0.49
1:A:377:ASP:O	1:A:380:GLN:N	2.46	0.49
1:A:397:MET:O	1:A:398:PHE:C	2.50	0.49
1:A:440:ALA:O	1:A:443:TRP:HB3	2.12	0.49
2:B:1:VAL:O	2:B:1:VAL:CG1	2.60	0.49
1:A:59:GLY:O	1:A:62:ALA:N	2.39	0.49
1:A:247:ILE:O	1:A:247:ILE:HG22	2.13	0.49
2:B:4:VAL:HA	2:B:83:SER:HB3	1.95	0.49
2:B:27:GLU:N	2:B:27:GLU:OE1	2.45	0.49
1:A:73:ILE:HA	1:A:254:ILE:CG2	2.43	0.49
1:A:189:TYR:HA	1:A:195:PRO:O	2.13	0.49
1:A:418:ARG:NH1	1:A:425:GLY:O	2.46	0.49
1:A:103:PHE:C	1:A:107:LEU:HD22	2.32	0.48
1:A:108:GLY:HA2	1:A:153:HIS:HD2	1.78	0.48
2:B:27:GLU:HB3	2:B:30:VAL:HA	1.95	0.48
1:A:56:VAL:HA	1:A:138:GLN:HE22	1.78	0.48
1:A:65:THR:CG2	1:A:66:VAL:N	2.77	0.48
1:A:81:ILE:HG13	1:A:163:LEU:HB2	1.95	0.48
2:B:22:TRP:O	2:B:56:THR:HG23	2.13	0.48
1:A:68:ILE:HD13	1:A:71:MET:HG3	1.96	0.48
1:A:288:SER:O	1:A:292:ILE:CG2	2.42	0.48
1:A:339:VAL:CG2	1:A:370:ALA:O	2.61	0.48
1:A:55:ALA:CB	1:A:58:LEU:HD21	2.42	0.48
1:A:73:ILE:N	1:A:254:ILE:CG2	2.76	0.48
1:A:259:PHE:CD2	1:A:262:ALA:HB3	2.48	0.48
1:A:26:PRO:HB3	1:A:167:ARG:CZ	2.44	0.48
1:A:65:THR:HG23	1:A:66:VAL:CG1	2.44	0.48
1:A:66:VAL:HA	1:A:69:THR:CG2	2.44	0.48
1:A:74:MET:CE	1:A:103:PHE:HB3	2.44	0.48
1:A:180:ASN:OD1	1:A:206:THR:HA	2.14	0.48
1:A:292:ILE:HD12	1:A:293:LEU:HD12	1.96	0.48
1:A:365:THR:CA	1:A:368:LEU:HD11	2.43	0.48
2:B:19:LEU:HD22	2:B:57:ALA:O	2.14	0.48
2:B:67:ASP:OD2	2:B:68:TYR:N	2.46	0.48
1:A:82:ALA:HB1	1:A:306:VAL:HG13	1.95	0.48
1:A:230:PHE:CD1	1:A:233:THR:HG21	2.48	0.48
1:A:271:LEU:HD13	1:A:415:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:HG23	1:A:340:LEU:CD1	2.44	0.48
1:A:343:VAL:HG22	1:A:371:GLY:N	2.28	0.48
1:A:73:ILE:N	1:A:254:ILE:HG23	2.29	0.48
1:A:103:PHE:HA	1:A:106:ILE:CG2	2.40	0.48
1:A:163:LEU:HD22	1:A:306:VAL:CG2	2.44	0.48
1:A:180:ASN:HD22	1:A:181:VAL:N	2.11	0.48
1:A:199:GLY:O	1:A:200:ALA:HB2	2.14	0.48
1:A:96:THR:O	1:A:99:GLN:N	2.47	0.48
1:A:102:TRP:CZ3	1:A:235:LYS:HG2	2.49	0.48
2:B:4:VAL:CG1	2:B:84:PRO:O	2.61	0.48
2:B:31:TYR:HB3	2:B:75:ARG:CB	2.40	0.47
2:B:17:SER:OG	2:B:18:LEU:N	2.48	0.47
2:B:65:GLY:HA2	2:B:91:THR:OG1	2.14	0.47
1:A:71:MET:CE	1:A:159:TYR:OH	2.63	0.47
1:A:143:THR:CG2	1:A:144:SER:N	2.77	0.47
1:A:143:THR:HG23	1:A:144:SER:N	2.28	0.47
1:A:17:ILE:HG22	1:A:18:ARG:H	1.80	0.47
1:A:116:TRP:O	1:A:117:ALA:C	2.52	0.47
1:A:339:VAL:HA	1:A:342:LEU:HG	1.95	0.47
1:A:372:LEU:HB3	1:A:431:ILE:CG2	2.27	0.47
2:B:8:LEU:HD13	2:B:87:ILE:CG1	2.45	0.47
1:A:142:PHE:O	1:A:146:ALA:HB3	2.15	0.47
1:A:241:TRP:NE1	1:A:243:VAL:HG22	2.30	0.47
1:A:268:ILE:CG1	1:A:287:ILE:CD1	2.92	0.47
1:A:314:ARG:O	1:A:316:GLU:N	2.47	0.47
1:A:317:PHE:O	1:A:318:SER:HB2	2.15	0.47
1:A:333:VAL:O	1:A:337:ILE:HG23	2.15	0.47
1:A:364:SER:C	1:A:366:VAL:N	2.68	0.47
1:A:372:LEU:HD22	1:A:431:ILE:HG21	1.97	0.47
1:A:416:ALA:O	1:A:417:TYR:CB	2.62	0.47
1:A:32:VAL:HG12	1:A:32:VAL:O	2.13	0.47
1:A:43:VAL:HG13	1:A:44:MET:CE	2.44	0.47
1:A:132:VAL:O	1:A:133:GLU:CG	2.60	0.47
1:A:369:PHE:CD2	1:A:424:TYR:HB3	2.49	0.47
2:B:36:TYR:CA	2:B:70:ILE:HD11	2.36	0.47
1:A:106:ILE:HG22	1:A:107:LEU:N	2.30	0.47
1:A:151:MET:CB	1:A:211:TRP:CD2	2.98	0.47
1:A:272:ILE:HD12	1:A:281:ALA:HB2	1.95	0.47
1:A:463:LEU:O	2:B:3:SER:CB	2.62	0.47
1:A:164:ASN:O	1:A:165:ARG:HD3	2.14	0.47
1:A:372:LEU:HD22	1:A:427:TRP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:HG23	2:B:51:PRO:O	2.13	0.47
1:A:16:GLU:C	1:A:17:ILE:HD12	2.36	0.46
1:A:317:PHE:HB3	1:A:452:LEU:HG	1.96	0.46
2:B:76:SER:O	2:B:77:TYR:C	2.54	0.46
1:A:40:VAL:HG11	1:A:180:ASN:ND2	2.30	0.46
1:A:72:GLY:O	1:A:73:ILE:C	2.54	0.46
1:A:98:ARG:HD3	1:A:229:PRO:O	2.16	0.46
1:A:110:PHE:O	1:A:111:GLY:C	2.51	0.46
1:A:260:LEU:C	1:A:262:ALA:N	2.65	0.46
1:A:26:PRO:HB3	1:A:167:ARG:NH1	2.30	0.46
1:A:183:LEU:CD2	1:A:209:VAL:HG23	2.46	0.46
1:A:225:LYS:HE2	1:A:226:PHE:CE2	2.51	0.46
1:A:339:VAL:HG21	1:A:375:PRO:CD	2.27	0.46
1:A:343:VAL:HA	1:A:367:LEU:HB3	1.98	0.46
1:A:410:LEU:C	1:A:412:GLY:H	2.19	0.46
2:B:63:SER:CB	2:B:64:PRO:HD2	2.45	0.46
1:A:372:LEU:HD22	1:A:431:ILE:CG1	2.45	0.46
1:A:89:LYS:HG3	1:A:92:GLU:CB	2.46	0.46
1:A:141:LEU:HD21	1:A:145:LEU:HD22	1.97	0.46
1:A:216:ALA:HA	1:A:219:ILE:CG1	2.43	0.46
1:A:283:GLN:O	1:A:283:GLN:NE2	2.47	0.46
1:A:418:ARG:CG	1:A:422:GLY:HA3	2.27	0.46
1:A:439:VAL:O	1:A:441:LEU:N	2.49	0.46
2:B:13:ALA:HB3	2:B:15:PRO:HG3	1.97	0.46
1:A:40:VAL:HG22	1:A:177:PHE:CD1	2.51	0.46
1:A:388:ARG:HB3	1:A:394:LYS:HB3	1.98	0.46
2:B:7:LYS:C	2:B:8:LEU:HD23	2.36	0.46
1:A:138:GLN:O	1:A:139:TYR:C	2.54	0.46
1:A:329:VAL:C	1:A:332:TRP:HB3	2.36	0.46
2:B:31:TYR:O	2:B:32:TYR:CD2	2.68	0.46
1:A:136:MET:O	1:A:139:TYR:HB2	2.15	0.46
1:A:145:LEU:HD22	1:A:203:GLY:CA	2.46	0.46
2:B:50:VAL:CG1	2:B:51:PRO:HD3	2.45	0.46
1:A:95:GLU:HA	1:A:98:ARG:HD3	1.98	0.46
1:A:230:PHE:CD1	1:A:233:THR:CG2	2.99	0.46
1:A:257:SER:OG	1:A:398:PHE:HA	2.15	0.46
2:B:36:TYR:HA	2:B:70:ILE:CG1	2.46	0.46
1:A:40:VAL:HG22	1:A:177:PHE:CB	2.45	0.45
1:A:94:GLY:HA2	1:A:227:PHE:CZ	2.51	0.45
1:A:268:ILE:HB	1:A:287:ILE:HD13	1.98	0.45
2:B:18:LEU:HB2	2:B:59:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ALA:HB1	2:B:53:SER:CA	2.46	0.45
1:A:77:LEU:C	1:A:79:PRO:HD2	2.37	0.45
1:A:103:PHE:CD2	1:A:106:ILE:HG22	2.51	0.45
1:A:192:PHE:O	1:A:193:GLY:O	2.34	0.45
1:A:409:LEU:HD23	1:A:410:LEU:HD11	1.98	0.45
1:A:415:LEU:HA	1:A:418:ARG:HD3	1.98	0.45
2:B:4:VAL:HG23	2:B:6:THR:HG23	1.89	0.45
1:A:109:ILE:CD1	1:A:110:PHE:CE2	2.99	0.45
1:A:317:PHE:HD2	1:A:455:SER:HB2	1.82	0.45
1:A:340:LEU:O	1:A:344:LEU:HB2	2.16	0.45
1:A:397:MET:O	1:A:400:HIS:ND1	2.47	0.45
2:B:28:TYR:O	2:B:29:VAL:C	2.51	0.45
1:A:163:LEU:HB3	1:A:306:VAL:HG22	1.99	0.45
1:A:298:GLN:O	1:A:382:ILE:CG2	2.64	0.45
1:A:426:PHE:CA	1:A:428:THR:HG22	2.47	0.45
2:B:27:GLU:HG3	2:B:52:GLY:O	2.16	0.45
1:A:70:PHE:O	1:A:73:ILE:HB	2.15	0.45
1:A:106:ILE:O	1:A:109:ILE:HG13	2.16	0.45
1:A:227:PHE:CD2	1:A:227:PHE:O	2.70	0.45
1:A:271:LEU:HD13	1:A:426:PHE:CE2	2.52	0.45
1:A:180:ASN:HA	1:A:209:VAL:HG21	1.98	0.45
1:A:95:GLU:O	1:A:99:GLN:CG	2.65	0.45
2:B:69:THR:O	2:B:70:ILE:HG13	2.17	0.45
1:A:73:ILE:CA	1:A:254:ILE:HG21	2.46	0.45
1:A:109:ILE:O	1:A:109:ILE:HD12	2.17	0.45
1:A:113:ILE:HG23	1:A:113:ILE:O	2.16	0.45
1:A:31:GLN:CG	1:A:296:ILE:HA	2.47	0.45
1:A:104:GLY:HA2	1:A:153:HIS:HB3	1.99	0.45
2:B:24:ALA:C	2:B:53:SER:OG	2.54	0.45
1:A:136:MET:C	1:A:138:GLN:H	2.20	0.44
1:A:147:MET:N	1:A:148:PRO:HD2	2.32	0.44
1:A:201:GLY:HA2	1:A:204:VAL:HG13	1.99	0.44
1:A:292:ILE:HG13	1:A:293:LEU:N	2.32	0.44
1:A:133:GLU:CG	1:A:133:GLU:O	2.66	0.44
1:A:322:TYR:HE1	1:A:449:SER:CB	2.31	0.44
1:A:133:GLU:HG2	1:A:133:GLU:O	2.18	0.44
1:A:150:ALA:O	1:A:152:VAL:N	2.48	0.44
1:A:359:VAL:CG1	1:A:360:LEU:HD22	2.42	0.44
1:A:388:ARG:O	1:A:391:LYS:N	2.50	0.44
1:A:116:TRP:HH2	1:A:147:MET:CA	2.27	0.44
1:A:147:MET:CE	1:A:207:MET:SD	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:O	1:A:43:VAL:N	2.49	0.44
1:A:120:THR:N	1:A:121:PRO:CD	2.81	0.44
2:B:27:GLU:HB3	2:B:30:VAL:HG23	2.00	0.44
2:B:35:THR:C	2:B:70:ILE:HG12	2.36	0.44
2:B:75:ARG:NH2	2:B:79:TRP:CE2	2.86	0.44
1:A:94:GLY:O	1:A:98:ARG:N	2.50	0.44
1:A:95:GLU:HA	1:A:98:ARG:CD	2.48	0.44
2:B:68:TYR:H	2:B:90:ARG:HB3	1.82	0.44
1:A:71:MET:HE2	1:A:159:TYR:OH	2.18	0.44
1:A:224:GLU:HG2	1:A:225:LYS:H	1.82	0.44
1:A:364:SER:OG	1:A:367:LEU:HD12	2.18	0.44
1:A:397:MET:O	1:A:400:HIS:HB3	2.17	0.44
1:A:40:VAL:HG11	1:A:180:ASN:CG	2.39	0.44
1:A:183:LEU:CD2	1:A:209:VAL:CG2	2.95	0.44
1:A:216:ALA:HA	1:A:219:ILE:CD1	2.47	0.44
1:A:332:TRP:CE3	1:A:332:TRP:O	2.71	0.44
1:A:342:LEU:CD1	1:A:374:GLN:OE1	2.66	0.44
1:A:416:ALA:O	1:A:417:TYR:HB3	2.16	0.44
1:A:103:PHE:C	1:A:105:LEU:H	2.16	0.44
1:A:225:LYS:HG2	1:A:226:PHE:HD2	1.82	0.44
1:A:315:ARG:NH2	2:B:11:VAL:HG11	2.32	0.44
1:A:372:LEU:HD11	1:A:424:TYR:O	2.18	0.44
1:A:391:LYS:C	1:A:393:THR:H	2.21	0.44
1:A:260:LEU:O	1:A:263:SER:N	2.49	0.43
1:A:403:ALA:O	1:A:407:CYS:CB	2.66	0.43
2:B:11:VAL:HG12	2:B:19:LEU:HD12	1.99	0.43
2:B:17:SER:HA	2:B:61:GLY:CA	2.47	0.43
2:B:71:THR:HG22	2:B:72:VAL:N	2.33	0.43
1:A:17:ILE:HG22	1:A:18:ARG:N	2.33	0.43
1:A:268:ILE:HD13	1:A:287:ILE:HD13	1.86	0.43
1:A:330:SER:O	1:A:333:VAL:HB	2.18	0.43
2:B:5:PRO:HD2	2:B:83:SER:O	2.18	0.43
1:A:132:VAL:CG1	1:A:133:GLU:H	2.25	0.43
1:A:339:VAL:HG22	1:A:370:ALA:O	2.19	0.43
1:A:373:PHE:HB3	1:A:431:ILE:HG22	2.00	0.43
1:A:411:PRO:HG3	1:A:429:ALA:CA	2.49	0.43
1:A:428:THR:C	1:A:430:LEU:H	2.21	0.43
2:B:29:VAL:O	2:B:30:VAL:CG1	2.67	0.43
1:A:339:VAL:CA	1:A:342:LEU:HD12	2.39	0.43
1:A:437:ALA:C	1:A:439:VAL:N	2.71	0.43
2:B:3:SER:OG	2:B:4:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LEU:HD13	2:B:19:LEU:O	2.17	0.43
1:A:372:LEU:HD22	1:A:431:ILE:CG2	2.48	0.43
1:A:411:PRO:O	1:A:426:PHE:O	2.36	0.43
1:A:418:ARG:CZ	1:A:425:GLY:HA3	2.48	0.43
1:A:78:ASN:N	1:A:79:PRO:CD	2.82	0.43
1:A:172:VAL:HG13	1:A:173:SER:N	2.34	0.43
1:A:285:VAL:O	1:A:289:LEU:HD23	2.18	0.43
2:B:26:GLY:O	2:B:53:SER:CB	2.67	0.43
1:A:418:ARG:HG3	1:A:419:PHE:H	1.82	0.43
1:A:180:ASN:C	1:A:180:ASN:HD22	2.23	0.43
2:B:64:PRO:HB2	2:B:65:GLY:H	1.66	0.43
1:A:78:ASN:C	1:A:163:LEU:HD13	2.38	0.43
1:A:183:LEU:O	1:A:183:LEU:HD12	2.19	0.43
1:A:186:ILE:O	1:A:190:GLY:HA3	2.19	0.43
1:A:268:ILE:HD12	1:A:268:ILE:C	2.39	0.43
1:A:346:ARG:O	1:A:348:PRO:CD	2.67	0.43
1:A:424:TYR:O	1:A:427:TRP:HB2	2.19	0.43
1:A:442:VAL:HG23	1:A:445:LEU:HD23	2.01	0.43
1:A:89:LYS:HG3	1:A:92:GLU:HB2	1.99	0.42
1:A:308:ILE:HD12	1:A:390:TYR:CA	2.49	0.42
2:B:76:SER:O	2:B:78:TYR:O	2.36	0.42
1:A:51:GLU:HB3	1:A:54:ALA:HB2	2.00	0.42
1:A:154:ARG:NH2	1:A:215:LEU:CD2	2.82	0.42
1:A:265:PHE:O	1:A:269:VAL:HB	2.19	0.42
1:A:90:THR:HA	1:A:93:ALA:HB3	1.99	0.42
1:A:115:MET:O	1:A:118:ALA:HB2	2.13	0.42
1:A:207:MET:SD	1:A:207:MET:O	2.77	0.42
1:A:292:ILE:HD12	1:A:293:LEU:CD1	2.49	0.42
1:A:426:PHE:HA	1:A:428:THR:HG22	2.01	0.42
1:A:155:ALA:HB2	1:A:214:ALA:CA	2.48	0.42
1:A:317:PHE:CD2	1:A:455:SER:HB2	2.55	0.42
2:B:16:THR:HG23	2:B:17:SER:H	1.83	0.42
1:A:32:VAL:O	1:A:35:VAL:HG12	2.19	0.42
1:A:65:THR:CG2	1:A:66:VAL:H	2.32	0.42
1:A:172:VAL:C	1:A:174:PHE:H	2.22	0.42
1:A:254:ILE:CD1	1:A:388:ARG:HD2	2.50	0.42
2:B:50:VAL:CB	2:B:51:PRO:CD	2.98	0.42
1:A:74:MET:C	1:A:76:ALA:N	2.72	0.42
1:A:77:LEU:HD12	1:A:250:ILE:HD13	2.02	0.42
1:A:252:ALA:HB3	1:A:253:PRO:HD3	2.02	0.42
1:A:301:GLY:O	1:A:305:THR:CG2	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HG3	1:A:419:PHE:N	2.35	0.42
2:B:34:ILE:HA	2:B:71:THR:O	2.20	0.42
1:A:295:MET:HG2	1:A:296:ILE:N	2.34	0.42
1:A:339:VAL:CG2	1:A:374:GLN:HB3	2.49	0.42
2:B:23:ASP:O	2:B:55:SER:OG	2.26	0.42
1:A:85:TYR:HD1	1:A:310:PHE:CE1	2.37	0.42
1:A:117:ALA:O	1:A:118:ALA:C	2.57	0.42
1:A:143:THR:O	1:A:147:MET:HB3	2.20	0.42
1:A:292:ILE:CD1	1:A:293:LEU:HD12	2.49	0.42
2:B:13:ALA:C	2:B:15:PRO:HD3	2.41	0.42
2:B:13:ALA:HB2	2:B:18:LEU:HG	2.01	0.42
2:B:60:SER:O	2:B:62:LEU:N	2.52	0.42
1:A:210:PHE:O	1:A:214:ALA:N	2.53	0.41
1:A:209:VAL:HG12	1:A:209:VAL:O	2.20	0.41
1:A:308:ILE:HD12	1:A:390:TYR:N	2.35	0.41
1:A:376:ALA:HB1	1:A:435:THR:HG21	2.02	0.41
2:B:69:THR:OG1	2:B:88:ASN:HB2	2.20	0.41
1:A:19:LEU:C	1:A:21:THR:N	2.74	0.41
1:A:43:VAL:HG22	1:A:43:VAL:O	2.20	0.41
1:A:118:ALA:O	1:A:120:THR:N	2.53	0.41
2:B:29:VAL:O	2:B:30:VAL:HB	2.19	0.41
1:A:76:ALA:HB1	1:A:394:LYS:HZ1	1.85	0.41
1:A:175:ALA:HA	1:A:178:VAL:HG12	2.03	0.41
1:A:236:PHE:HE2	1:A:239:PRO:O	2.03	0.41
1:A:247:ILE:HA	1:A:250:ILE:HG13	2.02	0.41
1:A:37:ILE:C	1:A:39:PHE:N	2.73	0.41
1:A:68:ILE:O	1:A:68:ILE:HG22	2.19	0.41
1:A:116:TRP:N	1:A:116:TRP:HE3	2.18	0.41
1:A:364:SER:OG	1:A:367:LEU:CD1	2.68	0.41
1:A:384:SER:O	1:A:386:ALA:N	2.43	0.41
2:B:67:ASP:OD2	2:B:67:ASP:C	2.59	0.41
2:B:81:TRP:CD1	2:B:81:TRP:N	2.89	0.41
1:A:100:GLY:C	1:A:157:HIS:CD2	2.93	0.41
1:A:407:CYS:HB3	1:A:433:SER:HB2	2.02	0.41
2:B:8:LEU:HD13	2:B:87:ILE:CD1	2.48	0.41
1:A:24:ALA:HB1	1:A:27:MET:HB2	2.03	0.41
1:A:152:VAL:HG12	1:A:210:PHE:CG	2.56	0.41
1:A:274:PRO:C	1:A:276:GLY:N	2.74	0.41
1:A:311:SER:HA	1:A:314:ARG:HB2	2.03	0.41
1:A:371:GLY:O	1:A:375:PRO:HD2	2.21	0.41
1:A:391:LYS:C	1:A:393:THR:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:HG12	2:B:48:PHE:HB2	2.02	0.41
1:A:40:VAL:HG12	1:A:44:MET:CE	2.44	0.41
1:A:209:VAL:HA	1:A:212:PHE:HB3	2.02	0.41
1:A:306:VAL:C	1:A:308:ILE:N	2.63	0.41
1:A:308:ILE:HG13	1:A:309:GLY:H	1.86	0.41
1:A:304:GLY:O	1:A:307:ARG:N	2.54	0.41
1:A:334:LEU:N	1:A:334:LEU:HD22	2.36	0.41
1:A:396:PRO:HA	1:A:398:PHE:HB3	2.03	0.41
1:A:458:ALA:HB1	2:B:8:LEU:CB	2.48	0.41
2:B:75:ARG:HD2	2:B:80:GLY:O	2.21	0.41
1:A:272:ILE:CG2	1:A:281:ALA:HA	2.51	0.40
2:B:31:TYR:CE1	2:B:75:ARG:NH1	2.88	0.40
1:A:64:ALA:HA	1:A:67:TYR:HB3	2.03	0.40
1:A:76:ALA:HB2	1:A:254:ILE:HG21	2.02	0.40
2:B:85:ILE:O	2:B:85:ILE:CG2	2.68	0.40
1:A:254:ILE:HB	1:A:394:LYS:HE2	2.03	0.40
1:A:255:GLY:O	1:A:259:PHE:N	2.54	0.40
1:A:284:GLN:HA	1:A:287:ILE:HG12	2.03	0.40
2:B:27:GLU:CG	2:B:30:VAL:HG23	2.46	0.40
1:A:55:ALA:O	1:A:138:GLN:NE2	2.54	0.40
1:A:148:PRO:HG3	1:A:207:MET:CB	2.51	0.40
1:A:220:TYR:HD2	1:A:222:ALA:HB3	1.86	0.40
1:A:387:LEU:HD13	1:A:387:LEU:HA	1.82	0.40
1:A:395:VAL:HG12	1:A:396:PRO:HD2	2.04	0.40
1:A:428:THR:OG1	1:A:429:ALA:N	2.55	0.40
1:A:82:ALA:CB	1:A:306:VAL:HG13	2.51	0.40
1:A:163:LEU:O	1:A:164:ASN:CB	2.69	0.40
1:A:230:PHE:HE1	1:A:233:THR:HG21	1.80	0.40
1:A:266:SER:O	1:A:266:SER:OG	2.39	0.40
1:A:268:ILE:HD12	1:A:269:VAL:CG2	2.49	0.40
1:A:321:ARG:HH21	1:A:390:TYR:HB3	1.86	0.40
1:A:436:ILE:O	1:A:436:ILE:HG13	2.21	0.40
2:B:4:VAL:HG12	2:B:83:SER:HB3	2.02	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	457/459 (100%)	258 (56%)	121 (26%)	78 (17%)	0	3
2	B	89/99 (90%)	52 (58%)	19 (21%)	18 (20%)	0	2
All	All	546/558 (98%)	310 (57%)	140 (26%)	96 (18%)	0	2

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	41	ASP
1	A	58	LEU
1	A	64	ALA
1	A	80	MET
1	A	105	LEU
1	A	118	ALA
1	A	139	TYR
1	A	164	ASN
1	A	166	PRO
1	A	192	PHE
1	A	193	GLY
1	A	194	MET
1	A	234	ALA
1	A	236	PHE
1	A	238	LYS
1	A	261	GLU
1	A	277	GLU
1	A	278	ASP
1	A	297	PRO
1	A	298	GLN
1	A	305	THR
1	A	307	ARG
1	A	347	SER
1	A	354	ASN

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Mol	Chain	Res	Type
1	A	361	SER
1	A	372	LEU
1	A	378	PHE
1	A	386	ALA
1	A	392	VAL
1	A	398	PHE
1	A	417	TYR
2	B	11	VAL
2	B	15	PRO
2	B	30	VAL
2	B	44	PRO
2	B	51	PRO
2	B	61	GLY
2	B	77	TYR
2	B	79	TRP
2	B	90	ARG
1	A	14	LEU
1	A	17	ILE
1	A	20	LEU
1	A	75	ALA
1	A	79	PRO
1	A	104	GLY
1	A	127	THR
1	A	130	ASP
1	A	131	TYR
1	A	132	VAL
1	A	149	ALA
1	A	158	ALA
1	A	200	ALA
1	A	229	PRO
1	A	244	PHE
1	A	275	PHE
1	A	291	GLY
1	A	348	PRO
1	A	380	GLN
1	A	388	ARG
1	A	389	GLY
1	A	396	PRO
1	A	405	TRP
1	A	442	VAL
2	B	5	PRO
2	B	38	GLU

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Mol	Chain	Res	Type
2	B	52	GLY
2	B	62	LEU
2	B	64	PRO
1	A	12	VAL
1	A	237	GLY
1	A	242	ALA
1	A	385	TYR
1	A	460	SER
2	B	56	THR
1	A	151	MET
1	A	165	ARG
1	A	173	SER
1	A	232	LEU
1	A	358	ALA
1	A	421	MET
1	A	440	ALA
1	A	97	GLY
1	A	314	ARG
1	A	344	LEU
1	A	353	TYR
2	B	24	ALA
2	B	83	SER
1	A	284	GLN
1	A	73	ILE
1	A	219	ILE
2	B	84	PRO
1	A	47	GLY
1	A	119	ILE
1	A	274	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	353/353 (100%)	243 (69%)	110 (31%)	0 2
2	B	78/85 (92%)	54 (69%)	24 (31%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	431/438 (98%)	297 (69%)	134 (31%)	0 2

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	14	LEU
1	A	15	LYS
1	A	18	ARG
1	A	20	LEU
1	A	25	LEU
1	A	39	PHE
1	A	44	MET
1	A	53	LEU
1	A	60	SER
1	A	61	SER
1	A	63	PHE
1	A	65	THR
1	A	71	MET
1	A	80	MET
1	A	81	ILE
1	A	89	LYS
1	A	95	GLU
1	A	102	TRP
1	A	103	PHE
1	A	105	LEU
1	A	106	ILE
1	A	107	LEU
1	A	112	MET
1	A	113	ILE
1	A	116	TRP
1	A	123	ARG
1	A	124	ASN
1	A	126	LEU
1	A	127	THR
1	A	136	MET
1	A	140	MET
1	A	147	MET
1	A	151	MET
1	A	153	HIS
1	A	154	ARG
1	A	159	TYR

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Mol	Chain	Res	Type
1	A	165	ARG
1	A	167	ARG
1	A	173	SER
1	A	180	ASN
1	A	183	LEU
1	A	184	ASN
1	A	197	LEU
1	A	204	VAL
1	A	206	THR
1	A	207	MET
1	A	210	PHE
1	A	212	PHE
1	A	215	LEU
1	A	218	TRP
1	A	224	GLU
1	A	225	LYS
1	A	228	ARG
1	A	232	LEU
1	A	235	LYS
1	A	238	LYS
1	A	248	TRP
1	A	249	LYS
1	A	257	SER
1	A	259	PHE
1	A	260	LEU
1	A	271	LEU
1	A	283	GLN
1	A	292	ILE
1	A	294	TYR
1	A	295	MET
1	A	296	ILE
1	A	299	SER
1	A	302	SER
1	A	305	THR
1	A	307	ARG
1	A	311	SER
1	A	312	LEU
1	A	321	ARG
1	A	323	ILE
1	A	329	VAL
1	A	334	LEU
1	A	336	VAL

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Mol	Chain	Res	Type
1	A	337	ILE
1	A	338	THR
1	A	340	LEU
1	A	347	SER
1	A	353	TYR
1	A	362	ILE
1	A	369	PHE
1	A	374	GLN
1	A	377	ASP
1	A	378	PHE
1	A	379	THR
1	A	382	ILE
1	A	384	SER
1	A	387	LEU
1	A	388	ARG
1	A	390	TYR
1	A	395	VAL
1	A	397	MET
1	A	407	CYS
1	A	417	TYR
1	A	427	TRP
1	A	428	THR
1	A	431	ILE
1	A	434	LEU
1	A	435	THR
1	A	436	ILE
1	A	439	VAL
1	A	441	LEU
1	A	447	LYS
1	A	452	LEU
1	A	460	SER
2	B	2	SER
2	B	6	THR
2	B	8	LEU
2	B	16	THR
2	B	18	LEU
2	B	19	LEU
2	B	20	ILE
2	B	21	SER
2	B	25	ARG
2	B	28	TYR
2	B	34	ILE

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Mol	Chain	Res	Type
2	B	36	TYR
2	B	38	GLU
2	B	39	THR
2	B	46	GLN
2	B	50	VAL
2	B	53	SER
2	B	55	SER
2	B	58	THR
2	B	70	ILE
2	B	75	ARG
2	B	78	TYR
2	B	90	ARG
2	B	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	184	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	459/459 (100%)	-0.30	24 (5%)	27	23	93, 203, 346, 432	0
2	B	91/99 (91%)	-0.35	5 (5%)	25	21	104, 178, 267, 302	0
All	All	550/558 (98%)	-0.31	29 (5%)	26	22	93, 200, 342, 432	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	SER	11.6
2	B	1	VAL	9.5
1	A	350	ALA	7.7
1	A	349	LEU	7.5
1	A	463	LEU	6.5
1	A	9	SER	6.0
1	A	5	LEU	4.6
1	A	239	PRO	4.4
1	A	6	ASP	4.2
1	A	352	MET	4.0
1	A	462	GLY	3.7
1	A	87	ALA	3.5
1	A	351	SER	3.5
1	A	380	GLN	3.5
1	A	88	GLY	3.3
1	A	379	THR	3.1
2	B	89	TYR	3.0
1	A	130	ASP	2.9
1	A	348	PRO	2.6
1	A	421	MET	2.6
1	A	7	ARG	2.6
1	A	326	VAL	2.4
1	A	419	PHE	2.3
1	A	20	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	457	LYS	2.3
2	B	3	SER	2.3
1	A	440	ALA	2.1
2	B	9	GLU	2.1
1	A	460	SER	2.1

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

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)

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CS	A	501	1/1	0.98	0.06	127,127,127,127	0

6.5 Other polymers (i)

There are no such residues in this entry.