Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 12:49 AM EST

PDB ID	:	4HUM
Title	:	MATE transporter NorM-NG in complex with ethidium and monobody
Authors	:	Lu, M.
Deposited on	:	2012-11-02
Resolution	:	3.49 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:

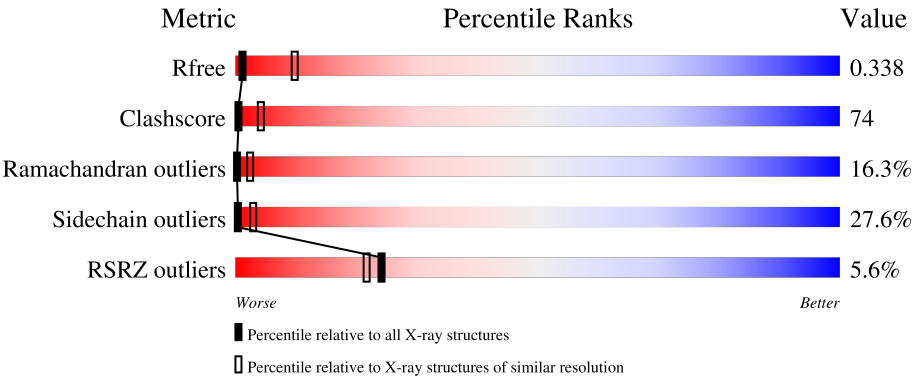
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.49 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 21% 52% 24% .
2	B	99	6% 12% 44% 31% . 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4239 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			

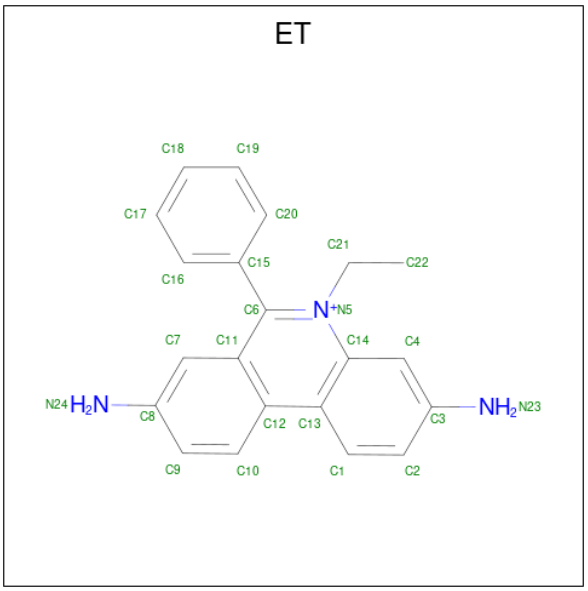
There are 4 discrepancies between the modelled and reference sequences:

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 ETHIDIUM (three-letter code: ET) (formula: $C_{21}H_{20}N_3$).



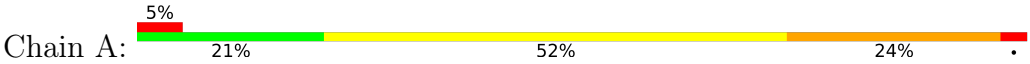
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 24 21 3	0	0

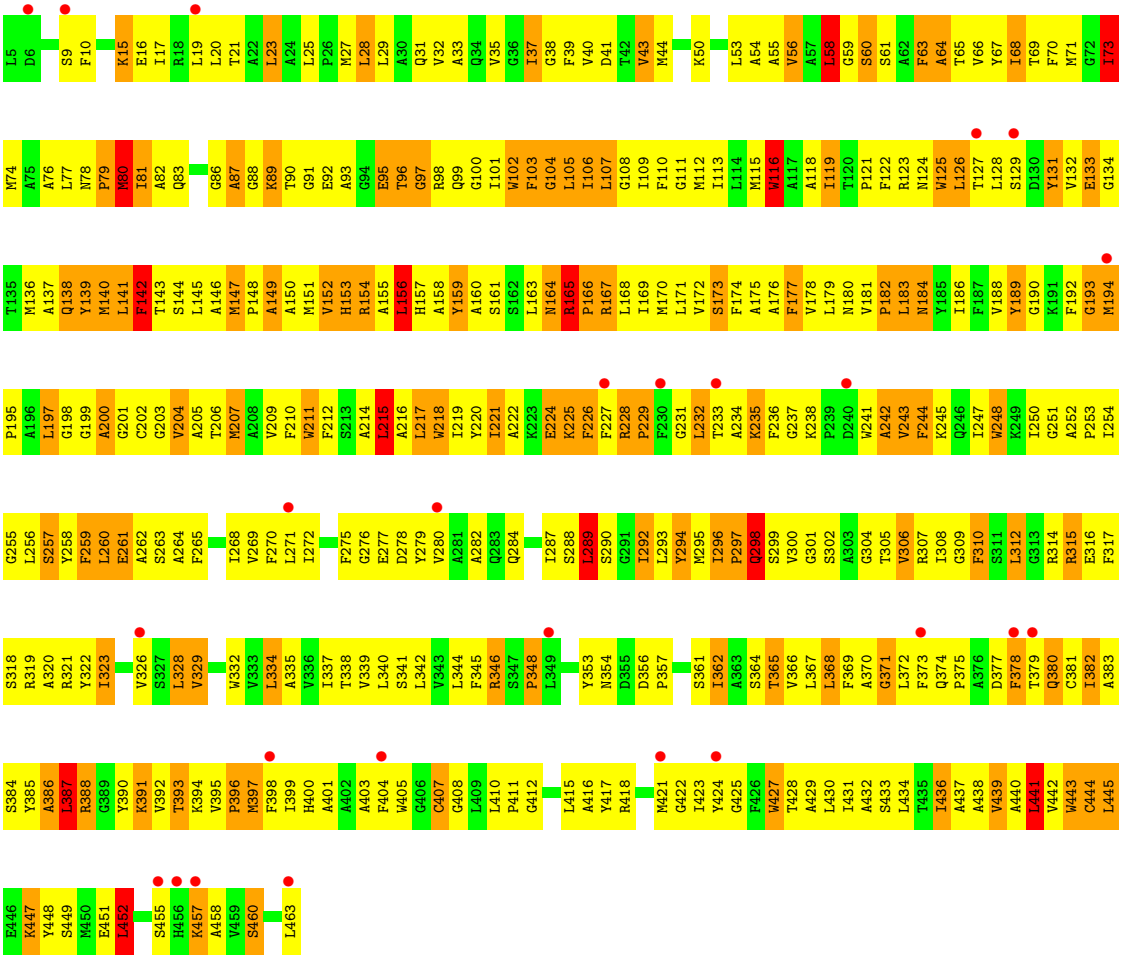
3 Residue-property plots (i)

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: Multidrug efflux protein

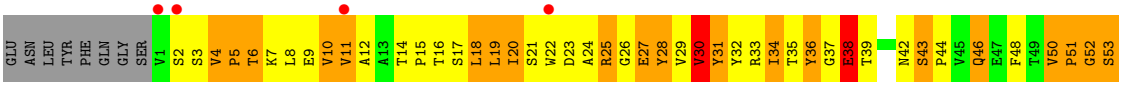
Chain A:





• Molecule 2: Protein B

Chain B:




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	119.03Å 119.03Å 227.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.49 52.73 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.49) 99.1 (52.73-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.314 , 0.331 0.330 , 0.338	Depositor DCC
R_{free} test set	1231 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	126.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 111.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.180 for -h,-k,l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	4239	wwPDB-VP
Average B, all atoms (Å^2)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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 (i)

5.1 Standard geometry (i)

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

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	0.72	6/3605 (0.2%)	0.94	5/4898 (0.1%)
2	B	0.81	0/729	1.19	4/1004 (0.4%)
All	All	0.73	6/4334 (0.1%)	0.98	9/5902 (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	9
2	B	0	2
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	TRP	CD2-CE2	5.57	1.48	1.41
1	A	443	TRP	CD2-CE2	5.51	1.48	1.41
1	A	125	TRP	CD2-CE2	5.42	1.47	1.41
1	A	102	TRP	CD2-CE2	5.34	1.47	1.41
1	A	116	TRP	CD2-CE2	5.15	1.47	1.41
1	A	427	TRP	CD2-CE2	5.02	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	30	VAL	CB-CA-C	-6.27	99.48	111.40
2	B	30	VAL	C-N-CA	-6.07	106.53	121.70
1	A	444	CYS	CA-CB-SG	6.00	124.81	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ALA	N-CA-C	-5.97	94.89	111.00
2	B	33	ARG	N-CA-C	-5.73	95.53	111.00
2	B	30	VAL	N-CA-C	5.34	125.43	111.00
1	A	156	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	289	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	328	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	GLN	Peptide
1	A	194	MET	Peptide
1	A	215	LEU	Peptide
1	A	220	TYR	Peptide
1	A	226	PHE	Peptide
1	A	338	THR	Peptide
1	A	387	LEU	Peptide
1	A	452	LEU	Peptide
1	A	54	ALA	Peptide
2	B	27	GLU	Peptide
2	B	76	SER	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	3587	521	0
2	B	707	0	681	127	0
3	A	24	0	20	3	0
All	All	4239	0	4288	633	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 74.

All (633) 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:460:SER:O	2:B:8:LEU:HD12	1.39	1.21
2:B:36:TYR:HA	2:B:70:ILE:HD11	1.23	1.17
1:A:78:ASN:HA	1:A:163:LEU:HD13	1.31	1.12
2:B:4:VAL:HG22	2:B:6:THR:HG23	1.11	1.11
1:A:144:SER:HB3	1:A:204:VAL:HG12	1.29	1.10
1:A:460:SER:O	2:B:8:LEU:CD1	1.98	1.10
1:A:44:MET:HE3	1:A:180:ASN:HD21	1.17	1.10
1:A:411:PRO:HB3	1:A:428:THR:HG23	1.23	1.09
1:A:137:ALA:O	1:A:199:GLY:O	1.71	1.08
2:B:30:VAL:O	2:B:30:VAL:HG22	1.33	1.08
1:A:158:ALA:HB2	1:A:217:LEU:CD1	1.84	1.06
1:A:145:LEU:HD13	1:A:203:GLY:O	1.56	1.06
2:B:67:ASP:HA	2:B:90:ARG:HB3	1.37	1.06
1:A:145:LEU:HD12	1:A:207:MET:HB3	1.33	1.05
2:B:8:LEU:HD13	2:B:87:ILE:HD11	1.06	1.04
1:A:365:THR:HB	1:A:423:ILE:HG21	1.40	1.04
2:B:10:VAL:HG12	2:B:18:LEU:HD22	1.36	1.03
1:A:265:PHE:CE2	3:A:501:ET:H9	1.94	1.03
1:A:193:GLY:O	1:A:195:PRO:HD3	1.58	1.02
1:A:411:PRO:HG3	1:A:429:ALA:HB3	1.42	1.02
2:B:50:VAL:HG12	2:B:51:PRO:CD	1.91	1.01
1:A:136:MET:O	1:A:139:TYR:HB2	1.58	1.00
2:B:30:VAL:O	2:B:30:VAL:CG2	2.10	0.97
1:A:439:VAL:HG23	1:A:440:ALA:H	1.27	0.97
1:A:218:TRP:HA	1:A:218:TRP:CE3	2.01	0.95
2:B:4:VAL:CG2	2:B:6:THR:HG23	1.95	0.95
1:A:144:SER:CB	1:A:204:VAL:HG12	1.97	0.94
2:B:4:VAL:HG22	2:B:6:THR:CG2	1.98	0.94
2:B:8:LEU:HD13	2:B:87:ILE:CD1	1.95	0.94
1:A:372:LEU:HB3	1:A:431:ILE:HG21	1.48	0.93
1:A:112:MET:CE	1:A:150:ALA:HB2	1.99	0.92
1:A:90:THR:HA	1:A:93:ALA:HB3	1.51	0.92
1:A:148:PRO:HB2	1:A:152:VAL:HG11	1.53	0.91
1:A:73:ILE:O	1:A:76:ALA:HB3	1.70	0.91
1:A:215:LEU:N	1:A:215:LEU:HD23	1.85	0.91
1:A:158:ALA:HB2	1:A:217:LEU:HD11	1.49	0.91
2:B:50:VAL:HG12	2:B:51:PRO:HD3	1.50	0.91
1:A:429:ALA:O	1:A:433:SER:HB3	1.71	0.91
1:A:145:LEU:HD11	1:A:206:THR:HG22	1.53	0.90
2:B:8:LEU:CD1	2:B:87:ILE:HD11	1.97	0.90
1:A:44:MET:SD	1:A:206:THR:OG1	2.30	0.90
1:A:315:ARG:HG3	1:A:317:PHE:CE1	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ALA:O	2:B:53:SER:OG	1.90	0.89
1:A:188:VAL:HA	1:A:198:GLY:HA2	1.55	0.89
1:A:78:ASN:HA	1:A:163:LEU:CD1	2.01	0.89
1:A:164:ASN:O	1:A:166:PRO:HD3	1.75	0.87
1:A:168:LEU:HA	1:A:171:LEU:HD13	1.57	0.86
1:A:102:TRP:O	1:A:106:ILE:HB	1.75	0.86
1:A:127:THR:HG22	1:A:128:LEU:H	1.41	0.85
2:B:36:TYR:CA	2:B:70:ILE:HD11	2.05	0.85
1:A:155:ALA:HB2	1:A:214:ALA:HA	1.58	0.85
1:A:259:PHE:HA	1:A:262:ALA:HB3	1.56	0.85
1:A:119:ILE:HG12	1:A:142:PHE:CD2	2.10	0.85
1:A:181:VAL:HB	1:A:182:PRO:CD	2.07	0.85
1:A:218:TRP:HA	1:A:218:TRP:HE3	1.40	0.85
1:A:224:GLU:HG2	1:A:225:LYS:H	1.39	0.85
1:A:65:THR:O	1:A:69:THR:HG22	1.77	0.85
1:A:141:LEU:CD2	1:A:203:GLY:HA3	2.05	0.84
1:A:248:TRP:CZ3	1:A:252:ALA:HB2	2.13	0.84
1:A:44:MET:CE	1:A:180:ASN:HD21	1.89	0.84
1:A:411:PRO:HB3	1:A:428:THR:CG2	2.08	0.84
2:B:19:LEU:HA	2:B:58:THR:HG22	1.58	0.84
2:B:37:GLY:H	2:B:70:ILE:CD1	1.92	0.83
1:A:339:VAL:HG21	1:A:375:PRO:HD3	1.60	0.82
1:A:44:MET:HE3	1:A:180:ASN:ND2	1.94	0.82
2:B:38:GLU:HA	2:B:68:TYR:HA	1.62	0.81
1:A:193:GLY:O	1:A:195:PRO:CD	2.28	0.81
1:A:252:ALA:HB3	1:A:253:PRO:HD3	1.60	0.80
1:A:441:LEU:O	1:A:443:TRP:N	2.12	0.80
1:A:214:ALA:C	1:A:215:LEU:HD23	2.02	0.80
1:A:144:SER:HB3	1:A:204:VAL:CG1	2.10	0.80
1:A:79:PRO:HG2	1:A:80:MET:H	1.46	0.80
1:A:151:MET:SD	1:A:211:TRP:CE3	2.75	0.80
1:A:145:LEU:HD11	1:A:206:THR:CG2	2.11	0.80
1:A:95:GLU:O	1:A:99:GLN:HG2	1.82	0.80
1:A:329:VAL:HA	1:A:332:TRP:CB	2.12	0.79
2:B:50:VAL:HG12	2:B:51:PRO:HD2	1.61	0.79
1:A:447:LYS:O	1:A:448:TYR:HD1	1.66	0.79
1:A:242:ALA:HA	1:A:245:LYS:H	1.46	0.78
1:A:154:ARG:NH2	1:A:215:LEU:HD22	1.98	0.78
1:A:432:ALA:O	1:A:436:ILE:HG23	1.82	0.78
1:A:158:ALA:HB2	1:A:217:LEU:CG	2.13	0.78
1:A:288:SER:O	1:A:292:ILE:HG23	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:O	2:B:70:ILE:HD12	1.84	0.77
1:A:183:LEU:HA	1:A:186:ILE:HD12	1.67	0.77
2:B:10:VAL:HG12	2:B:18:LEU:CD2	2.14	0.77
1:A:429:ALA:O	1:A:433:SER:CB	2.32	0.77
1:A:251:GLY:O	1:A:254:ILE:HG22	1.85	0.76
1:A:254:ILE:HB	1:A:394:LYS:NZ	1.99	0.76
1:A:439:VAL:HG23	1:A:440:ALA:N	1.99	0.76
1:A:254:ILE:O	1:A:258:TYR:N	2.19	0.76
1:A:89:LYS:HG3	1:A:92:GLU:HB2	1.68	0.76
1:A:436:ILE:O	1:A:439:VAL:HG22	1.84	0.75
1:A:400:HIS:CE1	1:A:401:ALA:HB2	2.21	0.75
1:A:290:SER:O	1:A:294:TYR:HB3	1.87	0.75
1:A:96:THR:O	1:A:99:GLN:N	2.19	0.75
2:B:67:ASP:HA	2:B:90:ARG:CB	2.16	0.75
2:B:69:THR:HA	2:B:88:ASN:HA	1.69	0.75
1:A:372:LEU:HD11	1:A:424:TYR:HD1	1.52	0.74
1:A:87:ALA:HB1	1:A:89:LYS:HZ2	1.52	0.74
2:B:12:ALA:O	2:B:18:LEU:HD23	1.87	0.74
1:A:429:ALA:HA	1:A:432:ALA:HB3	1.68	0.74
2:B:63:SER:HB3	2:B:64:PRO:CD	2.18	0.74
1:A:112:MET:CE	1:A:150:ALA:CB	2.65	0.73
1:A:264:ALA:O	1:A:268:ILE:HG12	1.88	0.73
1:A:87:ALA:HB1	1:A:89:LYS:NZ	2.03	0.73
1:A:424:TYR:HA	1:A:427:TRP:CD1	2.24	0.73
2:B:65:GLY:HA2	2:B:91:THR:HG21	1.71	0.73
1:A:377:ASP:HB2	1:A:434:LEU:HD21	1.70	0.72
1:A:384:SER:O	1:A:388:ARG:HG3	1.89	0.72
1:A:257:SER:OG	1:A:398:PHE:HA	1.89	0.72
1:A:32:VAL:HG22	1:A:296:ILE:HD11	1.70	0.72
1:A:321:ARG:HH22	1:A:391:LYS:HB2	1.53	0.72
1:A:403:ALA:O	1:A:407:CYS:HB2	1.90	0.72
1:A:394:LYS:HA	1:A:397:MET:HB2	1.70	0.72
1:A:159:TYR:HB3	1:A:169:ILE:HD13	1.72	0.72
2:B:87:ILE:HG22	2:B:88:ASN:N	2.04	0.72
1:A:148:PRO:O	1:A:150:ALA:N	2.23	0.71
1:A:297:PRO:O	1:A:299:SER:N	2.23	0.71
1:A:318:SER:C	1:A:320:ALA:H	1.92	0.71
1:A:373:PHE:HB3	1:A:431:ILE:HG22	1.70	0.71
1:A:60:SER:HB3	1:A:141:LEU:HD11	1.69	0.71
1:A:329:VAL:HA	1:A:332:TRP:HB3	1.73	0.71
1:A:439:VAL:CG2	1:A:440:ALA:H	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:HA	2:B:70:ILE:CD1	2.12	0.71
1:A:60:SER:HB3	1:A:141:LEU:CD1	2.21	0.71
1:A:384:SER:HA	1:A:387:LEU:HB2	1.73	0.71
2:B:4:VAL:HG21	2:B:85:ILE:HB	1.73	0.70
1:A:265:PHE:HE2	3:A:501:ET:H9	1.54	0.70
1:A:368:LEU:HD12	1:A:423:ILE:CG2	2.22	0.70
1:A:394:LYS:HA	1:A:397:MET:CB	2.20	0.70
1:A:100:GLY:O	1:A:103:PHE:N	2.25	0.70
1:A:159:TYR:CB	1:A:169:ILE:HD13	2.22	0.69
2:B:11:VAL:CG1	2:B:19:LEU:HD12	2.21	0.69
1:A:460:SER:O	2:B:8:LEU:CG	2.40	0.69
2:B:37:GLY:H	2:B:70:ILE:HD12	1.57	0.69
2:B:50:VAL:CG1	2:B:51:PRO:HD3	2.20	0.69
1:A:216:ALA:HA	1:A:219:ILE:CG1	2.21	0.69
1:A:372:LEU:HD11	1:A:424:TYR:HB2	1.75	0.69
1:A:146:ALA:N	1:A:148:PRO:HD2	2.08	0.68
1:A:256:LEU:HB3	1:A:398:PHE:HE1	1.59	0.68
1:A:397:MET:O	1:A:400:HIS:ND1	2.26	0.68
1:A:455:SER:HB3	2:B:11:VAL:HG23	1.76	0.68
1:A:77:LEU:HA	1:A:80:MET:HG3	1.75	0.68
1:A:457:LYS:O	2:B:10:VAL:HG23	1.93	0.68
1:A:68:ILE:HA	1:A:71:MET:HB3	1.75	0.68
1:A:87:ALA:CB	1:A:89:LYS:NZ	2.57	0.68
2:B:50:VAL:CG1	2:B:51:PRO:CD	2.69	0.67
1:A:78:ASN:CA	1:A:163:LEU:HD13	2.18	0.67
1:A:89:LYS:HG2	1:A:92:GLU:HB3	1.75	0.67
2:B:87:ILE:HG22	2:B:88:ASN:H	1.59	0.67
1:A:225:LYS:HD3	1:A:226:PHE:CD2	2.29	0.67
1:A:115:MET:O	1:A:118:ALA:HB3	1.95	0.67
1:A:216:ALA:HA	1:A:219:ILE:HG12	1.77	0.66
1:A:297:PRO:HB3	1:A:378:PHE:CE2	2.30	0.66
1:A:248:TRP:HZ3	1:A:252:ALA:HB2	1.55	0.66
1:A:154:ARG:HH21	1:A:215:LEU:HD22	1.58	0.66
1:A:315:ARG:NH2	2:B:11:VAL:HG11	2.09	0.66
2:B:32:TYR:HA	2:B:73:TYR:O	1.96	0.66
1:A:308:ILE:HD11	1:A:386:ALA:HA	1.76	0.66
1:A:44:MET:HE1	1:A:184:ASN:HB2	1.78	0.66
1:A:66:VAL:HA	1:A:69:THR:HG22	1.78	0.66
1:A:287:ILE:HG21	1:A:427:TRP:HH2	1.60	0.66
1:A:372:LEU:HD11	1:A:424:TYR:CD1	2.30	0.66
1:A:43:VAL:HG11	1:A:181:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB2	1:A:170:MET:HA	1.78	0.66
1:A:322:TYR:HE1	1:A:449:SER:HB3	1.61	0.65
1:A:364:SER:HA	1:A:366:VAL:HG22	1.77	0.65
2:B:18:LEU:HB2	2:B:59:ILE:HD11	1.78	0.65
1:A:259:PHE:HA	1:A:262:ALA:CB	2.26	0.65
1:A:321:ARG:HH21	1:A:390:TYR:HB3	1.62	0.64
1:A:224:GLU:HG2	1:A:225:LYS:N	2.11	0.64
2:B:11:VAL:HG12	2:B:19:LEU:HD12	1.77	0.64
1:A:441:LEU:C	1:A:443:TRP:H	1.99	0.64
1:A:102:TRP:CZ3	1:A:235:LYS:HG2	2.32	0.64
1:A:387:LEU:HD21	1:A:444:CYS:O	1.98	0.64
1:A:31:GLN:HG3	1:A:296:ILE:HA	1.80	0.63
1:A:141:LEU:HD22	1:A:203:GLY:HA3	1.79	0.63
2:B:29:VAL:O	2:B:30:VAL:HB	1.98	0.63
2:B:63:SER:HB3	2:B:64:PRO:HD3	1.80	0.63
2:B:78:TYR:C	2:B:80:GLY:H	2.02	0.63
1:A:89:LYS:HG2	1:A:89:LYS:O	1.96	0.63
1:A:132:VAL:HG13	1:A:133:GLU:N	2.13	0.63
1:A:19:LEU:HB3	1:A:326:VAL:HG11	1.80	0.63
1:A:112:MET:HE2	1:A:150:ALA:H	1.64	0.63
1:A:181:VAL:HB	1:A:182:PRO:HD2	1.78	0.62
1:A:317:PHE:CD2	1:A:452:LEU:HG	2.33	0.62
1:A:403:ALA:O	1:A:407:CYS:CB	2.46	0.62
1:A:447:LYS:HD2	1:A:448:TYR:CE1	2.34	0.62
1:A:280:VAL:HG13	1:A:423:ILE:HD11	1.82	0.62
1:A:364:SER:C	1:A:366:VAL:H	2.02	0.62
1:A:15:LYS:HA	1:A:322:TYR:CD2	2.34	0.62
1:A:136:MET:O	1:A:139:TYR:CB	2.41	0.62
1:A:328:LEU:O	1:A:332:TRP:HB2	1.99	0.62
1:A:458:ALA:HB3	2:B:8:LEU:C	2.20	0.62
1:A:181:VAL:HB	1:A:182:PRO:HD3	1.82	0.62
1:A:158:ALA:HB2	1:A:217:LEU:HG	1.82	0.62
1:A:263:SER:C	1:A:265:PHE:H	2.02	0.61
1:A:80:MET:SD	1:A:247:ILE:HD11	2.40	0.61
1:A:112:MET:HE1	1:A:150:ALA:HB2	1.81	0.61
2:B:4:VAL:CG2	2:B:85:ILE:HB	2.29	0.61
1:A:63:PHE:C	1:A:65:THR:H	2.04	0.61
2:B:75:ARG:NH2	2:B:79:TRP:CH2	2.68	0.61
1:A:369:PHE:HB3	1:A:372:LEU:HD12	1.83	0.61
1:A:112:MET:HE1	1:A:150:ALA:CB	2.30	0.61
1:A:322:TYR:CE1	1:A:449:SER:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TRP:HH2	1:A:147:MET:HA	1.66	0.61
1:A:253:PRO:HB2	1:A:394:LYS:HD3	1.81	0.61
2:B:27:GLU:HG3	2:B:52:GLY:O	2.01	0.61
1:A:127:THR:HG22	1:A:128:LEU:N	2.14	0.60
1:A:458:ALA:HB1	2:B:8:LEU:CB	2.31	0.60
1:A:40:VAL:O	1:A:43:VAL:N	2.34	0.60
1:A:145:LEU:HD12	1:A:207:MET:CB	2.22	0.60
1:A:408:GLY:HA2	1:A:411:PRO:HG2	1.82	0.60
1:A:346:ARG:HG2	1:A:367:LEU:HD11	1.84	0.60
2:B:59:ILE:HD12	2:B:61:GLY:H	1.67	0.60
1:A:140:MET:CE	1:A:197:LEU:HD11	2.32	0.60
1:A:365:THR:HA	1:A:368:LEU:HD21	1.83	0.60
2:B:68:TYR:O	2:B:88:ASN:O	2.19	0.60
1:A:31:GLN:O	1:A:296:ILE:HG13	2.02	0.59
1:A:98:ARG:HD3	1:A:229:PRO:O	2.02	0.59
1:A:254:ILE:HB	1:A:394:LYS:HZ1	1.66	0.59
2:B:65:GLY:HA2	2:B:91:THR:CG2	2.31	0.59
2:B:75:ARG:NE	2:B:79:TRP:O	2.35	0.59
1:A:148:PRO:HB2	1:A:152:VAL:CG1	2.31	0.59
1:A:232:LEU:C	1:A:234:ALA:H	2.06	0.59
1:A:250:ILE:O	1:A:394:LYS:NZ	2.34	0.59
1:A:80:MET:SD	1:A:247:ILE:CD1	2.91	0.59
2:B:4:VAL:HA	2:B:83:SER:HB3	1.85	0.59
1:A:318:SER:C	1:A:320:ALA:N	2.54	0.59
2:B:34:ILE:HG12	2:B:48:PHE:HB2	1.85	0.59
1:A:272:ILE:HG22	1:A:280:VAL:O	2.03	0.59
1:A:40:VAL:HG22	1:A:177:PHE:HD1	1.69	0.58
1:A:172:VAL:C	1:A:174:PHE:H	2.06	0.58
1:A:306:VAL:O	1:A:308:ILE:N	2.35	0.58
1:A:318:SER:HA	1:A:321:ARG:H	1.68	0.58
1:A:140:MET:HE2	1:A:197:LEU:HD11	1.86	0.58
1:A:332:TRP:HD1	1:A:379:THR:HG21	1.67	0.58
2:B:26:GLY:O	2:B:53:SER:HA	2.02	0.58
1:A:122:PHE:O	1:A:122:PHE:CD2	2.56	0.58
1:A:202:CYS:O	1:A:205:ALA:HB3	2.03	0.58
2:B:9:GLU:O	2:B:22:TRP:NE1	2.36	0.58
2:B:74:ALA:O	2:B:81:TRP:HE3	1.87	0.58
1:A:365:THR:HA	1:A:368:LEU:HD11	1.86	0.57
1:A:458:ALA:HB1	2:B:8:LEU:HB2	1.86	0.57
1:A:410:LEU:C	1:A:412:GLY:H	2.08	0.57
1:A:255:GLY:HA2	1:A:258:TYR:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG13	1:A:198:GLY:CA	2.35	0.57
2:B:35:THR:CG2	2:B:71:THR:HB	2.35	0.57
1:A:44:MET:CE	1:A:184:ASN:HB2	2.35	0.57
1:A:103:PHE:O	1:A:106:ILE:N	2.35	0.57
1:A:115:MET:HB3	1:A:146:ALA:HB1	1.87	0.57
1:A:447:LYS:O	1:A:451:GLU:HG2	2.04	0.57
1:A:372:LEU:CD1	1:A:424:TYR:HB2	2.34	0.56
1:A:31:GLN:HE22	1:A:300:VAL:HG23	1.71	0.56
1:A:89:LYS:H	1:A:89:LYS:HD3	1.68	0.56
1:A:89:LYS:CG	1:A:92:GLU:CB	2.83	0.56
1:A:132:VAL:HG13	1:A:133:GLU:H	1.70	0.56
1:A:215:LEU:N	1:A:215:LEU:CD2	2.60	0.56
1:A:329:VAL:HA	1:A:332:TRP:HB2	1.87	0.56
1:A:335:ALA:O	1:A:375:PRO:HB3	2.06	0.56
1:A:16:GLU:HA	1:A:19:LEU:HD12	1.87	0.56
1:A:242:ALA:HA	1:A:245:LYS:N	2.18	0.56
1:A:63:PHE:O	1:A:65:THR:N	2.38	0.56
1:A:141:LEU:HD21	1:A:203:GLY:HA3	1.86	0.56
2:B:35:THR:HG23	2:B:71:THR:HB	1.86	0.56
1:A:89:LYS:HG3	1:A:92:GLU:CB	2.34	0.56
1:A:321:ARG:NH2	1:A:391:LYS:HB2	2.19	0.56
1:A:70:PHE:CD2	1:A:107:LEU:HD12	2.40	0.56
1:A:142:PHE:O	1:A:146:ALA:HB2	2.06	0.56
1:A:66:VAL:HA	1:A:69:THR:CG2	2.36	0.56
1:A:447:LYS:C	1:A:448:TYR:HD1	2.09	0.56
1:A:89:LYS:CG	1:A:92:GLU:HB3	2.35	0.55
1:A:371:GLY:O	1:A:375:PRO:HD2	2.06	0.55
1:A:388:ARG:O	1:A:391:LYS:O	2.23	0.55
1:A:411:PRO:HG3	1:A:429:ALA:CB	2.27	0.55
1:A:415:LEU:HD11	1:A:423:ILE:HD12	1.87	0.55
1:A:369:PHE:C	1:A:371:GLY:H	2.10	0.55
1:A:158:ALA:CB	1:A:217:LEU:HG	2.36	0.55
1:A:73:ILE:HG13	1:A:251:GLY:CA	2.36	0.55
1:A:172:VAL:O	1:A:174:PHE:N	2.38	0.55
1:A:164:ASN:O	1:A:165:ARG:HD3	2.06	0.55
1:A:227:PHE:CD2	1:A:227:PHE:O	2.60	0.55
2:B:50:VAL:CB	2:B:51:PRO:CD	2.85	0.55
1:A:73:ILE:O	1:A:76:ALA:CB	2.49	0.55
1:A:105:LEU:O	1:A:109:ILE:HG23	2.06	0.55
1:A:140:MET:HB3	1:A:200:ALA:CB	2.37	0.55
1:A:441:LEU:C	1:A:443:TRP:N	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:O	1:A:329:VAL:HG13	2.07	0.54
2:B:4:VAL:HG12	2:B:83:SER:HB3	1.89	0.54
2:B:4:VAL:HG21	2:B:85:ILE:CB	2.38	0.54
2:B:4:VAL:HG21	2:B:85:ILE:CG1	2.37	0.54
2:B:87:ILE:CG2	2:B:88:ASN:N	2.71	0.54
1:A:99:GLN:NE2	1:A:234:ALA:O	2.41	0.54
1:A:209:VAL:HA	1:A:212:PHE:HB3	1.90	0.54
2:B:7:LYS:HB2	2:B:23:ASP:HB2	1.88	0.54
2:B:87:ILE:CG2	2:B:88:ASN:H	2.20	0.54
1:A:59:GLY:O	1:A:61:SER:N	2.41	0.54
1:A:103:PHE:HA	1:A:106:ILE:HG22	1.90	0.54
1:A:404:PHE:HA	1:A:433:SER:OG	2.08	0.54
1:A:95:GLU:HB2	1:A:98:ARG:HE	1.73	0.54
1:A:315:ARG:HH21	2:B:11:VAL:HG11	1.72	0.54
1:A:157:HIS:HA	1:A:160:ALA:HB3	1.89	0.54
1:A:167:ARG:C	1:A:169:ILE:H	2.12	0.54
1:A:184:ASN:HA	1:A:205:ALA:HB1	1.90	0.54
1:A:339:VAL:HA	1:A:342:LEU:HD12	1.90	0.53
1:A:77:LEU:C	1:A:79:PRO:HD2	2.28	0.53
1:A:144:SER:O	1:A:207:MET:HG2	2.07	0.53
1:A:282:ALA:HB2	1:A:362:ILE:HD12	1.91	0.53
1:A:77:LEU:HD12	1:A:77:LEU:N	2.23	0.53
2:B:3:SER:O	2:B:83:SER:HB2	2.09	0.53
1:A:346:ARG:O	1:A:348:PRO:HD3	2.09	0.53
1:A:428:THR:C	1:A:430:LEU:H	2.11	0.53
1:A:447:LYS:CD	1:A:448:TYR:CE1	2.92	0.53
2:B:72:VAL:HG12	2:B:85:ILE:HG22	1.90	0.53
1:A:250:ILE:HA	1:A:394:LYS:HD2	1.90	0.53
1:A:43:VAL:O	1:A:43:VAL:HG13	2.08	0.53
1:A:89:LYS:C	1:A:91:GLY:H	2.11	0.53
1:A:138:GLN:C	1:A:140:MET:N	2.62	0.53
1:A:174:PHE:C	1:A:176:ALA:H	2.12	0.53
1:A:290:SER:O	1:A:294:TYR:CB	2.57	0.52
1:A:460:SER:O	2:B:8:LEU:HG	2.08	0.52
1:A:142:PHE:O	1:A:146:ALA:CB	2.57	0.52
2:B:65:GLY:HA2	2:B:91:THR:CB	2.39	0.52
1:A:177:PHE:CD2	1:A:178:VAL:N	2.77	0.52
2:B:27:GLU:HG3	2:B:52:GLY:HA2	1.90	0.52
2:B:78:TYR:O	2:B:80:GLY:N	2.42	0.52
1:A:282:ALA:CB	1:A:362:ILE:HD12	2.38	0.52
1:A:59:GLY:C	1:A:61:SER:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:O	1:A:297:PRO:HB2	2.10	0.52
1:A:408:GLY:HA3	1:A:430:LEU:HG	1.91	0.52
1:A:284:GLN:HA	1:A:287:ILE:CG1	2.40	0.52
1:A:33:ALA:CB	1:A:170:MET:HA	2.39	0.52
1:A:254:ILE:HG23	1:A:255:GLY:N	2.24	0.52
1:A:308:ILE:HB	1:A:390:TYR:CD1	2.44	0.51
2:B:24:ALA:HB3	2:B:53:SER:O	2.10	0.51
1:A:294:TYR:CZ	1:A:298:GLN:HB2	2.44	0.51
1:A:377:ASP:O	1:A:380:GLN:N	2.44	0.51
1:A:224:GLU:CG	1:A:225:LYS:N	2.73	0.51
1:A:132:VAL:CG1	1:A:133:GLU:H	2.23	0.51
1:A:164:ASN:C	1:A:166:PRO:HD3	2.31	0.51
1:A:268:ILE:HD12	1:A:269:VAL:HG23	1.93	0.51
1:A:334:LEU:HA	1:A:337:ILE:HG13	1.92	0.51
1:A:368:LEU:HD12	1:A:423:ILE:HG22	1.91	0.51
2:B:29:VAL:HG12	2:B:30:VAL:HG12	1.93	0.51
1:A:112:MET:HG2	1:A:116:TRP:CH2	2.45	0.51
1:A:148:PRO:HB3	1:A:207:MET:HB2	1.92	0.51
1:A:180:ASN:O	1:A:184:ASN:N	2.32	0.51
1:A:384:SER:C	1:A:386:ALA:H	2.12	0.51
1:A:427:TRP:CD1	1:A:427:TRP:N	2.79	0.51
2:B:76:SER:O	2:B:78:TYR:O	2.29	0.51
1:A:183:LEU:O	1:A:184:ASN:C	2.49	0.51
1:A:217:LEU:O	1:A:218:TRP:C	2.46	0.51
1:A:375:PRO:HA	1:A:378:PHE:HB2	1.93	0.51
1:A:101:ILE:HD11	1:A:217:LEU:HD22	1.92	0.51
1:A:99:GLN:CD	1:A:241:TRP:HE1	2.15	0.51
2:B:59:ILE:HD12	2:B:61:GLY:N	2.26	0.51
1:A:381:CYS:O	1:A:384:SER:N	2.44	0.50
1:A:79:PRO:CG	1:A:80:MET:H	2.20	0.50
1:A:99:GLN:HG3	1:A:243:VAL:CG2	2.41	0.50
1:A:140:MET:HB3	1:A:200:ALA:HB1	1.92	0.50
1:A:356:ASP:OD1	3:A:501:ET:H212	2.12	0.50
2:B:67:ASP:CA	2:B:90:ARG:HB3	2.25	0.50
1:A:455:SER:O	2:B:11:VAL:HA	2.12	0.50
2:B:14:THR:C	2:B:16:THR:H	2.15	0.50
2:B:29:VAL:H	2:B:76:SER:HA	1.77	0.50
1:A:132:VAL:CG1	1:A:133:GLU:N	2.74	0.50
2:B:37:GLY:N	2:B:70:ILE:CD1	2.68	0.50
1:A:216:ALA:HA	1:A:219:ILE:HG13	1.93	0.50
1:A:95:GLU:O	1:A:99:GLN:CG	2.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:C	1:A:244:PHE:N	2.65	0.50
1:A:128:LEU:O	1:A:129:SER:HB3	2.12	0.50
2:B:37:GLY:H	2:B:70:ILE:HD11	1.73	0.50
1:A:32:VAL:O	1:A:35:VAL:HG12	2.11	0.49
1:A:19:LEU:O	1:A:21:THR:N	2.45	0.49
1:A:103:PHE:O	1:A:105:LEU:N	2.45	0.49
1:A:225:LYS:C	1:A:225:LYS:CD	2.81	0.49
1:A:339:VAL:CG2	1:A:375:PRO:HD3	2.37	0.49
1:A:344:LEU:HD22	1:A:345:PHE:CD2	2.48	0.49
1:A:154:ARG:HG2	1:A:155:ALA:N	2.28	0.49
1:A:200:ALA:O	1:A:203:GLY:N	2.39	0.49
2:B:74:ALA:O	2:B:81:TRP:CE3	2.64	0.49
1:A:254:ILE:HD11	1:A:388:ARG:HH11	1.78	0.49
1:A:67:TYR:O	1:A:69:THR:N	2.46	0.49
1:A:68:ILE:HA	1:A:71:MET:CB	2.42	0.49
1:A:126:LEU:HD13	1:A:270:PHE:CZ	2.48	0.49
1:A:300:VAL:O	1:A:304:GLY:N	2.44	0.49
2:B:4:VAL:CA	2:B:83:SER:HB3	2.42	0.49
2:B:27:GLU:HG3	2:B:52:GLY:C	2.33	0.49
2:B:32:TYR:HB2	2:B:50:VAL:HG23	1.94	0.49
2:B:37:GLY:N	2:B:70:ILE:HD11	2.27	0.49
2:B:36:TYR:HB3	2:B:46:GLN:HG3	1.94	0.49
1:A:159:TYR:C	1:A:161:SER:H	2.16	0.49
1:A:372:LEU:HD22	1:A:431:ILE:CD1	2.43	0.49
1:A:104:GLY:O	1:A:105:LEU:HB2	2.12	0.48
1:A:148:PRO:HG3	1:A:207:MET:CB	2.43	0.48
1:A:152:VAL:HG12	1:A:210:PHE:HB3	1.95	0.48
1:A:397:MET:HA	1:A:400:HIS:HB3	1.95	0.48
1:A:112:MET:HE2	1:A:150:ALA:CB	2.41	0.48
1:A:243:VAL:HG23	1:A:243:VAL:O	2.13	0.48
1:A:295:MET:HE2	1:A:295:MET:HB3	1.70	0.48
1:A:19:LEU:C	1:A:21:THR:N	2.67	0.48
1:A:28:LEU:O	1:A:32:VAL:HG23	2.14	0.48
1:A:82:ALA:HB1	1:A:310:PHE:HB2	1.94	0.48
1:A:78:ASN:N	1:A:79:PRO:HD2	2.28	0.48
1:A:79:PRO:O	1:A:80:MET:C	2.51	0.48
1:A:388:ARG:HB3	1:A:394:LYS:HB3	1.94	0.48
1:A:77:LEU:HD22	1:A:157:HIS:CE1	2.49	0.48
2:B:20:ILE:HD11	2:B:59:ILE:HG23	1.96	0.48
1:A:372:LEU:CD1	1:A:427:TRP:HB2	2.43	0.48
1:A:418:ARG:HG2	1:A:422:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:38:GLY:C	2.52	0.48
1:A:81:ILE:CD1	1:A:161:SER:HA	2.44	0.48
1:A:112:MET:HE3	1:A:150:ALA:HB2	1.92	0.48
1:A:294:TYR:O	1:A:294:TYR:CG	2.66	0.48
1:A:33:ALA:HB2	1:A:170:MET:CA	2.42	0.48
1:A:102:TRP:HZ3	1:A:235:LYS:HG2	1.78	0.48
1:A:116:TRP:N	1:A:116:TRP:HE3	2.12	0.48
1:A:177:PHE:CD2	1:A:177:PHE:C	2.87	0.48
1:A:218:TRP:CE3	1:A:221:ILE:HD11	2.49	0.48
1:A:458:ALA:HB1	2:B:8:LEU:HB3	1.95	0.48
1:A:248:TRP:CE3	1:A:252:ALA:HB2	2.48	0.48
1:A:56:VAL:HA	1:A:138:GLN:OE1	2.13	0.47
1:A:145:LEU:HD13	1:A:203:GLY:C	2.32	0.47
1:A:308:ILE:HD12	1:A:390:TYR:HB2	1.95	0.47
2:B:63:SER:CB	2:B:64:PRO:HD3	2.44	0.47
1:A:65:THR:CG2	1:A:66:VAL:N	2.77	0.47
1:A:364:SER:C	1:A:366:VAL:N	2.68	0.47
2:B:59:ILE:HD12	2:B:61:GLY:CA	2.44	0.47
1:A:37:ILE:HG13	1:A:38:GLY:N	2.28	0.47
1:A:87:ALA:CB	1:A:89:LYS:HZ1	2.27	0.47
1:A:96:THR:O	1:A:97:GLY:C	2.52	0.47
1:A:395:VAL:HB	1:A:396:PRO:HD3	1.96	0.47
2:B:4:VAL:HG11	2:B:84:PRO:O	2.14	0.47
1:A:231:GLY:O	1:A:232:LEU:C	2.53	0.47
1:A:301:GLY:O	1:A:385:TYR:O	2.32	0.47
1:A:381:CYS:C	1:A:383:ALA:N	2.67	0.47
1:A:31:GLN:HE22	1:A:300:VAL:HA	1.80	0.47
1:A:242:ALA:O	1:A:243:VAL:HG22	2.15	0.47
1:A:318:SER:O	1:A:322:TYR:N	2.43	0.47
2:B:4:VAL:CG1	2:B:84:PRO:O	2.62	0.47
2:B:7:LYS:O	2:B:8:LEU:HD23	2.14	0.47
1:A:151:MET:SD	1:A:211:TRP:CD2	3.08	0.47
1:A:221:ILE:HD13	1:A:228:ARG:HG3	1.96	0.47
1:A:298:GLN:HA	1:A:382:ILE:CG2	2.45	0.47
1:A:437:ALA:C	1:A:439:VAL:N	2.65	0.47
1:A:441:LEU:O	1:A:444:CYS:N	2.48	0.47
2:B:4:VAL:HG21	2:B:85:ILE:HD13	1.96	0.47
1:A:197:LEU:O	1:A:201:GLY:HA3	2.15	0.47
1:A:40:VAL:HG22	1:A:177:PHE:HB2	1.96	0.47
1:A:56:VAL:HA	1:A:138:GLN:HE22	1.80	0.47
1:A:74:MET:CE	1:A:103:PHE:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:O	1:A:261:GLU:HG3	2.14	0.47
1:A:292:ILE:O	1:A:293:LEU:HD23	2.15	0.47
1:A:297:PRO:HB3	1:A:378:PHE:CZ	2.50	0.47
1:A:23:LEU:HD12	1:A:25:LEU:HD12	1.97	0.46
1:A:100:GLY:C	1:A:102:TRP:N	2.67	0.46
1:A:184:ASN:HA	1:A:205:ALA:CB	2.43	0.46
1:A:256:LEU:HB3	1:A:398:PHE:CE1	2.46	0.46
1:A:400:HIS:CE1	1:A:401:ALA:CB	2.96	0.46
2:B:71:THR:HG22	2:B:72:VAL:N	2.29	0.46
1:A:141:LEU:HD23	1:A:200:ALA:O	2.16	0.46
1:A:160:ALA:HA	1:A:163:LEU:HD11	1.97	0.46
1:A:263:SER:C	1:A:265:PHE:N	2.68	0.46
1:A:155:ALA:HB2	1:A:214:ALA:CA	2.38	0.46
1:A:173:SER:HA	1:A:176:ALA:HB3	1.98	0.46
1:A:276:GLY:O	1:A:280:VAL:HB	2.15	0.46
1:A:19:LEU:C	1:A:21:THR:H	2.18	0.46
1:A:110:PHE:O	1:A:111:GLY:C	2.53	0.46
1:A:279:TYR:HB3	1:A:362:ILE:HG22	1.97	0.46
2:B:51:PRO:HB2	2:B:52:GLY:H	1.55	0.46
1:A:458:ALA:HB3	2:B:8:LEU:O	2.16	0.46
1:A:70:PHE:HD2	1:A:107:LEU:HG	1.80	0.46
2:B:27:GLU:CG	2:B:52:GLY:HA2	2.46	0.46
1:A:58:LEU:HD12	1:A:138:GLN:CD	2.36	0.46
1:A:437:ALA:C	1:A:439:VAL:H	2.19	0.46
1:A:87:ALA:HB3	1:A:89:LYS:NZ	2.31	0.46
1:A:116:TRP:CH2	1:A:147:MET:HA	2.50	0.46
1:A:144:SER:CB	1:A:204:VAL:CG1	2.81	0.46
1:A:158:ALA:HA	1:A:217:LEU:HD21	1.97	0.46
2:B:35:THR:O	2:B:70:ILE:HG13	2.16	0.46
1:A:366:VAL:HA	1:A:369:PHE:CZ	2.51	0.45
1:A:253:PRO:HB3	1:A:394:LYS:O	2.15	0.45
1:A:29:LEU:HB3	1:A:170:MET:SD	2.56	0.45
1:A:158:ALA:CB	1:A:217:LEU:HD11	2.33	0.45
1:A:284:GLN:HA	1:A:287:ILE:HG12	1.97	0.45
1:A:372:LEU:CB	1:A:431:ILE:HG21	2.34	0.45
1:A:127:THR:CG2	1:A:128:LEU:H	2.19	0.45
1:A:172:VAL:HG21	1:A:216:ALA:CB	2.47	0.45
1:A:381:CYS:O	1:A:385:TYR:N	2.41	0.45
2:B:78:TYR:C	2:B:80:GLY:N	2.68	0.45
1:A:332:TRP:HA	1:A:335:ALA:CB	2.46	0.45
1:A:334:LEU:HA	1:A:337:ILE:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD12	1:A:341:SER:N	2.32	0.45
1:A:368:LEU:CD1	1:A:423:ILE:CG2	2.94	0.45
1:A:218:TRP:CE3	1:A:218:TRP:CA	2.86	0.45
1:A:82:ALA:O	1:A:310:PHE:HA	2.17	0.45
1:A:315:ARG:HG3	1:A:317:PHE:HE1	1.70	0.45
2:B:21:SER:HA	2:B:56:THR:HA	1.99	0.45
1:A:98:ARG:CD	1:A:229:PRO:O	2.64	0.45
1:A:138:GLN:O	1:A:140:MET:N	2.50	0.45
1:A:184:ASN:ND2	1:A:202:CYS:HA	2.32	0.45
1:A:254:ILE:HG23	1:A:255:GLY:H	1.82	0.45
1:A:408:GLY:CA	1:A:430:LEU:HG	2.47	0.45
1:A:289:LEU:HA	1:A:292:ILE:HG12	1.99	0.44
1:A:71:MET:HG2	1:A:156:LEU:HD22	1.98	0.44
1:A:83:GLN:HA	1:A:309:GLY:O	2.18	0.44
1:A:86:GLY:HA3	1:A:314:ARG:N	2.32	0.44
1:A:112:MET:HE2	1:A:150:ALA:N	2.32	0.44
1:A:254:ILE:CD1	1:A:388:ARG:HH11	2.29	0.44
1:A:259:PHE:CA	1:A:262:ALA:HB3	2.39	0.44
1:A:151:MET:HB2	1:A:211:TRP:CE2	2.52	0.44
1:A:188:VAL:HG13	1:A:198:GLY:O	2.17	0.44
1:A:259:PHE:CD2	1:A:262:ALA:HB3	2.52	0.44
1:A:40:VAL:HG22	1:A:177:PHE:CD1	2.50	0.44
1:A:81:ILE:HD12	1:A:81:ILE:O	2.18	0.44
1:A:369:PHE:HD2	1:A:424:TYR:HB3	1.83	0.44
2:B:73:TYR:CE2	2:B:84:PRO:HB3	2.53	0.44
2:B:20:ILE:O	2:B:57:ALA:O	2.35	0.44
1:A:73:ILE:HG13	1:A:251:GLY:C	2.38	0.44
1:A:65:THR:CG2	1:A:66:VAL:H	2.30	0.44
1:A:232:LEU:C	1:A:234:ALA:N	2.71	0.44
1:A:346:ARG:CG	1:A:367:LEU:HD11	2.48	0.44
2:B:67:ASP:HA	2:B:90:ARG:CG	2.48	0.44
2:B:90:ARG:HB2	2:B:91:THR:H	1.43	0.44
1:A:260:LEU:HD23	1:A:261:GLU:N	2.33	0.43
1:A:77:LEU:HD22	1:A:157:HIS:NE2	2.33	0.43
1:A:89:LYS:HG2	1:A:92:GLU:CB	2.44	0.43
1:A:149:ALA:HA	1:A:152:VAL:HG22	1.99	0.43
1:A:372:LEU:HD22	1:A:431:ILE:HD13	2.00	0.43
1:A:428:THR:HG23	1:A:429:ALA:H	1.82	0.43
1:A:78:ASN:N	1:A:79:PRO:CD	2.81	0.43
1:A:374:GLN:HB3	1:A:375:PRO:HD3	1.99	0.43
1:A:452:LEU:HD12	1:A:455:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HA	1:A:152:VAL:CG2	2.49	0.43
1:A:159:TYR:HB2	1:A:169:ILE:HD13	1.97	0.43
1:A:297:PRO:O	1:A:298:GLN:C	2.56	0.43
1:A:203:GLY:HA2	1:A:206:THR:HB	2.01	0.43
1:A:394:LYS:HA	1:A:397:MET:HB3	1.97	0.43
1:A:458:ALA:CB	2:B:8:LEU:HB2	2.47	0.43
1:A:312:LEU:HD22	1:A:390:TYR:HE2	1.84	0.43
1:A:108:GLY:HA3	1:A:150:ALA:HA	2.00	0.43
1:A:284:GLN:HA	1:A:287:ILE:HG13	2.00	0.43
1:A:382:ILE:O	1:A:382:ILE:HG13	2.18	0.43
1:A:387:LEU:HD12	1:A:393:THR:HB	1.99	0.43
1:A:408:GLY:HA3	1:A:430:LEU:CD2	2.49	0.43
1:A:35:VAL:HB	1:A:295:MET:HE3	2.01	0.42
1:A:58:LEU:HD12	1:A:138:GLN:NE2	2.34	0.42
1:A:143:THR:HG23	1:A:144:SER:N	2.33	0.42
1:A:211:TRP:CD1	1:A:211:TRP:N	2.87	0.42
1:A:339:VAL:HG21	1:A:375:PRO:CD	2.39	0.42
1:A:387:LEU:CD1	1:A:393:THR:HB	2.49	0.42
1:A:158:ALA:CB	1:A:217:LEU:CG	2.91	0.42
1:A:178:VAL:O	1:A:182:PRO:HG2	2.19	0.42
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.92	0.42
1:A:300:VAL:HG12	1:A:382:ILE:HD12	2.01	0.42
1:A:415:LEU:HD12	1:A:423:ILE:HA	2.00	0.42
1:A:108:GLY:O	1:A:112:MET:HB2	2.18	0.42
1:A:188:VAL:HA	1:A:198:GLY:CA	2.36	0.42
2:B:30:VAL:O	2:B:31:TYR:HD2	2.02	0.42
2:B:75:ARG:HD2	2:B:80:GLY:C	2.40	0.42
1:A:73:ILE:HG22	1:A:74:MET:N	2.34	0.42
1:A:79:PRO:O	1:A:82:ALA:N	2.50	0.42
1:A:180:ASN:HB2	1:A:209:VAL:HG11	2.01	0.42
1:A:254:ILE:HG13	1:A:258:TYR:CD1	2.55	0.42
1:A:29:LEU:HB2	1:A:167:ARG:HG3	2.02	0.42
1:A:79:PRO:CG	1:A:80:MET:N	2.83	0.42
1:A:177:PHE:HD2	1:A:178:VAL:N	2.16	0.42
1:A:425:GLY:O	1:A:428:THR:HG22	2.19	0.42
2:B:25:ARG:NH1	2:B:28:TYR:CE2	2.88	0.42
1:A:254:ILE:HB	1:A:394:LYS:HZ3	1.82	0.42
1:A:387:LEU:HD12	1:A:393:THR:CG2	2.50	0.42
2:B:29:VAL:HG23	2:B:77:TYR:N	2.34	0.42
2:B:5:PRO:HG3	2:B:74:ALA:HB2	2.01	0.42
1:A:89:LYS:C	1:A:91:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TYR:HD1	1:A:190:GLY:N	2.18	0.42
1:A:260:LEU:C	1:A:262:ALA:H	2.23	0.42
1:A:148:PRO:O	1:A:152:VAL:HG13	2.20	0.42
1:A:167:ARG:HD3	1:A:167:ARG:N	2.35	0.42
2:B:61:GLY:O	2:B:62:LEU:C	2.58	0.42
1:A:377:ASP:O	1:A:378:PHE:C	2.57	0.41
1:A:379:THR:O	1:A:381:CYS:N	2.53	0.41
1:A:172:VAL:HG21	1:A:216:ALA:HB3	2.02	0.41
1:A:269:VAL:HG12	1:A:269:VAL:O	2.20	0.41
2:B:27:GLU:HG3	2:B:52:GLY:CA	2.50	0.41
1:A:153:HIS:HD1	1:A:153:HIS:HA	1.73	0.41
1:A:235:LYS:HB2	1:A:241:TRP:HB3	2.02	0.41
1:A:252:ALA:HB3	1:A:253:PRO:CD	2.40	0.41
1:A:298:GLN:HA	1:A:382:ILE:HG22	2.01	0.41
1:A:440:ALA:O	1:A:443:TRP:HB3	2.21	0.41
1:A:99:GLN:OE1	1:A:241:TRP:CD1	2.74	0.41
1:A:99:GLN:OE1	1:A:241:TRP:NE1	2.53	0.41
1:A:392:VAL:HG12	1:A:392:VAL:O	2.21	0.41
2:B:65:GLY:HA2	2:B:91:THR:HB	2.02	0.41
1:A:50:LYS:HD2	1:A:50:LYS:HA	1.94	0.41
1:A:95:GLU:O	1:A:98:ARG:HG2	2.20	0.41
1:A:214:ALA:CB	1:A:215:LEU:HD23	2.51	0.41
1:A:248:TRP:HZ3	1:A:252:ALA:CB	2.29	0.41
1:A:441:LEU:H	1:A:441:LEU:HD23	1.85	0.41
1:A:70:PHE:HD2	1:A:107:LEU:CD1	2.33	0.41
1:A:225:LYS:C	1:A:225:LYS:HD2	2.40	0.41
2:B:17:SER:OG	2:B:18:LEU:N	2.52	0.41
1:A:31:GLN:HE22	1:A:300:VAL:CA	2.34	0.41
1:A:346:ARG:HD2	1:A:367:LEU:HD11	2.03	0.41
1:A:387:LEU:HD22	1:A:387:LEU:HA	1.94	0.41
1:A:98:ARG:HA	1:A:101:ILE:HG22	2.02	0.41
1:A:346:ARG:CD	1:A:367:LEU:HD11	2.51	0.41
1:A:253:PRO:O	1:A:257:SER:HB2	2.21	0.41
1:A:372:LEU:HD21	1:A:424:TYR:CD1	2.56	0.41
1:A:373:PHE:O	1:A:377:ASP:HB3	2.21	0.41
2:B:17:SER:HA	2:B:61:GLY:HA3	2.02	0.41
1:A:74:MET:HE3	1:A:107:LEU:HD22	2.02	0.41
1:A:334:LEU:HD22	1:A:334:LEU:H	1.85	0.41
1:A:346:ARG:CD	1:A:364:SER:HB2	2.51	0.41
1:A:159:TYR:C	1:A:159:TYR:CD1	2.95	0.40
1:A:329:VAL:CA	1:A:332:TRP:HB3	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ALA:HB1	2:B:32:TYR:OH	2.20	0.40
1:A:247:ILE:HA	1:A:250:ILE:HD11	2.04	0.40
1:A:387:LEU:O	1:A:391:LYS:N	2.55	0.40
1:A:428:THR:C	1:A:430:LEU:N	2.74	0.40
2:B:16:THR:O	2:B:61:GLY:O	2.39	0.40
2:B:76:SER:HB2	2:B:82:TYR:CD2	2.56	0.40
1:A:63:PHE:CD2	1:A:64:ALA:N	2.89	0.40
1:A:77:LEU:N	1:A:77:LEU:CD1	2.84	0.40
1:A:126:LEU:HD13	1:A:270:PHE:HZ	1.85	0.40
1:A:400:HIS:CD2	1:A:404:PHE:CE1	3.09	0.40
1:A:31:GLN:HE22	1:A:300:VAL:CB	2.35	0.40
1:A:40:VAL:O	1:A:41:ASP:C	2.60	0.40
1:A:245:LYS:O	1:A:248:TRP:HB2	2.22	0.40
1:A:320:ALA:O	1:A:323:ILE:HG12	2.22	0.40
2:B:11:VAL:HG13	2:B:12:ALA:H	1.86	0.40
1:A:232:LEU:O	1:A:234:ALA:N	2.41	0.40
1:A:340:LEU:O	1:A:344:LEU:HB2	2.21	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%)	242 (53%)	142 (31%)	73 (16%)	0	2
2	B	89/99 (90%)	55 (62%)	18 (20%)	16 (18%)	0	2
All	All	546/558 (98%)	297 (54%)	160 (29%)	89 (16%)	0	2

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PHE

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Mol	Chain	Res	Type
1	A	80	MET
1	A	105	LEU
1	A	139	TYR
1	A	149	ALA
1	A	164	ASN
1	A	165	ARG
1	A	194	MET
1	A	233	THR
1	A	236	PHE
1	A	238	LYS
1	A	297	PRO
1	A	298	GLN
1	A	354	ASN
1	A	361	SER
1	A	378	PHE
1	A	396	PRO
1	A	441	LEU
1	A	442	VAL
1	A	445	LEU
2	B	11	VAL
2	B	15	PRO
2	B	30	VAL
2	B	52	GLY
2	B	61	GLY
2	B	77	TYR
2	B	79	TRP
2	B	90	ARG
1	A	20	LEU
1	A	60	SER
1	A	64	ALA
1	A	73	ILE
1	A	142	PHE
1	A	200	ALA
1	A	229	PRO
1	A	242	ALA
1	A	278	ASP
1	A	307	ARG
1	A	380	GLN
1	A	386	ALA
1	A	416	ALA
2	B	5	PRO
2	B	51	PRO

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Mol	Chain	Res	Type
2	B	62	LEU
2	B	64	PRO
1	A	58	LEU
1	A	79	PRO
1	A	119	ILE
1	A	131	TYR
1	A	166	PRO
1	A	173	SER
1	A	192	PHE
1	A	193	GLY
1	A	237	GLY
1	A	244	PHE
1	A	275	PHE
1	A	319	ARG
1	A	405	TRP
2	B	38	GLU
2	B	44	PRO
1	A	17	ILE
1	A	97	GLY
1	A	104	GLY
1	A	134	GLY
1	A	175	ALA
1	A	184	ASN
1	A	222	ALA
1	A	260	LEU
1	A	353	TYR
1	A	357	PRO
1	A	371	GLY
1	A	417	TYR
1	A	438	ALA
2	B	42	ASN
2	B	43	SER
1	A	68	ILE
1	A	87	ALA
1	A	88	GLY
1	A	125	TRP
1	A	261	GLU
1	A	277	GLU
1	A	316	GLU
1	A	365	THR
1	A	370	ALA
1	A	348	PRO

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Mol	Chain	Res	Type
1	A	121	PRO
1	A	182	PRO
1	A	439	VAL
1	A	306	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	353/353 (100%)	261 (74%)	92 (26%)	0 3
2	B	78/85 (92%)	51 (65%)	27 (35%)	0 1
All	All	431/438 (98%)	312 (72%)	119 (28%)	0 3

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	15	LYS
1	A	23	LEU
1	A	27	MET
1	A	28	LEU
1	A	37	ILE
1	A	39	PHE
1	A	43	VAL
1	A	53	LEU
1	A	56	VAL
1	A	58	LEU
1	A	63	PHE
1	A	73	ILE
1	A	80	MET
1	A	81	ILE
1	A	89	LYS
1	A	95	GLU
1	A	96	THR
1	A	103	PHE

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Mol	Chain	Res	Type
1	A	106	ILE
1	A	107	LEU
1	A	113	ILE
1	A	116	TRP
1	A	123	ARG
1	A	124	ASN
1	A	126	LEU
1	A	131	TYR
1	A	133	GLU
1	A	140	MET
1	A	141	LEU
1	A	142	PHE
1	A	147	MET
1	A	152	VAL
1	A	153	HIS
1	A	154	ARG
1	A	156	LEU
1	A	159	TYR
1	A	165	ARG
1	A	167	ARG
1	A	177	PHE
1	A	179	LEU
1	A	183	LEU
1	A	189	TYR
1	A	197	LEU
1	A	204	VAL
1	A	207	MET
1	A	215	LEU
1	A	217	LEU
1	A	218	TRP
1	A	221	ILE
1	A	224	GLU
1	A	225	LYS
1	A	228	ARG
1	A	232	LEU
1	A	235	LYS
1	A	243	VAL
1	A	248	TRP
1	A	257	SER
1	A	259	PHE
1	A	289	LEU
1	A	292	ILE

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Mol	Chain	Res	Type
1	A	294	TYR
1	A	296	ILE
1	A	298	GLN
1	A	302	SER
1	A	305	THR
1	A	310	PHE
1	A	312	LEU
1	A	315	ARG
1	A	323	ILE
1	A	329	VAL
1	A	334	LEU
1	A	346	ARG
1	A	362	ILE
1	A	368	LEU
1	A	382	ILE
1	A	387	LEU
1	A	388	ARG
1	A	391	LYS
1	A	393	THR
1	A	397	MET
1	A	399	ILE
1	A	407	CYS
1	A	421	MET
1	A	436	ILE
1	A	441	LEU
1	A	445	LEU
1	A	447	LYS
1	A	452	LEU
1	A	457	LYS
1	A	460	SER
1	A	463	LEU
2	B	2	SER
2	B	4	VAL
2	B	6	THR
2	B	10	VAL
2	B	18	LEU
2	B	19	LEU
2	B	20	ILE
2	B	25	ARG
2	B	28	TYR
2	B	31	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	43	SER
2	B	46	GLN
2	B	50	VAL
2	B	53	SER
2	B	60	SER
2	B	70	ILE
2	B	72	VAL
2	B	75	ARG
2	B	76	SER
2	B	78	TYR
2	B	83	SER
2	B	90	ARG
2	B	91	THR

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

Mol	Chain	Res	Type
1	A	31	GLN
1	A	124	ASN
1	A	180	ASN
1	A	184	ASN
2	B	42	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ET	A	501	-	26,27,27	2.02	3 (11%)	33,39,39	1.23	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ET	A	501	-	-	0/2/6/6	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ET	C11-C6	5.67	1.50	1.40
3	A	501	ET	C14-N5	5.31	1.45	1.38
3	A	501	ET	C13-C14	4.92	1.51	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ET	C4-C14-C13	-3.70	115.92	120.61
3	A	501	ET	C13-C14-N5	2.71	121.00	118.53
3	A	501	ET	C11-C6-N5	2.63	121.58	118.79

There are no chirality outliers.

There are no torsion outliers.

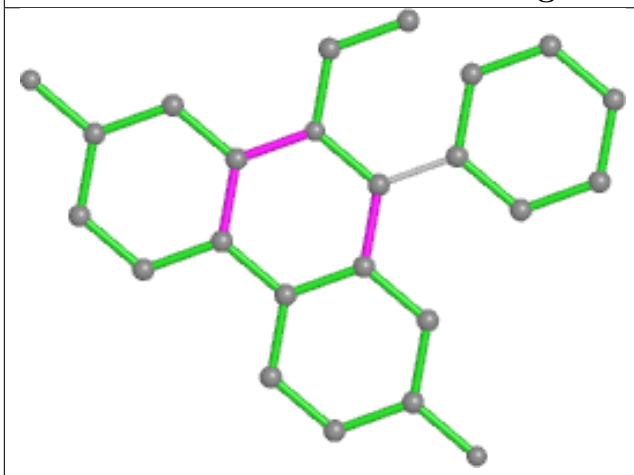
There are no ring outliers.

1 monomer is involved in 3 short contacts:

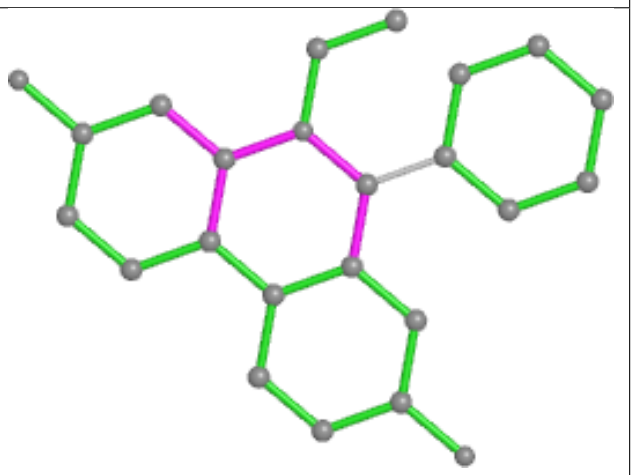
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ET	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

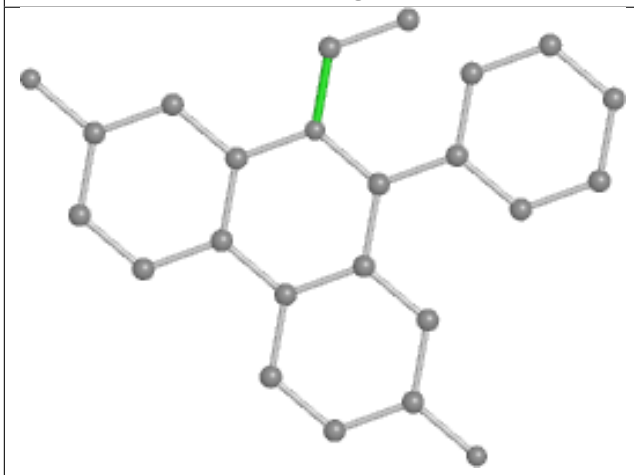
Ligand ET A 501



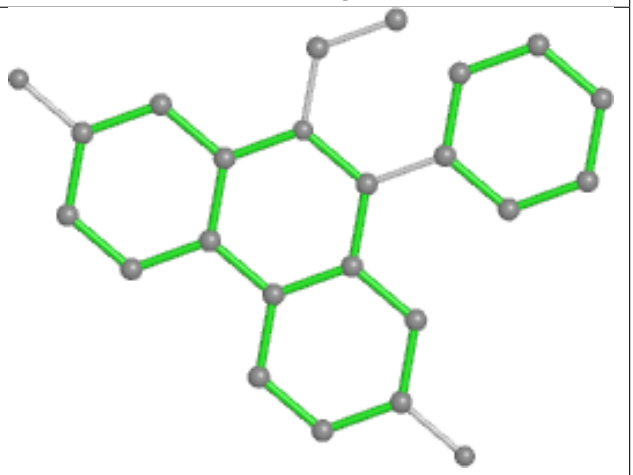
Bond lengths



Bond angles



Torsions



Rings

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%)	-0.02	25 (5%)	25	23	81, 185, 317, 399	0
2	B	91/99 (91%)	-0.06	6 (6%)	18	17	74, 159, 230, 277	0
All	All	550/558 (98%)	-0.03	31 (5%)	24	22	74, 181, 312, 399	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	SER	14.3
2	B	1	VAL	12.9
1	A	463	LEU	5.2
1	A	9	SER	5.0
1	A	457	LYS	4.8
1	A	240	ASP	4.5
2	B	89	TYR	4.3
1	A	456	HIS	4.0
1	A	349	LEU	3.9
2	B	11	VAL	3.9
1	A	230	PHE	3.8
1	A	194	MET	3.6
1	A	455	SER	3.6
1	A	271	LEU	3.3
1	A	227	PHE	3.0
1	A	6	ASP	2.8
1	A	129	SER	2.8
1	A	404	PHE	2.7
1	A	19	LEU	2.7
1	A	378	PHE	2.6
2	B	22	TRP	2.6
2	B	77	TYR	2.6
1	A	127	THR	2.4
1	A	379	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	280	VAL	2.4
1	A	421	MET	2.3
1	A	233	THR	2.2
1	A	326	VAL	2.2
1	A	398	PHE	2.1
1	A	424	TYR	2.0
1	A	373	PHE	2.0

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)

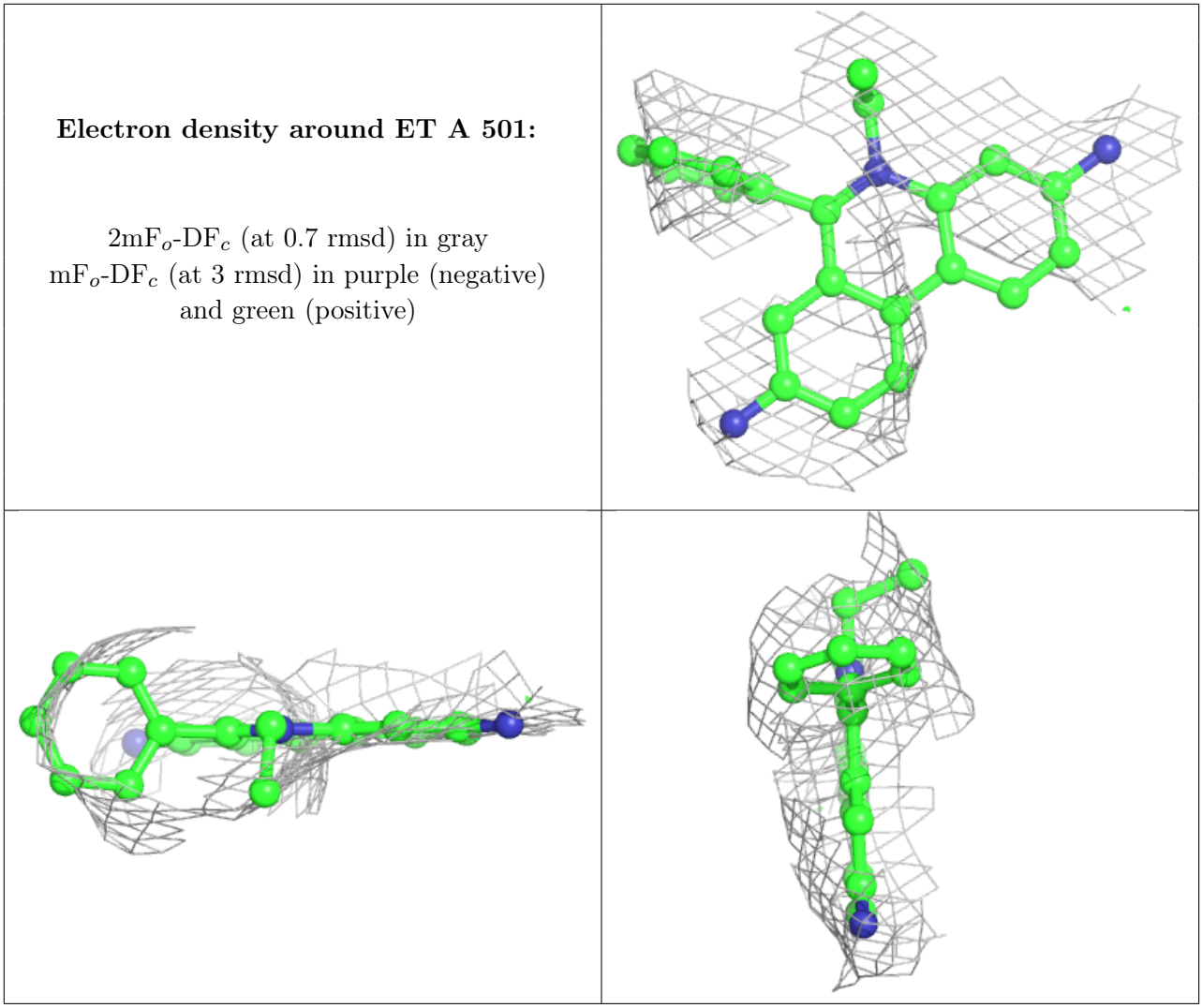
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ET	A	501	24/24	0.74	0.36	193,270,307,317	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ET A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.