Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 03:10 PM BST

PDB ID	:	4F35
Title	:	Crystal Structure of a bacterial dicarboxylate/sodium symporter
Authors	:	Mancusso, R.L.; Gregorio, G.G.; Liu, Q.; Wang, D.N.
Deposited on	:	2012-05-08
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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	:	2.13.1
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)	:	2.13.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
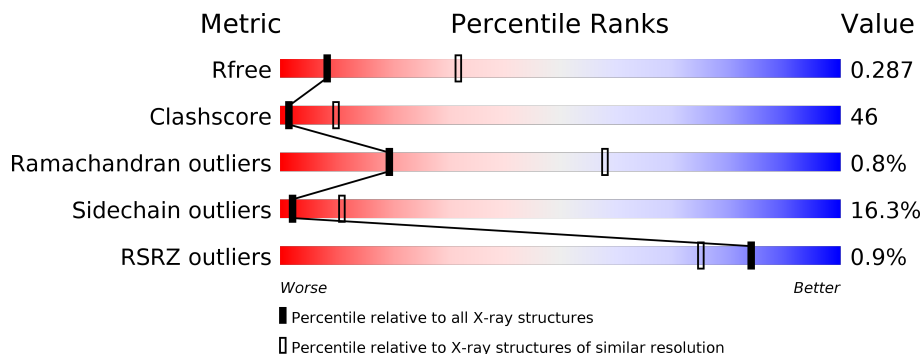
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	449	42% 43% 11% •
1	B	449	39% 44% 9% 8%
1	C	449	37% 49% 9% •
1	D	449	39% 49% 7% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	B	501	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12390 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 Transporter, NadC family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	430	Total	C	N	O	S	Se	3	0	0
			3076	2046	479	526	3	22			
1	B	414	Total	C	N	O	S	Se	0	0	0
			2980	1991	457	508	3	21			
1	A	434	Total	C	N	O	S	Se	0	0	0
			3110	2068	481	536	3	22			
1	C	430	Total	C	N	O	S	Se	0	0	0
			3113	2077	482	529	3	22			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).

BNG
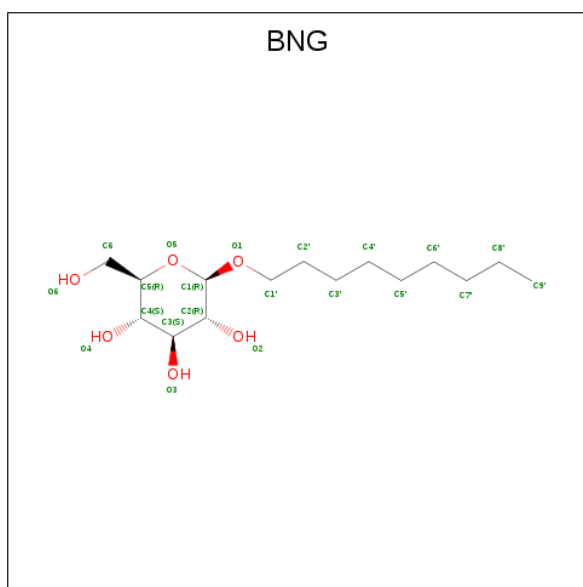
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 21	C 15	O 6	0	0
3	B	1	Total 21	C 15	O 6	0	0
3	C	1	Total 21	C 15	O 6	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

CIT
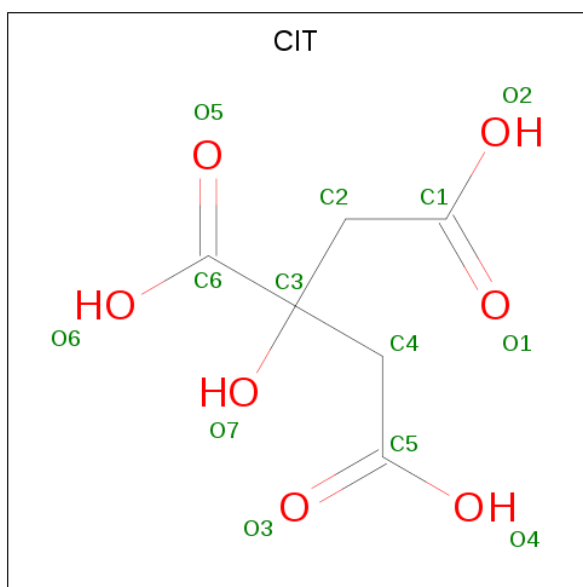
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 13	C 6	O 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0
4	C	1	Total 13	C 6	O 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total 3	O 3	0	0
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.
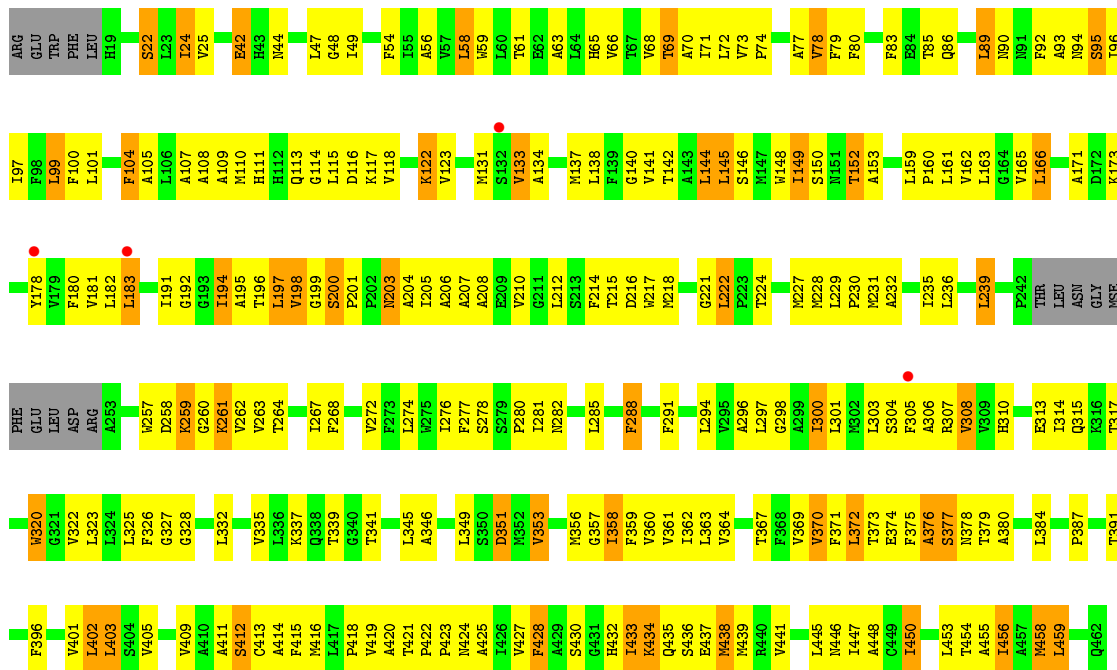
• Molecule 1: Transporter, NadC family
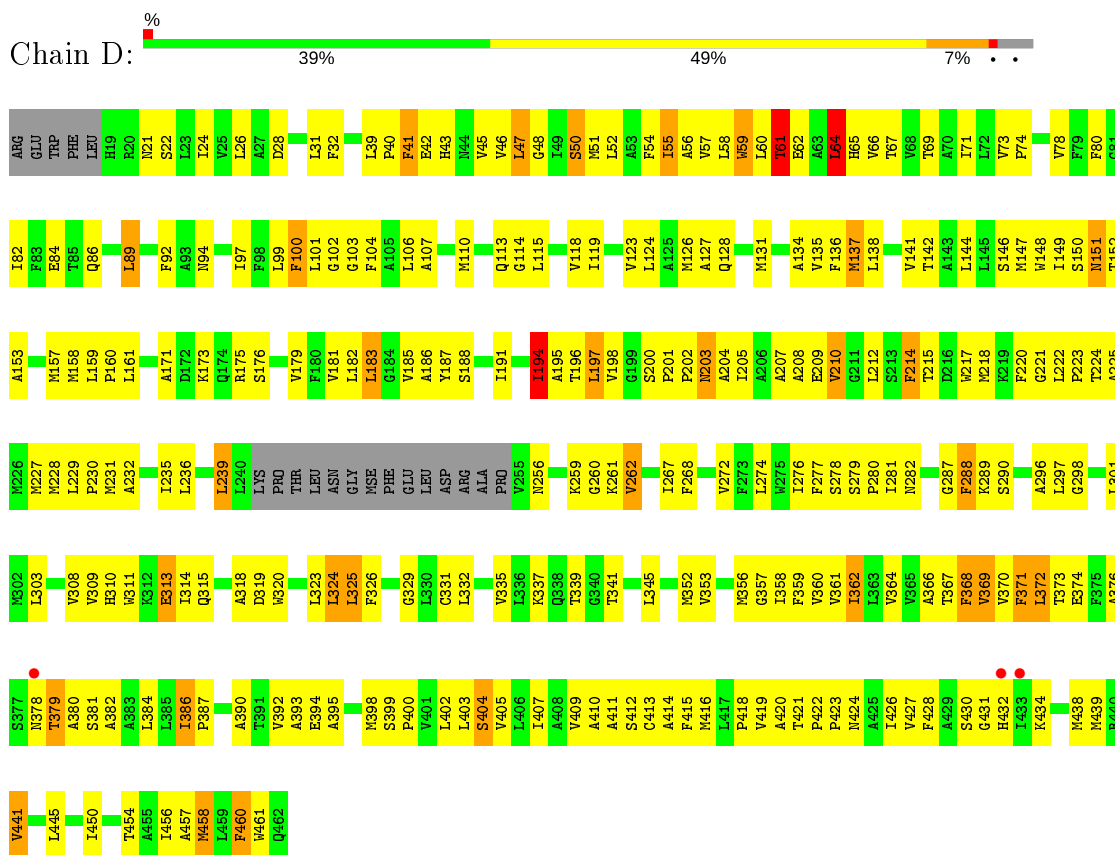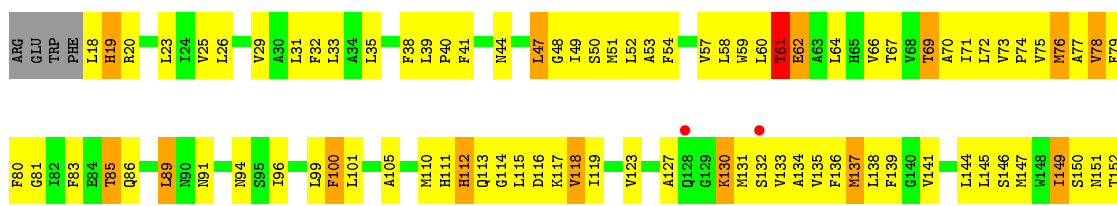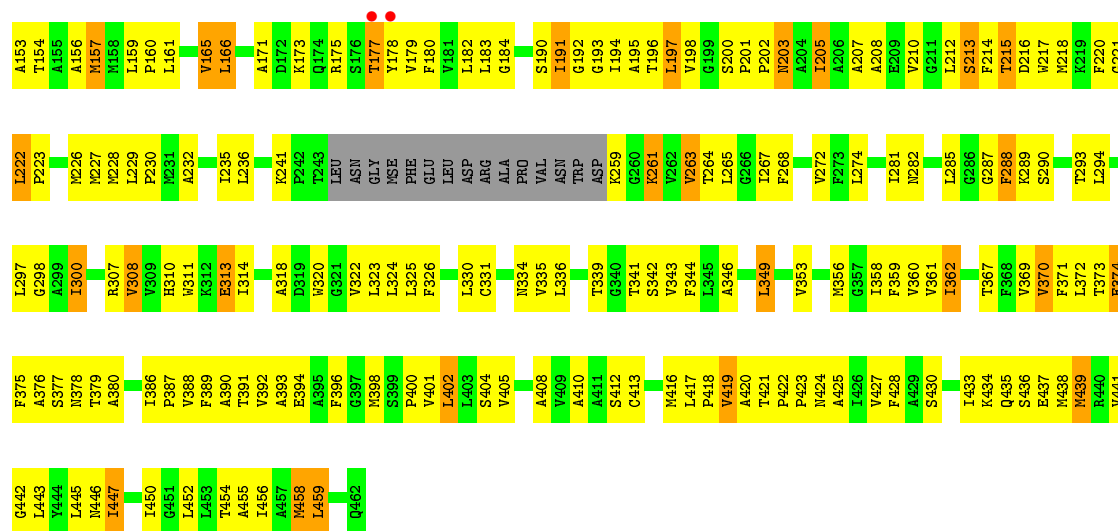

• Molecule 1: Transporter, NadC family

• Molecule 1: Transporter, NadC family

Chain A:

• Molecule 1: Transporter, NadC family

Chain C:
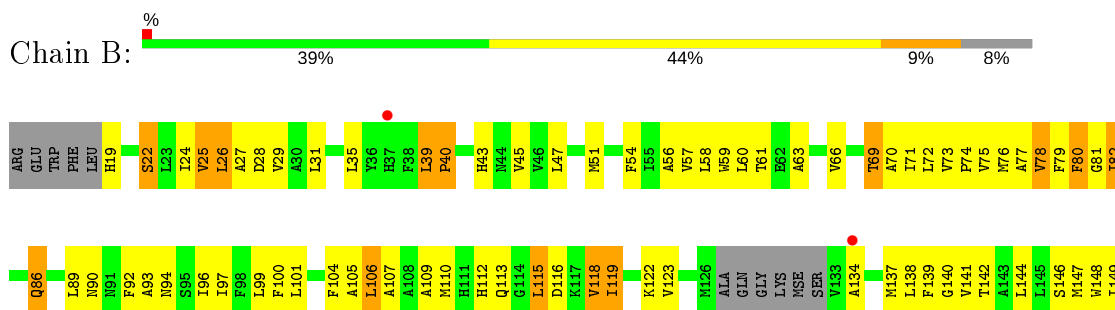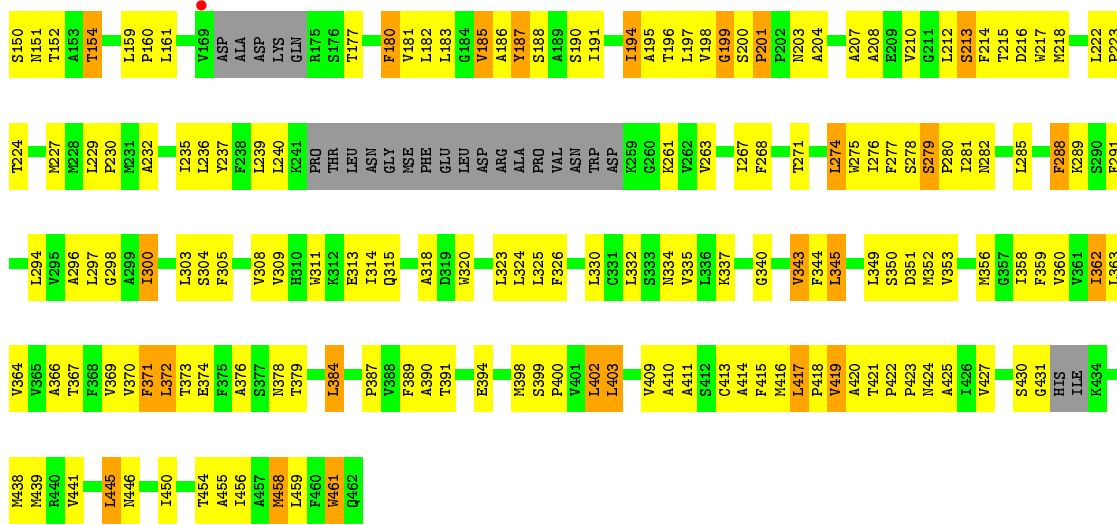
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.33Å 100.87Å 164.57Å 90.00° 101.74° 90.00°	Depositor
Resolution (Å)	44.38 – 3.20 44.38 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.38-3.20) 96.6 (44.38-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.53 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.228 , 0.291 0.223 , 0.287	Depositor DCC
R_{free} test set	2026 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å^2)	93.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 100.4	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12390	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NA, BNG, CIT

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	0.47	0/3153	0.71	2/4278 (0.0%)
1	B	0.42	0/3024	0.67	2/4106 (0.0%)
1	C	0.50	0/3163	0.73	1/4292 (0.0%)
1	D	0.50	0/3119	0.74	2/4231 (0.0%)
All	All	0.47	0/12459	0.71	7/16907 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	3
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	GLY	N-CA-C	-6.01	98.08	113.10
1	D	325	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	199	GLY	N-CA-C	-5.39	99.61	113.10
1	B	402	LEU	CA-CB-CG	-5.20	103.33	115.30
1	C	402	LEU	CA-CB-CG	-5.11	103.55	115.30
1	D	256	ASN	N-CA-C	5.04	124.62	111.00
1	A	259	LYS	N-CA-C	5.04	124.60	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	ILE	Peptide
1	C	430	SER	Peptide
1	C	61	THR	Peptide
1	D	371	PHE	Peptide
1	D	61	THR	Peptide
1	D	64	LEU	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	3110	0	3137	280	0
1	B	2980	0	3005	296	0
1	C	3113	0	3139	284	0
1	D	3076	0	3109	293	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	21	0	30	5	0
3	C	21	0	30	1	0
3	D	21	0	30	3	0
4	A	13	0	5	3	0
4	B	13	0	5	6	0
4	C	13	0	5	5	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	1	0
All	All	12390	0	12495	1133	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 46.

All (1133) 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:419:VAL:HG11	1:A:425:ALA:HB2	1.25	1.13
1:C:420:ALA:HB1	1:C:421:THR:HA	1.36	1.07
1:B:420:ALA:HB1	1:B:421:THR:HA	1.38	1.06
1:C:200:SER:HB2	1:C:201:PRO:HD2	1.37	1.04
1:A:377:SER:HB3	1:A:380:ALA:HB3	1.40	1.03
1:B:373:THR:HG21	1:B:416:MSE:HE2	1.41	1.02
1:B:372:LEU:HD13	1:B:414:ALA:HB2	1.38	1.01
1:A:372:LEU:HA	1:A:376:ALA:HA	1.39	1.01
1:C:372:LEU:O	1:C:376:ALA:HB2	1.59	1.01
1:A:61:THR:HG23	1:A:63:ALA:H	1.23	1.00
1:D:259:LYS:HG2	1:D:261:LYS:HE3	1.42	1.00
1:C:191:ILE:HG12	1:C:228:MSE:HE3	1.44	0.98
1:D:71:ILE:HD13	1:C:300:ILE:HD11	1.41	0.98
1:A:196:THR:HG22	1:A:198:VAL:H	1.27	0.98
1:D:42:GLU:HG2	1:D:43:HIS:H	1.26	0.98
1:A:108:ALA:HB2	1:A:317:THR:HG21	1.44	0.97
1:D:372:LEU:HD21	1:D:378:ASN:HA	1.47	0.97
1:C:196:THR:HG22	1:C:198:VAL:H	1.28	0.97
1:A:372:LEU:HD22	1:A:372:LEU:O	1.64	0.96
1:C:151:ASN:HD21	1:C:200:SER:HB3	1.28	0.96
1:C:362:ILE:HD11	1:C:454:THR:HA	1.47	0.96
1:B:318:ALA:HB3	1:B:320:TRP:CZ3	2.01	0.95
1:B:90:ASN:HD22	1:A:90:ASN:HD22	1.14	0.95
1:D:58:LEU:HD11	1:D:64:LEU:HD23	1.48	0.94
1:A:235:ILE:O	1:A:239:LEU:HB2	1.67	0.93
1:B:282:ASN:OD1	1:B:288:PHE:HB2	1.68	0.93
1:B:282:ASN:HD21	1:B:288:PHE:H	1.13	0.92
1:C:419:VAL:HG21	1:C:425:ALA:HB2	1.52	0.90
1:D:368:PHE:O	1:D:371:PHE:HB3	1.71	0.90
1:A:71:ILE:O	1:A:74:PRO:HD2	1.71	0.90
1:A:371:PHE:O	1:A:372:LEU:HB3	1.71	0.89
1:C:434:LYS:CB	1:C:437:GLU:HB2	2.03	0.88
1:C:418:PRO:HD3	1:C:438:MSE:SE	2.23	0.88
1:D:103:GLY:HA3	1:D:198:VAL:HG11	1.57	0.87
1:D:203:ASN:HB3	1:D:217:TRP:CZ2	2.10	0.87
1:B:372:LEU:O	1:B:376:ALA:HB2	1.74	0.86
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.57	0.85
1:A:419:VAL:HB	1:A:420:ALA:HA	1.57	0.85
1:C:356:MSE:HE3	1:C:360:VAL:HG12	1.59	0.85
1:D:51:MSE:CE	1:D:335:VAL:HG11	2.07	0.85
1:D:367:THR:HG23	1:D:450:ILE:HD13	1.58	0.85
1:A:97:ILE:H	1:A:97:ILE:HD12	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:HD13	1:C:229:LEU:HA	1.59	0.84
1:B:80:PHE:CE2	3:B:503:BNG:H3'1	2.11	0.84
1:D:191:ILE:HG12	1:D:228:MSE:HE2	1.59	0.84
1:A:419:VAL:HG11	1:A:425:ALA:CB	2.07	0.83
1:A:357:GLY:HA3	1:A:361:VAL:HG23	1.60	0.83
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.61	0.83
1:B:196:THR:OG1	1:B:198:VAL:O	1.96	0.83
1:B:200:SER:HB2	1:B:201:PRO:HD2	1.59	0.82
1:B:236:LEU:HD23	1:B:441:VAL:HG11	1.61	0.82
1:B:315:GLN:HA	1:B:320:TRP:CH2	2.15	0.81
1:B:282:ASN:ND2	1:B:288:PHE:H	1.78	0.81
1:D:159:LEU:HB3	1:D:160:PRO:HD3	1.63	0.81
1:D:376:ALA:HB3	1:D:420:ALA:H	1.46	0.81
1:A:59:TRP:NE1	1:A:69:THR:OG1	2.13	0.81
1:D:372:LEU:CD2	1:D:378:ASN:HA	2.11	0.81
1:A:282:ASN:OD1	1:A:288:PHE:HB2	1.81	0.81
1:C:80:PHE:CE2	3:C:503:BNG:H4'2	2.15	0.80
1:B:152:THR:HG22	1:B:423:PRO:HD3	1.62	0.80
1:B:229:LEU:HB3	1:B:230:PRO:HD3	1.63	0.80
1:C:418:PRO:HA	1:C:419:VAL:HG23	1.63	0.80
1:B:123:VAL:HG13	1:B:137:MSE:HE2	1.64	0.80
1:C:367:THR:OG1	1:C:450:ILE:HD11	1.82	0.80
1:A:207:ALA:HA	1:A:212:LEU:HB2	1.62	0.80
1:B:367:THR:HA	1:B:450:ILE:HD13	1.63	0.80
1:A:346:ALA:HA	1:A:396:PHE:HE2	1.47	0.79
1:B:79:PHE:O	1:B:80:PHE:HB2	1.80	0.79
1:C:151:ASN:ND2	1:C:200:SER:HB3	1.97	0.79
1:D:357:GLY:HA3	1:D:361:VAL:HG23	1.62	0.79
1:A:420:ALA:HB1	1:A:421:THR:HA	1.64	0.79
1:A:418:PRO:HD3	1:A:438:MSE:SE	2.32	0.79
1:C:419:VAL:HG13	1:C:420:ALA:HA	1.63	0.79
1:B:99:LEU:HD12	1:B:197:LEU:HD22	1.63	0.78
1:A:315:GLN:HA	1:A:320:TRP:CH2	2.17	0.78
1:C:130:LYS:HE3	1:C:130:LYS:HA	1.65	0.78
1:C:127:ALA:HB1	1:C:133:VAL:HG23	1.64	0.78
1:B:300:ILE:HD11	1:A:71:ILE:HD13	1.64	0.78
1:A:267:ILE:HD12	1:A:303:LEU:HD23	1.65	0.78
1:B:372:LEU:HD22	1:B:376:ALA:HB1	1.65	0.78
1:D:46:VAL:O	1:D:50:SER:HB2	1.84	0.77
1:C:78:VAL:O	1:C:81:GLY:N	2.16	0.77
1:A:258:ASP:HA	1:A:261:LYS:HD3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:HE2	1:A:391:THR:HG22	1.64	0.77
1:B:358:ILE:O	1:B:362:ILE:HG23	1.85	0.77
1:B:210:VAL:HG12	1:B:400:PRO:HB2	1.65	0.77
1:C:57:VAL:O	1:C:60:LEU:O	2.02	0.77
1:B:159:LEU:HB3	1:B:160:PRO:HD3	1.66	0.77
1:A:349:LEU:O	1:A:353:VAL:HG13	1.85	0.76
1:B:232:ALA:HA	1:B:445:LEU:HD11	1.67	0.76
1:B:418:PRO:HB3	1:B:419:VAL:HG13	1.67	0.76
1:A:92:PHE:HD2	1:A:327:GLY:HA3	1.49	0.76
1:A:210:VAL:HG11	1:A:401:VAL:HA	1.66	0.76
1:D:220:PHE:HD1	1:D:460:PHE:CE2	2.04	0.76
1:C:119:ILE:O	1:C:123:VAL:HG12	1.85	0.76
1:A:150:SER:HB3	1:A:153:ALA:HB3	1.68	0.75
1:A:413:CYS:HB3	1:A:415:PHE:CE2	2.20	0.75
1:B:394:GLU:HG2	1:B:400:PRO:HG3	1.67	0.75
1:A:47:LEU:HD11	1:A:80:PHE:HD1	1.50	0.75
1:A:196:THR:N	1:A:217:TRP:HZ3	1.85	0.75
1:D:373:THR:HG22	1:D:374:GLU:H	1.50	0.75
1:A:419:VAL:CG1	1:A:425:ALA:HB2	2.13	0.75
1:A:434:LYS:NZ	1:A:434:LYS:HB3	2.02	0.74
1:B:352:MSE:O	1:B:356:MSE:HG3	1.86	0.74
1:B:349:LEU:O	1:B:353:VAL:HG13	1.86	0.74
1:B:414:ALA:HB3	1:B:421:THR:HG23	1.69	0.74
1:A:48:GLY:HA3	1:A:341:THR:OG1	1.88	0.74
1:B:208:ALA:HB1	1:B:330:LEU:HD11	1.70	0.74
1:C:144:LEU:HA	1:C:147:MSE:HE3	1.68	0.74
1:B:72:LEU:HD13	1:A:301:LEU:HD22	1.69	0.74
1:D:200:SER:HB2	1:D:201:PRO:CD	2.17	0.74
1:D:67:THR:O	1:D:71:ILE:HD12	1.88	0.74
1:A:315:GLN:HG3	1:A:320:TRP:CZ3	2.23	0.74
1:D:373:THR:HG22	1:D:374:GLU:N	2.03	0.74
1:C:110:MSE:HG2	1:C:115:LEU:HD23	1.69	0.73
1:A:196:THR:HG23	1:A:214:PHE:HE1	1.53	0.73
1:A:356:MSE:HE3	1:A:360:VAL:HG12	1.68	0.73
1:A:162:VAL:O	1:A:166:LEU:HD22	1.87	0.73
1:C:362:ILE:CD1	1:C:454:THR:HA	2.16	0.73
1:D:200:SER:HB2	1:D:201:PRO:HD3	1.69	0.73
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.71	0.73
1:A:108:ALA:HB2	1:A:317:THR:CG2	2.18	0.73
1:D:123:VAL:O	1:D:126:MSE:HB3	1.88	0.73
1:D:392:VAL:O	1:D:395:ALA:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HD11	1:A:61:THR:HG21	1.69	0.72
1:D:370:VAL:O	1:D:373:THR:HB	1.89	0.72
1:C:200:SER:HB2	1:C:201:PRO:CD	2.17	0.72
1:A:285:LEU:O	1:A:285:LEU:HD23	1.90	0.72
1:A:99:LEU:HD22	1:A:296:ALA:HB2	1.72	0.72
1:C:213:SER:H	1:C:216:ASP:HB2	1.54	0.72
1:C:373:THR:HG22	1:C:417:LEU:HG	1.71	0.72
1:D:114:GLY:O	1:D:118:VAL:HG12	1.90	0.72
1:A:339:THR:OG1	1:A:341:THR:OG1	2.04	0.72
1:C:282:ASN:OD1	1:C:288:PHE:HB2	1.90	0.72
1:D:236:LEU:HD12	1:D:441:VAL:HG21	1.71	0.71
1:A:141:VAL:O	1:A:145:LEU:HB2	1.91	0.71
1:C:194:ILE:O	1:C:195:ALA:HB3	1.91	0.71
1:A:134:ALA:O	1:A:138:LEU:HB2	1.90	0.71
1:B:109:ALA:HA	1:B:309:VAL:HG22	1.72	0.71
1:D:372:LEU:HD21	1:D:378:ASN:CA	2.20	0.71
1:B:106:LEU:HD12	1:B:268:PHE:HD1	1.55	0.71
1:C:390:ALA:HB2	1:C:404:SER:OG	1.90	0.71
1:D:86:GLN:HE22	1:C:94:ASN:HA	1.56	0.71
1:B:139:PHE:O	1:B:142:THR:HG22	1.91	0.70
1:A:372:LEU:HD21	1:A:411:ALA:O	1.90	0.70
1:B:337:LYS:HE2	1:B:391:THR:HG22	1.73	0.70
1:D:131:MSE:O	1:D:134:ALA:N	2.24	0.70
1:A:107:ALA:HA	1:A:110:MSE:HE2	1.73	0.70
1:D:259:LYS:HG3	1:D:261:LYS:H	1.56	0.70
1:D:71:ILE:HD13	1:C:300:ILE:CD1	2.19	0.70
1:B:340:GLY:O	1:B:343:VAL:N	2.25	0.70
1:B:182:LEU:HD22	1:B:427:VAL:HB	1.73	0.70
1:D:402:LEU:HD23	1:D:403:LEU:N	2.07	0.70
1:A:92:PHE:HE2	1:A:328:GLY:N	1.89	0.70
1:A:346:ALA:HA	1:A:396:PHE:CE2	2.27	0.70
1:B:332:LEU:HA	1:B:335:VAL:HG12	1.73	0.69
1:C:151:ASN:O	1:C:154:THR:HG22	1.92	0.69
1:A:66:VAL:HG13	1:A:325:LEU:HD13	1.73	0.69
1:D:259:LYS:CG	1:D:261:LYS:HE3	2.22	0.69
1:D:42:GLU:HG2	1:D:43:HIS:N	2.03	0.69
1:B:372:LEU:HG	1:B:411:ALA:HA	1.74	0.69
1:B:106:LEU:O	1:B:110:MSE:HE2	1.92	0.69
1:C:115:LEU:O	1:C:118:VAL:HG13	1.93	0.68
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.75	0.68
1:A:267:ILE:CD1	1:A:303:LEU:HD23	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:HA	1:B:320:TRP:HH2	1.58	0.68
1:C:198:VAL:HG23	1:C:198:VAL:O	1.92	0.68
1:D:430:SER:C	1:D:432:HIS:H	1.94	0.68
1:B:152:THR:HG23	4:B:501:CIT:H41	1.76	0.68
1:A:58:LEU:HA	1:A:61:THR:HG22	1.76	0.68
1:A:166:LEU:O	1:A:166:LEU:HD23	1.94	0.67
1:D:127:ALA:C	1:D:128:GLN:HG2	2.15	0.67
1:C:212:LEU:HD22	1:C:216:ASP:HB3	1.76	0.67
1:D:323:LEU:HA	1:D:326:PHE:HD2	1.59	0.67
1:D:362:ILE:HG21	1:D:458:MSE:HE1	1.76	0.67
1:B:311:TRP:HB3	1:A:65:HIS:CD2	2.30	0.67
1:C:145:LEU:HD22	1:C:149:ILE:HD11	1.77	0.67
1:C:447:ILE:HA	1:C:450:ILE:HG22	1.77	0.67
1:B:45:VAL:HG11	1:B:344:PHE:CD1	2.30	0.67
1:D:47:LEU:HD21	1:D:80:PHE:HB3	1.74	0.67
1:B:455:ALA:O	1:B:459:LEU:HB2	1.95	0.67
1:A:384:LEU:O	1:A:387:PRO:HD2	1.95	0.67
1:B:194:ILE:HA	1:B:203:ASN:HD21	1.60	0.67
1:A:430:SER:O	1:A:430:SER:OG	2.08	0.67
1:C:25:VAL:O	1:C:29:VAL:HG23	1.95	0.67
1:A:373:THR:HG23	1:A:415:PHE:O	1.95	0.66
1:B:115:LEU:O	1:B:119:ILE:HG12	1.95	0.66
1:B:360:VAL:O	1:B:364:VAL:HG23	1.95	0.66
1:D:420:ALA:HB1	1:D:421:THR:HA	1.75	0.66
1:B:372:LEU:O	1:B:372:LEU:HD22	1.96	0.66
1:A:97:ILE:H	1:A:97:ILE:CD1	2.09	0.66
1:D:21:ASN:HA	1:D:24:ILE:HD12	1.78	0.66
1:C:196:THR:HG22	1:C:198:VAL:N	2.07	0.66
1:A:403:LEU:HD23	1:A:403:LEU:N	2.11	0.66
1:A:418:PRO:HG3	1:A:428:PHE:CE1	2.30	0.66
1:C:146:SER:HB2	1:C:154:THR:HG21	1.78	0.66
1:D:201:PRO:HD2	1:D:202:PRO:HD2	1.76	0.66
1:D:152:THR:HG23	1:D:422:PRO:HB2	1.78	0.65
1:B:24:ILE:O	1:B:27:ALA:HB3	1.96	0.65
1:A:97:ILE:N	1:A:97:ILE:HD12	2.12	0.65
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.78	0.65
1:A:332:LEU:HA	1:A:335:VAL:HG22	1.77	0.65
1:B:372:LEU:HD11	1:B:411:ALA:O	1.97	0.65
1:C:418:PRO:HG3	1:C:428:PHE:CD2	2.32	0.65
1:C:141:VAL:O	1:C:145:LEU:HB2	1.97	0.65
1:C:358:ILE:O	1:C:362:ILE:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:MSE:HE3	1:D:335:VAL:HG11	1.79	0.65
1:B:376:ALA:HB3	1:B:420:ALA:HB3	1.79	0.65
1:D:320:TRP:CE3	1:D:323:LEU:HD12	2.32	0.64
1:D:360:VAL:O	1:D:364:VAL:HG23	1.95	0.64
1:B:384:LEU:O	1:B:387:PRO:HD2	1.98	0.64
1:D:101:LEU:HD13	1:D:323:LEU:HD11	1.78	0.64
1:A:100:PHE:CE1	1:A:198:VAL:HG13	2.31	0.64
1:A:277:PHE:HB3	1:A:281:ILE:HD13	1.79	0.64
1:C:379:THR:OG1	4:C:501:CIT:H22	1.98	0.64
1:A:357:GLY:CA	1:A:358:ILE:C	2.66	0.64
1:C:331:CYS:O	1:C:335:VAL:HG23	1.98	0.64
1:C:394:GLU:HG3	1:C:400:PRO:HG3	1.78	0.64
1:C:69:THR:O	1:C:72:LEU:HB3	1.98	0.64
1:A:92:PHE:CD2	1:A:327:GLY:HA3	2.32	0.64
1:B:372:LEU:CD1	1:B:414:ALA:HB2	2.20	0.64
1:B:372:LEU:O	1:B:376:ALA:CB	2.44	0.63
1:C:259:LYS:CB	1:C:261:LYS:HE3	2.27	0.63
1:D:267:ILE:HD13	1:D:303:LEU:HD23	1.78	0.63
1:D:194:ILE:CG1	1:D:195:ALA:N	2.62	0.63
1:A:320:TRP:CD1	1:A:323:LEU:HD12	2.33	0.63
1:C:123:VAL:HG22	1:C:137:MSE:HG3	1.79	0.63
1:C:48:GLY:HA3	1:C:341:THR:OG1	1.98	0.63
1:D:372:LEU:HG	1:D:414:ALA:HB2	1.81	0.63
1:A:163:LEU:O	1:A:166:LEU:O	2.17	0.63
1:B:461:TRP:CE3	1:B:461:TRP:HA	2.34	0.63
1:C:261:LYS:HD2	1:C:261:LYS:H	1.62	0.63
1:C:310:HIS:O	1:C:313:GLU:HG2	1.99	0.63
1:D:182:LEU:HB3	1:D:427:VAL:HB	1.81	0.63
1:B:82:ILE:HD13	1:B:335:VAL:HG23	1.81	0.62
1:C:79:PHE:O	1:C:80:PHE:HB2	1.98	0.62
1:B:418:PRO:HD3	1:B:438:MSE:SE	2.49	0.62
1:C:115:LEU:O	1:C:119:ILE:HG13	1.99	0.62
1:A:315:GLN:HG3	1:A:320:TRP:HZ3	1.62	0.62
1:A:335:VAL:O	1:A:339:THR:HG23	1.98	0.62
1:B:362:ILE:HG21	1:B:458:MSE:HE1	1.81	0.62
1:C:105:ALA:HA	1:C:314:ILE:HD12	1.80	0.62
1:A:232:ALA:HB1	1:A:445:LEU:HD21	1.81	0.62
1:C:145:LEU:HD22	1:C:149:ILE:CD1	2.29	0.62
1:C:222:LEU:HD22	1:C:222:LEU:O	1.99	0.62
1:A:458:MSE:HA	1:A:458:MSE:HE3	1.80	0.62
1:B:109:ALA:HA	1:B:309:VAL:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:VAL:O	1:C:267:ILE:HG13	1.99	0.62
1:B:105:ALA:HA	1:B:314:ILE:HD12	1.81	0.62
1:C:213:SER:N	1:C:216:ASP:HB2	2.13	0.62
1:C:201:PRO:O	1:C:205:ILE:CG1	2.47	0.62
1:C:212:LEU:CD2	1:C:216:ASP:HB3	2.29	0.62
1:D:422:PRO:O	1:D:426:ILE:HG12	2.00	0.62
1:A:201:PRO:HB2	1:A:379:THR:HG23	1.81	0.62
1:B:151:ASN:O	1:B:154:THR:HG22	1.99	0.62
1:D:403:LEU:O	1:D:407:ILE:HG13	2.00	0.62
1:C:203:ASN:OD1	1:C:203:ASN:N	2.33	0.62
1:D:309:VAL:CG2	1:D:313:GLU:HG3	2.30	0.62
1:D:366:ALA:O	1:D:369:VAL:N	2.31	0.62
1:D:201:PRO:CD	1:D:202:PRO:HD2	2.29	0.61
1:A:447:ILE:HA	1:A:450:ILE:HG23	1.80	0.61
1:B:194:ILE:O	1:B:195:ALA:HB3	1.99	0.61
1:B:28:ASP:HB2	1:B:57:VAL:HG11	1.81	0.61
1:D:42:GLU:CG	1:D:43:HIS:H	2.04	0.61
1:C:191:ILE:CG1	1:C:228:MSE:HE3	2.26	0.61
1:D:267:ILE:HG21	1:D:303:LEU:CD2	2.30	0.61
1:D:259:LYS:O	1:D:262:VAL:HG12	2.00	0.61
1:D:73:VAL:HG12	1:D:331:CYS:SG	2.40	0.61
1:A:196:THR:HG22	1:A:198:VAL:N	2.09	0.61
1:A:22:SER:O	1:A:25:VAL:N	2.33	0.61
1:D:207:ALA:CB	1:D:212:LEU:HB2	2.30	0.61
1:D:362:ILE:HG12	1:D:454:THR:HG23	1.82	0.61
1:B:101:LEU:O	1:B:101:LEU:HD23	1.99	0.61
1:C:362:ILE:HG12	1:C:458:MSE:CE	2.31	0.61
1:D:115:LEU:HA	1:D:118:VAL:CG1	2.31	0.61
1:B:267:ILE:HG21	1:B:303:LEU:HG	1.81	0.61
1:B:308:VAL:HG12	1:B:309:VAL:HG23	1.83	0.61
1:C:111:HIS:O	1:C:114:GLY:N	2.29	0.61
1:D:194:ILE:HG13	1:D:195:ALA:N	2.16	0.61
1:A:203:ASN:HB3	1:A:217:TRP:CZ2	2.35	0.60
1:C:418:PRO:CD	1:C:438:MSE:SE	2.99	0.60
1:D:185:VAL:HG12	1:D:186:ALA:N	2.16	0.60
1:A:203:ASN:N	1:A:203:ASN:OD1	2.32	0.60
1:B:374:GLU:O	1:B:374:GLU:HG3	2.01	0.60
1:C:194:ILE:HG13	1:C:195:ALA:N	2.15	0.60
1:A:206:ALA:O	1:A:210:VAL:HG22	2.00	0.60
1:A:24:ILE:HG12	1:A:63:ALA:HB2	1.83	0.60
1:D:376:ALA:HB1	1:D:420:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:O	1:B:147:MSE:HE2	2.01	0.60
1:C:423:PRO:O	1:C:427:VAL:HG22	2.02	0.60
1:C:152:THR:HG23	4:C:501:CIT:O4	2.02	0.60
1:D:430:SER:O	1:D:432:HIS:N	2.34	0.60
1:D:74:PRO:HG2	1:D:92:PHE:CE1	2.37	0.60
1:A:47:LEU:HD11	1:A:80:PHE:CD1	2.33	0.60
1:B:267:ILE:HD12	1:B:303:LEU:HD23	1.84	0.60
1:D:277:PHE:O	1:D:280:PRO:HD2	2.00	0.60
1:A:133:VAL:O	1:A:137:MSE:HB2	2.02	0.60
1:C:419:VAL:HG21	1:C:425:ALA:CB	2.28	0.60
1:C:442:GLY:O	1:C:446:ASN:HB2	2.01	0.60
1:A:180:PHE:CD2	1:A:180:PHE:O	2.55	0.60
1:B:378:ASN:HD21	1:B:421:THR:HG21	1.66	0.60
1:D:201:PRO:N	1:D:202:PRO:HD2	2.16	0.60
1:C:455:ALA:O	1:C:459:LEU:HD12	2.02	0.60
1:D:432:HIS:C	1:D:434:LYS:H	2.04	0.60
1:C:325:LEU:CD2	1:C:379:THR:HG22	2.31	0.60
1:A:196:THR:HG23	1:A:214:PHE:CE1	2.35	0.59
1:C:197:LEU:HD12	1:C:214:PHE:HA	1.82	0.59
1:A:201:PRO:HG2	1:A:379:THR:OG1	2.02	0.59
1:C:419:VAL:HG13	1:C:420:ALA:CA	2.32	0.59
1:B:152:THR:HG23	4:B:501:CIT:C4	2.31	0.59
1:D:80:PHE:CZ	3:D:502:BNG:H3'1	2.37	0.59
1:B:93:ALA:HB2	1:A:93:ALA:HB2	1.84	0.59
1:B:118:VAL:O	1:B:122:LYS:N	2.30	0.59
1:C:367:THR:O	1:C:370:VAL:HG23	2.03	0.59
1:D:282:ASN:OD1	1:D:288:PHE:HB2	2.02	0.59
1:A:282:ASN:HD21	1:A:288:PHE:H	1.49	0.59
1:B:70:ALA:HB2	1:B:325:LEU:HD12	1.83	0.59
1:B:239:LEU:HD13	1:B:441:VAL:HA	1.84	0.59
1:D:67:THR:HG21	1:C:311:TRP:CZ2	2.38	0.59
1:B:31:LEU:HG	1:B:35:LEU:HD11	1.85	0.59
1:D:183:LEU:HG	1:D:187:TYR:CZ	2.38	0.59
1:A:372:LEU:HD22	1:A:376:ALA:HB1	1.84	0.59
1:A:152:THR:HB	1:A:422:PRO:HG2	1.84	0.59
1:A:231:MSE:HE3	1:A:448:ALA:HB1	1.84	0.59
1:B:410:ALA:O	1:B:413:CYS:HB2	2.03	0.59
1:C:232:ALA:HA	1:C:445:LEU:CD1	2.32	0.59
1:D:135:VAL:O	1:D:138:LEU:HB2	2.02	0.59
1:A:357:GLY:HA3	1:A:358:ILE:C	2.22	0.59
1:B:149:ILE:HD13	1:B:154:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:O	1:C:226:MSE:HG2	2.02	0.59
1:C:282:ASN:HD21	1:C:288:PHE:H	1.49	0.59
1:D:335:VAL:O	1:D:339:THR:HG23	2.02	0.59
1:A:370:VAL:O	1:A:371:PHE:HB3	2.02	0.59
1:A:372:LEU:HD23	1:A:378:ASN:HA	1.85	0.59
1:D:366:ALA:O	1:D:369:VAL:HB	2.02	0.59
1:A:420:ALA:HB1	1:A:421:THR:CA	2.32	0.59
1:B:372:LEU:HD21	1:B:378:ASN:HA	1.85	0.59
1:A:434:LYS:HZ3	1:A:434:LYS:HB3	1.68	0.58
1:C:175:ARG:O	1:C:179:VAL:O	2.21	0.58
1:C:215:THR:HA	1:C:218:MSE:HB3	1.84	0.58
1:D:203:ASN:HB3	1:D:217:TRP:CE2	2.38	0.58
1:B:214:PHE:HE2	1:B:218:MSE:SE	2.36	0.58
1:B:373:THR:CG2	1:B:416:MSE:HE2	2.26	0.58
1:C:123:VAL:HG11	1:C:141:VAL:CG2	2.32	0.58
1:C:144:LEU:O	1:C:147:MSE:HB2	2.02	0.58
1:C:447:ILE:O	1:C:450:ILE:HG22	2.03	0.58
1:C:73:VAL:HB	1:C:74:PRO:HD3	1.84	0.58
1:C:210:VAL:HG12	1:C:400:PRO:HB2	1.86	0.58
1:A:294:LEU:O	1:A:298:GLY:N	2.28	0.58
1:C:183:LEU:HD11	1:C:438:MSE:HG2	1.85	0.58
1:D:65:HIS:CG	1:D:66:VAL:H	2.21	0.58
1:B:43:HIS:HE1	3:B:503:BNG:H4	1.69	0.58
1:C:336:LEU:HB3	1:C:342:SER:OG	2.04	0.58
1:D:200:SER:O	1:D:203:ASN:OD1	2.22	0.58
1:A:282:ASN:HB2	1:A:291:PHE:CD2	2.39	0.57
1:A:297:LEU:O	1:A:300:ILE:HG23	2.04	0.57
1:B:123:VAL:HG11	1:B:141:VAL:HG23	1.84	0.57
1:B:123:VAL:HG13	1:B:137:MSE:CE	2.35	0.57
1:B:378:ASN:OD1	1:B:421:THR:HG22	2.04	0.57
1:C:135:VAL:HG23	1:C:136:PHE:N	2.20	0.57
1:C:180:PHE:O	1:C:184:GLY:N	2.20	0.57
1:D:80:PHE:CE1	3:D:502:BNG:H5'1	2.39	0.57
1:A:267:ILE:HG21	1:A:303:LEU:CD2	2.35	0.57
1:A:424:ASN:O	1:A:427:VAL:HG22	2.05	0.57
1:B:461:TRP:HE3	1:B:461:TRP:HA	1.69	0.57
1:D:59:TRP:CD1	1:D:69:THR:HG21	2.39	0.57
1:D:115:LEU:O	1:D:119:ILE:HG13	2.04	0.57
1:C:362:ILE:HD11	1:C:454:THR:CA	2.30	0.57
1:A:372:LEU:O	1:A:376:ALA:HB2	2.05	0.57
1:B:350:SER:O	1:B:353:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:CD1	1:D:376:ALA:HB1	2.34	0.57
1:B:419:VAL:HG12	1:B:421:THR:O	2.04	0.57
1:D:203:ASN:ND2	1:D:217:TRP:CH2	2.71	0.57
1:A:372:LEU:CD2	1:A:372:LEU:O	2.47	0.57
1:A:78:VAL:HA	1:A:83:PHE:O	2.05	0.57
1:B:279:SER:HB3	1:B:280:PRO:HD3	1.87	0.57
1:D:372:LEU:HD21	1:D:378:ASN:CB	2.35	0.56
1:D:432:HIS:C	1:D:434:LYS:N	2.56	0.56
1:C:282:ASN:ND2	1:C:288:PHE:H	2.03	0.56
1:B:318:ALA:HB3	1:B:320:TRP:CH2	2.38	0.56
1:C:201:PRO:O	1:C:205:ILE:HG13	2.04	0.56
1:C:40:PRO:HG2	1:C:41:PHE:H	1.70	0.56
1:A:200:SER:HB2	1:A:201:PRO:HD2	1.86	0.56
1:C:110:MSE:CG	1:C:115:LEU:HD23	2.34	0.56
1:D:61:THR:OG1	1:D:62:GLU:N	2.37	0.56
1:A:351:ASP:OD1	1:A:351:ASP:N	2.39	0.56
1:B:418:PRO:CB	1:B:419:VAL:HG13	2.36	0.56
1:D:56:ALA:HB2	1:D:384:LEU:HD11	1.87	0.56
1:B:86:GLN:OE1	1:A:95:SER:N	2.39	0.56
1:D:183:LEU:HB3	1:D:236:LEU:HD21	1.85	0.56
1:D:207:ALA:HA	1:D:212:LEU:HB2	1.87	0.56
1:D:267:ILE:HG21	1:D:303:LEU:HD21	1.87	0.56
1:D:279:SER:HB3	1:D:280:PRO:HD3	1.87	0.56
1:B:320:TRP:O	1:B:324:LEU:HD13	2.05	0.56
1:C:114:GLY:O	1:C:118:VAL:HG12	2.06	0.56
1:D:210:VAL:HG11	1:D:404:SER:OG	2.06	0.56
1:B:194:ILE:HB	1:B:217:TRP:HH2	1.70	0.56
1:B:282:ASN:HD21	1:B:288:PHE:N	1.95	0.56
1:C:373:THR:HG21	1:C:416:MSE:HE2	1.87	0.56
1:A:86:GLN:O	1:A:89:LEU:N	2.39	0.56
1:D:214:PHE:O	1:D:214:PHE:HD2	1.89	0.56
1:D:194:ILE:HG12	1:D:225:ALA:HB2	1.88	0.56
1:D:99:LEU:O	1:D:99:LEU:HD12	2.06	0.56
1:A:78:VAL:HG12	1:A:79:PHE:N	2.21	0.56
1:B:146:SER:HA	1:B:149:ILE:CD1	2.35	0.56
4:B:501:CIT:O2	4:B:501:CIT:H42	2.06	0.56
1:B:39:LEU:HD13	1:B:40:PRO:HD2	1.87	0.55
1:D:374:GLU:C	1:D:376:ALA:H	2.09	0.55
1:A:195:ALA:O	1:A:218:MSE:HG3	2.06	0.55
1:A:92:PHE:CE2	1:A:328:GLY:N	2.74	0.55
1:B:100:PHE:CD1	1:B:198:VAL:HG12	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:PHE:CD2	1:C:214:PHE:C	2.80	0.55
1:A:77:ALA:O	1:A:78:VAL:HB	2.05	0.55
1:D:150:SER:HB3	1:D:153:ALA:HB3	1.88	0.55
1:A:24:ILE:HD12	1:A:24:ILE:O	2.07	0.55
1:B:325:LEU:HD23	1:B:379:THR:HG22	1.88	0.55
1:D:203:ASN:N	1:D:203:ASN:OD1	2.37	0.55
1:B:66:VAL:CG1	1:B:325:LEU:HD13	2.36	0.55
1:B:372:LEU:HD22	1:B:376:ALA:CB	2.34	0.55
1:A:145:LEU:HD13	1:A:149:ILE:HG13	1.89	0.55
1:A:285:LEU:C	1:A:285:LEU:HD23	2.27	0.55
1:A:227:MSE:O	1:A:230:PRO:HD2	2.06	0.55
1:B:213:SER:H	1:B:216:ASP:HB2	1.72	0.55
1:B:31:LEU:O	1:B:35:LEU:HD12	2.07	0.55
1:B:413:CYS:O	1:B:415:PHE:CD2	2.60	0.55
1:B:414:ALA:HB3	1:B:421:THR:CG2	2.35	0.55
1:B:418:PRO:HG3	1:B:438:MSE:SE	2.57	0.55
1:C:152:THR:HG22	1:C:423:PRO:HD3	1.89	0.55
1:C:159:LEU:HB3	1:C:160:PRO:HD3	1.88	0.55
1:D:341:THR:O	1:D:345:LEU:HG	2.07	0.55
1:B:373:THR:HG23	1:B:415:PHE:O	2.07	0.55
1:D:418:PRO:HB3	1:D:424:ASN:HB3	1.88	0.55
1:A:111:HIS:O	1:A:114:GLY:N	2.40	0.54
1:A:268:PHE:O	1:A:272:VAL:HG23	2.07	0.54
1:A:372:LEU:C	1:A:372:LEU:HD13	2.28	0.54
1:A:373:THR:HG21	1:A:416:MSE:HB2	1.88	0.54
1:C:132:SER:O	1:C:135:VAL:HG22	2.07	0.54
1:D:103:GLY:HA3	1:D:198:VAL:CG1	2.35	0.54
1:D:268:PHE:O	1:D:272:VAL:HG23	2.06	0.54
1:D:372:LEU:CD2	1:D:411:ALA:O	2.55	0.54
1:C:38:PHE:O	1:C:39:LEU:C	2.46	0.54
1:D:372:LEU:HA	1:D:376:ALA:HA	1.88	0.54
1:A:362:ILE:HG13	1:A:454:THR:HG23	1.87	0.54
1:B:183:LEU:HD11	1:B:438:MSE:HE3	1.90	0.54
1:B:227:MSE:O	1:B:230:PRO:HD2	2.06	0.54
1:C:435:GLN:O	1:C:439:MSE:HG3	2.07	0.54
1:C:362:ILE:HG12	1:C:458:MSE:HE1	1.87	0.54
1:A:70:ALA:HB2	1:A:325:LEU:HD12	1.89	0.54
1:D:430:SER:C	1:D:432:HIS:N	2.60	0.54
1:B:194:ILE:HG21	1:B:409:VAL:HG23	1.89	0.54
1:B:152:THR:CG2	4:B:501:CIT:H41	2.38	0.54
1:C:127:ALA:HA	1:C:137:MSE:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LEU:HD21	1:C:379:THR:HG22	1.89	0.54
1:D:357:GLY:HA3	1:D:361:VAL:CG2	2.34	0.54
1:A:194:ILE:HG22	1:A:195:ALA:H	1.73	0.54
1:A:282:ASN:ND2	1:A:288:PHE:H	2.06	0.54
1:A:358:ILE:O	1:A:361:VAL:N	2.39	0.54
1:A:94:ASN:O	1:A:97:ILE:HD13	2.07	0.54
1:B:107:ALA:HA	1:B:110:MSE:CE	2.36	0.54
1:C:436:SER:HA	1:C:439:MSE:HG3	1.88	0.54
1:B:107:ALA:HA	1:B:110:MSE:HE3	1.88	0.54
1:B:90:ASN:HD22	1:A:90:ASN:ND2	1.96	0.54
1:D:227:MSE:O	1:D:230:PRO:HD2	2.07	0.54
1:A:258:ASP:N	1:A:259:LYS:CB	2.71	0.54
1:A:298:GLY:O	1:A:301:LEU:HB2	2.08	0.54
1:D:229:LEU:HB3	1:D:230:PRO:HD3	1.90	0.54
1:D:289:LYS:O	1:C:85:THR:OG1	2.17	0.54
1:A:276:ILE:HG22	1:A:277:PHE:CD2	2.44	0.53
1:C:220:PHE:CD2	1:C:405:VAL:HG21	2.43	0.53
1:C:418:PRO:HA	1:C:419:VAL:CG2	2.37	0.53
1:D:194:ILE:HG13	1:D:195:ALA:H	1.73	0.53
1:D:309:VAL:HG23	1:D:313:GLU:HG3	1.89	0.53
1:D:239:LEU:HD13	1:D:441:VAL:HG23	1.90	0.53
1:A:196:THR:HG22	1:A:198:VAL:O	2.09	0.53
1:A:86:GLN:HG3	1:A:90:ASN:OD1	2.08	0.53
1:B:101:LEU:HD23	1:B:101:LEU:C	2.28	0.53
1:B:424:ASN:CG	1:B:438:MSE:HE1	2.28	0.53
1:A:307:ARG:O	1:A:307:ARG:HG2	2.08	0.53
1:A:54:PHE:HE2	1:A:72:LEU:HD21	1.73	0.53
1:D:104:PHE:CD1	1:D:318:ALA:HA	2.44	0.53
1:D:58:LEU:HD11	1:D:64:LEU:CD2	2.31	0.53
1:B:134:ALA:O	1:B:138:LEU:HG	2.09	0.53
1:B:370:VAL:O	1:B:371:PHE:HB3	2.07	0.53
1:B:60:LEU:O	1:B:61:THR:OG1	2.26	0.53
1:C:150:SER:O	1:C:154:THR:HB	2.09	0.53
1:C:182:LEU:O	1:C:427:VAL:HG11	2.08	0.53
1:C:235:ILE:HD12	1:C:445:LEU:HD12	1.90	0.53
1:C:371:PHE:O	1:C:371:PHE:CG	2.61	0.53
1:D:61:THR:O	1:D:62:GLU:HG3	2.08	0.53
1:A:178:TYR:CB	1:A:432:HIS:H	2.22	0.53
1:A:377:SER:HB3	1:A:380:ALA:CB	2.25	0.53
1:A:325:LEU:CD2	1:A:379:THR:HG22	2.38	0.53
1:B:78:VAL:HG12	1:B:79:PHE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:CG2	1:C:198:VAL:O	2.57	0.53
1:D:418:PRO:HD3	1:D:438:MSE:SE	2.59	0.53
1:B:106:LEU:O	1:B:109:ALA:HB3	2.08	0.53
1:B:372:LEU:HD13	1:B:414:ALA:CB	2.27	0.53
1:C:127:ALA:HB1	1:C:133:VAL:CG2	2.38	0.53
1:C:123:VAL:CG1	1:C:141:VAL:HG21	2.39	0.53
1:C:227:MSE:O	1:C:230:PRO:HD2	2.08	0.53
1:C:232:ALA:HA	1:C:445:LEU:HD11	1.91	0.53
1:B:188:SER:HB2	1:B:229:LEU:HD11	1.91	0.53
1:B:200:SER:HB2	1:B:201:PRO:CD	2.32	0.53
1:B:204:ALA:CB	1:B:326:PHE:CZ	2.92	0.53
1:B:389:PHE:HD1	1:B:403:LEU:HD13	1.74	0.53
1:C:116:ASP:OD1	1:C:117:LYS:N	2.42	0.53
1:A:359:PHE:HD1	1:A:458:MSE:SE	2.42	0.53
1:C:86:GLN:O	1:C:86:GLN:HG3	2.09	0.53
1:D:272:VAL:O	1:D:276:ILE:HG13	2.09	0.53
1:A:212:LEU:HD22	1:A:216:ASP:HB3	1.89	0.52
1:A:42:GLU:OE1	1:A:44:ASN:HB2	2.09	0.52
1:D:97:ILE:HD12	1:D:97:ILE:N	2.24	0.52
1:A:456:ILE:HA	1:A:459:LEU:HD22	1.92	0.52
1:B:390:ALA:O	1:B:394:GLU:HG3	2.09	0.52
1:D:195:ALA:N	1:D:217:TRP:HZ3	2.08	0.52
1:A:376:ALA:HB3	1:A:420:ALA:HB3	1.91	0.52
1:B:378:ASN:HD21	1:B:421:THR:CG2	2.22	0.52
1:B:77:ALA:O	1:B:78:VAL:HB	2.09	0.52
1:C:31:LEU:O	1:C:31:LEU:HD12	2.09	0.52
1:C:54:PHE:C	1:C:54:PHE:CD2	2.81	0.52
1:D:382:ALA:O	1:D:386:ILE:HG12	2.10	0.52
1:D:394:GLU:HG3	1:D:400:PRO:HG3	1.91	0.52
1:D:220:PHE:CD1	1:D:460:PHE:CE2	2.93	0.52
1:A:108:ALA:CB	1:A:317:THR:HG21	2.28	0.52
1:B:279:SER:HB3	1:B:280:PRO:CD	2.40	0.52
1:C:265:LEU:O	1:C:268:PHE:HB3	2.10	0.52
1:C:210:VAL:HG21	1:C:401:VAL:HG22	1.91	0.52
1:D:379:THR:HG22	1:D:380:ALA:N	2.23	0.52
1:C:386:ILE:HD11	1:C:408:ALA:HB2	1.91	0.52
1:C:428:PHE:HZ	1:C:435:GLN:HB3	1.72	0.52
1:D:373:THR:O	1:D:376:ALA:HB2	2.10	0.52
1:D:52:LEU:HD12	1:D:52:LEU:O	2.10	0.52
1:B:187:TYR:CZ	1:B:415:PHE:HB3	2.45	0.52
1:B:197:LEU:HD12	1:B:214:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:O	1:B:75:VAL:HG23	2.09	0.52
1:C:377:SER:HB3	1:C:380:ALA:HB3	1.90	0.52
1:D:142:THR:HG23	1:D:158:MSE:HG3	1.92	0.52
1:D:422:PRO:N	1:D:423:PRO:HD2	2.25	0.52
1:D:74:PRO:HG2	1:D:92:PHE:HE1	1.74	0.52
1:A:274:LEU:O	1:A:278:SER:N	2.43	0.52
1:B:72:LEU:O	1:B:76:MSE:HG3	2.10	0.52
1:B:94:ASN:O	1:B:97:ILE:HB	2.10	0.52
1:C:35:LEU:HD22	1:C:39:LEU:HD22	1.91	0.52
1:A:315:GLN:HA	1:A:320:TRP:CZ3	2.45	0.52
1:D:151:ASN:OD1	1:D:151:ASN:N	2.42	0.52
1:D:405:VAL:O	1:D:409:VAL:HG23	2.10	0.52
1:B:151:ASN:HB2	4:B:501:CIT:C5	2.40	0.52
1:B:24:ILE:HG21	1:B:63:ALA:HB2	1.92	0.52
1:C:123:VAL:HG11	1:C:141:VAL:HG21	1.92	0.52
1:D:57:VAL:O	1:D:61:THR:HG23	2.10	0.52
1:A:196:THR:N	1:A:217:TRP:CZ3	2.72	0.51
1:A:96:ILE:HG13	1:A:208:ALA:HA	1.92	0.51
1:C:100:PHE:CD1	1:C:198:VAL:HG12	2.44	0.51
1:C:18:LEU:CB	1:C:19:HIS:HA	2.40	0.51
1:D:107:ALA:HA	1:D:110:MSE:HG2	1.92	0.51
1:C:23:LEU:O	1:C:26:LEU:N	2.43	0.51
1:D:201:PRO:HD2	1:D:202:PRO:CD	2.38	0.51
1:B:235:ILE:HD12	1:B:445:LEU:HD12	1.91	0.51
1:A:298:GLY:HA2	1:A:301:LEU:HD12	1.92	0.51
1:B:139:PHE:HA	1:B:142:THR:HG22	1.92	0.51
1:B:359:PHE:O	1:B:363:LEU:HB2	2.11	0.51
1:B:389:PHE:HD1	1:B:403:LEU:CD1	2.23	0.51
1:D:311:TRP:NE1	1:D:315:GLN:OE1	2.44	0.51
1:A:197:LEU:HD12	1:A:214:PHE:HA	1.92	0.51
1:A:277:PHE:O	1:A:280:PRO:HD2	2.11	0.51
1:D:288:PHE:O	1:D:289:LYS:HB2	2.10	0.51
1:D:298:GLY:HA2	1:D:301:LEU:HD12	1.92	0.51
1:C:202:PRO:HA	1:C:205:ILE:HG13	1.92	0.51
1:A:138:LEU:HD22	1:A:165:VAL:HG11	1.93	0.51
1:B:180:PHE:CD2	1:B:181:VAL:N	2.78	0.51
1:C:178:TYR:HA	1:C:182:LEU:CB	2.41	0.51
1:C:390:ALA:HB1	1:C:400:PRO:HB3	1.92	0.51
1:C:388:VAL:HG12	1:C:389:PHE:CD2	2.46	0.51
1:D:56:ALA:HB1	1:D:384:LEU:HD21	1.92	0.51
1:B:123:VAL:HG11	1:B:141:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:THR:CG2	1:B:422:PRO:HB2	2.40	0.51
1:B:147:MSE:O	1:B:198:VAL:O	2.28	0.51
1:C:282:ASN:OD1	1:C:288:PHE:N	2.44	0.51
1:D:205:ILE:O	1:D:208:ALA:HB3	2.11	0.51
1:B:418:PRO:CG	1:B:438:MSE:SE	3.09	0.51
1:C:369:VAL:HG11	1:C:450:ILE:HB	1.93	0.51
1:D:147:MSE:O	1:D:196:THR:OG1	2.22	0.51
1:D:372:LEU:HD13	1:D:376:ALA:HB1	1.90	0.51
1:D:236:LEU:HD12	1:D:441:VAL:CG2	2.39	0.50
1:D:372:LEU:O	1:D:373:THR:C	2.49	0.50
1:C:394:GLU:CG	1:C:400:PRO:HG3	2.41	0.50
1:C:422:PRO:O	1:C:423:PRO:C	2.47	0.50
1:C:428:PHE:HZ	1:C:435:GLN:CB	2.24	0.50
1:C:362:ILE:HD12	1:C:362:ILE:O	2.12	0.50
1:C:58:LEU:HD23	1:C:64:LEU:HD12	1.93	0.50
1:B:106:LEU:HD21	1:B:271:THR:HG21	1.93	0.50
1:C:235:ILE:HD12	1:C:445:LEU:CD1	2.40	0.50
1:C:373:THR:CG2	1:C:417:LEU:HG	2.41	0.50
1:D:60:LEU:C	1:D:61:THR:O	2.48	0.50
1:A:372:LEU:N	1:A:374:GLU:H	2.10	0.50
1:B:31:LEU:HG	1:B:35:LEU:CD1	2.42	0.50
1:D:337:LYS:HD3	5:D:601:HOH:O	2.09	0.50
1:D:372:LEU:CA	1:D:376:ALA:HA	2.42	0.50
1:A:152:THR:HG22	4:A:501:CIT:H41	1.93	0.50
1:D:127:ALA:O	1:D:128:GLN:HG2	2.12	0.50
1:D:309:VAL:HG22	1:D:313:GLU:HG3	1.94	0.50
1:D:47:LEU:HD21	1:D:80:PHE:CB	2.40	0.50
1:B:332:LEU:HA	1:B:335:VAL:CG1	2.41	0.50
1:A:371:PHE:O	1:A:371:PHE:CD2	2.64	0.50
1:B:369:VAL:HG11	1:B:450:ILE:HG12	1.94	0.50
1:D:195:ALA:N	1:D:217:TRP:CZ3	2.79	0.50
1:D:386:ILE:HB	1:D:387:PRO:HD3	1.94	0.50
1:A:325:LEU:HD23	1:A:379:THR:HG22	1.93	0.50
1:B:110:MSE:HG2	1:B:115:LEU:HD23	1.94	0.50
1:C:195:ALA:N	1:C:217:TRP:CZ3	2.80	0.50
1:D:220:PHE:HD1	1:D:460:PHE:CZ	2.29	0.50
1:A:405:VAL:O	1:A:409:VAL:HG23	2.12	0.49
1:B:227:MSE:SE	1:B:456:ILE:HD11	2.61	0.49
1:D:201:PRO:HG2	1:D:379:THR:OG1	2.12	0.49
1:A:162:VAL:HA	1:A:165:VAL:HG12	1.93	0.49
1:A:195:ALA:N	1:A:217:TRP:CH2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:H	1:A:374:GLU:H	1.60	0.49
1:B:185:VAL:CG1	1:B:186:ALA:N	2.75	0.49
1:B:324:LEU:N	1:B:324:LEU:HD12	2.26	0.49
1:B:372:LEU:HG	1:B:411:ALA:CA	2.40	0.49
1:A:191:ILE:HG12	1:A:228:MSE:HE2	1.94	0.49
1:A:358:ILE:N	1:A:358:ILE:HD12	2.26	0.49
1:B:356:MSE:HE3	1:B:360:VAL:HG12	1.93	0.49
1:D:106:LEU:HD12	1:D:303:LEU:HD11	1.93	0.49
1:A:413:CYS:HB3	1:A:415:PHE:HE2	1.75	0.49
1:A:421:THR:HG23	1:A:423:PRO:HD2	1.94	0.49
1:B:372:LEU:CD2	1:B:378:ASN:HA	2.43	0.49
1:C:152:THR:HG23	4:C:501:CIT:C5	2.42	0.49
1:C:127:ALA:CA	1:C:137:MSE:HE2	2.43	0.49
1:D:86:GLN:NE2	1:C:94:ASN:HA	2.25	0.49
1:A:357:GLY:CA	1:A:361:VAL:HG23	2.37	0.49
1:B:25:VAL:O	1:B:28:ASP:N	2.46	0.49
1:C:31:LEU:HD11	1:C:35:LEU:HD11	1.94	0.49
1:D:135:VAL:HG23	1:D:136:PHE:N	2.28	0.49
1:A:231:MSE:HE3	1:A:448:ALA:CB	2.43	0.49
1:B:19:HIS:HA	1:B:22:SER:HB2	1.93	0.49
1:D:104:PHE:CE1	1:D:319:ASP:N	2.67	0.49
1:D:214:PHE:CD2	1:D:214:PHE:C	2.86	0.49
1:D:182:LEU:O	1:D:427:VAL:HG11	2.13	0.49
1:D:416:MSE:HE3	1:D:439:MSE:HG3	1.95	0.49
1:C:196:THR:CG2	1:C:198:VAL:O	2.60	0.49
1:A:191:ILE:O	1:A:194:ILE:HG12	2.13	0.49
1:A:263:VAL:HG13	1:A:308:VAL:HG21	1.94	0.49
1:D:362:ILE:HD12	1:D:457:ALA:HB3	1.95	0.49
1:A:146:SER:C	1:A:148:TRP:H	2.15	0.49
1:A:260:GLY:O	1:A:263:VAL:HG12	2.13	0.49
1:B:57:VAL:O	1:B:60:LEU:O	2.31	0.49
1:C:325:LEU:CD2	1:C:379:THR:CG2	2.91	0.49
1:B:180:PHE:HD2	1:B:181:VAL:N	2.10	0.48
1:C:264:THR:OG1	1:C:308:VAL:HG21	2.13	0.48
1:D:175:ARG:HB2	1:D:179:VAL:CB	2.43	0.48
1:A:455:ALA:O	1:A:459:LEU:HD13	2.13	0.48
1:B:288:PHE:O	1:B:289:LYS:HB3	2.13	0.48
1:C:156:ALA:O	1:C:160:PRO:HD3	2.13	0.48
1:C:161:LEU:O	1:C:165:VAL:HG22	2.13	0.48
1:C:67:THR:O	1:C:71:ILE:HG13	2.12	0.48
1:A:146:SER:O	1:A:148:TRP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HD13	1:A:441:VAL:HA	1.94	0.48
1:B:151:ASN:HB2	4:B:501:CIT:O3	2.13	0.48
1:B:43:HIS:CE1	3:B:503:BNG:H62	2.48	0.48
1:C:374:GLU:O	1:C:375:PHE:C	2.50	0.48
1:D:323:LEU:O	1:D:326:PHE:HB2	2.12	0.48
1:D:80:PHE:CE2	3:D:502:BNG:H3'1	2.49	0.48
1:D:65:HIS:CG	1:D:66:VAL:N	2.81	0.48
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.94	0.48
1:A:263:VAL:HG13	1:A:264:THR:N	2.29	0.48
1:A:282:ASN:HB2	1:A:291:PHE:CG	2.49	0.48
1:A:377:SER:O	1:A:380:ALA:N	2.46	0.48
1:A:65:HIS:HB3	1:A:68:VAL:HG23	1.94	0.48
1:B:150:SER:O	1:B:154:THR:HB	2.13	0.48
1:A:369:VAL:HG12	1:A:370:VAL:N	2.26	0.48
1:B:115:LEU:O	1:B:118:VAL:HG13	2.14	0.48
1:B:197:LEU:O	1:B:197:LEU:HD23	2.13	0.48
1:B:389:PHE:CD1	1:B:403:LEU:HD13	2.48	0.48
1:D:141:VAL:CG1	1:D:158:MSE:HE1	2.44	0.48
1:A:203:ASN:CB	1:A:217:TRP:CZ2	2.97	0.48
1:B:195:ALA:N	1:B:217:TRP:CZ3	2.81	0.48
1:B:362:ILE:O	1:B:366:ALA:HB2	2.14	0.48
1:B:420:ALA:CB	1:B:421:THR:HA	2.20	0.48
1:D:110:MSE:HE1	1:D:148:TRP:HB3	1.95	0.48
1:A:96:ILE:O	1:A:97:ILE:C	2.52	0.48
1:C:359:PHE:C	1:C:359:PHE:CD2	2.87	0.48
1:D:369:VAL:HG23	1:D:410:ALA:HB1	1.94	0.48
1:D:61:THR:O	1:D:62:GLU:CG	2.62	0.48
1:A:181:VAL:HG12	1:A:182:LEU:HD23	1.96	0.48
1:B:107:ALA:HB1	1:B:149:ILE:HG22	1.96	0.48
1:B:362:ILE:HD11	1:B:454:THR:HG23	1.96	0.48
1:C:367:THR:O	1:C:367:THR:HG22	2.13	0.48
1:C:51:MSE:HB3	1:C:51:MSE:HE2	1.71	0.48
1:D:113:GLN:O	1:D:261:LYS:HE2	2.14	0.48
1:D:186:ALA:HB2	1:D:427:VAL:HG11	1.95	0.48
1:A:403:LEU:CD2	1:A:403:LEU:N	2.77	0.48
1:D:228:MSE:CE	1:D:415:PHE:HZ	2.27	0.48
1:A:204:ALA:HB3	1:A:326:PHE:CE1	2.48	0.48
1:B:288:PHE:CZ	1:A:79:PHE:HA	2.49	0.48
1:B:313:GLU:HA	1:B:313:GLU:OE2	2.14	0.48
1:B:374:GLU:CG	1:B:374:GLU:O	2.61	0.48
1:C:139:PHE:CE1	1:C:184:GLY:HA3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:CD1	1:A:181:VAL:HG21	2.44	0.47
1:A:113:GLN:HG3	1:A:264:THR:OG1	2.14	0.47
1:B:99:LEU:CD1	1:B:197:LEU:HD22	2.37	0.47
1:C:171:ALA:C	1:C:173:LYS:N	2.67	0.47
1:C:229:LEU:HB3	1:C:230:PRO:CD	2.35	0.47
1:C:356:MSE:HE3	1:C:360:VAL:CG1	2.39	0.47
1:D:185:VAL:CG1	1:D:186:ALA:N	2.77	0.47
1:D:259:LYS:HG2	1:D:261:LYS:CE	2.30	0.47
1:D:73:VAL:HB	1:D:74:PRO:CD	2.44	0.47
1:A:108:ALA:HB2	1:A:317:THR:CB	2.43	0.47
1:A:195:ALA:C	1:A:217:TRP:HZ3	2.17	0.47
1:A:66:VAL:CG1	1:A:325:LEU:HD13	2.43	0.47
1:C:393:ALA:HB1	1:C:398:MSE:HG2	1.96	0.47
1:C:77:ALA:O	1:C:78:VAL:HB	2.14	0.47
1:D:134:ALA:HA	1:D:137:MSE:HB2	1.96	0.47
1:D:214:PHE:HD2	1:D:214:PHE:C	2.17	0.47
1:A:372:LEU:CD2	1:A:376:ALA:HB1	2.43	0.47
1:B:140:GLY:O	1:B:144:LEU:HB2	2.14	0.47
1:B:212:LEU:HD13	1:B:217:TRP:HD1	1.78	0.47
1:C:325:LEU:HD23	1:C:379:THR:CG2	2.44	0.47
1:A:262:VAL:HG13	1:A:263:VAL:N	2.28	0.47
1:A:297:LEU:HA	1:A:300:ILE:CG2	2.43	0.47
1:A:414:ALA:CB	1:A:421:THR:H	2.27	0.47
1:B:106:LEU:HD11	1:B:268:PHE:HA	1.97	0.47
1:B:148:TRP:CD1	1:B:268:PHE:HZ	2.33	0.47
1:B:80:PHE:CZ	3:B:503:BNG:H5'2	2.49	0.47
1:C:194:ILE:CA	1:C:217:TRP:HH2	2.28	0.47
1:C:23:LEU:O	1:C:26:LEU:HB2	2.14	0.47
1:D:159:LEU:CB	1:D:160:PRO:HD3	2.38	0.47
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.96	0.47
1:D:353:VAL:HA	1:D:356:MSE:HB3	1.96	0.47
1:D:41:PHE:CD2	1:D:41:PHE:N	2.82	0.47
1:A:379:THR:OG1	4:A:501:CIT:H22	2.14	0.47
1:A:416:MSE:HG2	1:A:439:MSE:HA	1.95	0.47
1:A:79:PHE:O	1:A:80:PHE:HB2	2.14	0.47
1:B:274:LEU:O	1:B:278:SER:N	2.47	0.47
1:B:56:ALA:CB	1:B:384:LEU:HD21	2.44	0.47
1:C:113:GLN:HG3	1:C:308:VAL:HG22	1.95	0.47
1:C:191:ILE:HG12	1:C:228:MSE:CE	2.30	0.47
1:D:124:LEU:CD2	1:D:161:LEU:HD11	2.45	0.47
1:D:369:VAL:CG2	1:D:413:CYS:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:PHE:C	1:B:180:PHE:CD2	2.87	0.47
1:B:35:LEU:O	1:B:39:LEU:HB2	2.15	0.47
1:B:66:VAL:HG13	1:B:325:LEU:HD13	1.96	0.47
1:C:359:PHE:O	1:C:359:PHE:CD2	2.67	0.47
1:D:201:PRO:O	1:D:202:PRO:C	2.52	0.47
1:A:257:TRP:O	1:A:258:ASP:HB3	2.15	0.47
1:B:289:LYS:HE3	1:B:289:LYS:HB2	1.66	0.47
1:B:320:TRP:CD1	1:A:320:TRP:CD2	3.03	0.47
1:C:194:ILE:HA	1:C:217:TRP:HH2	1.78	0.47
1:D:31:LEU:O	1:D:31:LEU:HD12	2.14	0.47
1:D:32:PHE:CE1	1:D:50:SER:HB3	2.49	0.47
1:B:149:ILE:C	1:B:149:ILE:HD12	2.35	0.47
1:B:275:TRP:HZ2	1:B:296:ALA:HB2	1.80	0.47
1:C:356:MSE:HE2	1:C:361:VAL:HG22	1.95	0.47
1:D:430:SER:OG	1:D:431:GLY:N	2.48	0.47
1:D:48:GLY:HA3	1:D:341:THR:OG1	2.14	0.47
1:B:139:PHE:HE2	1:B:185:VAL:N	2.13	0.47
1:C:410:ALA:O	1:C:413:CYS:HB2	2.15	0.47
1:D:207:ALA:CA	1:D:212:LEU:HB2	2.45	0.47
1:A:210:VAL:HG23	1:A:212:LEU:HG	1.95	0.47
1:A:195:ALA:HB1	1:A:222:LEU:HD23	1.96	0.47
1:B:54:PHE:C	1:B:54:PHE:CD2	2.87	0.47
1:C:194:ILE:O	1:C:195:ALA:CB	2.56	0.47
1:C:195:ALA:N	1:C:217:TRP:HZ3	2.12	0.47
1:B:191:ILE:HD11	1:B:232:ALA:HB2	1.97	0.47
1:B:419:VAL:HG11	1:B:425:ALA:HB2	1.97	0.47
1:D:110:MSE:HB2	1:D:115:LEU:HB3	1.97	0.47
1:D:419:VAL:CB	1:D:420:ALA:HA	2.45	0.47
1:D:362:ILE:HD11	1:D:454:THR:HA	1.97	0.47
1:A:140:GLY:O	1:A:144:LEU:HB2	2.16	0.46
1:B:421:THR:OG1	1:B:423:PRO:HD2	2.15	0.46
1:C:281:ILE:O	1:C:285:LEU:HG	2.14	0.46
1:D:191:ILE:HD13	1:D:228:MSE:HG2	1.97	0.46
1:A:315:GLN:HA	1:A:320:TRP:HH2	1.74	0.46
1:A:371:PHE:O	1:A:371:PHE:CG	2.67	0.46
1:D:124:LEU:HD22	1:D:161:LEU:HD11	1.96	0.46
1:A:200:SER:CB	1:A:201:PRO:HD2	2.45	0.46
1:B:372:LEU:CD2	1:B:376:ALA:HB1	2.40	0.46
1:D:28:ASP:OD2	1:D:54:PHE:HA	2.15	0.46
1:D:51:MSE:O	1:D:55:ILE:HB	2.16	0.46
1:A:325:LEU:O	1:A:326:PHE:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ALA:O	1:A:377:SER:C	2.51	0.46
1:C:213:SER:H	1:C:216:ASP:CB	2.24	0.46
1:D:194:ILE:O	1:D:195:ALA:HB3	2.16	0.46
1:D:282:ASN:HD21	1:D:288:PHE:H	1.63	0.46
1:B:149:ILE:O	1:B:149:ILE:HD12	2.16	0.46
1:B:66:VAL:HG13	1:B:325:LEU:CD1	2.45	0.46
1:C:96:ILE:HG13	1:C:208:ALA:HA	1.96	0.46
1:C:369:VAL:HG13	1:C:446:ASN:OD1	2.16	0.46
1:C:61:THR:OG1	1:C:62:GLU:N	2.49	0.46
1:D:323:LEU:HA	1:D:326:PHE:CD2	2.45	0.46
1:A:422:PRO:HG2	1:A:423:PRO:HD3	1.98	0.46
1:C:135:VAL:O	1:C:138:LEU:HB2	2.16	0.46
1:C:421:THR:OG1	1:C:423:PRO:HD2	2.16	0.46
4:C:501:CIT:H21	4:C:501:CIT:O3	2.16	0.46
1:B:194:ILE:O	1:B:195:ALA:CB	2.63	0.46
1:B:362:ILE:O	1:B:366:ALA:CB	2.63	0.46
1:C:131:MSE:O	1:C:132:SER:C	2.54	0.46
1:D:171:ALA:HB1	1:D:173:LYS:H	1.81	0.46
1:D:58:LEU:CD1	1:D:64:LEU:HD23	2.33	0.46
1:A:70:ALA:O	1:A:74:PRO:HD3	2.16	0.46
1:C:130:LYS:HB3	1:C:131:MSE:H	1.59	0.46
1:C:161:LEU:HA	1:C:161:LEU:HD12	1.82	0.46
1:C:452:LEU:O	1:C:456:ILE:HG13	2.15	0.46
1:D:210:VAL:HG23	1:D:210:VAL:O	2.15	0.46
1:D:102:GLY:HA3	1:D:296:ALA:HB1	1.98	0.46
1:B:180:PHE:HB2	1:B:240:LEU:CD1	2.46	0.46
1:C:150:SER:HB3	1:C:153:ALA:HB3	1.97	0.46
1:D:386:ILE:O	1:D:387:PRO:C	2.55	0.46
1:D:64:LEU:HD13	1:D:64:LEU:HA	1.44	0.46
1:A:94:ASN:HB3	1:A:97:ILE:CD1	2.45	0.46
1:B:152:THR:HG22	1:B:423:PRO:CD	2.40	0.46
1:C:223:PRO:HA	1:C:226:MSE:CG	2.46	0.46
1:D:141:VAL:HG12	1:D:158:MSE:CE	2.45	0.46
1:A:107:ALA:HA	1:A:110:MSE:CE	2.42	0.45
1:C:420:ALA:HB1	1:C:421:THR:CA	2.26	0.45
1:C:232:ALA:HA	1:C:445:LEU:HD13	1.96	0.45
1:D:183:LEU:HD11	1:D:438:MSE:HG3	1.97	0.45
1:A:161:LEU:O	1:A:165:VAL:HG12	2.15	0.45
1:B:214:PHE:CE2	1:B:218:MSE:SE	3.17	0.45
1:B:210:VAL:CG1	1:B:400:PRO:HB2	2.43	0.45
1:B:187:TYR:CD1	1:B:415:PHE:HD1	2.34	0.45

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:MSE:CE	1:A:448:ALA:HB1	2.46	0.45
1:B:146:SER:HA	1:B:149:ILE:HD12	1.98	0.45
1:C:356:MSE:HE2	1:C:361:VAL:HA	1.99	0.45
1:C:40:PRO:O	1:C:41:PHE:C	2.53	0.45
1:A:310:HIS:HB2	1:A:313:GLU:HG2	1.99	0.45
1:B:213:SER:N	1:B:216:ASP:HB2	2.32	0.45
1:A:239:LEU:HD13	1:A:441:VAL:HG22	1.99	0.45
1:A:414:ALA:HB1	1:A:421:THR:H	1.82	0.45
1:A:182:LEU:O	1:A:427:VAL:HG11	2.16	0.45
1:B:372:LEU:CD1	1:B:411:ALA:O	2.63	0.45
1:D:393:ALA:O	1:D:398:MSE:HB3	2.17	0.45
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.71	0.45
1:C:294:LEU:O	1:C:298:GLY:N	2.43	0.45
1:D:39:LEU:HD22	1:D:41:PHE:HE2	1.81	0.45
1:A:137:MSE:O	1:A:141:VAL:HG23	2.16	0.45
1:C:261:LYS:O	1:C:264:THR:N	2.50	0.45
1:D:288:PHE:CZ	1:C:79:PHE:HD1	2.35	0.45
1:D:274:LEU:O	1:D:278:SER:N	2.50	0.45
1:A:131:MSE:O	1:A:134:ALA:N	2.50	0.45
1:B:207:ALA:HA	1:B:212:LEU:HB2	1.98	0.45
1:D:141:VAL:HG12	1:D:158:MSE:HE2	1.99	0.45
1:D:100:PHE:CE1	1:D:198:VAL:HA	2.51	0.45
1:D:188:SER:OG	1:D:229:LEU:HD11	2.16	0.45
1:D:376:ALA:CB	1:D:420:ALA:H	2.21	0.45
1:A:267:ILE:HG21	1:A:303:LEU:HD23	1.98	0.45
1:A:78:VAL:HG12	1:A:79:PHE:H	1.82	0.45
1:B:372:LEU:HD21	1:B:378:ASN:CG	2.37	0.45
1:D:386:ILE:HG23	1:D:404:SER:HB3	1.99	0.45
1:C:418:PRO:CA	1:C:419:VAL:HG23	2.40	0.45
1:A:377:SER:O	1:A:378:ASN:C	2.55	0.44
1:B:187:TYR:HD2	1:B:236:LEU:HD11	1.82	0.44
1:C:208:ALA:HB1	1:C:330:LEU:HD21	1.98	0.44
1:C:52:LEU:HD22	1:C:336:LEU:HD21	1.99	0.44
1:A:171:ALA:HB1	1:A:173:LYS:O	2.17	0.44
1:A:66:VAL:HG13	1:A:325:LEU:CD1	2.43	0.44
1:B:320:TRP:O	1:B:324:LEU:CD1	2.65	0.44
1:C:157:MSE:O	1:C:160:PRO:HD2	2.17	0.44
1:C:83:PHE:HZ	1:C:334:ASN:HB3	1.82	0.44
1:A:197:LEU:CD1	1:A:214:PHE:HA	2.47	0.44
1:A:372:LEU:HA	1:A:376:ALA:CA	2.29	0.44
1:B:180:PHE:HE1	1:B:237:TYR:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LEU:O	1:C:376:ALA:CB	2.48	0.44
1:D:235:ILE:O	1:D:239:LEU:HB2	2.17	0.44
1:D:66:VAL:CG1	1:D:325:LEU:HD23	2.47	0.44
1:D:97:ILE:H	1:D:97:ILE:CD1	2.30	0.44
1:A:101:LEU:O	1:A:104:PHE:HB2	2.18	0.44
1:A:445:LEU:O	1:A:448:ALA:HB3	2.17	0.44
1:B:277:PHE:O	1:B:281:ILE:HG13	2.17	0.44
1:B:186:ALA:HB2	1:B:427:VAL:CG1	2.47	0.44
1:B:86:GLN:OE1	1:A:94:ASN:HA	2.18	0.44
1:C:261:LYS:HD2	1:C:261:LYS:N	2.32	0.44
1:C:79:PHE:O	1:C:80:PHE:CB	2.65	0.44
1:D:222:LEU:HB3	1:D:223:PRO:CD	2.47	0.44
1:D:279:SER:HB3	1:D:280:PRO:CD	2.47	0.44
1:D:372:LEU:HD21	1:D:411:ALA:O	2.16	0.44
1:A:159:LEU:CB	1:A:160:PRO:HD3	2.45	0.44
1:C:147:MSE:HA	1:C:192:GLY:O	2.17	0.44
1:C:318:ALA:HB3	1:C:320:TRP:NE1	2.33	0.44
1:C:388:VAL:HG12	1:C:389:PHE:HD2	1.82	0.44
1:B:201:PRO:O	1:B:204:ALA:HB3	2.18	0.44
1:B:214:PHE:CD2	1:B:214:PHE:C	2.91	0.44
1:B:418:PRO:CA	1:B:419:VAL:HG13	2.47	0.44
1:B:367:THR:CA	1:B:450:ILE:HD13	2.40	0.44
1:B:82:ILE:CD1	1:B:335:VAL:HG23	2.46	0.44
1:C:221:GLY:O	1:C:222:LEU:C	2.55	0.44
1:C:293:THR:O	1:C:297:LEU:N	2.43	0.44
1:C:52:LEU:HD12	1:C:52:LEU:HA	1.72	0.44
1:D:110:MSE:HE3	1:D:149:ILE:HG13	1.99	0.44
1:D:26:LEU:HD23	1:D:26:LEU:HA	1.78	0.44
1:A:24:ILE:CG1	1:A:63:ALA:HB2	2.46	0.44
1:B:51:MSE:HG2	1:B:76:MSE:CE	2.48	0.44
1:C:201:PRO:O	1:C:205:ILE:HG12	2.16	0.44
1:A:401:VAL:O	1:A:405:VAL:HG23	2.18	0.44
1:A:453:LEU:HA	1:A:456:ILE:HD11	2.00	0.44
1:B:180:PHE:HB2	1:B:240:LEU:HD11	1.99	0.44
1:B:152:THR:HG22	1:B:422:PRO:HB2	2.00	0.44
1:C:369:VAL:HG23	1:C:413:CYS:HB2	2.00	0.44
1:C:419:VAL:CG1	1:C:420:ALA:HA	2.43	0.44
1:D:426:ILE:O	1:D:428:PHE:N	2.51	0.44
1:A:306:ALA:C	1:A:308:VAL:H	2.20	0.44
1:B:320:TRP:CD1	1:A:320:TRP:CG	3.06	0.44
1:B:371:PHE:C	1:B:371:PHE:CD2	2.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:HB1	1:B:384:LEU:HD21	1.99	0.44
1:C:346:ALA:HB1	1:C:396:PHE:CE1	2.53	0.44
1:D:161:LEU:O	1:D:161:LEU:HD12	2.18	0.44
1:D:303:LEU:HA	1:D:303:LEU:HD23	1.87	0.44
1:D:67:THR:HG21	1:C:311:TRP:CE2	2.53	0.44
1:A:109:ALA:HB2	1:A:303:LEU:HD13	2.01	0.43
1:B:80:PHE:CD2	3:B:503:BNG:H3'1	2.51	0.43
1:C:112:HIS:ND1	1:C:112:HIS:C	2.71	0.43
1:C:137:MSE:O	1:C:141:VAL:HG23	2.18	0.43
1:C:358:ILE:HD13	1:C:458:MSE:SE	2.68	0.43
1:D:94:ASN:HA	1:C:86:GLN:HE22	1.83	0.43
1:D:372:LEU:C	1:D:376:ALA:HA	2.39	0.43
1:D:86:GLN:O	1:D:89:LEU:N	2.51	0.43
1:A:433:ILE:HG13	1:A:437:GLU:OE1	2.18	0.43
1:A:458:MSE:HA	1:A:458:MSE:CE	2.46	0.43
1:B:402:LEU:HA	1:B:402:LEU:HD12	1.57	0.43
1:B:232:ALA:HB1	1:B:445:LEU:HD21	2.00	0.43
1:D:195:ALA:HA	1:D:221:GLY:C	2.38	0.43
1:A:297:LEU:HA	1:A:300:ILE:HG23	2.00	0.43
1:B:313:GLU:CA	1:B:313:GLU:OE2	2.66	0.43
1:B:430:SER:O	1:B:431:GLY:C	2.57	0.43
1:B:418:PRO:CD	1:B:438:MSE:SE	3.17	0.43
1:B:149:ILE:C	1:B:149:ILE:CD1	2.87	0.43
1:B:345:LEU:HA	1:B:345:LEU:HD12	1.77	0.43
1:C:356:MSE:HE2	1:C:361:VAL:CG2	2.48	0.43
1:D:418:PRO:HB3	1:D:424:ASN:CB	2.49	0.43
1:A:78:VAL:C	1:A:79:PHE:O	2.50	0.43
1:B:198:VAL:HA	1:B:199:GLY:HA2	1.84	0.43
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.84	0.43
1:A:146:SER:C	1:A:148:TRP:N	2.72	0.43
1:A:372:LEU:CD2	1:A:378:ASN:OD1	2.67	0.43
1:A:346:ALA:CA	1:A:396:PHE:CE2	3.00	0.43
1:B:110:MSE:HB2	1:B:110:MSE:HE3	1.95	0.43
1:B:418:PRO:HA	1:B:419:VAL:HG13	2.00	0.43
1:B:416:MSE:HG2	1:B:439:MSE:HA	1.99	0.43
1:B:69:THR:O	1:B:72:LEU:HB3	2.19	0.43
1:D:207:ALA:HB1	1:D:212:LEU:HB2	1.99	0.43
1:D:289:LYS:O	1:D:290:SER:HB2	2.18	0.43
1:D:55:ILE:HG22	1:D:56:ALA:N	2.34	0.43
1:A:162:VAL:HA	1:A:165:VAL:CG1	2.49	0.43
1:C:191:ILE:C	1:C:193:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LEU:HD23	1:C:326:PHE:CE2	2.54	0.43
1:C:76:MSE:C	1:C:77:ALA:O	2.55	0.43
1:D:402:LEU:C	1:D:402:LEU:HD23	2.38	0.43
1:A:378:ASN:ND2	1:A:412:SER:HA	2.33	0.43
1:C:390:ALA:HB2	1:C:404:SER:HG	1.81	0.43
1:A:374:GLU:O	1:A:375:PHE:C	2.55	0.43
1:B:195:ALA:H	1:B:217:TRP:HH2	1.65	0.43
1:C:349:LEU:HD12	1:C:353:VAL:HG13	2.01	0.43
1:C:236:LEU:HD12	1:C:441:VAL:HG11	2.01	0.43
1:D:149:ILE:HG22	1:D:150:SER:HB3	2.00	0.43
1:D:142:THR:HG23	1:D:158:MSE:CG	2.48	0.43
1:A:114:GLY:O	1:A:118:VAL:HG13	2.19	0.43
1:A:123:VAL:HG11	1:A:141:VAL:HG22	2.00	0.43
1:A:435:GLN:HB3	1:A:439:MSE:SE	2.69	0.43
1:A:71:ILE:C	1:A:74:PRO:HD2	2.38	0.43
1:B:374:GLU:HB3	1:B:417:LEU:HD21	2.01	0.43
1:C:376:ALA:O	1:C:377:SER:HB3	2.19	0.43
1:D:146:SER:O	1:D:148:TRP:N	2.52	0.43
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.89	0.42
1:B:334:ASN:O	1:B:335:VAL:C	2.56	0.42
1:B:78:VAL:O	1:B:81:GLY:N	2.40	0.42
1:B:78:VAL:HG12	1:B:79:PHE:H	1.84	0.42
1:C:311:TRP:CZ3	1:C:314:ILE:HG21	2.54	0.42
1:C:387:PRO:O	1:C:391:THR:HG23	2.18	0.42
1:D:51:MSE:HE1	1:D:82:ILE:CD1	2.48	0.42
1:A:115:LEU:HA	1:A:118:VAL:HG22	2.01	0.42
1:A:236:LEU:HA	1:A:236:LEU:HD12	1.83	0.42
1:B:26:LEU:HD23	1:A:305:PHE:HZ	1.84	0.42
1:A:447:ILE:CA	1:A:450:ILE:HG23	2.47	0.42
1:C:44:ASN:O	1:C:339:THR:HB	2.19	0.42
1:A:159:LEU:HB3	1:A:160:PRO:CD	2.45	0.42
1:B:144:LEU:O	1:B:144:LEU:HD13	2.19	0.42
1:B:281:ILE:O	1:B:285:LEU:HG	2.18	0.42
1:C:135:VAL:CG2	1:C:136:PHE:N	2.82	0.42
1:C:263:VAL:HG22	1:C:264:THR:N	2.34	0.42
1:D:194:ILE:CD1	1:D:224:THR:HG22	2.49	0.42
1:B:416:MSE:HB3	1:B:417:LEU:H	1.53	0.42
1:B:96:ILE:HD13	1:B:96:ILE:HA	1.73	0.42
1:C:76:MSE:O	1:C:79:PHE:O	2.38	0.42
1:C:77:ALA:O	1:C:78:VAL:CB	2.66	0.42
1:D:260:GLY:C	1:D:262:VAL:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:PHE:O	1:B:107:ALA:N	2.53	0.42
1:B:123:VAL:HB	1:B:141:VAL:HG21	2.01	0.42
1:B:182:LEU:O	1:B:185:VAL:HG12	2.19	0.42
1:C:356:MSE:HG3	1:C:361:VAL:HG23	2.02	0.42
1:D:218:MSE:CG	1:D:222:LEU:HB2	2.49	0.42
1:D:358:ILE:O	1:D:359:PHE:C	2.57	0.42
1:D:358:ILE:HD13	1:D:461:TRP:CH2	2.54	0.42
1:A:85:THR:O	1:A:86:GLN:C	2.57	0.42
1:A:99:LEU:HD13	1:A:99:LEU:O	2.19	0.42
1:B:229:LEU:HB3	1:B:230:PRO:CD	2.40	0.42
1:B:367:THR:O	1:B:370:VAL:HG22	2.20	0.42
1:C:70:ALA:O	1:C:74:PRO:HD3	2.19	0.42
1:D:432:HIS:O	1:D:434:LYS:N	2.52	0.42
1:D:445:LEU:HD12	1:D:445:LEU:HA	1.82	0.42
1:A:105:ALA:HB1	1:A:314:ILE:HD13	2.02	0.42
1:A:166:LEU:HD22	1:A:166:LEU:H	1.85	0.42
1:A:221:GLY:O	1:A:224:THR:HB	2.19	0.42
1:B:116:ASP:OD1	1:B:116:ASP:N	2.52	0.42
1:B:362:ILE:HD11	1:B:454:THR:HA	2.01	0.42
1:B:74:PRO:HG2	1:B:92:PHE:CE1	2.55	0.42
1:C:377:SER:O	1:C:378:ASN:C	2.57	0.42
1:C:424:ASN:ND2	1:C:438:MSE:HE1	2.35	0.42
1:C:48:GLY:O	1:C:52:LEU:N	2.45	0.42
1:C:66:VAL:HG13	1:C:325:LEU:HD13	2.00	0.42
1:C:89:LEU:C	1:C:91:ASN:N	2.72	0.42
1:D:41:PHE:O	1:D:42:GLU:C	2.58	0.42
1:A:433:ILE:CD1	1:A:436:SER:HB2	2.49	0.42
1:A:152:THR:CG2	4:A:501:CIT:H41	2.49	0.42
1:D:186:ALA:HB2	1:D:427:VAL:CG1	2.49	0.42
1:A:320:TRP:O	1:A:323:LEU:N	2.53	0.42
1:A:49:ILE:HG13	1:A:341:THR:HG23	2.00	0.42
1:B:305:PHE:C	1:B:305:PHE:CD1	2.92	0.42
1:C:196:THR:HG22	1:C:198:VAL:O	2.19	0.42
1:C:223:PRO:HA	1:C:226:MSE:HG2	2.01	0.42
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.52	0.42
1:D:204:ALA:HB3	1:D:326:PHE:CE1	2.54	0.42
1:D:232:ALA:O	1:D:236:LEU:HB2	2.20	0.42
1:D:362:ILE:HD13	1:D:458:MSE:HE3	2.02	0.42
1:D:97:ILE:CD1	1:D:97:ILE:N	2.83	0.42
1:C:392:VAL:C	1:C:394:GLU:N	2.74	0.41
1:C:99:LEU:CD2	1:C:197:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:LEU:HD23	1:D:297:LEU:HA	1.30	0.41
1:A:372:LEU:O	1:A:376:ALA:CB	2.68	0.41
1:B:222:LEU:N	1:B:223:PRO:HD2	2.35	0.41
1:B:363:LEU:HD12	1:B:454:THR:OG1	2.21	0.41
1:C:379:THR:HG1	4:C:501:CIT:H22	1.83	0.41
1:D:110:MSE:HE1	1:D:148:TRP:CB	2.50	0.41
1:D:115:LEU:HA	1:D:118:VAL:HG12	2.02	0.41
1:A:56:ALA:HB2	1:A:384:LEU:HD11	2.01	0.41
1:B:416:MSE:O	1:B:418:PRO:HD3	2.20	0.41
1:B:177:THR:O	1:B:180:PHE:N	2.50	0.41
1:B:151:ASN:HD22	1:B:200:SER:HB3	1.86	0.41
1:B:334:ASN:O	1:B:337:LYS:N	2.53	0.41
1:D:157:MSE:O	1:D:160:PRO:HD2	2.21	0.41
1:D:324:LEU:HD12	1:D:324:LEU:HA	1.67	0.41
1:D:239:LEU:HD13	1:D:441:VAL:CG2	2.50	0.41
1:B:186:ALA:HB2	1:B:427:VAL:HG13	2.03	0.41
1:B:446:ASN:O	1:B:450:ILE:HG13	2.20	0.41
1:C:18:LEU:C	1:C:20:ARG:N	2.72	0.41
1:C:195:ALA:HA	1:C:222:LEU:N	2.35	0.41
1:C:282:ASN:CG	1:C:288:PHE:H	2.23	0.41
1:C:89:LEU:O	1:C:91:ASN:N	2.54	0.41
1:D:289:LYS:HA	1:D:289:LYS:HD3	1.82	0.41
1:D:310:HIS:O	1:D:314:ILE:HG13	2.20	0.41
1:D:66:VAL:HG13	1:D:325:LEU:HD23	2.02	0.41
1:D:386:ILE:O	1:D:390:ALA:CB	2.68	0.41
1:D:415:PHE:O	1:D:416:MSE:HB2	2.20	0.41
1:A:122:LYS:HB2	1:A:122:LYS:HE3	1.87	0.41
1:C:183:LEU:HD11	1:C:438:MSE:CG	2.48	0.41
1:C:285:LEU:N	1:C:285:LEU:HD23	2.35	0.41
1:D:373:THR:CG2	1:D:374:GLU:N	2.75	0.41
1:D:41:PHE:O	1:D:46:VAL:HG23	2.21	0.41
1:D:42:GLU:CG	1:D:43:HIS:N	2.73	0.41
1:B:149:ILE:HD11	1:B:154:THR:OG1	2.21	0.41
1:B:146:SER:HB2	1:B:154:THR:HG21	2.03	0.41
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.75	0.41
1:B:372:LEU:O	1:B:414:ALA:HB2	2.20	0.41
1:C:41:PHE:CE2	1:C:344:PHE:HZ	2.39	0.41
1:D:392:VAL:O	1:D:393:ALA:C	2.58	0.41
1:D:416:MSE:O	1:D:438:MSE:SE	2.89	0.41
1:A:116:ASP:OD1	1:A:117:LYS:N	2.49	0.41
1:A:232:ALA:HA	1:A:445:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:CD1	1:A:441:VAL:HA	2.51	0.41
1:B:278:SER:HB2	1:B:291:PHE:HD2	1.85	0.41
1:B:418:PRO:HA	1:B:419:VAL:HA	1.91	0.41
1:C:416:MSE:HE2	1:C:416:MSE:HB3	1.97	0.41
1:C:447:ILE:CA	1:C:450:ILE:HG22	2.49	0.41
1:D:100:PHE:HE1	1:D:197:LEU:O	2.04	0.41
1:D:267:ILE:HG22	1:D:268:PHE:N	2.36	0.41
1:D:73:VAL:CB	1:D:74:PRO:HD3	2.49	0.41
1:B:194:ILE:CB	1:B:217:TRP:HH2	2.34	0.41
1:B:113:GLN:OE1	1:B:261:LYS:CB	2.69	0.41
1:B:294:LEU:O	1:B:298:GLY:N	2.53	0.41
1:B:152:THR:HG21	1:B:422:PRO:HB2	2.03	0.41
1:C:48:GLY:O	1:C:52:LEU:HB2	2.21	0.41
1:C:53:ALA:O	1:C:54:PHE:C	2.58	0.41
1:B:159:LEU:HB3	1:B:160:PRO:CD	2.44	0.41
1:C:322:VAL:HG12	1:C:323:LEU:N	2.36	0.41
1:C:67:THR:O	1:C:70:ALA:HB3	2.21	0.41
1:C:73:VAL:CB	1:C:74:PRO:HD3	2.48	0.41
1:D:368:PHE:HA	1:D:368:PHE:HD1	1.69	0.41
1:D:399:SER:HA	1:D:400:PRO:HD3	1.89	0.41
1:B:394:GLU:CG	1:B:400:PRO:HG3	2.42	0.41
1:C:134:ALA:O	1:C:138:LEU:HD23	2.22	0.41
1:C:32:PHE:O	1:C:33:LEU:C	2.58	0.41
1:C:402:LEU:HD12	1:C:402:LEU:HA	1.69	0.41
1:D:146:SER:O	1:D:147:MSE:C	2.59	0.41
1:D:195:ALA:O	1:D:218:MSE:HG3	2.21	0.41
1:A:183:LEU:HA	1:A:183:LEU:HD12	1.79	0.40
1:B:79:PHE:HA	1:A:288:PHE:CZ	2.57	0.40
1:A:325:LEU:HD23	1:A:379:THR:CG2	2.50	0.40
1:B:371:PHE:CG	1:B:371:PHE:O	2.72	0.40
1:B:76:MSE:HB3	1:B:76:MSE:HE2	1.90	0.40
1:D:175:ARG:O	1:D:176:SER:CB	2.68	0.40
1:D:40:PRO:HD2	1:D:41:PHE:CE2	2.56	0.40
1:D:47:LEU:HD23	1:D:82:ILE:HD11	2.02	0.40
1:A:192:GLY:O	1:A:194:ILE:O	2.39	0.40
1:A:402:LEU:HA	1:A:402:LEU:HD22	1.83	0.40
1:C:123:VAL:HG11	1:C:141:VAL:HG22	2.01	0.40
1:C:194:ILE:HB	1:C:217:TRP:HH2	1.86	0.40
1:C:367:THR:HA	1:C:450:ILE:HD12	2.03	0.40
1:C:74:PRO:O	1:C:78:VAL:HG23	2.22	0.40
1:B:215:THR:OG1	1:B:276:ILE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:PHE:O	1:B:416:MSE:CB	2.69	0.40
1:C:166:LEU:HG	1:C:177:THR:HA	2.03	0.40
1:C:194:ILE:HA	1:C:217:TRP:CH2	2.55	0.40
1:C:264:THR:OG1	1:C:308:VAL:CG2	2.69	0.40
1:D:113:GLN:OE1	1:D:261:LYS:HA	2.21	0.40
1:D:200:SER:CB	1:D:201:PRO:CD	2.95	0.40
1:D:287:GLY:HA3	1:D:288:PHE:HA	1.43	0.40
1:D:460:PHE:HD1	1:D:460:PHE:HA	1.78	0.40
1:A:362:ILE:CG1	1:A:454:THR:HG23	2.50	0.40
1:B:26:LEU:HA	1:B:29:VAL:HB	2.03	0.40
1:B:66:VAL:HG12	1:B:325:LEU:HD13	2.02	0.40
1:B:367:THR:HA	1:B:450:ILE:CD1	2.43	0.40
1:B:39:LEU:HD13	1:B:40:PRO:CD	2.52	0.40
1:B:239:LEU:CD1	1:B:441:VAL:HA	2.52	0.40
1:C:287:GLY:HA3	1:C:288:PHE:HA	1.60	0.40
1:C:369:VAL:HG13	1:C:370:VAL:N	2.35	0.40
1:C:393:ALA:HB1	1:C:398:MSE:CG	2.52	0.40
1:C:47:LEU:HD13	1:C:47:LEU:HA	1.70	0.40
1:D:329:GLY:O	1:D:332:LEU:HB3	2.21	0.40
1:D:352:MSE:O	1:D:356:MSE:HB2	2.21	0.40
1:D:362:ILE:CD1	1:D:457:ALA:HB3	2.51	0.40
1:C:197:LEU:HD21	1:C:207:ALA:CB	2.52	0.40
1:C:323:LEU:HD23	1:C:323:LEU:HA	1.80	0.40
1:C:416:MSE:N	1:C:438:MSE:HE2	2.37	0.40
1:D:274:LEU:HD23	1:D:281:ILE:HD13	2.03	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	430/449 (96%)	355 (83%)	72 (17%)	3 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	404/449 (90%)	360 (89%)	40 (10%)	4 (1%)	15	54
1	C	426/449 (95%)	369 (87%)	53 (12%)	4 (1%)	17	56
1	D	426/449 (95%)	356 (84%)	68 (16%)	2 (0%)	29	67
All	All	1686/1796 (94%)	1440 (85%)	233 (14%)	13 (1%)	19	58

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	VAL
1	B	78	VAL
1	C	78	VAL
1	B	40	PRO
1	A	376	ALA
1	B	82	ILE
1	C	149	ILE
1	C	433	ILE
1	D	181	VAL
1	C	241	LYS
1	A	194	ILE
1	D	194	ILE
1	B	25	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	307/334 (92%)	253 (82%)	54 (18%)	2	9
1	B	297/334 (89%)	251 (84%)	46 (16%)	2	12
1	C	310/334 (93%)	256 (83%)	54 (17%)	2	10
1	D	303/334 (91%)	259 (86%)	44 (14%)	3	15
All	All	1217/1336 (91%)	1019 (84%)	198 (16%)	2	11

All (198) residues with a non-rotameric sidechain are listed below:

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Mol	Chain	Res	Type
1	D	22	SER
1	D	41	PHE
1	D	45	VAL
1	D	47	LEU
1	D	50	SER
1	D	55	ILE
1	D	59	TRP
1	D	61	THR
1	D	64	LEU
1	D	78	VAL
1	D	84	GLU
1	D	89	LEU
1	D	100	PHE
1	D	137	MSE
1	D	144	LEU
1	D	151	ASN
1	D	183	LEU
1	D	194	ILE
1	D	197	LEU
1	D	203	ASN
1	D	209	GLU
1	D	210	VAL
1	D	214	PHE
1	D	215	THR
1	D	231	MSE
1	D	239	LEU
1	D	262	VAL
1	D	288	PHE
1	D	308	VAL
1	D	313	GLU
1	D	324	LEU
1	D	362	ILE
1	D	368	PHE
1	D	369	VAL
1	D	372	LEU
1	D	379	THR
1	D	381	SER
1	D	386	ILE
1	D	404	SER
1	D	412	SER
1	D	441	VAL
1	D	456	ILE
1	D	458	MSE

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Mol	Chain	Res	Type
1	D	460	PHE
1	B	22	SER
1	B	26	LEU
1	B	39	LEU
1	B	47	LEU
1	B	58	LEU
1	B	59	TRP
1	B	69	THR
1	B	80	PHE
1	B	86	GLN
1	B	89	LEU
1	B	106	LEU
1	B	112	HIS
1	B	115	LEU
1	B	118	VAL
1	B	119	ILE
1	B	154	THR
1	B	161	LEU
1	B	180	PHE
1	B	185	VAL
1	B	187	TYR
1	B	190	SER
1	B	194	ILE
1	B	201	PRO
1	B	213	SER
1	B	224	THR
1	B	263	VAL
1	B	274	LEU
1	B	279	SER
1	B	288	PHE
1	B	300	ILE
1	B	304	SER
1	B	343	VAL
1	B	345	LEU
1	B	351	ASP
1	B	362	ILE
1	B	371	PHE
1	B	372	LEU
1	B	384	LEU
1	B	398	MSE
1	B	399	SER
1	B	403	LEU

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Mol	Chain	Res	Type
1	B	417	LEU
1	B	419	VAL
1	B	445	LEU
1	B	458	MSE
1	B	461	TRP
1	A	22	SER
1	A	24	ILE
1	A	42	GLU
1	A	58	LEU
1	A	69	THR
1	A	89	LEU
1	A	95	SER
1	A	99	LEU
1	A	104	PHE
1	A	122	LYS
1	A	133	VAL
1	A	142	THR
1	A	144	LEU
1	A	145	LEU
1	A	149	ILE
1	A	152	THR
1	A	166	LEU
1	A	183	LEU
1	A	197	LEU
1	A	198	VAL
1	A	200	SER
1	A	203	ASN
1	A	205	ILE
1	A	215	THR
1	A	222	LEU
1	A	239	LEU
1	A	261	LYS
1	A	288	PHE
1	A	300	ILE
1	A	304	SER
1	A	308	VAL
1	A	320	TRP
1	A	322	VAL
1	A	345	LEU
1	A	351	ASP
1	A	353	VAL
1	A	358	ILE

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Mol	Chain	Res	Type
1	A	363	LEU
1	A	364	VAL
1	A	367	THR
1	A	370	VAL
1	A	372	LEU
1	A	377	SER
1	A	402	LEU
1	A	403	LEU
1	A	412	SER
1	A	428	PHE
1	A	434	LYS
1	A	438	MSE
1	A	446	ASN
1	A	450	ILE
1	A	456	ILE
1	A	458	MSE
1	A	459	LEU
1	C	19	HIS
1	C	47	LEU
1	C	49	ILE
1	C	50	SER
1	C	59	TRP
1	C	61	THR
1	C	62	GLU
1	C	69	THR
1	C	75	VAL
1	C	76	MSE
1	C	85	THR
1	C	89	LEU
1	C	100	PHE
1	C	101	LEU
1	C	112	HIS
1	C	118	VAL
1	C	130	LYS
1	C	137	MSE
1	C	157	MSE
1	C	165	VAL
1	C	166	LEU
1	C	177	THR
1	C	190	SER
1	C	191	ILE
1	C	197	LEU

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Mol	Chain	Res	Type
1	C	203	ASN
1	C	205	ILE
1	C	213	SER
1	C	215	THR
1	C	222	LEU
1	C	261	LYS
1	C	263	VAL
1	C	272	VAL
1	C	274	LEU
1	C	288	PHE
1	C	289	LYS
1	C	290	SER
1	C	300	ILE
1	C	307	ARG
1	C	308	VAL
1	C	313	GLU
1	C	324	LEU
1	C	343	VAL
1	C	349	LEU
1	C	362	ILE
1	C	370	VAL
1	C	374	GLU
1	C	412	SER
1	C	419	VAL
1	C	439	MSE
1	C	443	LEU
1	C	447	ILE
1	C	458	MSE
1	C	459	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	282	ASN
1	A	94	ASN
1	C	151	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	BNG	D	502	-	21,21,21	1.23	2 (9%)	26,26,26	1.88	9 (34%)
4	CIT	A	501	-	3,12,12	1.40	0	3,17,17	2.08	1 (33%)
4	CIT	B	501	-	3,12,12	1.54	0	3,17,17	2.30	2 (66%)
4	CIT	C	501	-	3,12,12	1.31	1 (33%)	3,17,17	2.01	1 (33%)
3	BNG	C	503	-	21,21,21	1.22	3 (14%)	26,26,26	1.21	2 (7%)
3	BNG	B	503	-	21,21,21	1.34	3 (14%)	26,26,26	1.83	4 (15%)

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	BNG	D	502	-	-	6/12/32/32	0/1/1/1
4	CIT	A	501	-	-	6/6/16/16	-
4	CIT	B	501	-	-	4/6/16/16	-
4	CIT	C	501	-	-	1/6/16/16	-
3	BNG	C	503	-	-	4/12/32/32	0/1/1/1
3	BNG	B	503	-	-	8/12/32/32	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	BNG	C3-C2	-4.16	1.41	1.52
3	D	502	BNG	C3-C2	-3.99	1.42	1.52
3	C	503	BNG	C3-C2	-3.65	1.43	1.52
3	C	503	BNG	O5-C1	2.70	1.48	1.41
3	B	503	BNG	O5-C1	2.37	1.47	1.41
3	D	502	BNG	O5-C1	2.32	1.47	1.41
4	C	501	CIT	O7-C3	2.19	1.46	1.43
3	B	503	BNG	C4-C3	-2.16	1.46	1.52
3	C	503	BNG	C4-C3	-2.04	1.47	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	BNG	C1'-O1-C1	5.34	122.70	113.84
3	D	502	BNG	C1-C2-C3	3.64	117.58	110.00
3	D	502	BNG	C1'-O1-C1	3.64	119.87	113.84
3	B	503	BNG	O1-C1'-C2'	3.51	121.88	109.56
3	B	503	BNG	O1-C1-C2	3.48	113.73	108.30
4	A	501	CIT	C3-C4-C5	-3.46	109.44	114.98
4	B	501	CIT	C3-C4-C5	-3.42	109.52	114.98
3	D	502	BNG	O2-C2-C3	-3.41	102.45	110.35
4	C	501	CIT	C3-C4-C5	-3.36	109.60	114.98
3	D	502	BNG	C4-C3-C2	3.23	116.45	110.82
3	D	502	BNG	O1-C1'-C2'	2.89	119.69	109.56
3	B	503	BNG	O2-C2-C3	-2.84	103.77	110.35
3	D	502	BNG	O6-C6-C5	2.64	120.36	111.29
3	C	503	BNG	O1-C1'-C2'	2.62	118.75	109.56
3	C	503	BNG	O1-C1-C2	2.57	112.31	108.30
3	D	502	BNG	O5-C1-C2	2.49	115.61	110.35
3	D	502	BNG	C3-C4-C5	2.01	113.83	110.24
4	B	501	CIT	C3-C2-C1	-2.01	111.76	114.98
3	D	502	BNG	O1-C1-C2	2.01	111.44	108.30

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	CIT	C6-C3-C4-C5
3	C	503	BNG	C2-C1-O1-C1'
3	C	503	BNG	O5-C1-O1-C1'
3	B	503	BNG	O5-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
4	A	501	CIT	C2-C3-C4-C5
4	B	501	CIT	C2-C3-C4-C5
3	D	502	BNG	O5-C5-C6-O6
3	C	503	BNG	O1-C1'-C2'-C3'
3	D	502	BNG	O1-C1'-C2'-C3'
3	B	503	BNG	C5'-C6'-C7'-C8'
3	B	503	BNG	C2'-C3'-C4'-C5'
4	A	501	CIT	C1-C2-C3-O7
3	B	503	BNG	C1'-C2'-C3'-C4'
3	B	503	BNG	C4'-C5'-C6'-C7'
3	D	502	BNG	C6'-C7'-C8'-C9'
3	B	503	BNG	O5-C5-C6-O6
4	A	501	CIT	O7-C3-C4-C5
3	B	503	BNG	C2-C1-O1-C1'
3	C	503	BNG	C3'-C4'-C5'-C6'
4	A	501	CIT	C1-C2-C3-C4
4	B	501	CIT	O7-C3-C4-C5
4	C	501	CIT	C1-C2-C3-O7
3	D	502	BNG	C5'-C6'-C7'-C8'
4	A	501	CIT	C1-C2-C3-C6
4	B	501	CIT	C6-C3-C4-C5
3	D	502	BNG	C4'-C5'-C6'-C7'
3	D	502	BNG	C4-C5-C6-O6
4	B	501	CIT	C1-C2-C3-O7
3	B	503	BNG	C2'-C1'-O1-C1

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	BNG	3	0
4	A	501	CIT	3	0
4	B	501	CIT	6	0
4	C	501	CIT	5	0
3	C	503	BNG	1	0
3	B	503	BNG	5	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 BNG D 502

Bond lengths   Bond angles

Torsions   Rings

Ligand BNG C 503

Bond lengths   Bond angles

Torsions   Rings

Ligand BNG B 503

Bond lengths

Bond angles

Torsions

Rings
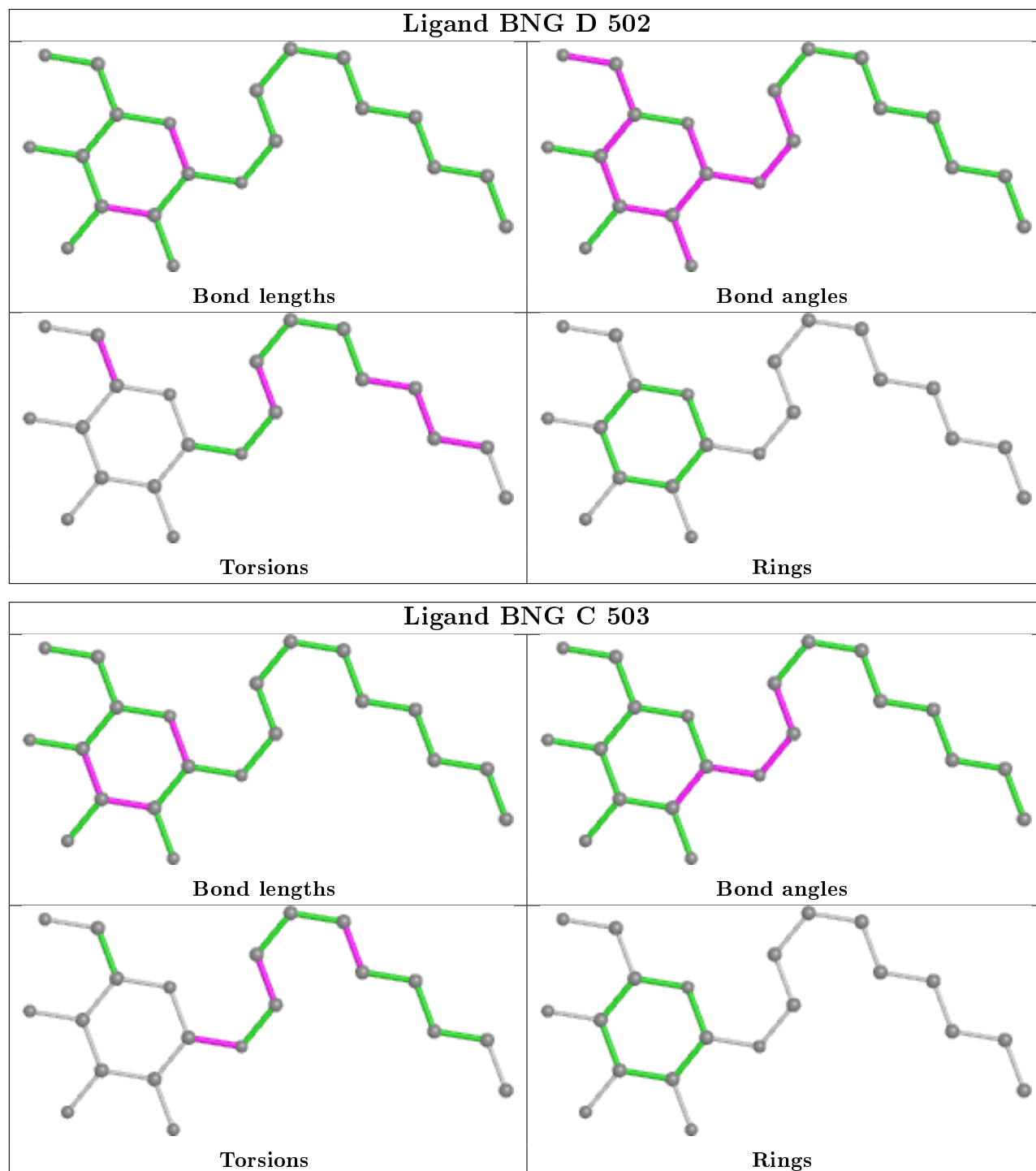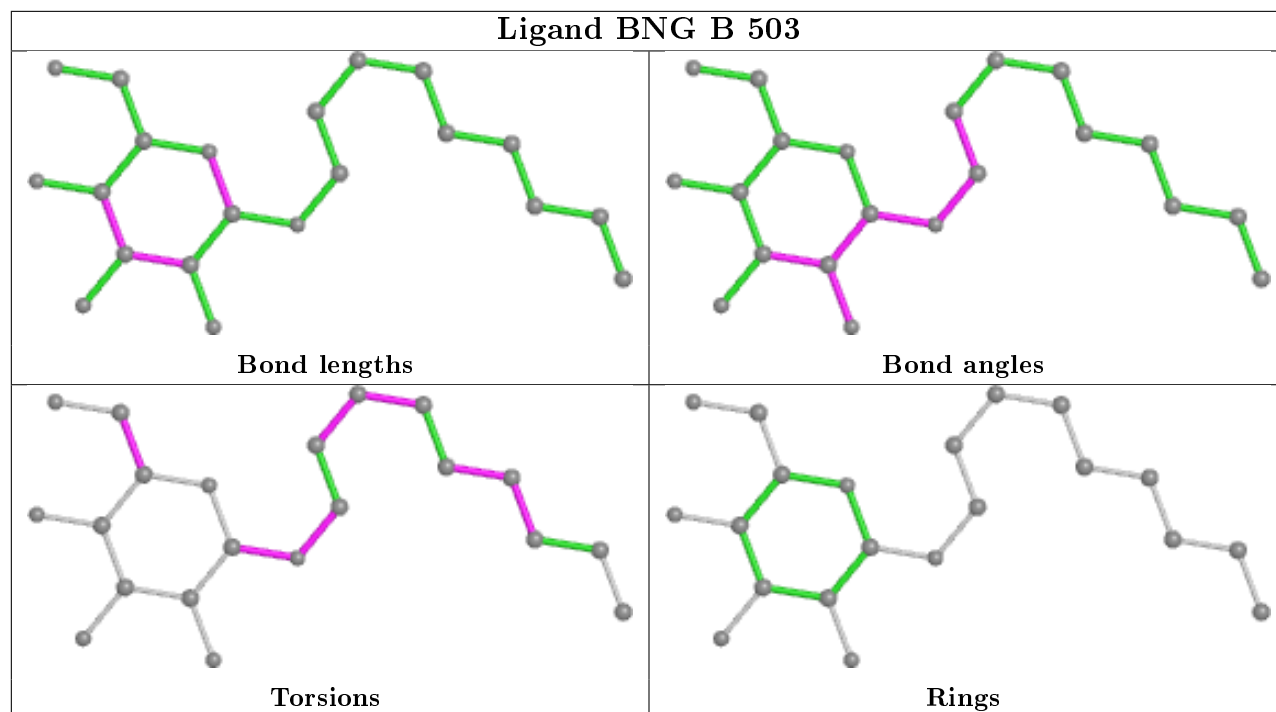
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	412/449 (91%)	-0.33	4 (0%)	82	72	57, 93, 150, 196	0
1	B	393/449 (87%)	-0.33	3 (0%)	86	78	61, 103, 160, 188	0
1	C	408/449 (90%)	-0.45	4 (0%)	82	72	53, 87, 139, 187	0
1	D	408/449 (90%)	-0.42	3 (0%)	87	81	48, 89, 142, 229	1 (0%)
All	All	1621/1796 (90%)	-0.38	14 (0%)	84	75	48, 93, 150, 229	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	THR	4.7
1	A	132	SER	3.7
1	D	432	HIS	3.5
1	C	132	SER	2.9
1	D	378	ASN	2.8
1	C	178	TYR	2.6
1	A	178	TYR	2.6
1	B	134	ALA	2.5
1	D	433	ILE	2.5
1	A	305	PHE	2.5
1	C	128	GLN	2.4
1	B	37	HIS	2.3
1	B	169	VAL	2.2
1	A	183	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

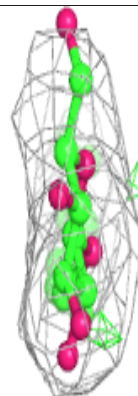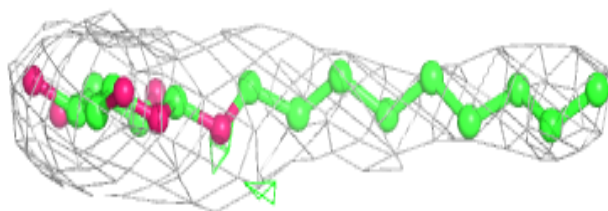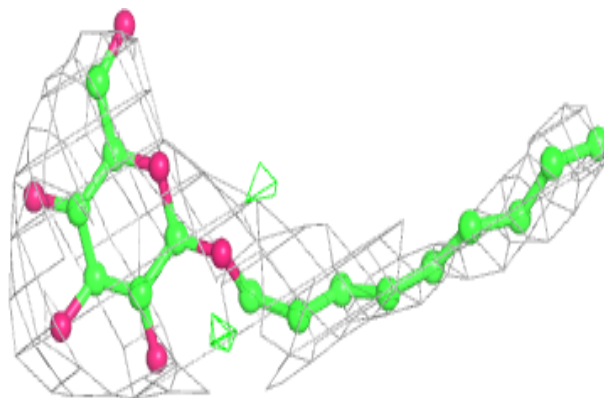| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BNG	B	503	21/21	0.77	0.33	62,175,190,333	0
4	CIT	B	501	13/13	0.83	0.37	127,135,161,164	0
3	BNG	C	503	21/21	0.87	0.31	58,111,159,160	0
3	BNG	D	502	21/21	0.88	0.35	75,100,143,143	0
4	CIT	A	501	13/13	0.92	0.40	101,117,130,136	0
4	CIT	C	501	13/13	0.92	0.25	88,110,139,149	0
2	NA	B	502	1/1	0.97	0.40	71,71,71,71	0
2	NA	C	502	1/1	0.97	0.19	53,53,53,53	0
2	NA	D	501	1/1	0.97	0.36	63,63,63,63	0
2	NA	A	502	1/1	0.98	0.52	77,77,77,77	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.
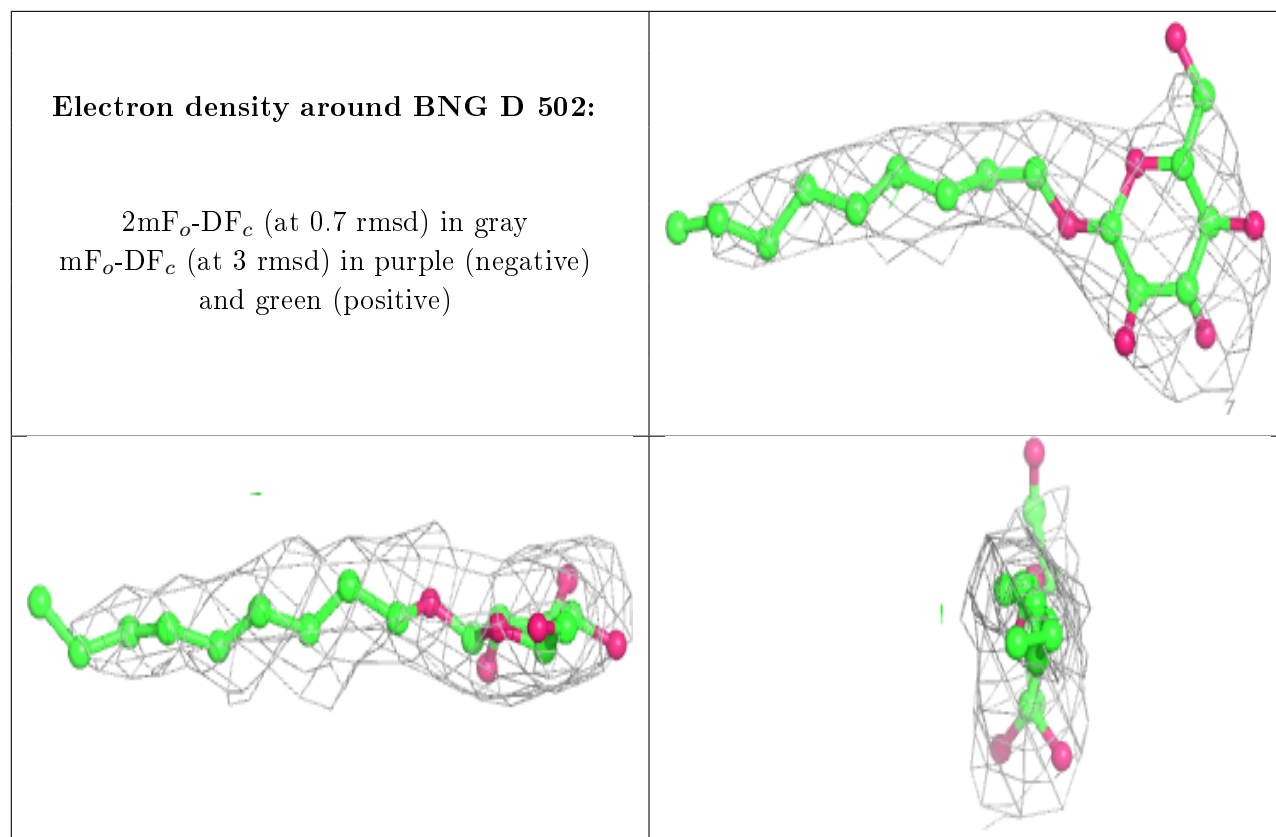
Electron density around BNG B 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
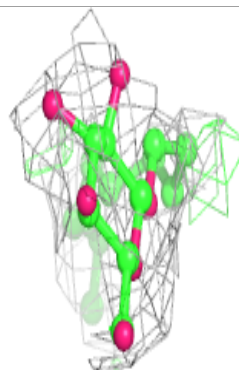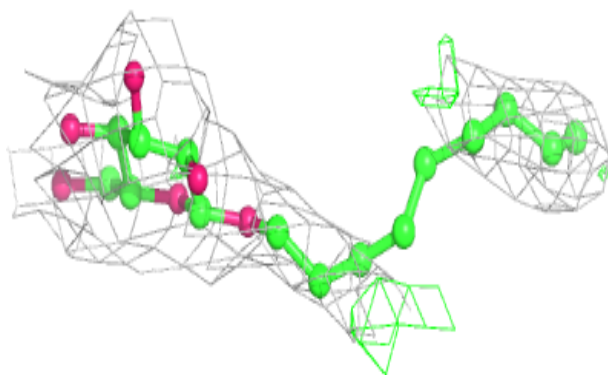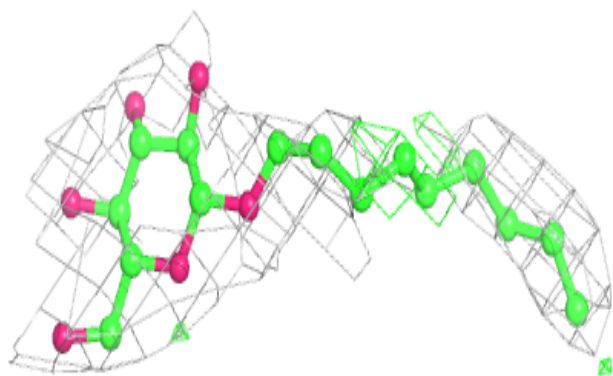
Electron density around BNG C 503:

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

Electron density around BNG D 502:

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

6.5 Other polymers (i)

There are no such residues in this entry.