Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:44 am BST

PDB ID	:	2PZY
Title	:	Structure of MK2 Complexed with Compound 76
Authors	:	White, A.; Wu, J.P.; Wang, J.; Abeywardane, A.; Andersen, D.; Emmanuel, M.; Gautschi, E.; Goldberg, D.R.; Kashem, M.A.; Lukas, S.; Mao, W.; Martin, L.; Morwick, T.; Moss, N.; Pargellis, C.; Patel, U.R.; Patnaude, L.; Peet, G.W.; Skow, D.; Snow, R.J.; Ward, Y.; Werneburg, B.
Deposited on	:	2007-05-18
Resolution	:	2.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		3.7%
Sidechain outliers		8.7%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
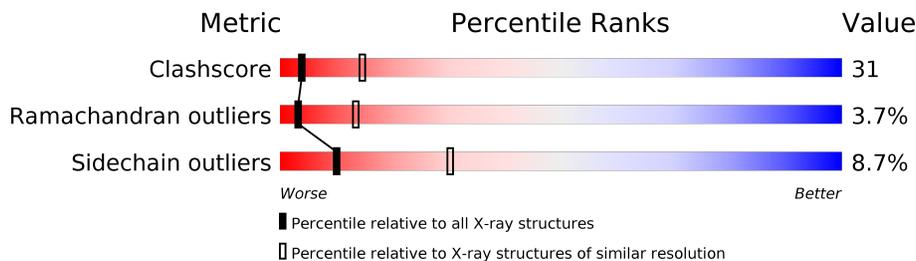
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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%

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	324	43% 42% 5% 10%
1	B	324	40% 41% 6% 13%
1	C	324	42% 44% 9% 5%
1	D	324	35% 46% 7% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9585 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2356	1509	405	425	17			
1	B	283	Total	C	N	O	S	0	0	0
			2300	1471	395	417	17			
1	C	307	Total	C	N	O	S	0	0	0
			2492	1590	428	456	18			
1	D	288	Total	C	N	O	S	0	0	0
			2340	1502	401	419	18			

- Molecule 2 is (4R)-N-[4-({[2-(DIMETHYLAMINO)ETHYL]AMINO}CARBONYL)-1,3-THIAZOL-2-YL]-4-METHYL-1-OXO-2,3,4,9-TETRAHYDRO-1H-BETA-CARBOLINE-6-CARBOXAMIDE (three-letter code: B18) (formula: $C_{21}H_{24}N_6O_3S$).


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	21	6	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 31	C 21	N 6	O 3	S 1	0	0

- Molecule 3 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).
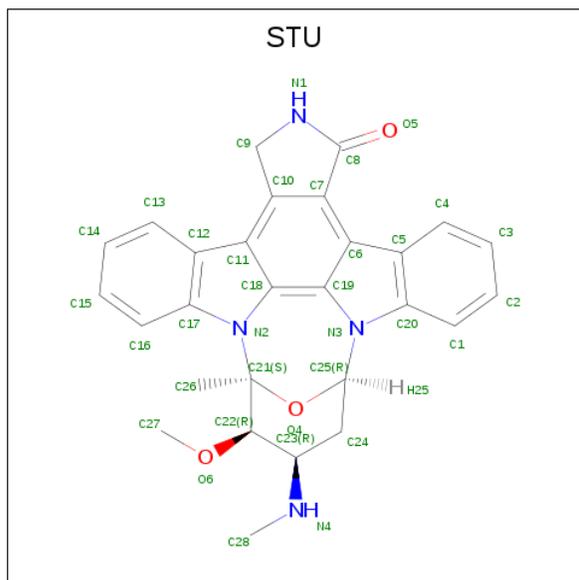
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 35	C 28	N 4	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: MAP kinase-activated protein kinase 2
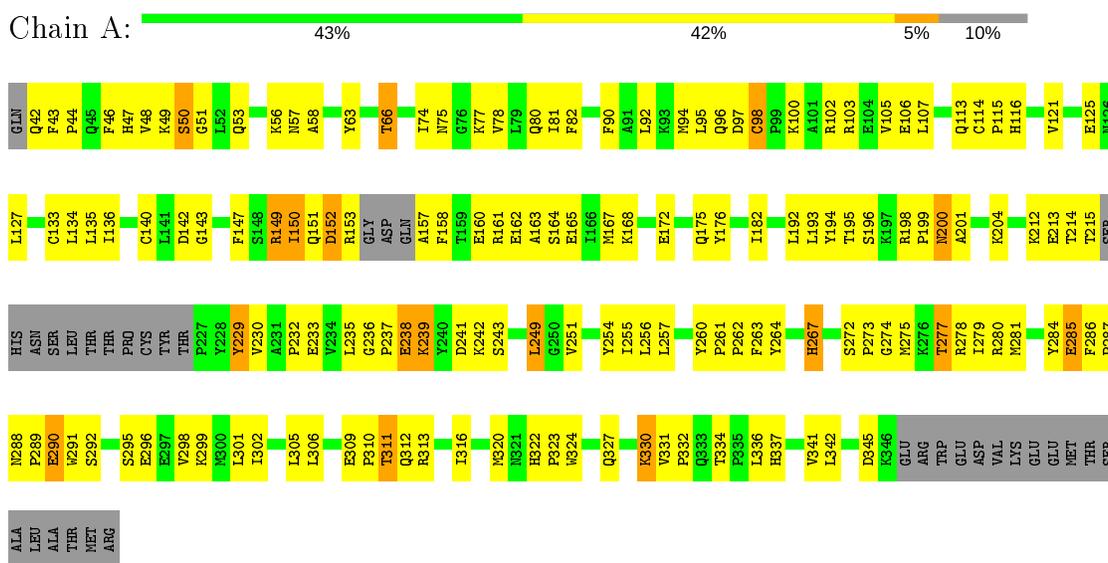
• Molecule 1: MAP kinase-activated protein kinase 2
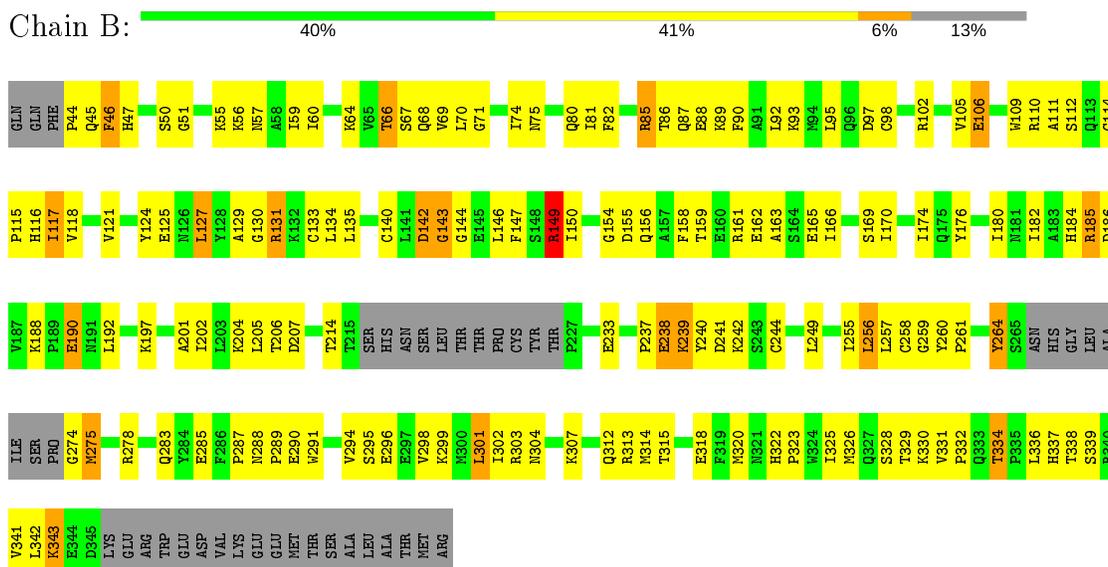
• Molecule 1: MAP kinase-activated protein kinase 2

Chain C:
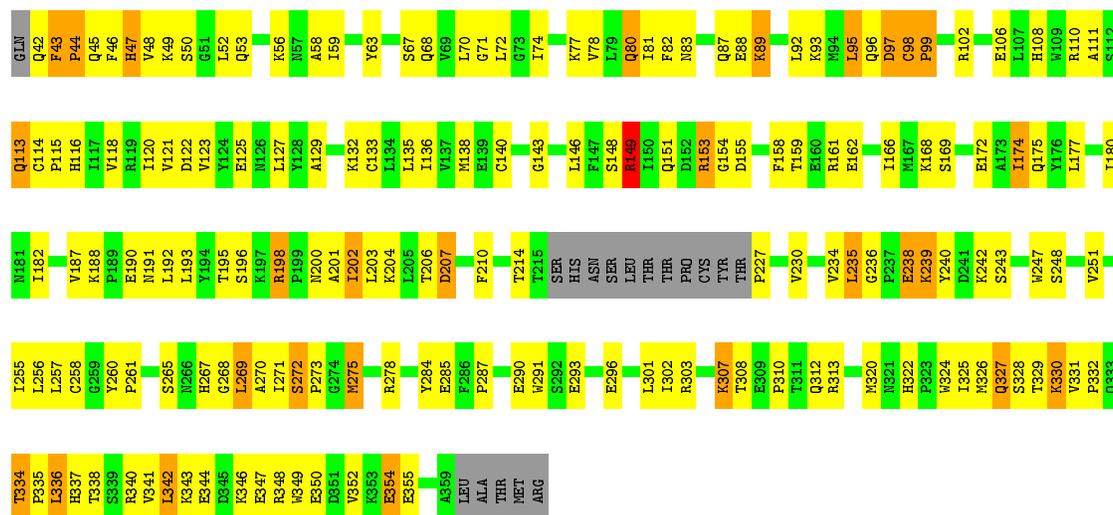
• Molecule 1: MAP kinase-activated protein kinase 2

Chain D:
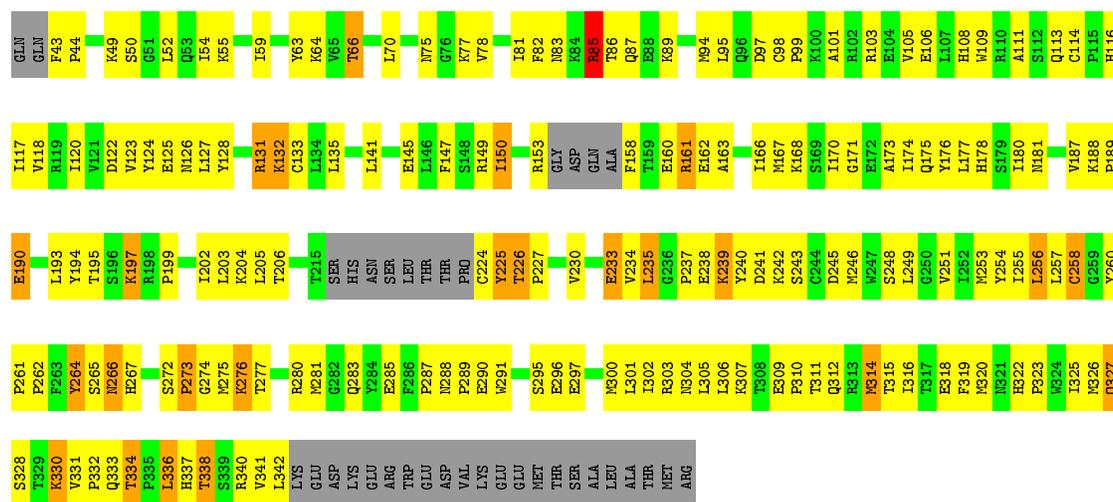
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	159.61Å 159.61Å 134.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.32 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (34.32-2.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9585	wwPDB-VP
Average B, all atoms (Å²)	72.0	wwPDB-VP

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: STU, B18

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	0.45	0/2409	0.60	0/3252
1	B	0.42	0/2350	0.63	0/3168
1	C	0.42	0/2548	0.61	0/3439
1	D	0.38	0/2394	0.57	0/3233
All	All	0.42	0/9701	0.60	0/13092

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	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	TYR	Sidechain
1	B	185	ARG	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	2356	0	2375	141	0
1	B	2300	0	2328	129	0
1	C	2492	0	2501	167	1
1	D	2340	0	2368	187	1
2	A	31	0	24	0	0
2	B	31	0	24	0	0
3	C	35	0	26	8	0
All	All	9585	0	9646	590	1

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 31.

All (590) 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:D:197:LYS:H	1:D:197:LYS:HD3	1.15	1.11
1:B:56:LYS:HG3	1:C:53:GLN:HG2	1.13	1.10
1:C:239:LYS:HG3	1:C:240:TYR:H	1.09	1.06
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.38	1.06
1:C:149:ARG:HG2	1:C:149:ARG:HH11	0.91	1.05
1:B:85:ARG:HH11	1:B:85:ARG:HG2	1.21	1.04
1:C:149:ARG:NH1	1:C:149:ARG:HG2	1.71	0.98
1:C:153:ARG:HA	1:C:153:ARG:HE	1.27	0.97
1:B:95:LEU:O	1:B:133:CYS:HB2	1.66	0.96
1:B:131:ARG:HH21	1:B:131:ARG:HG2	1.30	0.95
1:D:161:ARG:CZ	1:D:161:ARG:HB2	1.98	0.93
1:C:149:ARG:CG	1:C:149:ARG:HH11	1.82	0.93
1:B:56:LYS:HG3	1:C:53:GLN:CG	2.01	0.90
1:B:159:THR:HG22	1:B:162:GLU:HG3	1.54	0.88
1:D:160:GLU:HA	1:D:336:LEU:HD21	1.53	0.88
1:B:260:TYR:HE2	1:B:290:GLU:HG2	1.38	0.88
1:C:239:LYS:HG3	1:C:240:TYR:N	1.88	0.87
1:B:56:LYS:CG	1:C:53:GLN:HG2	2.01	0.86
1:D:54:ILE:HG22	1:D:55:LYS:H	1.40	0.86
1:A:153:ARG:HD3	1:A:157:ALA:HA	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LYS:CG	1:C:240:TYR:H	1.88	0.83
1:D:239:LYS:HD2	1:D:239:LYS:H	1.43	0.83
1:A:309:GLU:HB3	1:A:312:GLN:HE21	1.42	0.82
1:A:95:LEU:O	1:A:133:CYS:HB2	1.80	0.82
1:A:235:LEU:HD13	1:D:276:LYS:HZ2	1.45	0.82
1:C:116:HIS:CE1	1:C:169:SER:HB2	2.15	0.82
1:B:131:ARG:NH2	1:B:131:ARG:HG2	1.91	0.81
1:C:102:ARG:O	1:C:106:GLU:HG2	1.80	0.81
1:A:115:PRO:O	1:A:204:LYS:HE2	1.81	0.81
1:C:43:PHE:O	1:C:45:GLN:HG3	1.82	0.80
1:C:196:SER:OG	1:C:201:ALA:HB2	1.81	0.79
1:D:161:ARG:HB2	1:D:161:ARG:NH1	1.96	0.79
1:B:260:TYR:CE2	1:B:290:GLU:HG2	2.18	0.78
1:D:255:ILE:HG12	1:D:261:PRO:HA	1.64	0.78
1:D:161:ARG:HH22	1:D:330:LYS:N	1.82	0.78
1:B:70:LEU:HD21	1:B:80:GLN:HB2	1.65	0.78
1:D:54:ILE:HG22	1:D:55:LYS:N	1.98	0.78
1:C:115:PRO:O	1:C:204:LYS:HE2	1.84	0.77
1:B:85:ARG:HG2	1:B:85:ARG:NH1	1.98	0.76
1:A:257:LEU:O	1:A:336:LEU:HD22	1.84	0.76
1:A:260:TYR:OH	1:A:287:PRO:HG2	1.87	0.75
1:B:115:PRO:O	1:B:204:LYS:HE2	1.85	0.75
1:B:264:TYR:HA	1:B:275:MET:CE	2.16	0.75
1:A:114:CYS:HB2	1:A:176:TYR:CD2	2.22	0.74
1:C:133:CYS:SG	1:C:135:LEU:HD21	2.26	0.74
1:B:130:GLY:O	1:C:110:ARG:HD2	1.88	0.74
1:B:159:THR:HG22	1:B:162:GLU:CG	2.18	0.73
1:D:197:LYS:HD3	1:D:197:LYS:N	1.98	0.73
1:C:43:PHE:O	1:C:45:GLN:N	2.21	0.73
1:D:205:LEU:HD12	1:D:206:THR:H	1.54	0.73
1:C:328:SER:O	1:C:331:VAL:HG12	1.89	0.73
1:B:97:ASP:HB2	1:B:133:CYS:HA	1.71	0.72
1:C:43:PHE:HB3	1:C:44:PRO:HD2	1.70	0.72
1:D:95:LEU:O	1:D:133:CYS:HB2	1.89	0.72
1:D:188:LYS:HG3	1:D:190:GLU:HG2	1.70	0.72
1:B:339:SER:O	1:B:343:LYS:HB2	1.89	0.72
1:C:153:ARG:NE	1:C:153:ARG:HA	2.03	0.72
1:B:161:ARG:HG2	1:B:331:VAL:HG22	1.72	0.72
1:D:178:HIS:CG	1:D:242:LYS:HD3	2.25	0.72
1:A:311:THR:HG22	1:D:309:GLU:CD	2.10	0.71
1:B:57:ASN:HA	1:C:50:SER:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ARG:HH21	1:B:131:ARG:CG	2.04	0.71
1:D:66:THR:HG21	1:D:82:PHE:HE1	1.54	0.70
1:B:127:LEU:HD11	1:C:110:ARG:HG2	1.73	0.70
1:B:264:TYR:HA	1:B:275:MET:HE2	1.73	0.70
1:D:161:ARG:HD2	1:D:333:GLN:NE2	2.07	0.69
1:A:48:VAL:HG11	1:C:59:ILE:HG22	1.73	0.69
1:D:150:ILE:HG13	1:D:158:PHE:CE1	2.27	0.69
1:B:161:ARG:O	1:B:165:GLU:HG3	1.92	0.69
1:C:290:GLU:HA	1:C:337:HIS:CD2	2.28	0.69
1:D:171:GLY:HA3	1:D:320:MET:CE	2.22	0.69
1:C:108:HIS:ND1	1:C:120:ILE:HD11	2.08	0.68
1:A:251:VAL:O	1:A:255:ILE:HG13	1.93	0.68
1:A:309:GLU:CB	1:A:312:GLN:HE21	2.06	0.68
1:D:256:LEU:O	1:D:257:LEU:HD23	1.94	0.68
1:D:64:LYS:HG2	1:D:64:LYS:O	1.93	0.68
1:C:202:ILE:HD12	1:C:203:LEU:O	1.93	0.67
1:B:264:TYR:N	1:B:264:TYR:HD2	1.93	0.67
1:D:161:ARG:HA	1:D:331:VAL:CG2	2.25	0.67
1:C:98:CYS:HB2	1:C:99:PRO:CD	2.24	0.67
1:D:150:ILE:HG13	1:D:158:PHE:CD1	2.29	0.67
1:D:171:GLY:HA3	1:D:320:MET:HE1	1.74	0.67
1:B:186:ASP:OD2	1:B:188:LYS:HE2	1.95	0.66
1:A:102:ARG:HD3	1:A:134:LEU:HD11	1.78	0.66
1:A:143:GLY:O	1:A:149:ARG:HG3	1.96	0.66
1:C:337:HIS:O	1:C:341:VAL:HG23	1.96	0.66
1:D:153:ARG:HH21	1:D:158:PHE:HA	1.60	0.66
1:D:225:TYR:O	1:D:226:THR:HB	1.96	0.66
1:C:158:PHE:HA	1:C:162:GLU:OE2	1.96	0.65
1:C:190:GLU:OE2	1:C:190:GLU:N	2.29	0.65
1:B:70:LEU:CD2	1:B:80:GLN:HB2	2.26	0.65
1:B:307:LYS:HD2	1:B:312:GLN:HB3	1.78	0.65
1:C:118:VAL:CG1	1:C:206:THR:HG22	2.26	0.65
1:C:265:SER:N	1:C:275:MET:HG2	2.11	0.65
1:D:149:ARG:NH2	1:D:197:LYS:HA	2.10	0.65
1:B:301:LEU:HG	1:B:322:HIS:CD2	2.32	0.64
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.27	0.64
1:D:255:ILE:O	1:D:255:ILE:HG22	1.96	0.64
1:D:118:VAL:CG1	1:D:206:THR:HG22	2.26	0.64
1:A:160:GLU:N	1:A:336:LEU:HD12	2.13	0.64
1:B:264:TYR:N	1:B:264:TYR:CD2	2.65	0.64
1:B:143:GLY:HA2	1:B:197:LYS:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:TYR:HE2	1:A:290:GLU:HG2	1.62	0.63
1:A:274:GLY:O	1:A:278:ARG:HG3	1.98	0.63
1:C:52:LEU:HD21	1:C:123:VAL:HG21	1.80	0.63
1:A:327:GLN:OE1	1:A:330:LYS:HG2	1.97	0.63
1:C:301:LEU:HD22	1:C:322:HIS:CD2	2.33	0.63
1:C:326:MET:HA	1:C:326:MET:HE3	1.79	0.63
1:A:295:SER:HB3	1:A:298:VAL:HG23	1.81	0.63
1:D:160:GLU:CA	1:D:336:LEU:HD21	2.26	0.63
1:B:146:LEU:HD12	1:B:192:LEU:HD13	1.80	0.63
1:C:243:SER:OG	1:C:310:PRO:HB3	1.99	0.63
1:A:172:GLU:HG2	1:A:320:MET:HE1	1.81	0.62
1:A:236:GLY:HA3	1:D:280:ARG:HH21	1.65	0.62
1:A:49:LYS:HB2	1:A:113:GLN:HE22	1.63	0.62
1:B:118:VAL:HB	1:B:206:THR:HG22	1.81	0.62
1:B:82:PHE:CE2	1:B:89:LYS:HB3	2.35	0.62
1:B:85:ARG:CG	1:B:85:ARG:HH11	2.04	0.62
1:A:143:GLY:HA3	1:A:194:TYR:HB2	1.81	0.62
1:A:311:THR:HG22	1:D:309:GLU:CG	2.30	0.62
1:A:105:VAL:HG21	1:A:134:LEU:HD13	1.80	0.62
1:A:57:ASN:HA	1:B:50:SER:HB2	1.81	0.62
1:D:97:ASP:HB2	1:D:133:CYS:HA	1.82	0.62
1:C:260:TYR:OH	1:C:287:PRO:HG2	2.00	0.61
1:C:331:VAL:HG23	1:C:332:PRO:HD2	1.81	0.61
1:C:43:PHE:CB	1:C:44:PRO:HD2	2.30	0.61
1:D:303:ARG:O	1:D:307:LYS:HG2	2.00	0.61
1:D:150:ILE:CG1	1:D:158:PHE:CE1	2.83	0.61
1:A:214:THR:OG1	1:A:242:LYS:NZ	2.33	0.61
1:B:159:THR:CG2	1:B:162:GLU:HG3	2.29	0.61
1:C:98:CYS:HB2	1:C:99:PRO:HD2	1.81	0.61
1:D:266:ASN:O	1:D:273:PRO:O	2.19	0.61
1:A:214:THR:O	1:A:215:THR:HG23	2.01	0.61
1:A:323:PRO:C	1:A:327:GLN:HE21	2.04	0.61
1:C:146:LEU:HD11	1:C:166:ILE:HD13	1.83	0.60
1:A:152:ASP:O	1:A:153:ARG:HG3	2.01	0.60
1:D:43:PHE:CD1	1:D:44:PRO:HD2	2.35	0.60
1:C:148:SER:O	1:C:151:GLN:HG2	2.01	0.60
1:C:71:GLY:HA3	3:C:3:STU:O4	2.01	0.60
1:A:305:LEU:O	1:A:313:ARG:HD3	2.02	0.60
1:B:161:ARG:HA	1:B:331:VAL:CG2	2.31	0.60
1:D:103:ARG:HE	1:D:103:ARG:HA	1.66	0.60
1:B:296:GLU:O	1:B:296:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASN:O	1:D:87:GLN:HA	2.02	0.60
1:D:118:VAL:HG11	1:D:206:THR:HG22	1.82	0.59
1:C:81:ILE:HG21	1:C:92:LEU:HD22	1.82	0.59
1:D:161:ARG:HA	1:D:331:VAL:HG23	1.84	0.59
1:B:174:ILE:HG13	1:B:249:LEU:HD13	1.83	0.59
1:D:197:LYS:CD	1:D:197:LYS:H	1.97	0.59
1:A:96:GLN:HA	1:A:133:CYS:HB3	1.84	0.59
1:A:229:TYR:OH	1:D:188:LYS:HD3	2.02	0.59
1:B:150:ILE:HD12	1:B:158:PHE:CE1	2.37	0.59
1:D:227:PRO:O	1:D:230:VAL:HG12	2.03	0.58
1:D:303:ARG:HG3	1:D:303:ARG:HH11	1.68	0.58
1:A:255:ILE:HG12	1:A:261:PRO:HA	1.84	0.58
3:C:3:STU:H16	3:C:3:STU:H261	1.85	0.58
1:D:52:LEU:HB2	1:D:109:TRP:CD1	2.37	0.58
1:A:238:GLU:O	1:A:239:LYS:O	2.21	0.58
1:A:289:PRO:HA	1:A:292:SER:OG	2.02	0.58
1:D:106:GLU:OE2	1:D:106:GLU:HA	2.03	0.58
1:B:162:GLU:O	1:B:166:ILE:HG13	2.03	0.58
1:B:258:CYS:HB2	1:B:290:GLU:HB3	1.85	0.58
1:B:278:ARG:HG2	1:B:283:GLN:HB2	1.85	0.58
1:C:113:GLN:O	1:C:113:GLN:HG3	2.03	0.58
1:A:311:THR:HG22	1:D:309:GLU:HG2	1.86	0.58
1:D:167:MET:CB	1:D:325:ILE:HD11	2.34	0.58
1:C:138:MET:HE1	3:C:3:STU:H13	1.86	0.58
1:D:300:MET:HE2	1:D:300:MET:HA	1.85	0.58
1:C:158:PHE:O	1:C:336:LEU:HB2	2.04	0.57
1:D:258:CYS:HB2	1:D:260:TYR:CE2	2.39	0.57
1:D:161:ARG:HH22	1:D:330:LYS:H	1.48	0.57
1:B:159:THR:HG23	1:B:162:GLU:H	1.69	0.57
1:B:314:MET:HE2	1:B:318:GLU:HB2	1.86	0.57
1:C:78:VAL:HA	1:C:92:LEU:O	2.03	0.57
1:D:255:ILE:HD11	1:D:261:PRO:HB3	1.86	0.57
1:A:162:GLU:O	1:A:165:GLU:HG2	2.05	0.57
1:C:267:HIS:HA	1:C:273:PRO:HB3	1.85	0.57
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.87	0.57
1:D:54:ILE:CG2	1:D:55:LYS:H	2.14	0.57
1:A:232:PRO:HD2	1:A:233:GLU:OE2	2.05	0.57
1:A:161:ARG:HA	1:A:331:VAL:CG2	2.34	0.57
1:B:214:THR:OG1	1:B:242:LYS:NZ	2.37	0.57
1:C:154:GLY:O	1:C:155:ASP:HB2	2.05	0.57
1:A:153:ARG:HD3	1:A:157:ALA:CA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD11	1:C:80:GLN:HG2	1.86	0.57
1:A:160:GLU:HG3	1:A:324:TRP:HZ2	1.68	0.56
1:D:161:ARG:CZ	1:D:161:ARG:CB	2.78	0.56
1:D:66:THR:HG21	1:D:82:PHE:CE1	2.39	0.56
1:B:44:PRO:HB3	1:B:46:PHE:CZ	2.40	0.56
1:D:161:ARG:NH2	1:D:331:VAL:H	2.03	0.56
1:B:93:LYS:HE2	1:B:95:LEU:HD21	1.87	0.56
1:A:235:LEU:CD1	1:D:276:LYS:HZ2	2.17	0.56
1:D:337:HIS:O	1:D:338:THR:C	2.42	0.56
1:A:151:GLN:O	1:A:151:GLN:HG2	2.05	0.56
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.40	0.56
1:C:97:ASP:HB3	1:C:132:LYS:O	2.06	0.56
1:B:260:TYR:HB2	1:B:261:PRO:HD2	1.87	0.56
1:C:326:MET:HA	1:C:326:MET:CE	2.35	0.56
1:D:145:GLU:HG2	1:D:193:LEU:CD2	2.36	0.56
1:A:172:GLU:HG2	1:A:320:MET:CE	2.36	0.56
1:D:300:MET:CE	1:D:303:ARG:HD2	2.36	0.56
1:D:180:ILE:O	1:D:181:ASN:HB2	2.06	0.56
1:D:187:VAL:O	1:D:248:SER:HB3	2.06	0.56
1:D:327:GLN:HB3	1:D:330:LYS:HB3	1.87	0.56
1:C:118:VAL:HG11	1:C:206:THR:HG22	1.87	0.55
1:D:54:ILE:HG23	1:D:123:VAL:HG12	1.88	0.55
1:D:111:ALA:HB1	1:D:117:ILE:HD13	1.89	0.55
1:D:272:SER:HA	1:D:277:THR:HG21	1.89	0.55
1:C:195:THR:HG23	1:C:202:ILE:O	2.06	0.55
1:C:348:ARG:O	1:C:352:VAL:HG13	2.07	0.55
1:C:68:GLN:HA	1:C:68:GLN:NE2	2.22	0.55
1:B:114:CYS:HB2	1:B:176:TYR:CD2	2.43	0.55
1:B:85:ARG:CG	1:B:85:ARG:NH1	2.68	0.54
1:D:94:MET:HG2	1:D:135:LEU:HD22	1.88	0.54
1:C:327:GLN:HB2	1:C:330:LYS:HZ3	1.71	0.54
1:A:97:ASP:O	1:A:98:CYS:HB3	2.08	0.54
1:B:129:ALA:HA	1:C:47:HIS:CE1	2.41	0.54
1:D:178:HIS:CE1	1:D:242:LYS:HB3	2.42	0.54
1:B:105:VAL:HG21	1:B:134:LEU:HD23	1.89	0.54
1:B:97:ASP:OD2	1:B:102:ARG:NH2	2.40	0.54
1:D:149:ARG:HH22	1:D:197:LYS:HA	1.73	0.54
1:C:239:LYS:CG	1:C:240:TYR:N	2.60	0.54
1:A:337:HIS:HB3	1:A:341:VAL:HG23	1.89	0.54
1:B:97:ASP:OD1	1:B:98:CYS:N	2.41	0.54
1:D:75:ASN:O	1:D:95:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:PRO:HA	1:B:326:MET:HB3	1.89	0.53
1:B:330:LYS:HG2	1:B:330:LYS:O	2.08	0.53
1:C:207:ASP:CG	3:C:3:STU:H15	2.29	0.53
1:C:44:PRO:HA	1:C:46:PHE:CE1	2.43	0.53
1:D:260:TYR:OH	1:D:287:PRO:HG2	2.08	0.53
1:C:192:LEU:O	1:C:193:LEU:HD23	2.08	0.53
1:D:111:ALA:HB1	1:D:117:ILE:CD1	2.38	0.53
1:D:240:TYR:O	1:D:243:SER:HB3	2.09	0.53
1:C:202:ILE:HG13	1:C:202:ILE:O	2.07	0.53
1:C:96:GLN:NE2	1:C:96:GLN:H	2.07	0.53
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.43	0.53
1:B:264:TYR:HA	1:B:275:MET:HE3	1.90	0.53
1:D:86:THR:O	1:D:87:GLN:HB3	2.09	0.53
1:A:74:ILE:O	1:A:75:ASN:HB2	2.09	0.53
1:D:158:PHE:HE2	1:D:163:ALA:HB2	1.74	0.53
1:C:284:TYR:OH	1:C:303:ARG:HA	2.09	0.53
1:B:56:LYS:NZ	1:B:125:GLU:OE2	2.42	0.53
1:C:191:ASN:HA	3:C:3:STU:C27	2.39	0.53
1:D:167:MET:HB3	1:D:325:ILE:HD11	1.90	0.52
1:D:300:MET:HE2	1:D:303:ARG:HD2	1.91	0.52
1:A:196:SER:OG	1:A:201:ALA:HB2	2.09	0.52
1:B:257:LEU:HD12	1:B:302:ILE:HD11	1.92	0.52
1:D:264:TYR:N	1:D:264:TYR:CD2	2.73	0.52
1:D:87:GLN:HG3	1:D:87:GLN:O	2.10	0.52
1:A:332:PRO:HB3	1:A:334:THR:HG23	1.89	0.52
1:A:42:GLN:HB3	1:C:67:SER:OG	2.09	0.52
1:B:154:GLY:C	1:B:156:GLN:H	2.12	0.52
1:B:70:LEU:CG	1:B:80:GLN:HB2	2.39	0.52
1:B:285:GLU:O	1:B:287:PRO:HD3	2.10	0.52
1:B:66:THR:OG1	1:B:67:SER:N	2.41	0.52
1:C:70:LEU:HD11	1:C:80:GLN:CG	2.40	0.52
1:B:315:THR:OG1	1:B:318:GLU:HG3	2.10	0.52
1:A:332:PRO:CB	1:A:334:THR:HG23	2.39	0.51
1:A:96:GLN:HA	1:A:133:CYS:CB	2.39	0.51
1:B:299:LYS:O	1:B:303:ARG:HG3	2.11	0.51
1:D:285:GLU:O	1:D:287:PRO:HD3	2.10	0.51
1:C:151:GLN:NE2	1:C:343:LYS:HA	2.25	0.51
1:B:142:ASP:O	1:B:144:GLY:N	2.44	0.51
1:B:259:GLY:HA2	1:B:342:LEU:HD13	1.92	0.51
1:A:49:LYS:HD3	1:C:127:LEU:HD12	1.92	0.51
1:C:269:LEU:HD12	1:C:278:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:TYR:CE1	1:C:348:ARG:NH1	2.78	0.51
1:A:49:LYS:HD2	1:A:113:GLN:CD	2.31	0.51
1:C:166:ILE:HG21	1:C:256:LEU:HD11	1.91	0.51
1:D:255:ILE:HG12	1:D:261:PRO:CA	2.38	0.51
1:A:96:GLN:H	1:A:96:GLN:CD	2.13	0.51
1:D:320:MET:HA	1:D:325:ILE:HG21	1.91	0.51
1:A:337:HIS:O	1:A:341:VAL:HG23	2.10	0.51
1:A:66:THR:HG23	1:A:80:GLN:O	2.10	0.51
1:C:296:GLU:O	1:C:296:GLU:HG3	2.09	0.51
1:D:161:ARG:HH22	1:D:331:VAL:H	1.58	0.51
1:D:254:TYR:CG	1:D:262:PRO:HG3	2.45	0.51
1:D:289:PRO:O	1:D:290:GLU:C	2.49	0.51
1:C:136:ILE:HG22	1:C:138:MET:HG3	1.93	0.51
1:C:89:LYS:O	1:C:140:CYS:HB2	2.11	0.51
1:D:49:LYS:HG2	1:D:50:SER:N	2.26	0.51
1:A:289:PRO:O	1:A:291:TRP:N	2.44	0.50
1:B:64:LYS:N	1:B:82:PHE:O	2.39	0.50
1:C:202:ILE:HD11	1:C:204:LYS:HG2	1.92	0.50
1:B:180:ILE:HD11	1:B:182:ILE:HD12	1.91	0.50
1:C:214:THR:HB	1:C:238:GLU:HG3	1.93	0.50
1:D:101:ALA:O	1:D:105:VAL:HG23	2.11	0.50
1:D:195:THR:CG2	1:D:204:LYS:HE3	2.41	0.50
1:D:265:SER:HA	1:D:275:MET:HB2	1.93	0.50
1:A:267:HIS:ND1	1:A:273:PRO:HB2	2.27	0.50
1:D:161:ARG:NH2	1:D:330:LYS:N	2.57	0.50
1:A:233:GLU:CG	1:D:310:PRO:HG3	2.42	0.50
1:C:108:HIS:HE1	1:C:138:MET:HE2	1.76	0.50
1:D:98:CYS:HB2	1:D:99:PRO:CD	2.42	0.50
1:A:102:ARG:NH1	1:A:125:GLU:OE2	2.45	0.50
1:B:88:GLU:HG3	1:B:90:PHE:CE1	2.46	0.50
1:D:153:ARG:NH2	1:D:158:PHE:HA	2.27	0.50
1:B:118:VAL:O	1:B:118:VAL:HG13	2.12	0.50
1:B:116:HIS:CE1	1:B:169:SER:HB2	2.47	0.50
1:C:68:GLN:HA	1:C:68:GLN:HE21	1.76	0.50
1:D:258:CYS:HG	1:D:291:TRP:HZ2	1.57	0.50
1:D:296:GLU:HG3	1:D:296:GLU:O	2.12	0.50
1:D:97:ASP:H	1:D:133:CYS:HA	1.77	0.49
1:A:229:TYR:CZ	1:D:188:LYS:HB3	2.47	0.49
1:B:285:GLU:C	1:B:287:PRO:HD3	2.33	0.49
1:B:60:ILE:HG21	1:C:45:GLN:HB3	1.95	0.49
1:D:125:GLU:HG2	1:D:132:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HZ2	1:A:113:GLN:HB2	1.78	0.49
1:A:134:LEU:O	1:A:135:LEU:HD23	2.12	0.49
1:C:338:THR:HG22	1:C:342:LEU:HD12	1.94	0.49
1:A:254:TYR:CD1	1:A:262:PRO:HD3	2.48	0.49
1:C:272:SER:N	1:C:273:PRO:HD3	2.27	0.49
1:D:272:SER:N	1:D:273:PRO:HD3	2.27	0.49
1:D:277:THR:O	1:D:281:MET:HB2	2.13	0.49
1:D:195:THR:CG2	1:D:202:ILE:HG23	2.42	0.49
1:D:54:ILE:CG2	1:D:55:LYS:N	2.70	0.49
1:B:59:ILE:HD12	1:B:124:TYR:CD1	2.48	0.49
1:D:168:LYS:HD2	1:D:328:SER:HB2	1.94	0.49
1:A:296:GLU:HG3	1:A:296:GLU:O	2.13	0.49
1:C:198:ARG:H	1:C:198:ARG:HD3	1.77	0.49
1:C:240:TYR:O	1:C:243:SER:HB3	2.12	0.49
1:D:267:HIS:CE1	1:D:274:GLY:HA2	2.48	0.49
1:D:327:GLN:HG2	1:D:330:LYS:CE	2.43	0.49
1:A:58:ALA:H	1:B:50:SER:HB3	1.78	0.48
1:C:332:PRO:O	1:C:334:THR:N	2.42	0.48
1:D:63:TYR:HD1	1:D:83:ASN:HA	1.78	0.48
1:A:58:ALA:N	1:B:50:SER:HB3	2.28	0.48
1:C:325:ILE:HD12	1:C:325:ILE:N	2.28	0.48
1:D:315:THR:OG1	1:D:318:GLU:HG3	2.12	0.48
1:A:214:THR:HG21	1:A:242:LYS:NZ	2.28	0.48
1:B:298:VAL:O	1:B:302:ILE:HG13	2.14	0.48
1:B:88:GLU:HG3	1:B:90:PHE:HE1	1.78	0.48
1:C:192:LEU:HD23	1:C:204:LYS:O	2.13	0.48
1:C:70:LEU:HD21	1:C:80:GLN:HG3	1.95	0.48
1:A:230:VAL:HG13	1:A:235:LEU:HD11	1.95	0.48
1:C:251:VAL:O	1:C:255:ILE:HG13	2.13	0.48
1:D:114:CYS:HB2	1:D:176:TYR:CD2	2.48	0.48
1:D:85:ARG:HD3	1:D:86:THR:N	2.29	0.48
1:A:44:PRO:HB2	1:A:47:HIS:HB2	1.95	0.48
1:A:198:ARG:HG3	1:A:199:PRO:HD2	1.96	0.48
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.48	0.48
1:B:184:HIS:CD2	1:B:205:LEU:HD21	2.49	0.48
1:D:233:GLU:O	1:D:235:LEU:N	2.46	0.48
1:D:150:ILE:HD12	1:D:150:ILE:HA	1.76	0.48
1:D:246:MET:O	1:D:305:LEU:HD22	2.14	0.48
1:B:289:PRO:O	1:B:290:GLU:C	2.52	0.47
1:A:249:LEU:HA	1:A:249:LEU:HD12	1.67	0.47
1:A:302:ILE:HG22	1:A:302:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLU:O	1:B:239:LYS:O	2.32	0.47
1:C:350:GLU:O	1:C:354:GLU:HB3	2.13	0.47
1:D:170:ILE:O	1:D:174:ILE:HG12	2.14	0.47
1:A:233:GLU:HG3	1:D:310:PRO:HG3	1.97	0.47
1:D:240:TYR:HE2	1:D:311:THR:CG2	2.26	0.47
1:A:241:ASP:C	1:A:243:SER:N	2.66	0.47
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.73	0.47
1:B:163:ALA:HA	1:B:256:LEU:HD13	1.97	0.47
1:B:296:GLU:OE1	1:B:299:LYS:HD2	2.15	0.47
1:C:108:HIS:HE1	1:C:138:MET:CE	2.27	0.47
1:D:127:LEU:HD12	1:D:132:LYS:HA	1.97	0.47
1:D:153:ARG:NH2	1:D:162:GLU:OE2	2.47	0.47
1:D:288:ASN:HB3	1:D:289:PRO:HA	1.95	0.47
1:A:263:PHE:CG	1:A:279:ILE:HD13	2.49	0.47
1:C:265:SER:HB2	1:C:355:GLU:OE2	2.14	0.47
1:C:342:LEU:O	1:C:343:LYS:C	2.53	0.47
1:C:287:PRO:HD2	1:C:291:TRP:CD1	2.49	0.47
1:D:251:VAL:O	1:D:255:ILE:HG13	2.15	0.47
1:A:161:ARG:HA	1:A:331:VAL:HG21	1.96	0.47
1:A:175:GLN:HB2	1:A:316:ILE:HG13	1.95	0.47
1:A:330:LYS:CG	1:A:330:LYS:O	2.62	0.47
1:A:196:SER:H	1:A:201:ALA:HB1	1.80	0.47
1:A:56:LYS:O	1:B:51:GLY:N	2.47	0.47
1:B:80:GLN:HG2	1:B:81:ILE:N	2.30	0.47
1:D:108:HIS:O	1:D:108:HIS:HD2	1.97	0.47
1:A:49:LYS:NZ	1:A:113:GLN:HB2	2.30	0.46
1:A:63:TYR:CG	1:A:81:ILE:HD12	2.50	0.46
1:C:82:PHE:HA	1:C:88:GLU:O	2.15	0.46
1:A:167:MET:HG2	1:A:256:LEU:HD12	1.97	0.46
1:A:241:ASP:C	1:A:243:SER:H	2.19	0.46
1:C:322:HIS:HD2	1:C:324:TRP:HB3	1.79	0.46
1:A:158:PHE:HZ	1:A:163:ALA:HA	1.79	0.46
1:A:260:TYR:OH	1:A:287:PRO:CG	2.62	0.46
1:C:174:ILE:HD13	1:C:174:ILE:N	2.28	0.46
1:D:173:ALA:O	1:D:177:LEU:HG	2.16	0.46
1:D:255:ILE:CD1	1:D:261:PRO:HB3	2.45	0.46
1:A:286:PHE:HB3	1:A:291:TRP:CG	2.50	0.46
1:C:275:MET:HG3	1:C:355:GLU:OE2	2.16	0.46
1:D:332:PRO:O	1:D:334:THR:HG23	2.15	0.46
1:B:288:ASN:HB3	1:B:289:PRO:HA	1.97	0.46
1:C:102:ARG:O	1:C:106:GLU:CG	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:SER:HB3	1:A:298:VAL:CG2	2.45	0.46
1:A:49:LYS:HG2	1:A:50:SER:N	2.31	0.46
1:B:90:PHE:CD2	1:B:121:VAL:HG21	2.50	0.46
1:A:147:PHE:HB3	1:A:342:LEU:HD21	1.98	0.46
1:D:167:MET:HG3	1:D:253:MET:HE2	1.97	0.46
1:B:190:GLU:N	1:B:190:GLU:OE2	2.49	0.46
1:B:338:THR:O	1:B:342:LEU:HB2	2.16	0.46
1:D:167:MET:HB3	1:D:167:MET:HE2	1.75	0.46
1:D:239:LYS:CD	1:D:239:LYS:H	2.21	0.46
1:D:301:LEU:HD13	1:D:322:HIS:CD2	2.51	0.46
1:D:161:ARG:NH2	1:D:331:VAL:N	2.63	0.46
1:D:116:HIS:O	1:D:204:LYS:HA	2.16	0.46
1:C:308:THR:O	1:C:310:PRO:HD3	2.16	0.45
1:D:82:PHE:CD2	1:D:89:LYS:HB3	2.50	0.45
1:C:121:VAL:HG12	1:C:122:ASP:N	2.31	0.45
1:C:102:ARG:NH2	1:C:125:GLU:OE2	2.50	0.45
1:C:191:ASN:HA	3:C:3:STU:H272	1.98	0.45
1:C:214:THR:HG21	1:C:242:LYS:HG3	1.97	0.45
1:D:141:LEU:HD22	1:D:195:THR:HA	1.97	0.45
1:D:147:PHE:CE2	1:D:256:LEU:HG	2.51	0.45
1:A:49:LYS:HB2	1:A:113:GLN:NE2	2.30	0.45
1:C:43:PHE:HB3	1:C:44:PRO:CD	2.45	0.45
1:C:83:ASN:C	1:C:83:ASN:OD1	2.55	0.45
1:A:47:HIS:CE1	1:D:273:PRO:HG3	2.52	0.45
1:A:277:THR:O	1:A:281:MET:HG2	2.17	0.45
1:A:288:ASN:HB3	1:A:292:SER:OG	2.16	0.45
1:B:185:ARG:NH1	1:B:241:ASP:OD1	2.49	0.45
1:C:337:HIS:HA	1:C:340:ARG:NH1	2.32	0.45
1:D:64:LYS:CG	1:D:64:LYS:O	2.64	0.45
1:C:52:LEU:HD12	1:C:53:GLN:N	2.32	0.45
1:C:52:LEU:HD21	1:C:123:VAL:CG2	2.46	0.45
1:C:129:ALA:HB1	1:D:273:PRO:HG2	1.98	0.45
1:D:273:PRO:O	1:D:274:GLY:C	2.54	0.45
1:A:116:HIS:O	1:A:204:LYS:HA	2.17	0.45
1:A:212:LYS:HG2	1:A:213:GLU:N	2.32	0.45
1:A:289:PRO:O	1:A:290:GLU:C	2.54	0.45
1:C:175:GLN:HG2	1:C:175:GLN:O	2.15	0.45
1:A:95:LEU:HD11	1:A:136:ILE:HD11	1.97	0.45
1:A:260:TYR:CE2	1:A:290:GLU:HG2	2.49	0.45
1:B:314:MET:HE2	1:B:318:GLU:CB	2.47	0.45
1:C:235:LEU:HB3	1:C:236:GLY:H	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LYS:N	1:D:239:LYS:HD2	2.23	0.45
1:A:107:LEU:HD22	1:A:182:ILE:CD1	2.47	0.44
1:C:72:LEU:H	3:C:3:STU:H262	1.82	0.44
1:C:63:TYR:CD1	1:C:81:ILE:HD12	2.53	0.44
1:D:267:HIS:HE1	1:D:274:GLY:HA2	1.82	0.44
1:D:161:ARG:CA	1:D:331:VAL:HG23	2.46	0.44
1:D:70:LEU:HD12	1:D:78:VAL:HG12	1.98	0.44
1:D:82:PHE:HA	1:D:89:LYS:HA	1.99	0.44
1:D:258:CYS:HB2	1:D:290:GLU:HG2	1.99	0.44
1:D:161:ARG:CB	1:D:331:VAL:HG23	2.47	0.44
1:A:94:MET:HG2	1:A:135:LEU:HD22	1.99	0.44
1:A:78:VAL:HA	1:A:92:LEU:O	2.18	0.44
1:D:87:GLN:CG	1:D:87:GLN:O	2.65	0.44
1:B:190:GLU:N	1:B:190:GLU:CD	2.71	0.44
1:B:332:PRO:CB	1:B:334:THR:HG22	2.27	0.44
1:C:168:LYS:HB2	1:C:325:ILE:HG23	2.00	0.44
1:C:332:PRO:O	1:C:334:THR:HG23	2.17	0.44
1:C:49:LYS:HD2	1:C:113:GLN:HB2	2.00	0.44
1:D:338:THR:O	1:D:342:LEU:N	2.42	0.44
1:A:214:THR:HG21	1:A:242:LYS:HZ3	1.82	0.44
1:A:284:TYR:O	1:A:285:GLU:HB2	2.17	0.44
1:C:188:LYS:HG2	1:C:191:ASN:HD22	1.83	0.44
1:C:327:GLN:HE21	1:C:327:GLN:HB2	1.61	0.44
1:A:192:LEU:C	1:A:193:LEU:HD23	2.37	0.44
1:C:192:LEU:HA	1:C:204:LYS:O	2.17	0.44
1:D:225:TYR:CG	1:D:226:THR:N	2.85	0.44
1:D:304:ASN:O	1:D:314:MET:HB3	2.18	0.44
1:A:198:ARG:HG2	1:A:200:ASN:OD1	2.18	0.44
1:B:111:ALA:HB1	1:B:117:ILE:HD12	2.00	0.44
1:B:166:ILE:O	1:B:170:ILE:HG13	2.17	0.44
1:C:187:VAL:HG12	1:C:187:VAL:O	2.16	0.44
1:C:77:LYS:O	1:C:93:LYS:HA	2.17	0.44
1:D:147:PHE:HE2	1:D:256:LEU:HG	1.82	0.44
1:B:149:ARG:NH2	1:B:201:ALA:HB3	2.32	0.44
1:C:257:LEU:HD12	1:C:302:ILE:HD11	1.99	0.44
1:A:150:ILE:HG23	1:A:150:ILE:O	2.18	0.44
1:B:149:ARG:HH22	1:B:201:ALA:HB3	1.83	0.44
1:C:114:CYS:HA	1:C:115:PRO:HD3	1.82	0.44
1:C:159:THR:O	1:C:162:GLU:N	2.48	0.44
1:C:261:PRO:HD3	1:C:349:TRP:CE2	2.53	0.44
1:D:150:ILE:HD11	1:D:158:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:THR:HG21	1:A:82:PHE:HE1	1.82	0.43
1:C:285:GLU:HG3	1:C:287:PRO:HD3	2.00	0.43
1:D:205:LEU:HD12	1:D:206:THR:N	2.28	0.43
1:A:322:HIS:CE1	1:A:324:TRP:H	2.36	0.43
1:D:309:GLU:OE2	1:D:310:PRO:HD2	2.18	0.43
1:A:168:LYS:O	1:A:172:GLU:HG3	2.19	0.43
1:C:180:ILE:HD11	1:C:182:ILE:HD12	2.00	0.43
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.78	0.43
1:D:55:LYS:HD2	1:D:124:TYR:CE2	2.53	0.43
1:D:63:TYR:CG	1:D:81:ILE:HD12	2.53	0.43
1:C:43:PHE:CB	1:C:44:PRO:CD	2.97	0.43
1:A:158:PHE:O	1:A:336:LEU:HB2	2.18	0.43
1:B:328:SER:C	1:B:330:LYS:H	2.21	0.43
1:C:271:ILE:O	1:C:272:SER:HB2	2.17	0.43
1:D:194:TYR:CE1	1:D:203:LEU:HB2	2.53	0.43
1:A:102:ARG:HD3	1:A:102:ARG:HA	1.83	0.43
1:A:264:TYR:O	1:A:275:MET:HG2	2.18	0.43
1:A:322:HIS:HA	1:A:323:PRO:HD3	1.86	0.43
1:B:257:LEU:HD11	1:B:298:VAL:HG11	2.00	0.43
1:B:86:THR:O	1:B:87:GLN:HB2	2.19	0.43
1:D:128:TYR:HD2	1:D:131:ARG:NH1	2.17	0.43
1:B:274:GLY:C	1:B:278:ARG:HH21	2.21	0.43
1:C:192:LEU:C	1:C:193:LEU:HD23	2.39	0.43
1:C:44:PRO:O	1:C:48:VAL:HG23	2.19	0.43
1:A:51:GLY:O	1:C:56:LYS:HB3	2.18	0.43
1:A:50:SER:HB2	1:C:58:ALA:N	2.34	0.43
1:D:161:ARG:HD2	1:D:333:GLN:HE21	1.80	0.43
1:A:302:ILE:HG22	1:A:306:LEU:HD12	2.01	0.43
1:D:295:SER:C	1:D:297:GLU:H	2.22	0.43
1:C:80:GLN:HE21	1:C:80:GLN:HB3	1.57	0.43
1:D:109:TRP:HA	1:D:120:ILE:HD12	2.00	0.43
1:D:188:LYS:HB2	1:D:189:PRO:HD2	2.01	0.43
1:A:143:GLY:O	1:A:149:ARG:CG	2.66	0.42
1:B:337:HIS:O	1:B:341:VAL:HG23	2.19	0.42
1:B:56:LYS:O	1:C:50:SER:HB2	2.18	0.42
1:B:57:ASN:CA	1:C:50:SER:HB2	2.44	0.42
1:D:171:GLY:HA3	1:D:320:MET:HE3	1.98	0.42
1:D:323:PRO:HA	1:D:326:MET:HB3	2.01	0.42
1:C:255:ILE:HG12	1:C:261:PRO:HA	2.01	0.42
1:C:172:GLU:HA	1:C:320:MET:HE2	2.00	0.42
1:C:161:ARG:HB2	1:C:161:ARG:HE	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:O	1:A:238:GLU:O	2.36	0.42
1:A:164:SER:OG	1:A:324:TRP:O	2.37	0.42
1:A:43:PHE:CG	1:A:44:PRO:HD2	2.53	0.42
1:B:69:VAL:HG12	1:B:71:GLY:H	1.83	0.42
1:C:143:GLY:O	1:C:149:ARG:HD3	2.19	0.42
1:C:187:VAL:O	1:C:248:SER:HB3	2.20	0.42
1:C:336:LEU:C	1:C:338:THR:H	2.22	0.42
1:A:286:PHE:CE1	1:A:299:LYS:HB3	2.53	0.42
1:C:234:VAL:O	1:C:234:VAL:HG12	2.19	0.42
1:C:96:GLN:H	1:C:96:GLN:CD	2.23	0.42
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.81	0.42
1:D:86:THR:O	1:D:87:GLN:CB	2.68	0.42
1:D:125:GLU:HG2	1:D:125:GLU:O	2.20	0.42
1:D:302:ILE:O	1:D:302:ILE:HG22	2.20	0.42
1:D:226:THR:HA	1:D:227:PRO:HD3	1.78	0.42
1:D:253:MET:O	1:D:257:LEU:HG	2.18	0.42
1:C:238:GLU:O	1:C:239:LYS:O	2.37	0.42
1:B:154:GLY:C	1:B:156:GLN:N	2.74	0.42
1:B:304:ASN:O	1:B:313:ARG:HA	2.19	0.42
1:B:74:ILE:O	1:B:75:ASN:HB2	2.20	0.42
1:D:190:GLU:OE1	1:D:190:GLU:N	2.52	0.42
1:D:300:MET:CE	1:D:300:MET:HA	2.50	0.42
1:D:307:LYS:HD3	1:D:312:GLN:HB3	2.02	0.41
1:D:49:LYS:HD2	1:D:113:GLN:CD	2.40	0.41
1:B:264:TYR:H	1:B:264:TYR:HD2	1.64	0.41
1:C:196:SER:H	1:C:201:ALA:HB1	1.84	0.41
1:C:70:LEU:HA	1:C:70:LEU:HD23	1.72	0.41
1:D:245:ASP:O	1:D:249:LEU:HB2	2.21	0.41
1:D:55:LYS:HB2	1:D:124:TYR:CD2	2.55	0.41
1:A:100:LYS:HE2	1:A:103:ARG:HH12	1.86	0.41
1:B:320:MET:HA	1:B:325:ILE:HG21	2.02	0.41
1:B:55:LYS:O	1:B:124:TYR:HA	2.20	0.41
1:C:334:THR:HA	1:C:335:PRO:HD3	1.87	0.41
1:C:138:MET:CE	3:C:3:STU:H13	2.50	0.41
1:A:114:CYS:HA	1:A:115:PRO:HD3	1.79	0.41
1:B:291:TRP:HA	1:B:294:VAL:HG23	2.03	0.41
1:C:247:TRP:O	1:C:251:VAL:HG23	2.20	0.41
1:C:74:ILE:HG13	1:C:207:ASP:OD2	2.19	0.41
1:D:246:MET:HE1	1:D:316:ILE:HA	2.02	0.41
1:D:319:PHE:CE2	1:D:320:MET:HE2	2.56	0.41
1:A:198:ARG:HG3	1:A:199:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:OE1	1:C:56:LYS:HG3	2.20	0.41
1:B:109:TRP:O	1:B:112:SER:HB3	2.20	0.41
1:B:70:LEU:HG	1:B:80:GLN:HB2	2.02	0.41
1:C:307:LYS:HD3	1:C:312:GLN:OE1	2.20	0.41
1:A:53:GLN:HB2	1:C:56:LYS:HG3	2.03	0.41
1:C:95:LEU:N	1:C:95:LEU:HD12	2.36	0.41
1:B:68:GLN:NE2	1:B:80:GLN:OE1	2.54	0.41
1:C:188:LYS:HG2	1:C:191:ASN:ND2	2.35	0.41
1:C:227:PRO:O	1:C:230:VAL:HG12	2.21	0.41
1:A:143:GLY:HA3	1:A:194:TYR:CB	2.50	0.41
1:C:347:GLU:C	1:C:349:TRP:N	2.72	0.41
1:D:128:TYR:HD2	1:D:131:ARG:HH12	1.68	0.41
1:D:225:TYR:O	1:D:226:THR:CB	2.67	0.41
1:A:309:GLU:OE2	1:A:310:PRO:HD2	2.21	0.41
1:D:327:GLN:HG2	1:D:330:LYS:HD3	2.03	0.41
1:A:142:ASP:N	1:A:195:THR:O	2.31	0.41
1:A:175:GLN:HA	1:A:316:ILE:HG12	2.03	0.41
1:D:77:LYS:H	1:D:77:LYS:HG2	1.65	0.41
1:A:273:PRO:O	1:A:274:GLY:C	2.59	0.41
1:B:134:LEU:CD1	1:B:134:LEU:N	2.84	0.41
1:C:111:ALA:HB1	1:C:177:LEU:HD21	2.03	0.41
1:A:229:TYR:CE1	1:D:188:LYS:HB3	2.56	0.40
1:D:59:ILE:N	1:D:126:ASN:OD1	2.52	0.40
1:D:163:ALA:O	1:D:166:ILE:N	2.54	0.40
1:D:325:ILE:HG22	1:D:326:MET:N	2.36	0.40
1:B:106:GLU:O	1:B:110:ARG:HG3	2.22	0.40
1:B:134:LEU:N	1:B:134:LEU:HD12	2.35	0.40
1:B:56:LYS:HG3	1:C:53:GLN:HE21	1.86	0.40
1:A:147:PHE:CE1	1:A:255:ILE:HG21	2.57	0.40
1:B:147:PHE:CZ	1:B:255:ILE:CG2	3.05	0.40
1:D:145:GLU:HG2	1:D:193:LEU:HD22	2.02	0.40
1:A:161:ARG:HB2	1:A:331:VAL:HG23	2.02	0.40
1:B:185:ARG:O	1:B:185:ARG:HG3	2.21	0.40
1:C:149:ARG:CG	1:C:149:ARG:NH1	2.52	0.40
1:B:159:THR:HG22	1:B:162:GLU:CB	2.51	0.40
1:B:257:LEU:HA	1:B:336:LEU:HD23	2.03	0.40
1:D:302:ILE:HG22	1:D:306:LEU:HD12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ARG:NH2	1:D:233:GLU:OE1[2_545]	2.19	0.01

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	285/324 (88%)	248 (87%)	31 (11%)	6 (2%)	7	26
1	B	277/324 (86%)	238 (86%)	32 (12%)	7 (2%)	5	21
1	C	303/324 (94%)	244 (80%)	45 (15%)	14 (5%)	2	9
1	D	282/324 (87%)	228 (81%)	39 (14%)	15 (5%)	2	6
All	All	1147/1296 (88%)	958 (84%)	147 (13%)	42 (4%)	3	13

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	GLU
1	A	239	LYS
1	A	330	LYS
1	A	345	ASP
1	B	239	LYS
1	C	238	GLU
1	C	239	LYS
1	C	270	ALA
1	C	346	LYS
1	D	234	VAL
1	D	237	PRO
1	D	238	GLU
1	D	338	THR
1	B	143	GLY
1	B	155	ASP
1	C	207	ASP
1	C	268	GLY

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Mol	Chain	Res	Type
1	D	225	TYR
1	D	233	GLU
1	B	207	ASP
1	C	44	PRO
1	C	258	CYS
1	D	85	ARG
1	D	226	THR
1	D	266	ASN
1	D	314	MET
1	A	98	CYS
1	A	290	GLU
1	D	235	LEU
1	D	258	CYS
1	D	273	PRO
1	D	330	LYS
1	B	238	GLU
1	C	97	ASP
1	C	342	LEU
1	B	149	ARG
1	B	237	PRO
1	C	98	CYS
1	C	99	PRO
1	C	149	ARG
1	D	199	PRO
1	C	272	SER

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	261/293 (89%)	243 (93%)	18 (7%)	15	41
1	B	256/293 (87%)	231 (90%)	25 (10%)	8	24
1	C	276/293 (94%)	249 (90%)	27 (10%)	8	24
1	D	261/293 (89%)	239 (92%)	22 (8%)	11	31
All	All	1054/1172 (90%)	962 (91%)	92 (9%)	10	30

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	50	SER
1	A	66	THR
1	A	77	LYS
1	A	106	GLU
1	A	127	LEU
1	A	140	CYS
1	A	149	ARG
1	A	150	ILE
1	A	152	ASP
1	A	200	ASN
1	A	249	LEU
1	A	267	HIS
1	A	272	SER
1	A	277	THR
1	A	280	ARG
1	A	285	GLU
1	A	311	THR
1	B	45	GLN
1	B	46	PHE
1	B	47	HIS
1	B	66	THR
1	B	85	ARG
1	B	106	GLU
1	B	117	ILE
1	B	127	LEU
1	B	131	ARG
1	B	140	CYS
1	B	142	ASP
1	B	149	ARG
1	B	190	GLU
1	B	202	ILE
1	B	233	GLU
1	B	240	TYR
1	B	244	CYS
1	B	256	LEU
1	B	264	TYR
1	B	275	MET
1	B	295	SER
1	B	301	LEU
1	B	329	THR
1	B	334	THR

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Mol	Chain	Res	Type
1	B	343	LYS
1	C	42	GLN
1	C	43	PHE
1	C	47	HIS
1	C	80	GLN
1	C	87	GLN
1	C	89	LYS
1	C	95	LEU
1	C	113	GLN
1	C	149	ARG
1	C	153	ARG
1	C	174	ILE
1	C	198	ARG
1	C	200	ASN
1	C	202	ILE
1	C	210	PHE
1	C	235	LEU
1	C	269	LEU
1	C	275	MET
1	C	293	GLU
1	C	307	LYS
1	C	327	GLN
1	C	329	THR
1	C	330	LYS
1	C	334	THR
1	C	336	LEU
1	C	344	GLU
1	C	354	GLU
1	D	66	THR
1	D	85	ARG
1	D	122	ASP
1	D	131	ARG
1	D	132	LYS
1	D	150	ILE
1	D	161	ARG
1	D	175	GLN
1	D	190	GLU
1	D	197	LYS
1	D	224	CYS
1	D	239	LYS
1	D	241	ASP
1	D	256	LEU

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Mol	Chain	Res	Type
1	D	264	TYR
1	D	276	LYS
1	D	283	GLN
1	D	327	GLN
1	D	334	THR
1	D	336	LEU
1	D	340	ARG
1	D	341	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	108	HIS
1	A	113	GLN
1	A	151	GLN
1	A	288	ASN
1	A	312	GLN
1	A	337	HIS
1	B	45	GLN
1	B	68	GLN
1	B	83	ASN
1	B	113	GLN
1	B	181	ASN
1	B	333	GLN
1	C	47	HIS
1	C	53	GLN
1	C	68	GLN
1	C	80	GLN
1	C	87	GLN
1	C	96	GLN
1	C	108	HIS
1	C	151	GLN
1	C	191	ASN
1	C	266	ASN
1	C	304	ASN
1	C	322	HIS
1	C	327	GLN
1	D	47	HIS
1	D	57	ASN
1	D	96	GLN
1	D	175	GLN

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Mol	Chain	Res	Type
1	D	267	HIS
1	D	333	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are 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	$\#|Z| > 2$
2	B18	A	1	-	28,34,34	2.47	8 (28%)	31,49,49	1.05	3 (9%)
3	STU	C	3	-	30,42,42	1.94	4 (13%)	31,68,68	2.17	6 (19%)
2	B18	B	2	-	28,34,34	2.47	9 (32%)	31,49,49	1.02	2 (6%)

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
2	B18	A	1	-	-	2/12/31/31	0/4/4/4
3	STU	C	3	-	-	2/4/42/42	-
2	B18	B	2	-	-	3/12/31/31	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	STU	O6-C22	7.51	1.54	1.42
2	A	1	B18	C18-N17	6.92	1.48	1.36
2	B	2	B18	C18-N17	6.50	1.48	1.36
2	B	2	B18	C07-C03	5.73	1.46	1.40
2	A	1	B18	C07-C03	5.33	1.46	1.40
2	A	1	B18	C08-C13	-4.76	1.37	1.47
2	B	2	B18	C08-C13	-4.11	1.39	1.47
2	B	2	B18	C21-C23	-3.97	1.41	1.50
2	A	1	B18	C21-C23	-3.89	1.41	1.50
2	B	2	B18	C02-C01	3.48	1.43	1.37
2	B	2	B18	C11-N12	3.47	1.50	1.46
2	A	1	B18	C11-N12	3.30	1.49	1.46
2	A	1	B18	C02-C01	3.29	1.43	1.37
2	B	2	B18	C07-C10	3.17	1.55	1.51
2	A	1	B18	C07-C10	2.92	1.55	1.51
2	B	2	B18	C06-C01	2.86	1.44	1.39
2	B	2	B18	C05-C06	2.74	1.42	1.36
3	C	3	STU	C2-C1	2.72	1.42	1.36
3	C	3	STU	C5-C20	2.64	1.45	1.41
2	A	1	B18	C05-C06	2.37	1.41	1.36
3	C	3	STU	C24-C25	2.27	1.56	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	STU	C9-N1-C8	-5.09	108.95	113.85
3	C	3	STU	C26-C21-C22	-4.71	103.47	112.64
3	C	3	STU	C10-C9-N1	4.67	106.51	101.76
3	C	3	STU	C7-C8-N1	4.18	110.60	106.37
3	C	3	STU	O5-C8-C7	-3.87	124.73	129.32
2	A	1	B18	C08-N09-C04	3.19	110.44	103.90
2	B	2	B18	C08-N09-C04	3.17	110.41	103.90
3	C	3	STU	C24-C23-N4	-2.89	105.75	112.17
2	A	1	B18	O14-C13-C08	-2.62	119.25	124.37
2	B	2	B18	O14-C13-C08	-2.47	119.54	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	B18	C31-C10-C11	-2.42	107.02	112.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	STU	C24-C23-N4-C28
3	C	3	STU	C22-C23-N4-C28
2	A	1	B18	N24-C26-C27-N28
2	A	1	B18	C26-C27-N28-C30
2	B	2	B18	N24-C26-C27-N28
2	B	2	B18	C26-C27-N28-C29
2	B	2	B18	C26-C27-N28-C30

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	STU	8	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 B18 A 1

Bond lengths

Bond angles

Torsions

Rings

Ligand STU C 3

Bond lengths

Bond angles

Torsions

Rings

Ligand B18 B 2

Bond lengths

Bond angles

Torsions

Rings
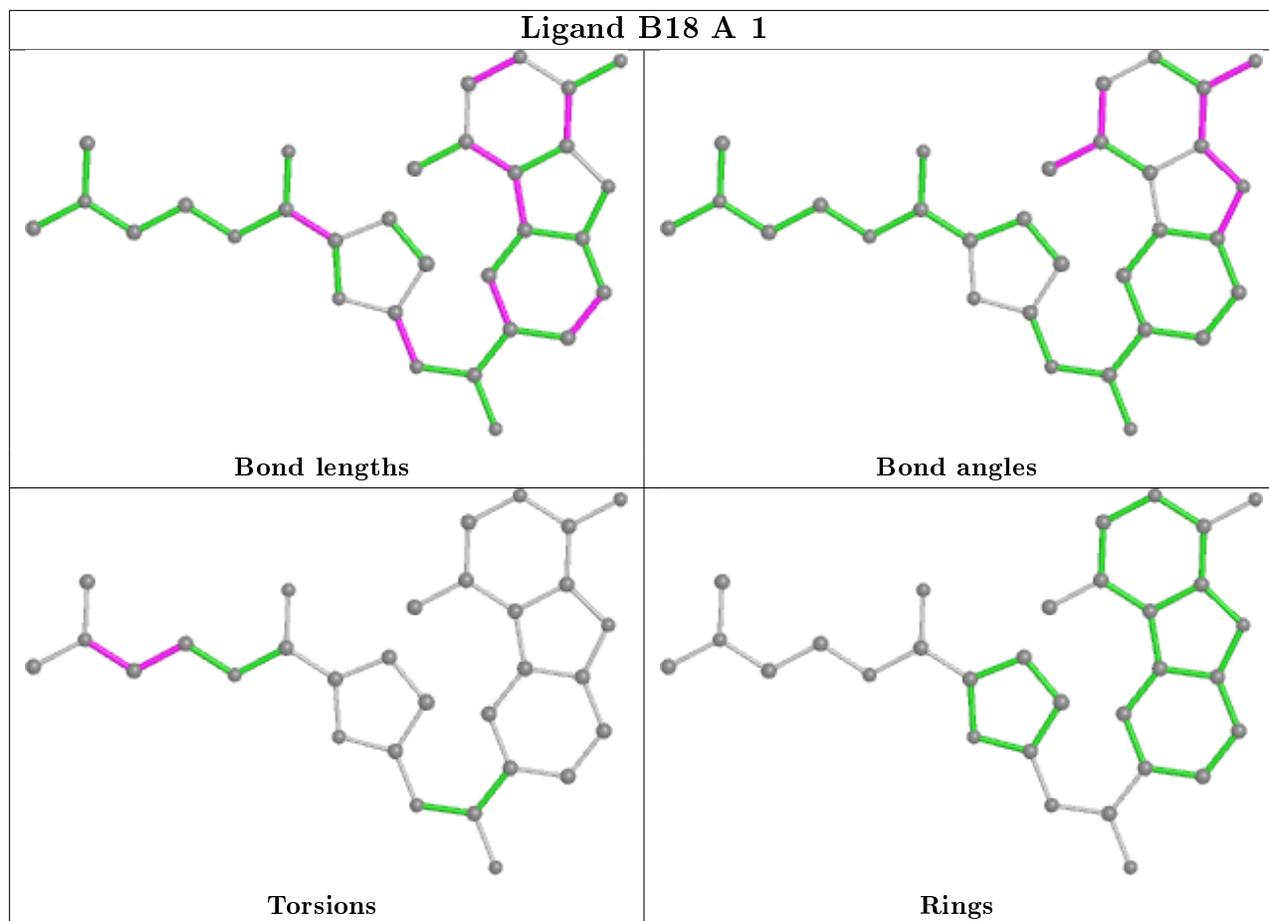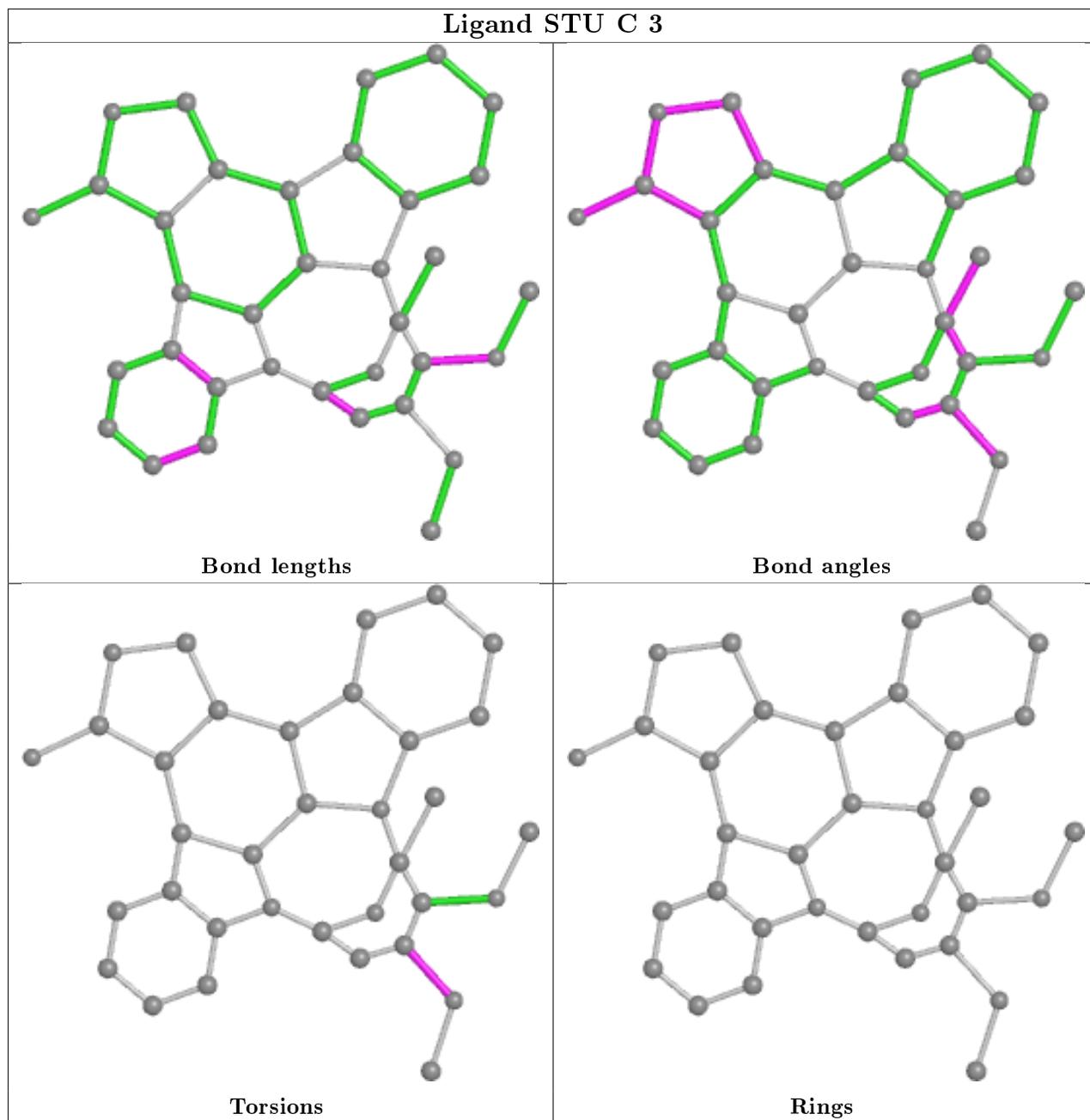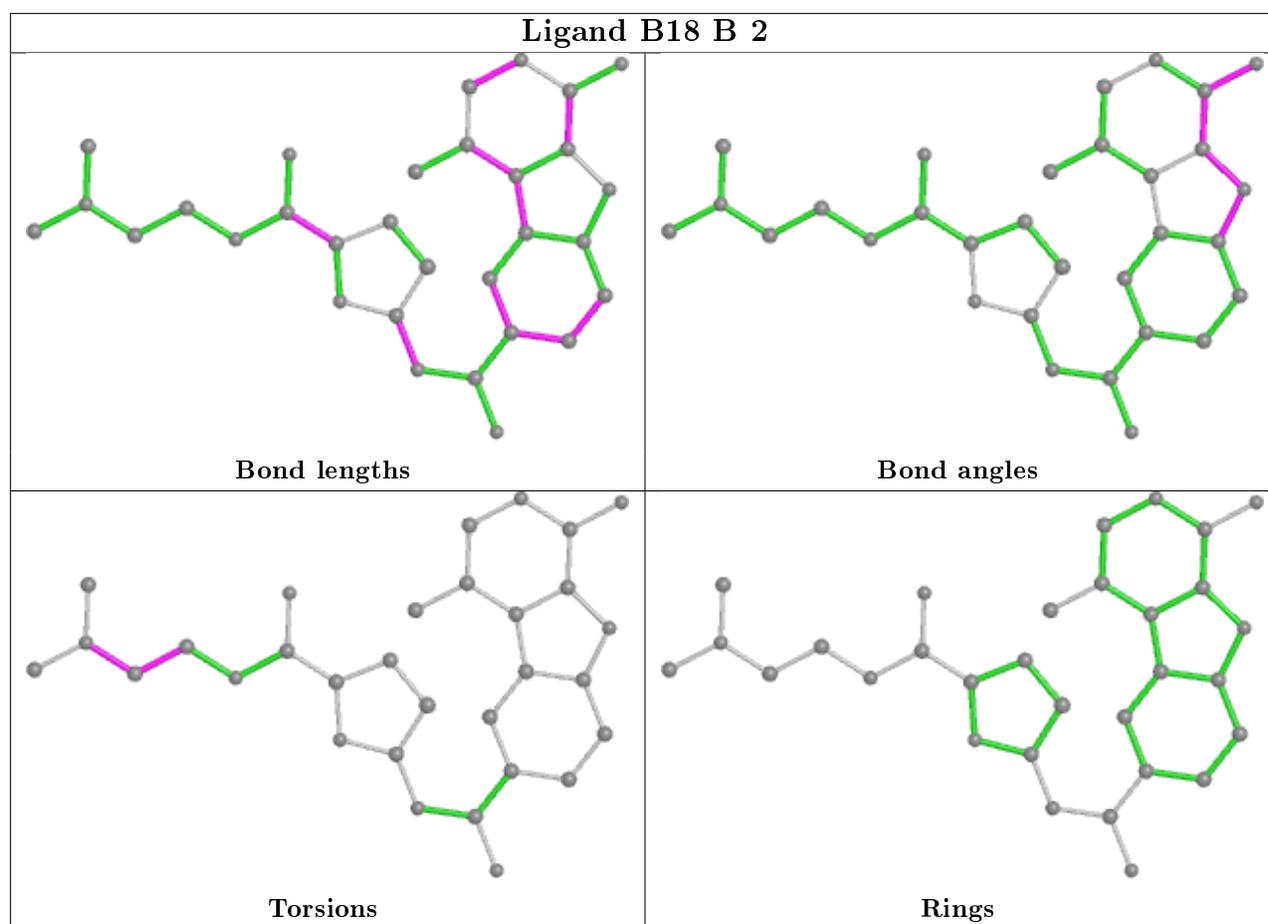
5.7 Other polymers (i)

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.