



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3JBR  
EMDB ID: : EMD-6475  
Title : Cryo-EM structure of the rabbit voltage-gated calcium channel Cav1.1 complex at 4.2 angstrom  
Authors : Wu, J.P.; Yan, Z.; Yan, N.  
Deposited on : 2015-09-29  
Resolution : 4.20 Å(reported)  
Based on PDB ID : 1T0J

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

---

MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

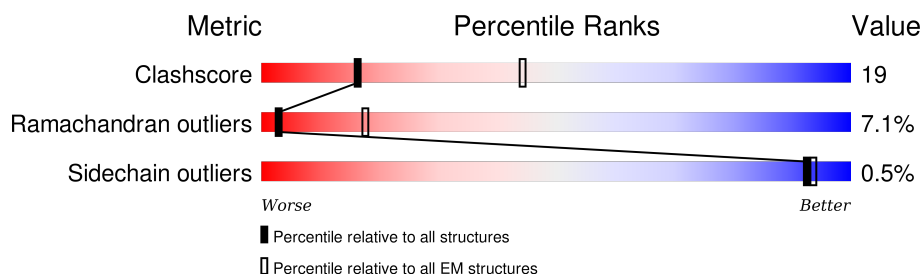
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1873	
2	B	356	
3	E	222	
4	F	1106	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16467 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1224	Total	C	N	O	S	0	0
			7601	4843	1330	1400	28		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	281	Total	C	N	O	S	0	0
			2210	1405	385	411	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLY	-	EXPRESSION TAG	UNP Q8VGC3
B	15	HIS	-	EXPRESSION TAG	UNP Q8VGC3
B	16	MET	-	EXPRESSION TAG	UNP Q8VGC3
B	201	MET	-	LINKER	UNP Q8VGC3

- Molecule 3 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	138	Total	C	N	O	0	0
			688	410	138	140		

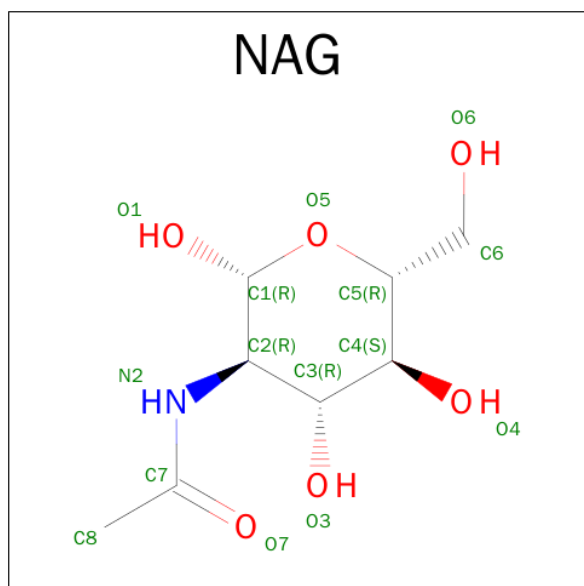
- Molecule 4 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	872	Total	C	N	O	S	0	0
			5735	3570	1042	1108	15		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



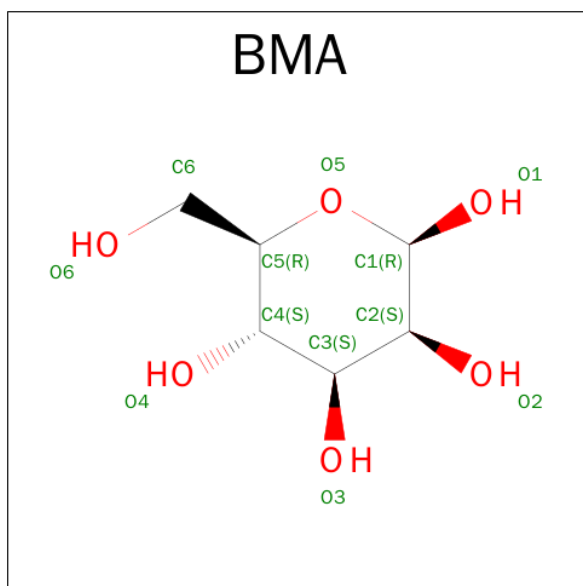
Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	

*Continued on next page...*

*Continued from previous page...*

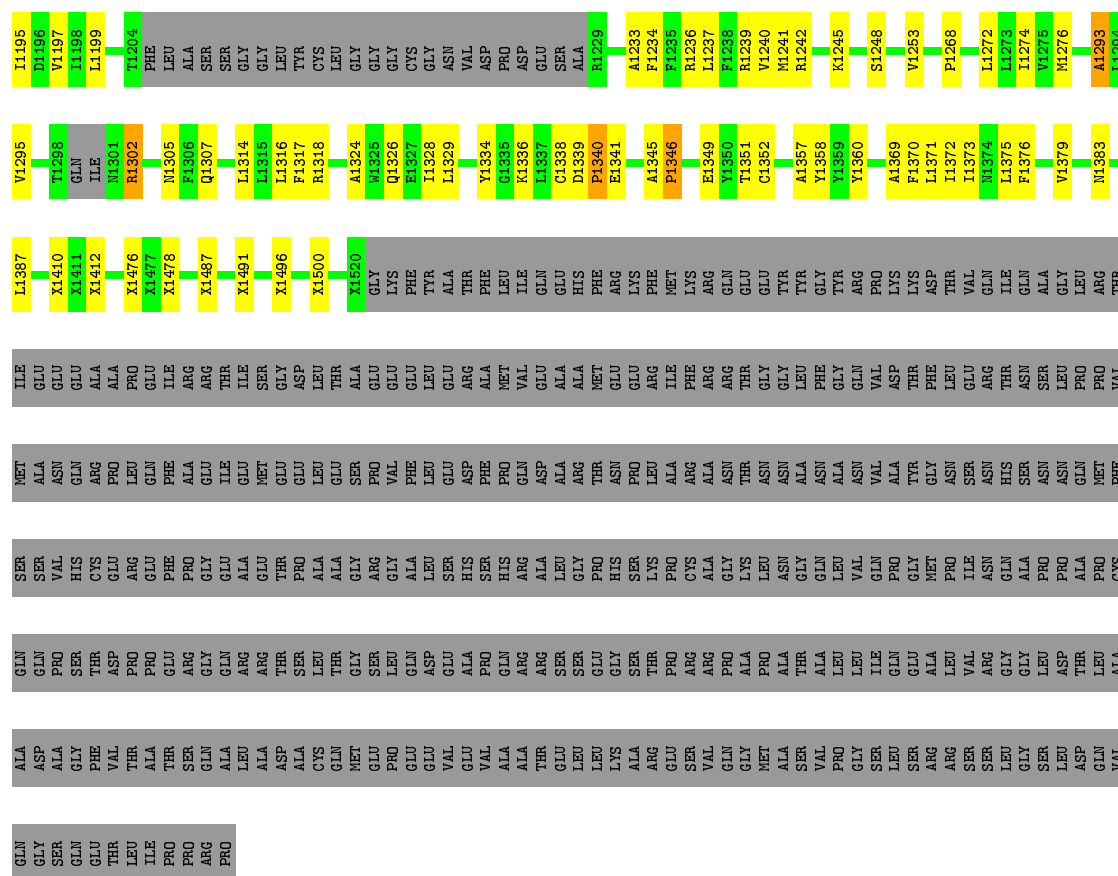
Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	
6	F	1	Total	C	N	O	0
			210	120	15	75	

- Molecule 7 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

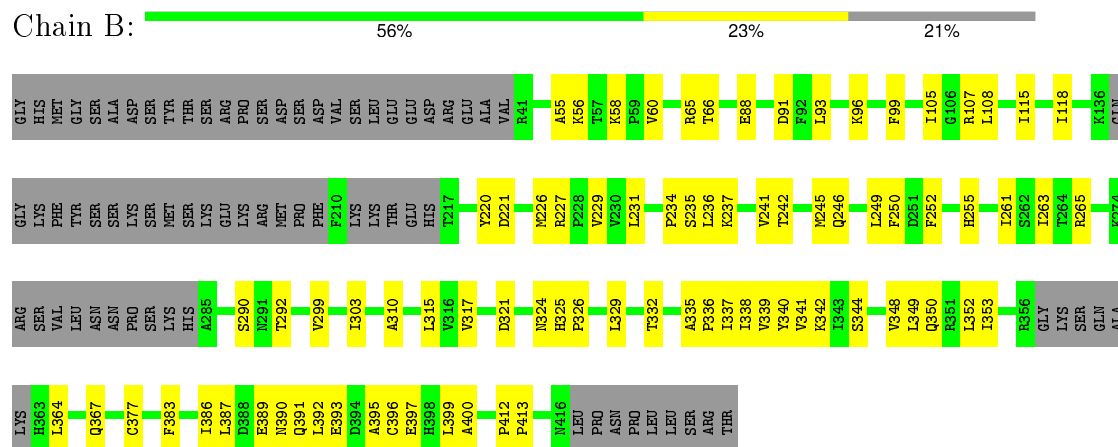


Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			22	12	10	
7	F	1	Total	C	O	0
			22	12	10	

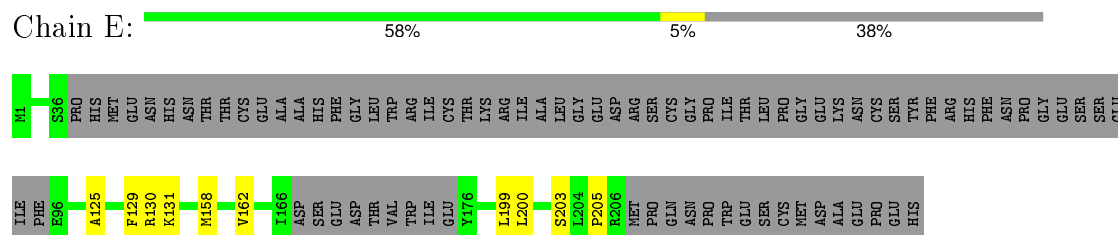




• Molecule 2: Voltage-dependent L-type calcium channel subunit beta-2



• Molecule 3: Voltage-dependent calcium channel gamma-1 subunit



- Chain F:  46% 29% 1% 21%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	353372	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	2.0	Depositor
Maximum defocus (nm)	3.3	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.45	0/7080	0.57	19/9723 (0.2%)
2	B	0.22	0/2252	0.40	0/3051
3	E	0.31	0/685	0.45	0/950
4	F	0.48	1/4603 (0.0%)	0.67	14/6265 (0.2%)
All	All	0.43	1/14620 (0.0%)	0.58	33/19989 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	627	PRO	N-CD	5.04	1.54	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	PRO	N-CA-CB	6.39	110.96	103.30
1	A	1346	PRO	N-CA-CB	6.35	110.92	103.30
1	A	457	PRO	N-CA-CB	6.34	110.91	103.30
1	A	73	PRO	N-CA-CB	6.10	110.62	103.30
1	A	253	PRO	N-CA-CB	6.10	110.62	103.30
1	A	242	PRO	N-CA-CB	6.08	110.60	103.30
4	F	135	PRO	N-CA-CB	6.07	110.59	103.30
4	F	553	PRO	N-CA-CB	6.01	110.51	103.30
1	A	1103	PRO	N-CA-CB	5.99	110.49	103.30
1	A	75	PRO	N-CA-CB	5.98	110.48	103.30
4	F	1059	PRO	N-CA-CB	5.95	110.44	103.30
4	F	171	PRO	N-CA-CB	5.95	110.44	103.30
4	F	653	PRO	N-CA-CB	5.94	110.42	103.30
1	A	821	PRO	N-CA-CB	5.93	110.42	103.30
4	F	142	PRO	N-CA-CB	5.93	110.42	103.30
4	F	1053	PRO	N-CA-CB	5.91	110.39	103.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1340	PRO	N-CA-CB	5.85	110.31	103.30
4	F	1046	PRO	N-CA-CB	5.84	110.30	103.30
4	F	1044	PRO	N-CA-CB	5.82	110.28	103.30
4	F	485	LEU	CA-CB-CG	-5.81	101.94	115.30
4	F	1028	PRO	N-CA-CB	5.80	110.26	103.30
1	A	904	PRO	N-CA-CB	5.80	110.26	103.30
4	F	626	LEU	C-N-CD	5.78	140.53	128.40
1	A	1268	PRO	N-CA-CB	5.74	110.19	103.30
4	F	74	PRO	N-CA-CB	5.74	110.19	103.30
1	A	521	PRO	N-CA-CB	5.71	110.15	103.30
1	A	268	PRO	N-CA-CB	5.69	110.13	103.30
1	A	1106	PRO	N-CA-CB	5.67	110.10	103.30
1	A	39	PRO	N-CA-CB	5.59	110.01	103.30
1	A	266	PRO	N-CA-CB	5.53	109.93	103.30
4	F	309	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	1033	PRO	N-CA-CB	5.10	109.42	103.30
1	A	244	PRO	N-CA-CB	5.04	109.35	103.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	7601	0	5495	201	0
2	B	2210	0	2208	65	0
3	E	688	0	336	4	0
4	F	5735	0	4413	281	0
5	A	1	0	0	0	0
6	F	210	0	195	11	0
7	F	22	0	20	2	0
All	All	16467	0	12667	542	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 19.

All (542) 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)
4:F:607:ARG:HA	4:F:627:PRO:HD3	1.21	1.14
4:F:607:ARG:HA	4:F:627:PRO:CD	1.84	1.07
4:F:626:LEU:O	4:F:628:THR:N	2.02	0.92
4:F:248:GLN:HE21	4:F:447:GLN:HG2	1.37	0.89
4:F:606:ASN:O	4:F:627:PRO:HD2	1.73	0.88
1:A:256:ILE:H	1:A:257:ASN:HA	1.39	0.87
1:A:1274:ILE:HA	1:A:1371:LEU:HD21	1.58	0.86
4:F:75:ASN:CB	4:F:630:SER:O	2.23	0.85
4:F:1008:VAL:HG12	4:F:1009:GLU:H	1.45	0.81
1:A:1373:ILE:HA	1:A:1376:PHE:HD2	1.43	0.81
4:F:601:TYR:HA	4:F:1017:ILE:HG21	1.64	0.79
4:F:238:TYR:HE1	4:F:243:ARG:HD2	1.48	0.77
1:A:367:MET:SD	2:B:352:LEU:HD23	2.24	0.77
4:F:523:VAL:HG12	4:F:524:LEU:HG	1.67	0.77
4:F:626:LEU:O	4:F:628:THR:HG22	1.85	0.75
4:F:169:HIS:HB3	4:F:216:LEU:HB2	1.69	0.75
4:F:570:ASN:HD21	4:F:594:VAL:HG21	1.52	0.75
1:A:983:MET:HG3	4:F:235:ILE:HD12	1.67	0.75
4:F:302:ASP:HB2	4:F:306:PHE:HE1	1.52	0.74
4:F:509:CYS:SG	4:F:561:LEU:N	2.60	0.74
4:F:346:LEU:O	4:F:353:ARG:NH1	2.22	0.73
2:B:226:MET:H	2:B:310:ALA:HB1	1.53	0.72
1:A:1070:GLU:OE2	1:A:1070:GLU:HA	1.88	0.72
1:A:1067:THR:HA	1:A:1070:GLU:HB2	1.71	0.71
4:F:182:LEU:HD23	4:F:185:LEU:HD12	1.72	0.71
1:A:1233:ALA:HA	1:A:1236:ARG:HE	1.56	0.71
4:F:437:VAL:HA	4:F:469:PHE:HE2	1.55	0.71
4:F:73:GLU:O	4:F:632:TYR:N	2.24	0.71
2:B:99:PHE:HB2	2:B:105:ILE:HG13	1.72	0.70
4:F:607:ARG:CA	4:F:627:PRO:HD3	2.11	0.70
4:F:238:TYR:CE1	4:F:243:ARG:HD2	2.27	0.70
2:B:325:HIS:NE2	2:B:377:CYS:SG	2.65	0.70
4:F:502:LEU:O	4:F:622:LEU:HB3	1.92	0.69
4:F:461:VAL:HG22	4:F:484:GLN:HA	1.73	0.69
4:F:883:UNK:HA	4:F:892:UNK:HA	1.75	0.69
2:B:231:LEU:O	2:B:246:GLN:NE2	2.25	0.69
4:F:345:GLN:O	4:F:348:ASN:ND2	2.26	0.69
4:F:356:CYS:SG	4:F:357:ASN:N	2.61	0.69
1:A:201:LEU:O	1:A:205:PHE:N	2.25	0.69
4:F:184:GLU:HA	4:F:187:TRP:NE1	2.08	0.68
4:F:606:ASN:O	4:F:627:PRO:CD	2.42	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:343:PHE:HE1	4:F:384:VAL:HG11	1.56	0.68
4:F:1009:GLU:O	4:F:1011:LEU:N	2.26	0.68
4:F:573:LYS:HA	4:F:576:ILE:HD12	1.76	0.68
4:F:212:SER:OG	4:F:213:ALA:N	2.25	0.67
4:F:1004:ARG:NH1	4:F:1035:ILE:O	2.28	0.67
4:F:500:LYS:HG2	4:F:501:ARG:O	1.94	0.67
1:A:365:GLY:O	1:A:368:SER:OG	2.11	0.67
2:B:229:VAL:HG22	2:B:337:ILE:HB	1.76	0.67
2:B:389:GLU:HB2	2:B:395:ALA:HB2	1.77	0.67
1:A:165:ARG:HB3	1:A:579:GLN:HE21	1.60	0.66
4:F:520:ASN:ND2	4:F:560:THR:O	2.29	0.66
4:F:502:LEU:HD12	4:F:512:GLY:HA3	1.78	0.66
4:F:516:ALA:HB3	4:F:1007:HIS:HE1	1.61	0.65
4:F:184:GLU:HA	4:F:187:TRP:HE1	1.60	0.65
1:A:1373:ILE:HA	1:A:1376:PHE:CD2	2.30	0.65
4:F:210:PHE:HB3	4:F:217:ALA:HB3	1.79	0.65
4:F:343:PHE:CE1	4:F:384:VAL:HG11	2.31	0.64
4:F:516:ALA:HB3	4:F:1007:HIS:CE1	2.32	0.64
4:F:1036:GLN:O	4:F:1038:GLU:N	2.30	0.64
4:F:225:TRP:NE1	4:F:236:ASP:OD1	2.31	0.64
4:F:335:TYR:OH	4:F:369:GLU:O	2.05	0.64
1:A:644:LEU:O	1:A:648:GLY:N	2.28	0.64
1:A:309:TRP:HA	1:A:311:TRP:CD1	2.32	0.64
4:F:242:ARG:HH11	4:F:425:THR:HG23	1.61	0.64
4:F:257:LEU:HB3	4:F:360:ILE:HG22	1.79	0.64
4:F:680:UNK:O	4:F:682:UNK:N	2.31	0.63
1:A:1034:VAL:O	1:A:1036:ASN:N	2.31	0.63
1:A:165:ARG:HB3	1:A:579:GLN:NE2	2.14	0.63
4:F:282:LEU:HB3	4:F:317:LYS:HZ3	1.64	0.62
1:A:90:GLU:HB3	1:A:171:ARG:HH12	1.63	0.62
1:A:1172:PHE:O	1:A:1174:ALA:N	2.33	0.62
4:F:999:CYS:HB2	4:F:1019:ILE:H	1.63	0.62
4:F:585:SER:HB2	4:F:611:TRP:HH2	1.63	0.62
4:F:449:THR:HG22	4:F:463:THR:H	1.64	0.62
4:F:98:ALA:HB1	4:F:199:ARG:HE	1.63	0.62
1:A:211:ALA:O	1:A:215:LEU:N	2.33	0.62
1:A:369:TRP:HZ3	2:B:392:LEU:HA	1.65	0.62
4:F:417:SER:OG	4:F:418:ILE:N	2.33	0.62
4:F:196:LYS:HD3	4:F:219:TYR:HB2	1.81	0.62
4:F:132:ASP:N	4:F:140:SER:O	2.33	0.61
2:B:234:PRO:HD2	2:B:242:THR:HG23	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:VAL:HG22	2:B:387:LEU:HD12	1.82	0.61
2:B:237:LYS:H	2:B:324:ASN:HD21	1.46	0.61
4:F:95:ARG:NH2	4:F:204:SER:O	2.32	0.61
4:F:311:GLN:HA	4:F:316:ASN:HD22	1.65	0.61
4:F:606:ASN:ND2	6:F:1211:NAG:O7	2.32	0.61
1:A:1370:PHE:HA	1:A:1373:ILE:HD12	1.82	0.61
4:F:500:LYS:HZ2	4:F:502:LEU:HD13	1.65	0.61
3:E:200:LEU:O	3:E:203:SER:OG	2.16	0.61
2:B:56:LYS:HA	2:B:115:ILE:HG13	1.83	0.60
4:F:607:ARG:HA	4:F:627:PRO:HD2	1.79	0.60
2:B:60:VAL:HA	2:B:96:LYS:HD3	1.83	0.60
1:A:309:TRP:O	1:A:312:ILE:HG22	2.01	0.60
4:F:1005:ILE:HG22	4:F:1007:HIS:H	1.65	0.60
4:F:379:ASN:HD21	4:F:382:LYS:HA	1.66	0.60
4:F:500:LYS:HE3	4:F:502:LEU:HB2	1.84	0.60
1:A:645:PHE:O	1:A:649:ASN:N	2.31	0.60
4:F:911:UNK:O	4:F:915:UNK:N	2.35	0.60
1:A:584:ARG:O	1:A:586:ASP:N	2.31	0.60
4:F:188:THR:HG23	4:F:189:SER:H	1.67	0.60
1:A:288:CYS:HA	1:A:294:TRP:HB3	1.83	0.60
1:A:131:PHE:CD1	1:A:164:LEU:HB3	2.37	0.59
4:F:297:ASN:C	4:F:299:ASN:H	2.04	0.59
4:F:263:SER:O	4:F:265:SER:N	2.36	0.59
1:A:995:PHE:HB3	1:A:1006:SER:HB2	1.85	0.59
4:F:402:GLN:NE2	4:F:1063:PHE:O	2.36	0.59
1:A:602:GLN:O	1:A:605:ILE:HG13	2.02	0.59
4:F:570:ASN:O	4:F:572:ILE:N	2.33	0.59
1:A:973:TYR:HE1	4:F:235:ILE:HG21	1.67	0.59
1:A:131:PHE:HA	1:A:164:LEU:HD22	1.85	0.59
2:B:252:PHE:HA	2:B:255:HIS:CD2	2.37	0.59
2:B:231:LEU:HA	2:B:339:VAL:HB	1.83	0.59
4:F:242:ARG:NH1	4:F:421:ILE:O	2.36	0.58
4:F:298:SER:N	4:F:332:ILE:O	2.37	0.58
1:A:944:CYS:O	1:A:948:GLN:HG2	2.04	0.58
4:F:1008:VAL:HG11	4:F:1013:ASN:HD22	1.67	0.58
1:A:1070:GLU:O	1:A:1074:THR:N	2.35	0.58
2:B:390:ASN:OD1	2:B:391:GLN:N	2.35	0.58
1:A:1237:LEU:O	1:A:1241:MET:HG2	2.04	0.58
4:F:463:THR:HG22	4:F:482:LYS:HA	1.85	0.58
4:F:256:MET:HG3	4:F:285:LEU:HD11	1.84	0.58
2:B:290:SER:OG	2:B:292:THR:OG1	2.19	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:UNK:O	1:A:1500:UNK:N	2.36	0.57
4:F:372:GLN:HA	4:F:375:PHE:CD2	2.39	0.57
4:F:359:ILE:HB	4:F:385:ARG:HB2	1.86	0.57
4:F:210:PHE:CD2	4:F:479:THR:HG22	2.40	0.57
1:A:592:VAL:O	1:A:594:ARG:N	2.36	0.57
4:F:614:VAL:HG12	4:F:616:GLY:H	1.70	0.57
4:F:470:ASN:HD22	4:F:473:GLY:H	1.53	0.57
4:F:569:GLU:OE2	4:F:571:ASP:N	2.36	0.57
2:B:88:GLU:N	2:B:91:ASP:OD2	2.37	0.57
2:B:265:ARG:NH2	2:B:321:ASP:OD2	2.38	0.57
6:F:1209:NAG:HO4	7:F:1217:BMA:HO2	1.51	0.57
1:A:363:LEU:HA	2:B:348:VAL:HG13	1.87	0.56
4:F:497:GLU:OE1	4:F:497:GLU:N	2.38	0.56
1:A:1067:THR:O	1:A:1071:GLN:N	2.34	0.56
2:B:241:VAL:O	2:B:245:MET:HG3	2.05	0.56
2:B:341:VAL:HA	2:B:387:LEU:HB2	1.87	0.56
1:A:322:SER:O	1:A:326:LEU:HG	2.04	0.56
4:F:131:ASP:HA	4:F:141:GLU:HA	1.86	0.56
4:F:662:UNK:O	4:F:666:UNK:N	2.38	0.56
6:F:1203:NAG:O4	6:F:1204:NAG:O7	2.19	0.56
2:B:299:VAL:O	2:B:303:ILE:HG12	2.04	0.56
4:F:206:LEU:O	4:F:220:TYR:OH	2.24	0.56
4:F:322:ASP:HA	4:F:325:ASN:ND2	2.20	0.56
4:F:1004:ARG:HG2	4:F:1014:THR:HG22	1.87	0.56
4:F:589:THR:HG21	4:F:610:THR:HA	1.88	0.56
1:A:216:GLU:O	1:A:220:GLY:N	2.35	0.56
2:B:261:ILE:HA	2:B:315:LEU:HB2	1.88	0.56
1:A:233:ILE:O	1:A:235:ALA:N	2.38	0.56
1:A:1043:ILE:HG22	1:A:1047:ILE:HD11	1.89	0.55
4:F:210:PHE:HE1	4:F:212:SER:HB2	1.71	0.55
1:A:1064:VAL:O	1:A:1067:THR:OG1	2.15	0.55
4:F:243:ARG:HH12	4:F:455:ALA:H	1.55	0.55
1:A:975:TYR:HE1	1:A:983:MET:HB3	1.71	0.55
4:F:307:GLN:O	4:F:308:HIS:ND1	2.40	0.55
2:B:350:GLN:HA	2:B:364:LEU:HD11	1.89	0.55
4:F:63:TYR:O	4:F:67:GLN:N	2.40	0.55
2:B:353:ILE:HD13	2:B:367:GLN:OE1	2.07	0.55
4:F:336:LYS:HA	4:F:339:PHE:CD2	2.41	0.55
1:A:34:LEU:O	1:A:36:LEU:N	2.40	0.55
4:F:264:GLY:N	4:F:331:GLY:O	2.36	0.55
1:A:1124:MET:HA	1:A:1127:LEU:HD12	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:O	1:A:222:MET:N	2.40	0.54
4:F:308:HIS:HB2	4:F:309:LEU:HG	1.89	0.54
2:B:387:LEU:HD21	2:B:399:LEU:HB2	1.89	0.54
4:F:298:SER:HB2	4:F:332:ILE:HG13	1.90	0.54
4:F:375:PHE:O	4:F:379:ASN:N	2.32	0.54
1:A:1158:THR:HG21	1:A:1197:VAL:HG21	1.90	0.54
4:F:602:ILE:HG22	4:F:603:ASP:O	2.08	0.54
4:F:259:LEU:HB3	4:F:296:PHE:HE1	1.72	0.54
1:A:1239:ARG:HG3	1:A:1242:ARG:CZ	2.38	0.54
2:B:252:PHE:CZ	2:B:396:CYS:HB3	2.43	0.54
1:A:1055:PHE:O	1:A:1059:ILE:HG13	2.08	0.54
1:A:322:SER:O	1:A:325:ILE:HG13	2.08	0.54
4:F:248:GLN:NE2	4:F:447:GLN:HG2	2.17	0.53
4:F:182:LEU:HA	4:F:185:LEU:HD12	1.89	0.53
1:A:656:PHE:CE2	1:A:1057:MET:HG3	2.44	0.53
4:F:505:ARG:N	4:F:509:CYS:O	2.29	0.53
4:F:1008:VAL:HG12	4:F:1009:GLU:N	2.20	0.53
4:F:62:ILE:O	4:F:66:TYR:N	2.39	0.53
4:F:530:GLN:HB2	4:F:531:PRO:HD3	1.91	0.53
4:F:557:GLU:HB3	4:F:558:PRO:HA	1.90	0.53
4:F:414:GLU:O	4:F:423:ILE:HG21	2.08	0.53
2:B:235:SER:OG	2:B:236:LEU:N	2.41	0.53
1:A:1120:PHE:HA	1:A:1123:LEU:HD12	1.90	0.53
1:A:1146:MET:HA	1:A:1149:ILE:HD12	1.90	0.53
1:A:1186:ASP:HA	1:A:1189:ILE:HD12	1.90	0.53
4:F:76:ASN:O	4:F:78:ARG:N	2.42	0.53
4:F:614:VAL:HB	4:F:618:ASP:O	2.08	0.52
1:A:1056:MET:HA	1:A:1059:ILE:HD12	1.92	0.52
4:F:256:MET:HB2	4:F:291:VAL:HG22	1.90	0.52
4:F:615:ASN:ND2	6:F:1203:NAG:O5	2.42	0.52
4:F:163:TYR:O	4:F:221:PRO:HD3	2.09	0.52
4:F:500:LYS:HE2	4:F:624:LEU:HD12	1.91	0.52
6:F:1203:NAG:O6	6:F:1204:NAG:O7	2.27	0.52
1:A:186:LEU:O	1:A:189:ILE:HG22	2.09	0.52
4:F:503:THR:OG1	4:F:511:ASN:OD1	2.15	0.52
4:F:411:TYR:CE2	4:F:427:GLU:HG3	2.44	0.52
1:A:186:LEU:HA	1:A:189:ILE:HG22	1.90	0.52
1:A:1336:LYS:C	1:A:1351:THR:HA	2.30	0.52
4:F:595:LYS:HA	4:F:604:LYS:HA	1.90	0.52
1:A:997:PHE:HE1	1:A:1006:SER:HB3	1.74	0.52
1:A:298:LEU:HA	1:A:314:PHE:HE2	1.74	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:PHE:HB2	1:A:597:PHE:CD2	2.45	0.52
4:F:188:THR:HG23	4:F:189:SER:N	2.24	0.52
1:A:993:ASN:O	1:A:995:PHE:N	2.36	0.52
4:F:427:GLU:HB3	4:F:431:VAL:HG23	1.91	0.52
1:A:1187:PHE:CE2	1:A:1191:ILE:HD11	2.43	0.52
4:F:192:ASP:O	4:F:196:LYS:HG2	2.09	0.52
1:A:661:VAL:O	1:A:664:LEU:HG	2.09	0.52
4:F:293:VAL:HG23	4:F:320:LEU:HD21	1.90	0.52
4:F:391:VAL:HG12	4:F:415:ILE:HB	1.91	0.52
1:A:1383:ASN:O	1:A:1387:LEU:N	2.25	0.52
1:A:1014:GLU:OE2	1:A:1324:ALA:HA	2.09	0.52
4:F:393:GLN:N	4:F:393:GLN:OE1	2.43	0.52
1:A:1334:TYR:CE1	1:A:1352:CYS:HA	2.44	0.52
4:F:191:LEU:HD11	4:F:195:PHE:HE2	1.74	0.52
4:F:178:SER:HB3	4:F:181:VAL:HG23	1.90	0.52
1:A:1002:SER:O	1:A:1005:MET:HB3	2.10	0.52
4:F:263:SER:OG	4:F:265:SER:OG	2.14	0.52
1:A:962:LYS:O	1:A:964:THR:N	2.43	0.52
1:A:287:GLN:O	1:A:290:THR:OG1	2.17	0.52
1:A:592:VAL:C	1:A:594:ARG:H	2.12	0.51
4:F:403:TRP:O	4:F:407:GLU:HB2	2.10	0.51
1:A:1369:ALA:O	1:A:1373:ILE:HG13	2.09	0.51
2:B:227:ARG:NE	2:B:335:ALA:O	2.24	0.51
1:A:954:PHE:O	1:A:956:SER:N	2.43	0.51
4:F:444:LYS:HD3	4:F:469:PHE:CE1	2.45	0.51
2:B:231:LEU:HD23	2:B:249:LEU:HD13	1.93	0.51
1:A:581:PHE:O	1:A:585:TYR:N	2.31	0.51
1:A:651:ILE:HA	1:A:654:ASN:ND2	2.25	0.51
1:A:1131:ASN:O	1:A:1135:LEU:HG	2.10	0.51
2:B:387:LEU:HD11	2:B:399:LEU:HD22	1.93	0.51
4:F:208:GLN:HA	4:F:481:LEU:HD23	1.92	0.51
1:A:1019:LEU:HG	1:A:1045:PHE:CZ	2.46	0.51
4:F:242:ARG:HE	4:F:425:THR:CG2	2.24	0.51
4:F:192:ASP:HB3	4:F:196:LYS:HE3	1.91	0.51
4:F:886:UNK:N	4:F:889:UNK:O	2.43	0.51
1:A:244:PRO:HA	1:A:304:ALA:HB2	1.92	0.51
4:F:167:ALA:HB3	4:F:218:ARG:HB2	1.92	0.51
4:F:570:ASN:HD22	4:F:573:LYS:HE3	1.76	0.51
2:B:263:ILE:HG12	2:B:317:VAL:HB	1.93	0.51
2:B:342:LYS:HE3	2:B:344:SER:HB2	1.93	0.51
4:F:352:SER:O	4:F:354:ALA:N	2.38	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:243:ARG:NH1	4:F:455:ALA:H	2.10	0.50
4:F:266:VAL:HB	4:F:270:THR:HG23	1.92	0.50
2:B:348:VAL:O	2:B:352:LEU:HG	2.11	0.50
4:F:320:LEU:O	4:F:324:VAL:HG23	2.12	0.50
1:A:124:VAL:HA	1:A:127:PHE:HD2	1.76	0.50
4:F:309:LEU:C	4:F:311:GLN:H	2.13	0.50
1:A:958:ASN:HD22	1:A:989:GLN:H	1.59	0.50
1:A:128:ILE:O	1:A:131:PHE:HB3	2.11	0.50
1:A:369:TRP:HE1	2:B:245:MET:HG2	1.77	0.50
4:F:576:ILE:HD13	4:F:609:TYR:OH	2.12	0.49
2:B:229:VAL:HB	2:B:317:VAL:HG22	1.94	0.49
2:B:252:PHE:HE2	2:B:400:ALA:HB2	1.78	0.49
4:F:99:LEU:HB3	4:F:466:LEU:CD2	2.42	0.49
1:A:268:PRO:C	1:A:271:GLY:H	2.15	0.49
4:F:580:MET:HG2	4:F:611:TRP:CZ3	2.47	0.49
4:F:274:ILE:HD11	4:F:363:PHE:HB2	1.92	0.49
4:F:312:ALA:O	4:F:314:VAL:N	2.43	0.49
1:A:1020:LEU:O	1:A:1024:ILE:HG12	2.12	0.49
2:B:66:THR:HG22	2:B:220:TYR:HE1	1.76	0.49
4:F:505:ARG:HG3	4:F:619:TYR:HE1	1.77	0.49
4:F:313:ASN:O	4:F:317:LYS:HB3	2.12	0.49
1:A:1006:SER:O	1:A:1009:THR:OG1	2.16	0.49
1:A:61:ILE:O	1:A:64:ASN:HB2	2.13	0.49
2:B:93:LEU:HB3	2:B:118:ILE:HD13	1.93	0.49
1:A:663:ASN:HD22	1:A:1061:VAL:HG12	1.78	0.49
1:A:1048:TYR:CZ	1:A:1052:ILE:HD11	2.48	0.49
1:A:1234:PHE:O	1:A:1237:LEU:HB3	2.13	0.49
4:F:281:MET:O	4:F:285:LEU:N	2.45	0.49
1:A:1163:LEU:O	1:A:1167:LEU:HG	2.13	0.49
1:A:942:PHE:HA	1:A:945:ILE:HD12	1.95	0.49
4:F:73:GLU:C	4:F:632:TYR:H	2.16	0.49
4:F:99:LEU:HB3	4:F:466:LEU:HD23	1.95	0.49
4:F:1006:PHE:CD1	4:F:1012:MET:HG3	2.48	0.49
4:F:61:ASP:O	4:F:65:LYS:N	2.42	0.49
4:F:594:VAL:HG22	4:F:595:LYS:O	2.12	0.49
1:A:1043:ILE:O	1:A:1047:ILE:HG13	2.12	0.49
1:A:964:THR:HA	1:A:1030:ASP:O	2.13	0.49
4:F:99:LEU:HD21	4:F:481:LEU:HG	1.94	0.49
4:F:109:VAL:HG12	4:F:187:TRP:HB2	1.94	0.48
1:A:89:LEU:HG	1:A:93:PHE:CE2	2.48	0.48
2:B:227:ARG:NH2	2:B:336:PRO:O	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:CYS:O	1:A:650:TYR:HB3	2.13	0.48
2:B:93:LEU:HD23	2:B:108:LEU:HA	1.94	0.48
4:F:214:THR:OG1	4:F:215:GLY:N	2.45	0.48
1:A:1015:GLY:HA3	1:A:1326:GLN:HE22	1.78	0.48
4:F:261:ASP:OD2	4:F:263:SER:OG	2.30	0.48
1:A:1127:LEU:HD13	1:A:1160:ILE:HG21	1.94	0.48
4:F:259:LEU:HD23	4:F:296:PHE:CE1	2.49	0.48
4:F:461:VAL:HG13	4:F:483:ASN:O	2.13	0.48
1:A:1144:GLU:O	1:A:1146:MET:N	2.46	0.48
1:A:597:PHE:HE1	1:A:606:SER:HB3	1.78	0.48
1:A:290:THR:HG21	1:A:616:TRP:HZ2	1.79	0.48
1:A:1019:LEU:HG	1:A:1045:PHE:HZ	1.78	0.48
1:A:581:PHE:HB2	1:A:597:PHE:HD2	1.78	0.48
4:F:186:ASN:HD21	6:F:1207:NAG:H2	1.79	0.48
2:B:326:PRO:HG3	2:B:383:PHE:CZ	2.49	0.48
2:B:340:TYR:HB2	2:B:383:PHE:CD1	2.49	0.48
4:F:238:TYR:OH	4:F:243:ARG:NH2	2.36	0.48
4:F:609:TYR:CB	4:F:624:LEU:HA	2.43	0.48
4:F:588:LYS:O	4:F:611:TRP:NE1	2.47	0.48
4:F:518:ASP:HB2	4:F:1007:HIS:CD2	2.47	0.48
4:F:609:TYR:HB2	4:F:624:LEU:HA	1.96	0.48
4:F:308:HIS:HA	4:F:309:LEU:HD23	1.95	0.48
4:F:494:VAL:HA	4:F:497:GLU:OE2	2.13	0.48
1:A:210:TYR:OH	1:A:320:LEU:HD12	2.13	0.48
4:F:88:ILE:O	4:F:92:LEU:HG	2.14	0.48
4:F:299:ASN:OD1	4:F:300:ALA:N	2.46	0.48
4:F:988:ASN:HD22	6:F:1205:NAG:C7	2.27	0.48
4:F:764:UNK:O	4:F:766:UNK:N	2.46	0.48
1:A:455:ASN:O	1:A:459:TRP:N	2.41	0.47
1:A:1147:ASN:O	1:A:1150:SER:OG	2.22	0.47
4:F:218:ARG:NH2	4:F:456:LEU:HD12	2.28	0.47
4:F:358:LYS:O	4:F:384:VAL:HA	2.14	0.47
1:A:131:PHE:HZ	1:A:168:ARG:HH21	1.61	0.47
4:F:460:LEU:HD23	4:F:517:ILE:HG23	1.96	0.47
1:A:179:VAL:HB	1:A:182:LEU:HD12	1.96	0.47
2:B:55:ALA:HA	2:B:58:LYS:HD2	1.96	0.47
1:A:1476:UNK:O	1:A:1478:UNK:N	2.48	0.47
4:F:606:ASN:O	4:F:627:PRO:CG	2.62	0.47
4:F:248:GLN:HE22	4:F:448:TRP:C	2.16	0.47
1:A:216:GLU:HG3	1:A:1240:VAL:HG21	1.97	0.47
1:A:606:SER:O	1:A:609:GLN:HB3	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:506:PHE:HB2	4:F:618:ASP:HB2	1.96	0.47
1:A:369:TRP:CD1	2:B:245:MET:HG2	2.50	0.47
1:A:79:ASN:HA	4:F:332:ILE:HA	1.97	0.47
1:A:964:THR:O	1:A:966:GLU:N	2.43	0.47
2:B:250:PHE:HE1	2:B:317:VAL:HG12	1.80	0.47
4:F:297:ASN:ND2	4:F:330:LYS:O	2.48	0.46
4:F:271:LEU:HA	4:F:274:ILE:HG22	1.97	0.46
1:A:1193:SER:O	1:A:1197:VAL:HG23	2.14	0.46
4:F:673:UNK:O	4:F:677:UNK:N	2.47	0.46
2:B:349:LEU:HA	2:B:352:LEU:HD12	1.98	0.46
1:A:61:ILE:HA	1:A:64:ASN:OD1	2.15	0.46
4:F:988:ASN:ND2	6:F:1205:NAG:O7	2.48	0.46
1:A:1066:VAL:O	1:A:1070:GLU:N	2.42	0.46
1:A:1009:THR:O	1:A:1012:THR:OG1	2.22	0.46
4:F:1006:PHE:HD1	4:F:1012:MET:HG3	1.79	0.46
4:F:1000:GLY:O	4:F:1001:ASN:ND2	2.48	0.46
4:F:524:LEU:HD21	4:F:1033:LEU:N	2.31	0.46
4:F:485:LEU:O	4:F:489:VAL:HG23	2.15	0.46
4:F:492:VAL:HG13	4:F:501:ARG:NH1	2.30	0.46
4:F:195:PHE:O	4:F:199:ARG:HG3	2.16	0.46
1:A:369:TRP:NE1	2:B:245:MET:HG2	2.29	0.46
4:F:263:SER:HA	4:F:297:ASN:HD22	1.81	0.46
4:F:1063:PHE:HA	4:F:1064:ASP:HA	1.64	0.46
4:F:281:MET:SD	4:F:363:PHE:HZ	2.39	0.46
1:A:649:ASN:O	1:A:653:LEU:HG	2.15	0.46
1:A:435:TYR:HA	1:A:436:TRP:HA	1.69	0.46
2:B:107:ARG:HB3	2:B:115:ILE:HD13	1.97	0.46
1:A:363:LEU:O	1:A:367:MET:HG2	2.16	0.46
4:F:524:LEU:HD21	4:F:1033:LEU:H	1.81	0.46
1:A:131:PHE:CE1	1:A:164:LEU:HB3	2.50	0.46
1:A:210:TYR:O	1:A:214:GLY:N	2.37	0.46
1:A:631:SER:OG	1:A:633:PRO:HD2	2.16	0.46
4:F:595:LYS:HB2	6:F:1212:NAG:H83	1.98	0.46
1:A:958:ASN:HA	1:A:959:ASP:HA	1.68	0.46
1:A:245:CYS:O	1:A:264:GLY:HA2	2.16	0.46
2:B:65:ARG:N	2:B:221:ASP:O	2.31	0.46
1:A:124:VAL:O	1:A:128:ILE:HG12	2.16	0.46
2:B:237:LYS:H	2:B:324:ASN:ND2	2.10	0.46
1:A:326:LEU:O	1:A:330:LEU:HG	2.16	0.46
2:B:393:GLU:O	2:B:397:GLU:HG2	2.16	0.46
4:F:254:LYS:HA	4:F:357:ASN:OD1	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:254:LYS:HG2	4:F:357:ASN:HD21	1.80	0.45
4:F:512:GLY:O	4:F:514:TYR:N	2.43	0.45
4:F:617:THR:HG22	4:F:618:ASP:OD1	2.16	0.45
4:F:858:UNK:O	4:F:862:UNK:HG2	2.17	0.45
1:A:1015:GLY:HA3	1:A:1326:GLN:NE2	2.31	0.45
4:F:509:CYS:N	4:F:561:LEU:O	2.49	0.45
4:F:587:GLU:O	4:F:589:THR:HG23	2.16	0.45
1:A:290:THR:HG21	1:A:616:TRP:CZ2	2.51	0.45
1:A:1151:ASP:O	1:A:1155:VAL:HG23	2.17	0.45
4:F:576:ILE:HD11	4:F:590:PHE:CZ	2.52	0.45
4:F:505:ARG:HG3	4:F:619:TYR:CE1	2.52	0.45
1:A:1272:LEU:O	1:A:1276:MET:N	2.44	0.45
4:F:591:ARG:HB3	4:F:608:THR:HG22	1.99	0.45
1:A:1487:UNK:O	1:A:1491:UNK:N	2.50	0.45
1:A:614:GLU:OE2	1:A:615:ASP:HB2	2.16	0.45
4:F:336:LYS:HB3	4:F:374:ILE:HD11	1.98	0.45
1:A:620:MET:O	1:A:624:ILE:HD12	2.16	0.45
1:A:73:PRO:HA	1:A:74:MET:HA	1.55	0.45
1:A:1142:GLN:HA	1:A:1143:SER:HA	1.63	0.45
4:F:568:LEU:HD12	4:F:596:SER:HA	1.97	0.45
4:F:449:THR:CG2	4:F:463:THR:H	2.26	0.45
4:F:219:TYR:O	4:F:220:TYR:CG	2.69	0.45
1:A:1057:MET:O	1:A:1061:VAL:HG23	2.17	0.45
1:A:969:ARG:HH21	4:F:177:GLY:HA3	1.81	0.45
1:A:1372:ILE:HG22	1:A:1376:PHE:CE2	2.52	0.45
4:F:102:LEU:HG	4:F:199:ARG:NH2	2.32	0.45
4:F:130:LYS:N	4:F:141:GLU:O	2.49	0.45
4:F:285:LEU:HD23	4:F:286:SER:O	2.17	0.45
2:B:66:THR:HG22	2:B:220:TYR:CE1	2.52	0.45
4:F:186:ASN:OD1	6:F:1207:NAG:H2	2.16	0.45
4:F:290:PHE:CD1	4:F:290:PHE:N	2.83	0.45
4:F:224:PRO:HA	4:F:225:TRP:HA	1.60	0.44
1:A:1033:PRO:HA	1:A:1034:VAL:HA	1.74	0.44
1:A:204:LEU:O	1:A:208:ILE:N	2.50	0.44
2:B:329:LEU:O	2:B:332:THR:OG1	2.23	0.44
4:F:86:ARG:HG2	4:F:90:LYS:HE3	2.00	0.44
1:A:1329:LEU:HD11	1:A:1358:TYR:CD1	2.52	0.44
4:F:333:THR:HG22	4:F:335:TYR:HB2	1.98	0.44
4:F:184:GLU:O	4:F:188:THR:HG22	2.17	0.44
1:A:1195:ILE:O	1:A:1199:LEU:HG	2.16	0.44
1:A:930:ASN:O	1:A:934:VAL:HG23	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:ARG:O	1:A:1305:ASN:ND2	2.51	0.44
2:B:65:ARG:HB3	2:B:221:ASP:HB2	2.00	0.44
4:F:1007:HIS:CG	4:F:1008:VAL:H	2.36	0.44
4:F:509:CYS:SG	4:F:560:THR:HA	2.58	0.44
1:A:664:LEU:O	1:A:668:GLU:N	2.45	0.44
1:A:1233:ALA:HB2	1:A:1236:ARG:HH21	1.83	0.44
4:F:453:LEU:HB2	4:F:557:GLU:OE2	2.18	0.44
1:A:286:TYR:O	1:A:290:THR:HG23	2.18	0.44
4:F:487:LEU:HD22	4:F:490:MET:SD	2.58	0.44
4:F:343:PHE:O	4:F:347:LEU:N	2.51	0.43
1:A:205:PHE:O	1:A:209:ILE:N	2.40	0.43
4:F:334:ASP:HB3	4:F:337:LYS:HB2	1.99	0.43
4:F:123:GLU:HA	4:F:124:VAL:HA	1.74	0.43
1:A:1123:LEU:O	1:A:1127:LEU:HG	2.17	0.43
1:A:366:TYR:HD2	2:B:348:VAL:HG11	1.82	0.43
4:F:462:ILE:HG13	4:F:485:LEU:HD11	2.00	0.43
1:A:647:CYS:O	1:A:651:ILE:HG13	2.18	0.43
4:F:297:ASN:C	4:F:299:ASN:N	2.70	0.43
1:A:942:PHE:HD1	1:A:1044:PHE:CE1	2.36	0.43
1:A:631:SER:OG	1:A:632:TYR:N	2.41	0.43
2:B:229:VAL:HB	2:B:317:VAL:HA	2.01	0.43
4:F:98:ALA:HB1	4:F:199:ARG:NE	2.31	0.43
4:F:196:LYS:HE2	4:F:196:LYS:HB3	1.81	0.43
4:F:117:GLU:O	4:F:119:PHE:N	2.51	0.43
1:A:1314:LEU:O	1:A:1317:PHE:N	2.48	0.43
2:B:55:ALA:HB1	2:B:105:ILE:HG21	2.01	0.43
4:F:600:ARG:HD3	4:F:600:ARG:HA	1.65	0.43
4:F:271:LEU:HD11	4:F:327:ILE:HG23	2.00	0.43
2:B:353:ILE:HB	2:B:364:LEU:HD13	1.99	0.43
1:A:1185:PHE:HA	1:A:1188:LEU:HD12	2.00	0.43
1:A:194:LEU:O	1:A:196:LEU:N	2.48	0.43
2:B:329:LEU:HB3	2:B:336:PRO:HG3	2.01	0.43
1:A:1046:ILE:O	1:A:1050:ILE:HG13	2.19	0.43
2:B:412:PRO:HA	2:B:413:PRO:HD3	1.92	0.43
4:F:334:ASP:O	4:F:336:LYS:N	2.51	0.43
1:A:90:GLU:HA	1:A:93:PHE:HD2	1.83	0.43
1:A:631:SER:H	1:A:635:VAL:HG23	1.83	0.43
1:A:458:LEU:O	1:A:462:HIS:N	2.31	0.43
3:E:125:ALA:O	3:E:129:PHE:N	2.52	0.43
1:A:1063:PHE:O	1:A:1067:THR:HG23	2.18	0.43
4:F:465:THR:HG22	4:F:480:ASN:HB3	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:158:MET:O	3:E:162:VAL:HG23	2.19	0.43
4:F:92:LEU:HD22	4:F:448:TRP:CH2	2.54	0.42
4:F:302:ASP:HB2	4:F:306:PHE:CE1	2.42	0.42
4:F:248:GLN:NE2	4:F:448:TRP:O	2.35	0.42
4:F:461:VAL:HG13	4:F:483:ASN:C	2.39	0.42
4:F:96:SER:O	4:F:100:VAL:HG23	2.19	0.42
1:A:226:CYS:N	1:A:274:HIS:HE2	2.17	0.42
4:F:622:LEU:HD12	4:F:623:ALA:H	1.83	0.42
4:F:390:SER:HB2	4:F:414:GLU:HG2	2.01	0.42
1:A:958:ASN:ND2	1:A:989:GLN:H	2.16	0.42
1:A:1318:ARG:CZ	1:A:1328:ILE:HD11	2.49	0.42
4:F:564:LEU:HD13	4:F:574:VAL:HG22	2.01	0.42
4:F:113:HIS:O	4:F:115:TRP:N	2.39	0.42
1:A:1008:PHE:O	1:A:1011:SER:HB3	2.19	0.42
4:F:596:SER:C	4:F:602:ILE:HG23	2.40	0.42
4:F:609:TYR:HB2	4:F:623:ALA:O	2.19	0.42
4:F:335:TYR:CE2	4:F:339:PHE:HE2	2.37	0.42
1:A:1239:ARG:HG3	1:A:1242:ARG:NH2	2.33	0.42
2:B:326:PRO:HB3	2:B:338:ILE:HG21	2.01	0.42
4:F:868:UNK:HA	4:F:869:UNK:HA	1.76	0.42
1:A:282:MET:HG2	1:A:286:TYR:CE2	2.55	0.42
4:F:236:ASP:OD1	4:F:238:TYR:HB3	2.19	0.42
4:F:86:ARG:O	4:F:90:LYS:HG3	2.20	0.42
4:F:485:LEU:HD23	4:F:485:LEU:HA	1.68	0.42
4:F:107:GLU:OE2	4:F:444:LYS:NZ	2.53	0.42
4:F:470:ASN:HD22	4:F:473:GLY:N	2.14	0.42
1:A:1178:PHE:O	1:A:1180:ASP:N	2.53	0.42
1:A:88:LYS:O	1:A:91:TYR:HB3	2.20	0.42
1:A:87:GLU:HA	1:A:90:GLU:OE1	2.20	0.42
4:F:595:LYS:HB3	4:F:602:ILE:HG21	2.02	0.42
1:A:89:LEU:O	1:A:92:PHE:HB3	2.20	0.42
4:F:359:ILE:CB	4:F:385:ARG:HB2	2.49	0.42
1:A:210:TYR:HD2	1:A:313:TYR:CE1	2.37	0.42
4:F:614:VAL:HG12	4:F:616:GLY:N	2.32	0.41
4:F:248:GLN:NE2	4:F:447:GLN:O	2.53	0.41
4:F:528:ASN:O	4:F:531:PRO:HD2	2.20	0.41
1:A:943:ALA:HB1	1:A:1000:VAL:HG13	2.02	0.41
1:A:1069:GLN:O	1:A:1073:GLU:N	2.49	0.41
4:F:256:MET:SD	4:F:359:ILE:HD11	2.60	0.41
1:A:357:GLN:O	1:A:361:GLU:HG2	2.19	0.41
1:A:589:ASP:HA	1:A:590:THR:HA	1.81	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:626:LEU:C	4:F:628:THR:N	2.73	0.41
1:A:1375:LEU:O	1:A:1379:VAL:HG23	2.20	0.41
1:A:309:TRP:HA	1:A:311:TRP:NE1	2.35	0.41
1:A:321:GLY:O	1:A:325:ILE:HG23	2.20	0.41
1:A:937:LEU:HA	1:A:940:PHE:HD2	1.84	0.41
4:F:489:VAL:HA	4:F:492:VAL:HB	2.02	0.41
4:F:488:GLY:O	4:F:492:VAL:HG23	2.20	0.41
4:F:505:ARG:HG2	4:F:506:PHE:N	2.36	0.41
1:A:1184:VAL:O	1:A:1188:LEU:HG	2.20	0.41
4:F:304:SER:O	4:F:305:CYS:SG	2.79	0.41
4:F:609:TYR:CG	4:F:624:LEU:HD23	2.55	0.41
1:A:1119:TYR:O	1:A:1123:LEU:HG	2.21	0.41
1:A:1293:ALA:N	1:A:1338:CYS:O	2.54	0.41
4:F:85:ALA:O	4:F:89:GLU:HG3	2.21	0.41
1:A:1410:UNK:O	1:A:1412:UNK:N	2.53	0.41
4:F:356:CYS:O	4:F:358:LYS:NZ	2.51	0.41
4:F:356:CYS:O	4:F:358:LYS:HG3	2.20	0.41
4:F:411:TYR:HB3	4:F:431:VAL:HG21	2.03	0.41
1:A:169:VAL:O	1:A:172:PRO:HD2	2.20	0.41
1:A:936:THR:O	1:A:939:GLN:HB2	2.21	0.41
4:F:606:ASN:C	4:F:627:PRO:HG3	2.41	0.41
4:F:437:VAL:HA	4:F:469:PHE:CE2	2.43	0.41
4:F:292:ASN:OD1	4:F:308:HIS:HB3	2.20	0.41
1:A:595:SER:HB3	1:A:605:ILE:HD11	2.03	0.41
1:A:969:ARG:HD2	4:F:177:GLY:HA3	2.03	0.41
1:A:1372:ILE:HA	1:A:1375:LEU:HD12	2.03	0.41
4:F:505:ARG:HB3	4:F:508:LEU:O	2.20	0.41
4:F:444:LYS:HD3	4:F:469:PHE:HE1	1.85	0.41
4:F:335:TYR:CE2	4:F:371:ALA:HB2	2.56	0.41
1:A:1166:ILE:O	1:A:1170:LEU:HG	2.21	0.41
3:E:199:LEU:O	3:E:203:SER:N	2.53	0.41
6:F:1209:NAG:O3	7:F:1217:BMA:O5	2.27	0.41
2:B:340:TYR:HD2	2:B:386:ILE:HG12	1.86	0.41
1:A:627:TYR:CD2	1:A:637:VAL:HG21	2.56	0.41
1:A:370:ILE:HD11	2:B:352:LEU:HB3	2.03	0.40
4:F:500:LYS:HZ1	4:F:502:LEU:HD22	1.86	0.40
4:F:460:LEU:HG	4:F:460:LEU:H	1.66	0.40
4:F:175:TYR:O	4:F:177:GLY:N	2.54	0.40
4:F:115:TRP:HA	4:F:183:ASN:OD1	2.21	0.40
1:A:1016:TRP:N	1:A:1017:PRO:HD2	2.35	0.40
1:A:165:ARG:O	1:A:168:ARG:HB3	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:282:LEU:HA	4:F:282:LEU:HD23	1.85	0.40
4:F:195:PHE:HA	4:F:198:ASN:ND2	2.37	0.40
1:A:632:TYR:H	1:A:633:PRO:HD2	1.86	0.40
1:A:1316:LEU:HD11	1:A:1360:TYR:OH	2.20	0.40
1:A:1245:LYS:O	1:A:1248:SER:HB2	2.21	0.40
1:A:521:PRO:HA	1:A:522:LEU:HA	1.59	0.40
4:F:568:LEU:HD11	4:F:597:GLN:H	1.87	0.40
4:F:554:LYS:O	4:F:555:SER:OG	2.31	0.40
1:A:642:ILE:O	1:A:646:VAL:HB	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1084/1873 (58%)	936 (86%)	75 (7%)	73 (7%)	1	25
2	B	272/356 (76%)	261 (96%)	11 (4%)	0	100	100
3	E	132/222 (60%)	127 (96%)	2 (2%)	3 (2%)	8	50
4	F	617/1106 (56%)	461 (75%)	83 (14%)	73 (12%)	0	9
All	All	2105/3557 (59%)	1785 (85%)	171 (8%)	149 (7%)	3	23

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	39	PRO
1	A	74	MET
1	A	75	PRO
1	A	242	PRO
1	A	244	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	248	THR
1	A	253	PRO
1	A	266	PRO
1	A	268	PRO
1	A	305	ILE
1	A	518	ALA
1	A	1033	PRO
1	A	1035	TYR
1	A	1106	PRO
1	A	1295	VAL
1	A	1307	GLN
1	A	1340	PRO
1	A	1346	PRO
3	E	130	ARG
4	F	56	VAL
4	F	73	GLU
4	F	74	PRO
4	F	117	GLU
4	F	121	SER
4	F	134	ASP
4	F	142	PRO
4	F	305	CYS
4	F	351	VAL
4	F	510	PRO
4	F	618	ASP
4	F	629	TYR
4	F	630	SER
4	F	638	ILE
4	F	1008	VAL
4	F	1035	ILE
4	F	1036	GLN
4	F	1046	PRO
4	F	1053	PRO
1	A	35	THR
1	A	50	TRP
1	A	51	LYS
1	A	78	ASP
1	A	107	ALA
1	A	262	ARG
1	A	263	GLY
1	A	273	THR
1	A	276	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	589	ASP
1	A	632	TYR
1	A	891	SER
1	A	962	LYS
1	A	963	MET
1	A	966	GLU
1	A	1138	GLN
1	A	1141	HIS
1	A	1173	LYS
3	E	205	PRO
4	F	72	VAL
4	F	77	ALA
4	F	138	ASN
4	F	141	GLU
4	F	264	GLY
4	F	308	HIS
4	F	314	VAL
4	F	347	LEU
4	F	349	TYR
4	F	356	CYS
4	F	409	LYS
4	F	441	ASP
4	F	458	LEU
4	F	470	ASN
4	F	520	ASN
4	F	522	TYR
4	F	639	GLU
4	F	1043	GLY
4	F	1062	CYS
1	A	79	ASN
1	A	131	PHE
1	A	234	VAL
1	A	251	GLY
1	A	466	ILE
1	A	468	ASN
1	A	541	TYR
1	A	631	SER
1	A	892	VAL
1	A	978	GLY
1	A	1145	GLU
1	A	1179	GLY
1	A	1293	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1341	GLU
1	A	1345	ALA
1	A	1357	ALA
3	E	131	LYS
4	F	118	ASP
4	F	125	VAL
4	F	164	GLN
4	F	265	SER
4	F	335	TYR
4	F	394	HIS
4	F	438	LEU
4	F	475	PHE
4	F	525	LEU
4	F	555	SER
4	F	571	ASP
4	F	1032	ARG
4	F	1037	ALA
4	F	1050	VAL
1	A	36	LEU
1	A	196	LEU
1	A	252	ARG
1	A	261	CYS
1	A	644	LEU
1	A	949	LEU
1	A	1171	ALA
1	A	1302	ARG
1	A	1349	GLU
4	F	163	TYR
4	F	251	ALA
4	F	311	GLN
4	F	330	LYS
4	F	353	ARG
4	F	557	GLU
4	F	627	PRO
4	F	1010	LYS
4	F	1047	CYS
1	A	241	LYS
1	A	254	CYS
1	A	258	GLY
1	A	308	GLU
1	A	977	ASP
1	A	994	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	F	186	ASN
4	F	348	ASN
4	F	380	LYS
4	F	495	SER
4	F	1007	HIS
1	A	837	ILE
1	A	866	ASN
4	F	137	LYS
4	F	220	TYR
4	F	395	ASN
1	A	1339	ASP
4	F	310	VAL
4	F	499	ILE
1	A	1253	VAL
4	F	634	ILE
4	F	327	ILE
1	A	73	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	430/1519 (28%)	428 (100%)	2 (0%)	92	96
2	B	240/315 (76%)	240 (100%)	0	100	100
3	E	3/192 (2%)	3 (100%)	0	100	100
4	F	417/706 (59%)	414 (99%)	3 (1%)	88	94
All	All	1090/2732 (40%)	1085 (100%)	5 (0%)	92	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	A	1070	GLU
4	F	359	ILE
4	F	626	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	F	628	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	GLN
1	A	654	ASN
1	A	663	ASN
1	A	958	ASN
1	A	1131	ASN
2	B	67	ASN
2	B	314	GLN
2	B	324	ASN
2	B	363	HIS
4	F	316	ASN
4	F	570	ASN
4	F	615	ASN
4	F	1007	HIS
4	F	1013	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z  > 2$
6	NAG	F	1201	-	14,14,15	0.23	0	15,19,21	0.46	0
6	NAG	F	1202	-	14,14,15	0.22	0	15,19,21	0.35	0
6	NAG	F	1203	-	14,14,15	0.30	0	15,19,21	0.27	0
6	NAG	F	1204	-	14,14,15	0.21	0	15,19,21	0.46	0
6	NAG	F	1205	-	14,14,15	0.22	0	15,19,21	0.31	0
6	NAG	F	1206	-	14,14,15	0.27	0	15,19,21	0.31	0
6	NAG	F	1207	-	14,14,15	0.25	0	15,19,21	0.34	0
6	NAG	F	1208	-	14,14,15	0.28	0	15,19,21	0.39	0
6	NAG	F	1209	-	14,14,15	0.26	0	15,19,21	0.31	0
6	NAG	F	1210	-	14,14,15	0.26	0	15,19,21	0.31	0
6	NAG	F	1211	-	14,14,15	0.25	0	15,19,21	0.28	0
6	NAG	F	1212	-	14,14,15	0.24	0	15,19,21	0.36	0
6	NAG	F	1213	-	14,14,15	0.29	0	15,19,21	0.27	0
6	NAG	F	1214	-	14,14,15	0.30	0	15,19,21	0.36	0
6	NAG	F	1215	-	14,14,15	0.28	0	15,19,21	0.39	0
7	BMA	F	1216	-	11,11,12	0.54	0	15,15,17	0.75	0
7	BMA	F	1217	-	11,11,12	0.62	0	15,15,17	0.69	0

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
6	NAG	F	1201	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1202	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1203	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1204	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1205	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1206	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1207	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1208	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1209	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1210	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1211	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1212	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1213	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1214	-	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1215	-	-	0/6/23/26	0/1/1/1
7	BMA	F	1216	-	-	0/2/19/22	0/1/1/1
7	BMA	F	1217	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1203	NAG	3	0
6	F	1204	NAG	2	0
6	F	1205	NAG	2	0
6	F	1207	NAG	2	0
6	F	1209	NAG	2	0
6	F	1211	NAG	1	0
6	F	1212	NAG	1	0
7	F	1217	BMA	2	0

## 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.