wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:54 PM BST

PDB ID	:	3JAF
EMDB ID:	:	EMD-6346
Title	:	Structure of alpha-1 glycine receptor by single particle electron cryo-microscopy, glycine/ivermectin-bound state
Authors	:	Du, J.; Lu, W.; Wu, S.P.; Cheng, Y.F.; Gouaux, E.
Deposited on	:	2015-06-08
Resolution	:	3.80 Å(reported)
Based on PDB ID	:	3RHW

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

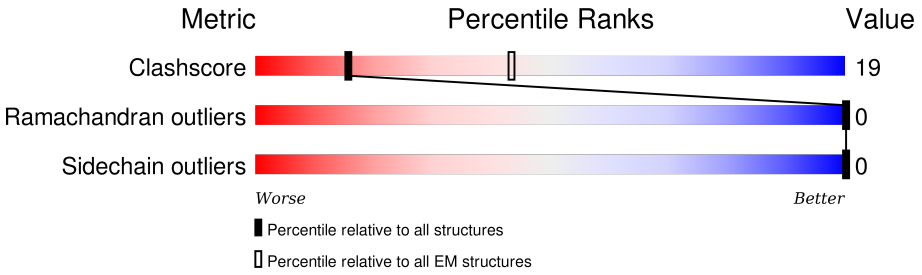
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	342	63% 37%
1	B	342	63% 37%
1	C	342	61% 39%
1	D	342	62% 38%
1	E	342	63% 37%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13865 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.

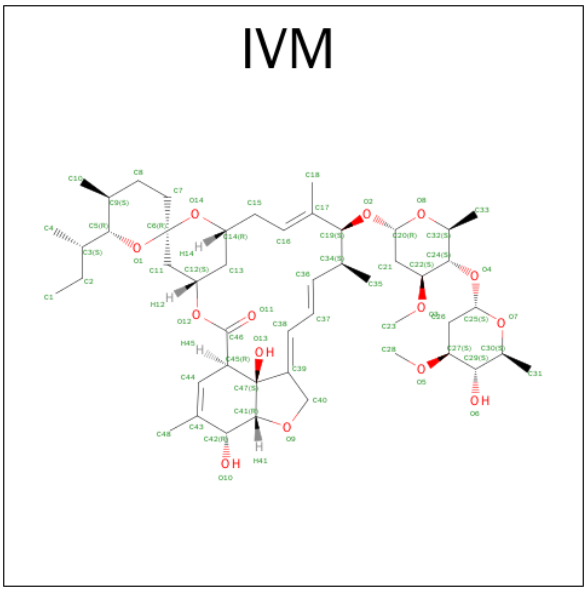
- Molecule 1 is a protein called Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	342	Total	C	N	O	S	0	0
			2683	1759	440	466	18		
1	B	342	Total	C	N	O	S	0	0
			2683	1759	440	466	18		
1	C	342	Total	C	N	O	S	0	0
			2683	1759	440	466	18		
1	D	342	Total	C	N	O	S	0	0
			2683	1759	440	466	18		
1	E	342	Total	C	N	O	S	0	0
			2683	1759	440	466	18		

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			28	16	2	10	
2	B	2	Total	C	N	O	0
			28	16	2	10	
2	C	2	Total	C	N	O	0
			28	16	2	10	
2	D	2	Total	C	N	O	0
			28	16	2	10	
2	E	2	Total	C	N	O	0
			28	16	2	10	

- Molecule 3 is (2AE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17AR,20R,20AR,20BS)-6'-[(2S)-BUTAN-2-YL]-20,20B-DIHYDROXY-5',6,8,19-TETRAMETHYL-17-OXO-3',4',5',6,6',10,11,14,15,17,17A,20,20A,20B-TETRADECAHYDRO-2H,7H-SPIRO[11,15-METHANOFURO[4,3,2-PQ][2,6]BENZODIOXACYCLOOCTADECINE-13,2'-PYRAN]-7-YL 2,6-DIDEOXY-4-O-(2,6-DIDEOXY-3-O-METHYL-ALPHA-L-ARABINO-HEXOPYRANOSYL)-3-O-METHYL-ALPHA-L-ARABINO-HEXOPYRANOSIDE (three-letter code: IVM) (formula: $C_{48}H_{74}O_{14}$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			62	48	14	
3	B	1	Total	C	O	0
			62	48	14	
3	C	1	Total	C	O	0
			62	48	14	
3	D	1	Total	C	O	0
			62	48	14	
3	E	1	Total	C	O	0
			62	48	14	

3 Residue-property plots (i)

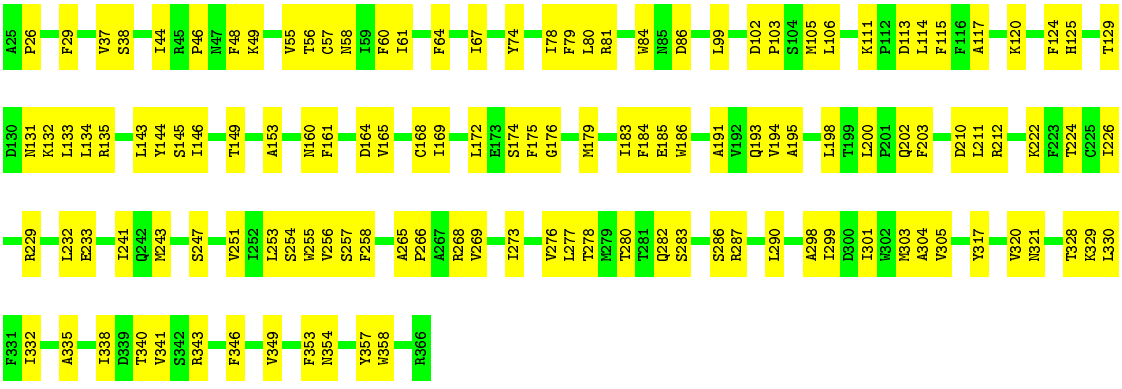
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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.

- Molecule 1: Glycine receptor subunit alphaZ1

Chain A:

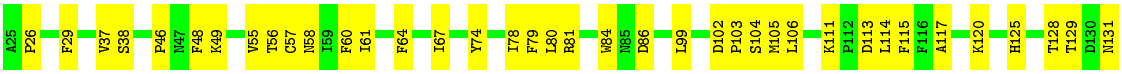
- Molecule 1: Glycine receptor subunit alphaZ1

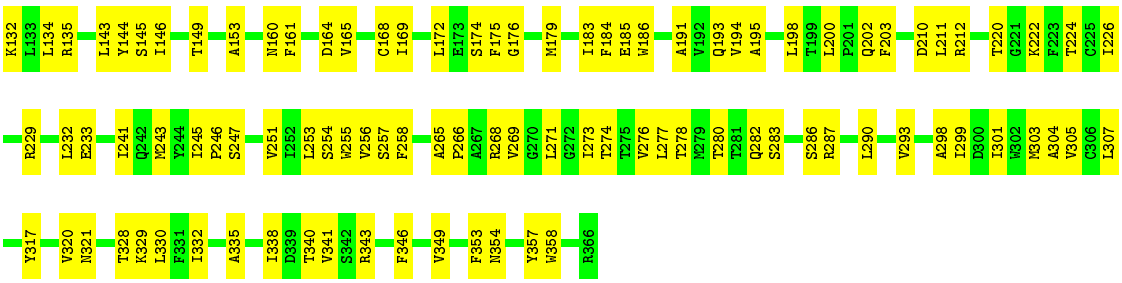
Chain B:



- Molecule 1: Glycine receptor subunit alphaZ1

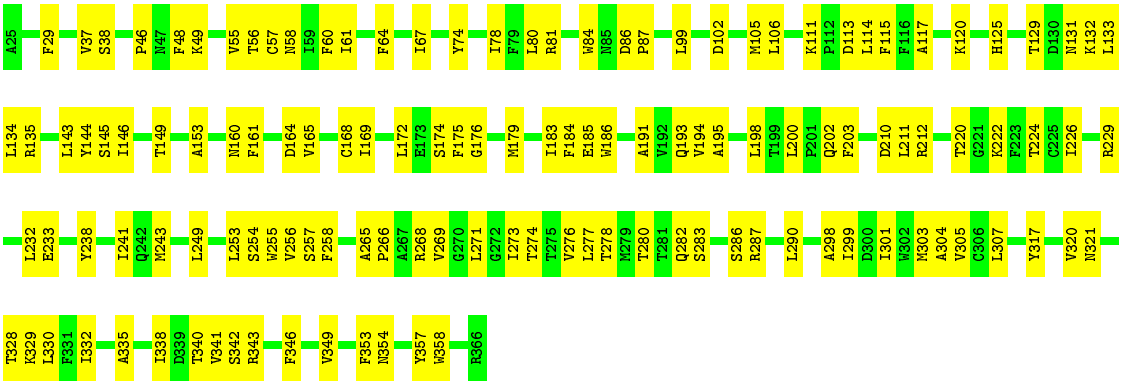
Chain C:





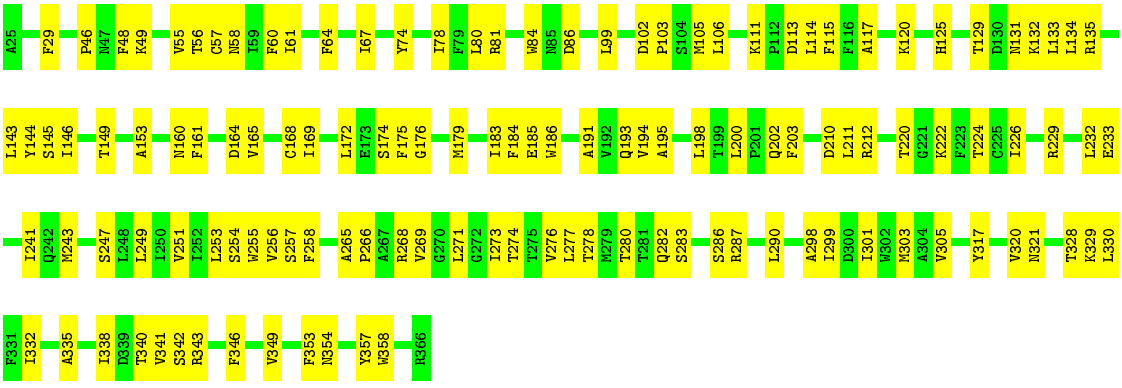
• Molecule 1: Glycine receptor subunit alphaZ1

Chain D:



• Molecule 1: Glycine receptor subunit alphaZ1

Chain E:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	56957	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	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: IVM, 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	0.28	0/2753	0.56	0/3749
1	B	0.28	0/2753	0.56	0/3749
1	C	0.28	0/2753	0.56	0/3749
1	D	0.28	0/2753	0.56	0/3749
1	E	0.28	0/2753	0.56	0/3749
All	All	0.28	0/13765	0.56	0/18745

There are no bond length outliers.

There are no bond angle outliers.

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	2683	0	2660	97	0
1	B	2683	0	2660	106	0
1	C	2683	0	2660	115	0
1	D	2683	0	2660	113	0
1	E	2683	0	2660	105	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	62	0	74	9	0
3	B	62	0	74	12	0
3	C	62	0	74	11	0
3	D	62	0	74	11	0
3	E	62	0	74	9	0
All	All	13865	0	13795	525	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 (525) 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:129:THR:HG21	1:E:113:ASP:HB2	1.57	0.85
1:B:283:SER:HB2	3:B:503:IVM:O10	1.81	0.81
1:C:113:ASP:HB2	1:D:129:THR:HG21	1.62	0.81
1:D:113:ASP:HB2	1:E:129:THR:HG21	1.63	0.80
1:A:114:LEU:HD21	1:A:172:LEU:HD23	1.64	0.80
1:D:114:LEU:HD21	1:D:172:LEU:HD23	1.64	0.79
1:C:114:LEU:HD11	1:C:172:LEU:HB3	1.65	0.79
1:D:114:LEU:HD11	1:D:172:LEU:HB3	1.65	0.79
1:B:114:LEU:HD11	1:B:172:LEU:HB3	1.65	0.78
1:C:114:LEU:HD21	1:C:172:LEU:HD23	1.64	0.78
1:B:114:LEU:HD21	1:B:172:LEU:HD23	1.64	0.78
1:E:114:LEU:HD21	1:E:172:LEU:HD23	1.64	0.78
1:E:114:LEU:HD11	1:E:172:LEU:HB3	1.65	0.78
1:A:114:LEU:HD11	1:A:172:LEU:HB3	1.65	0.77
1:B:210:ASP:OD2	1:B:212:ARG:NH2	2.21	0.74
1:C:210:ASP:OD2	1:C:212:ARG:NH2	2.21	0.74
1:E:210:ASP:OD2	1:E:212:ARG:NH2	2.21	0.74
1:D:210:ASP:OD2	1:D:212:ARG:NH2	2.20	0.73
1:D:132:LYS:HG2	1:D:146:ILE:HG22	1.71	0.73
1:C:283:SER:HB2	3:C:503:IVM:O10	1.88	0.72
1:E:132:LYS:HG2	1:E:146:ILE:HG22	1.71	0.72
1:A:210:ASP:OD2	1:A:212:ARG:NH2	2.20	0.72
1:D:283:SER:HB2	3:D:503:IVM:O10	1.89	0.72
1:C:132:LYS:HG2	1:C:146:ILE:HG22	1.71	0.71
1:B:132:LYS:HG2	1:B:146:ILE:HG22	1.71	0.71
1:A:132:LYS:HG2	1:A:146:ILE:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASP:HB2	1:C:129:THR:HG21	1.73	0.70
1:E:106:LEU:HD21	1:E:144:TYR:HE1	1.57	0.70
1:C:106:LEU:HD21	1:C:144:TYR:HE1	1.56	0.69
1:A:106:LEU:HD13	1:A:134:LEU:HD13	1.75	0.69
1:D:106:LEU:HD21	1:D:144:TYR:HE1	1.56	0.69
1:A:113:ASP:HB2	1:B:129:THR:HG21	1.75	0.69
1:E:106:LEU:HD13	1:E:134:LEU:HD13	1.75	0.69
1:B:106:LEU:HD21	1:B:144:TYR:HE1	1.57	0.69
1:B:106:LEU:HD13	1:B:134:LEU:HD13	1.75	0.69
1:A:305:VAL:HG11	1:A:353:PHE:CE2	2.28	0.69
1:D:305:VAL:HG11	1:D:353:PHE:CE2	2.28	0.69
1:B:305:VAL:HG11	1:B:353:PHE:CE2	2.28	0.69
1:C:305:VAL:HG11	1:C:353:PHE:CE2	2.28	0.69
1:D:106:LEU:HD13	1:D:134:LEU:HD13	1.75	0.68
1:D:165:VAL:HG22	1:D:233:GLU:HG2	1.75	0.68
1:A:165:VAL:HG22	1:A:233:GLU:HG2	1.75	0.68
1:A:106:LEU:HD21	1:A:144:TYR:HE1	1.56	0.68
1:C:106:LEU:HD13	1:C:134:LEU:HD13	1.75	0.68
1:C:165:VAL:HG22	1:C:233:GLU:HG2	1.75	0.68
1:E:305:VAL:HG11	1:E:353:PHE:CE2	2.28	0.68
1:B:165:VAL:HG22	1:B:233:GLU:HG2	1.75	0.68
1:E:165:VAL:HG22	1:E:233:GLU:HG2	1.75	0.67
1:D:161:PHE:CE1	1:D:290:LEU:HD21	2.31	0.66
1:E:161:PHE:CE1	1:E:290:LEU:HD21	2.31	0.66
1:B:161:PHE:CE1	1:B:290:LEU:HD21	2.31	0.66
1:D:67:ILE:HG12	1:D:74:TYR:HB2	1.77	0.66
1:C:67:ILE:HG12	1:C:74:TYR:HB2	1.77	0.66
1:A:161:PHE:CE1	1:A:290:LEU:HD21	2.31	0.66
1:B:340:THR:HA	1:B:343:ARG:HE	1.61	0.65
1:A:67:ILE:HG12	1:A:74:TYR:HB2	1.77	0.65
1:A:160:ASN:O	1:A:164:ASP:HB3	1.96	0.65
1:C:329:LYS:O	1:C:332:ILE:HG22	1.97	0.65
1:E:67:ILE:HG12	1:E:74:TYR:HB2	1.77	0.65
1:D:160:ASN:O	1:D:164:ASP:HB3	1.96	0.65
1:B:160:ASN:O	1:B:164:ASP:HB3	1.96	0.65
1:C:161:PHE:CE1	1:C:290:LEU:HD21	2.31	0.65
1:B:67:ILE:HG12	1:B:74:TYR:HB2	1.77	0.65
1:B:317:TYR:O	1:B:321:ASN:ND2	2.30	0.65
1:C:160:ASN:O	1:C:164:ASP:HB3	1.96	0.65
1:D:340:THR:HA	1:D:343:ARG:HE	1.61	0.65
1:E:160:ASN:O	1:E:164:ASP:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:HA	1:A:343:ARG:HE	1.61	0.65
1:A:329:LYS:O	1:A:332:ILE:HG22	1.97	0.65
1:B:329:LYS:O	1:B:332:ILE:HG22	1.97	0.65
1:C:340:THR:HA	1:C:343:ARG:HE	1.61	0.64
1:D:329:LYS:O	1:D:332:ILE:HG22	1.97	0.64
1:E:329:LYS:O	1:E:332:ILE:HG22	1.97	0.64
1:C:317:TYR:O	1:C:321:ASN:ND2	2.30	0.64
1:A:283:SER:HB2	3:A:503:IVM:O10	1.98	0.64
1:A:317:TYR:O	1:A:321:ASN:ND2	2.30	0.64
1:E:340:THR:HA	1:E:343:ARG:HE	1.61	0.64
1:C:174:SER:HB2	1:C:184:PHE:HE2	1.63	0.63
1:A:174:SER:HB2	1:A:184:PHE:HE2	1.63	0.63
1:D:317:TYR:O	1:D:321:ASN:ND2	2.30	0.63
3:D:503:IVM:C35	3:D:503:IVM:H32	2.29	0.62
1:E:174:SER:HB2	1:E:184:PHE:HE2	1.63	0.62
3:A:503:IVM:C35	3:A:503:IVM:H32	2.29	0.62
1:D:174:SER:HB2	1:D:184:PHE:HE2	1.63	0.62
1:B:174:SER:HB2	1:B:184:PHE:HE2	1.63	0.62
1:E:317:TYR:O	1:E:321:ASN:ND2	2.30	0.62
3:B:503:IVM:H32	3:B:503:IVM:C35	2.29	0.62
3:E:401:IVM:H32	3:E:401:IVM:C35	2.29	0.61
3:C:503:IVM:C35	3:C:503:IVM:H32	2.29	0.61
1:E:283:SER:HB2	3:E:401:IVM:O10	2.01	0.61
1:A:243:MET:HE1	1:A:286:SER:HB3	1.83	0.61
1:E:195:ALA:HB3	1:E:198:LEU:HB2	1.83	0.61
1:A:195:ALA:HB3	1:A:198:LEU:HB2	1.83	0.60
1:A:115:PHE:CE1	1:A:175:PHE:HB2	2.37	0.60
1:E:115:PHE:CE1	1:E:175:PHE:HB2	2.37	0.59
1:C:195:ALA:HB3	1:C:198:LEU:HB2	1.83	0.59
1:D:115:PHE:CE1	1:D:175:PHE:HB2	2.37	0.59
1:D:195:ALA:HB3	1:D:198:LEU:HB2	1.83	0.59
1:E:254:SER:O	1:E:257:SER:OG	2.13	0.59
1:B:115:PHE:CE1	1:B:175:PHE:HB2	2.37	0.59
1:B:195:ALA:HB3	1:B:198:LEU:HB2	1.83	0.59
1:D:243:MET:HE1	1:D:286:SER:HB3	1.85	0.59
1:B:179:MET:HB3	1:B:222:LYS:HE3	1.84	0.59
1:D:179:MET:HB3	1:D:222:LYS:HE3	1.84	0.59
1:A:254:SER:O	1:A:257:SER:OG	2.13	0.58
1:A:179:MET:HB3	1:A:222:LYS:HE3	1.84	0.58
1:D:46:PRO:HB3	1:D:86:ASP:HB3	1.85	0.58
1:C:46:PRO:HB3	1:C:86:ASP:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:PHE:CE1	1:C:175:PHE:HB2	2.37	0.58
1:B:175:PHE:HZ	1:C:145:SER:HG	1.52	0.58
1:E:46:PRO:HB3	1:E:86:ASP:HB3	1.86	0.58
1:B:46:PRO:HB3	1:B:86:ASP:HB3	1.86	0.58
3:D:503:IVM:H35A	3:D:503:IVM:H32	1.86	0.57
3:D:503:IVM:O7	3:D:503:IVM:H33	2.04	0.57
3:E:401:IVM:H35A	3:E:401:IVM:H32	1.86	0.57
3:E:401:IVM:H33	3:E:401:IVM:O7	2.04	0.57
1:B:287:ARG:NH2	1:C:241:ILE:HG22	2.20	0.57
3:B:503:IVM:H33	3:B:503:IVM:O7	2.04	0.57
1:A:46:PRO:HB3	1:A:86:ASP:HB3	1.86	0.57
1:E:179:MET:HB3	1:E:222:LYS:HE3	1.84	0.57
3:A:503:IVM:H33	3:A:503:IVM:O7	2.04	0.57
1:A:265:ALA:HA	1:A:317:TYR:OH	2.05	0.57
3:C:503:IVM:H35A	3:C:503:IVM:H32	1.86	0.57
1:C:179:MET:HB3	1:C:222:LYS:HE3	1.85	0.57
1:C:265:ALA:HA	1:C:317:TYR:OH	2.05	0.57
1:D:265:ALA:HA	1:D:317:TYR:OH	2.05	0.57
1:E:125:HIS:CE1	1:E:149:THR:HG1	2.23	0.57
3:C:503:IVM:H33	3:C:503:IVM:O7	2.04	0.57
1:E:265:ALA:HA	1:E:317:TYR:OH	2.05	0.57
1:B:304:ALA:HB1	3:B:503:IVM:H18B	1.87	0.57
1:C:243:MET:HE1	1:C:286:SER:HB3	1.86	0.57
1:B:283:SER:CB	3:B:503:IVM:O10	2.53	0.57
1:D:125:HIS:CE1	1:D:149:THR:HG1	2.23	0.56
1:B:265:ALA:HA	1:B:317:TYR:OH	2.05	0.56
3:A:503:IVM:H35A	3:A:503:IVM:H32	1.86	0.56
1:D:120:LYS:HD2	1:D:153:ALA:HB2	1.88	0.56
1:D:254:SER:O	1:D:257:SER:OG	2.13	0.56
1:A:125:HIS:CE1	1:A:149:THR:HG1	2.24	0.56
1:B:125:HIS:CE1	1:B:149:THR:HG1	2.24	0.56
1:A:120:LYS:HD2	1:A:153:ALA:HB2	1.88	0.56
1:B:120:LYS:HD2	1:B:153:ALA:HB2	1.88	0.56
3:B:503:IVM:H32	3:B:503:IVM:H35A	1.86	0.55
1:E:120:LYS:HD2	1:E:153:ALA:HB2	1.88	0.55
1:D:338:ILE:HA	1:D:341:VAL:HG12	1.88	0.55
1:C:287:ARG:HH12	3:C:503:IVM:C42	2.18	0.55
1:B:338:ILE:HA	1:B:341:VAL:HG12	1.88	0.55
1:C:120:LYS:HD2	1:C:153:ALA:HB2	1.88	0.55
1:C:338:ILE:HA	1:C:341:VAL:HG12	1.89	0.55
1:C:125:HIS:CE1	1:C:149:THR:HG1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ARG:HH12	3:D:503:IVM:C42	2.20	0.55
1:A:338:ILE:HA	1:A:341:VAL:HG12	1.88	0.55
1:E:338:ILE:HA	1:E:341:VAL:HG12	1.88	0.55
1:D:115:PHE:CD1	1:D:175:PHE:HB2	2.43	0.54
1:A:115:PHE:CD1	1:A:175:PHE:HB2	2.43	0.54
1:C:115:PHE:CD1	1:C:175:PHE:HB2	2.43	0.54
1:E:243:MET:HE1	1:E:286:SER:HB3	1.89	0.54
1:B:243:MET:HE1	1:B:286:SER:HB3	1.89	0.54
1:E:115:PHE:CD1	1:E:175:PHE:HB2	2.43	0.54
1:E:287:ARG:HH12	3:E:401:IVM:C42	2.21	0.54
1:B:115:PHE:CD1	1:B:175:PHE:HB2	2.43	0.53
1:B:287:ARG:HH12	3:B:503:IVM:C42	2.21	0.53
1:B:265:ALA:HB3	1:B:266:PRO:HD3	1.91	0.53
1:D:280:THR:O	1:D:283:SER:OG	2.22	0.53
1:A:265:ALA:HB3	1:A:266:PRO:HD3	1.91	0.53
1:C:254:SER:O	1:C:257:SER:OG	2.13	0.53
1:C:287:ARG:HH12	3:C:503:IVM:H42	1.73	0.53
1:E:265:ALA:HB3	1:E:266:PRO:HD3	1.91	0.53
1:C:265:ALA:HB3	1:C:266:PRO:HD3	1.91	0.53
1:E:265:ALA:O	1:E:269:VAL:HG23	2.09	0.53
1:C:243:MET:CE	1:C:286:SER:HB3	2.39	0.53
1:E:243:MET:CE	1:E:286:SER:HB3	2.39	0.53
1:D:243:MET:CE	1:D:286:SER:HB3	2.39	0.53
1:B:243:MET:CE	1:B:286:SER:HB3	2.39	0.52
1:D:265:ALA:O	1:D:269:VAL:HG23	2.09	0.52
1:C:265:ALA:O	1:C:269:VAL:HG23	2.09	0.52
1:A:265:ALA:O	1:A:269:VAL:HG23	2.09	0.52
1:D:265:ALA:HB3	1:D:266:PRO:HD3	1.91	0.52
1:A:133:LEU:HD21	1:E:220:THR:HG21	1.90	0.52
1:B:265:ALA:O	1:B:269:VAL:HG23	2.09	0.52
1:B:277:LEU:HD22	1:C:278:THR:HG21	1.92	0.52
1:B:280:THR:O	1:B:283:SER:OG	2.22	0.51
1:A:243:MET:CE	1:A:286:SER:HB3	2.39	0.51
1:B:273:ILE:HD11	1:C:271:LEU:HG	1.92	0.51
1:A:265:ALA:N	1:A:266:PRO:CD	2.74	0.51
1:E:29:PHE:HE2	1:E:99:LEU:HD22	1.76	0.51
1:E:287:ARG:HH12	3:E:401:IVM:H42	1.76	0.51
1:D:265:ALA:N	1:D:266:PRO:CD	2.74	0.51
1:B:29:PHE:HE2	1:B:99:LEU:HD22	1.76	0.51
1:C:265:ALA:N	1:C:266:PRO:CD	2.74	0.51
1:E:265:ALA:N	1:E:266:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:PHE:HD2	1:D:232:LEU:HB3	1.76	0.51
1:E:280:THR:O	1:E:283:SER:OG	2.22	0.51
1:A:106:LEU:HD21	1:A:144:TYR:CE1	2.43	0.51
1:B:265:ALA:N	1:B:266:PRO:CD	2.74	0.51
1:C:29:PHE:HE2	1:C:99:LEU:HD22	1.76	0.51
1:D:29:PHE:HE2	1:D:99:LEU:HD22	1.76	0.51
1:B:277:LEU:HD11	1:C:274:THR:CG2	2.41	0.50
1:B:203:PHE:HD2	1:B:232:LEU:HB3	1.76	0.50
1:B:106:LEU:CD2	1:B:132:LYS:HE2	2.41	0.50
1:B:254:SER:O	1:B:257:SER:OG	2.13	0.50
1:E:346:PHE:HA	1:E:349:VAL:HG12	1.94	0.50
1:A:203:PHE:HD2	1:A:232:LEU:HB3	1.76	0.50
1:C:203:PHE:HD2	1:C:232:LEU:HB3	1.76	0.50
1:C:106:LEU:CD2	1:C:132:LYS:HE2	2.42	0.50
1:A:106:LEU:CD2	1:A:132:LYS:HE2	2.42	0.50
1:C:106:LEU:HD21	1:C:144:TYR:CE1	2.43	0.50
1:B:106:LEU:HD21	1:B:144:TYR:CE1	2.43	0.50
1:A:113:ASP:OD2	1:A:176:GLY:HA3	2.12	0.50
1:B:346:PHE:HA	1:B:349:VAL:HG12	1.94	0.50
1:C:277:LEU:HD22	1:D:278:THR:HG21	1.93	0.50
1:E:113:ASP:OD2	1:E:176:GLY:HA3	2.12	0.50
1:B:60:PHE:HB3	1:B:81:ARG:HH22	1.77	0.50
1:D:80:LEU:O	1:D:145:SER:HA	2.12	0.50
1:B:61:ILE:HG22	1:B:78:ILE:HG22	1.94	0.50
1:D:354:ASN:OD1	1:D:358:TRP:NE1	2.45	0.50
1:D:346:PHE:HA	1:D:349:VAL:HG12	1.94	0.50
1:D:277:LEU:HD22	1:E:278:THR:HG21	1.94	0.50
1:C:183:ILE:HA	1:C:224:THR:HG21	1.94	0.50
1:A:29:PHE:HE2	1:A:99:LEU:HD22	1.76	0.50
1:E:61:ILE:HD11	1:E:194:VAL:HG22	1.93	0.50
1:D:106:LEU:CD2	1:D:132:LYS:HE2	2.42	0.49
1:D:287:ARG:HH12	3:D:503:IVM:H42	1.75	0.49
1:D:183:ILE:HA	1:D:224:THR:HG21	1.94	0.49
1:A:183:ILE:HA	1:A:224:THR:HG21	1.93	0.49
1:A:346:PHE:HA	1:A:349:VAL:HG12	1.94	0.49
1:C:61:ILE:HD11	1:C:194:VAL:HG22	1.94	0.49
1:A:61:ILE:HD11	1:A:194:VAL:HG22	1.94	0.49
1:B:80:LEU:O	1:B:145:SER:HA	2.12	0.49
1:E:106:LEU:CD2	1:E:132:LYS:HE2	2.42	0.49
1:B:113:ASP:OD2	1:B:176:GLY:HA3	2.12	0.49
1:B:61:ILE:HD11	1:B:194:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASN:OD1	1:A:358:TRP:NE1	2.45	0.49
1:E:203:PHE:HD2	1:E:232:LEU:HB3	1.76	0.49
1:C:346:PHE:HA	1:C:349:VAL:HG12	1.94	0.49
1:C:354:ASN:OD1	1:C:358:TRP:NE1	2.45	0.49
1:E:80:LEU:O	1:E:145:SER:HA	2.12	0.49
1:E:183:ILE:HA	1:E:224:THR:HG21	1.93	0.49
1:D:298:ALA:O	1:D:301:ILE:HG13	2.13	0.49
1:D:186:TRP:NE1	1:D:226:ILE:HB	2.28	0.49
1:A:186:TRP:NE1	1:A:226:ILE:HB	2.28	0.49
1:C:60:PHE:HB3	1:C:81:ARG:HH22	1.77	0.49
1:C:61:ILE:HG22	1:C:78:ILE:HG22	1.94	0.49
1:A:298:ALA:O	1:A:301:ILE:HG13	2.13	0.49
1:E:186:TRP:NE1	1:E:226:ILE:HB	2.28	0.49
1:E:298:ALA:O	1:E:301:ILE:HG13	2.13	0.49
1:D:113:ASP:OD2	1:D:176:GLY:HA3	2.12	0.49
1:A:106:LEU:HD23	1:A:132:LYS:HE2	1.95	0.49
1:B:354:ASN:OD1	1:B:358:TRP:NE1	2.45	0.49
1:B:278:THR:O	1:B:282:GLN:HG2	2.13	0.49
1:A:60:PHE:HB3	1:A:81:ARG:HH22	1.77	0.49
1:C:298:ALA:O	1:C:301:ILE:HG13	2.13	0.49
1:C:80:LEU:O	1:C:145:SER:HA	2.12	0.49
1:E:202:GLN:C	1:E:203:PHE:HD1	2.16	0.49
1:A:80:LEU:O	1:A:145:SER:HA	2.12	0.49
1:C:335:ALA:HA	1:C:338:ILE:HG22	1.95	0.49
1:A:61:ILE:HG22	1:A:78:ILE:HG22	1.94	0.49
1:E:354:ASN:OD1	1:E:358:TRP:NE1	2.45	0.49
1:B:183:ILE:HA	1:B:224:THR:HG21	1.94	0.49
1:A:278:THR:O	1:A:282:GLN:HG2	2.13	0.49
1:E:106:LEU:HD23	1:E:132:LYS:HE2	1.95	0.48
1:A:287:ARG:HH12	3:A:503:IVM:C42	2.26	0.48
1:A:202:GLN:C	1:A:203:PHE:HD1	2.16	0.48
1:E:61:ILE:HG22	1:E:78:ILE:HG22	1.94	0.48
1:B:186:TRP:NE1	1:B:226:ILE:HB	2.28	0.48
1:D:273:ILE:O	1:D:277:LEU:HG	2.13	0.48
1:C:186:TRP:NE1	1:C:226:ILE:HB	2.28	0.48
1:C:113:ASP:OD2	1:C:176:GLY:HA3	2.12	0.48
1:C:106:LEU:HD23	1:C:132:LYS:HE2	1.95	0.48
1:A:273:ILE:O	1:A:277:LEU:HG	2.13	0.48
1:D:61:ILE:HG22	1:D:78:ILE:HG22	1.94	0.48
1:B:202:GLN:C	1:B:203:PHE:HD1	2.16	0.48
1:E:273:ILE:O	1:E:277:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ASP:HB3	1:E:105:MET:HG2	1.96	0.48
1:B:298:ALA:O	1:B:301:ILE:HG13	2.13	0.48
1:D:102:ASP:HB3	1:D:105:MET:HG2	1.96	0.48
1:C:278:THR:O	1:C:282:GLN:HG2	2.13	0.48
1:E:278:THR:O	1:E:282:GLN:HG2	2.13	0.48
1:D:61:ILE:HD11	1:D:194:VAL:HG22	1.94	0.48
1:E:64:PHE:HB2	1:E:200:LEU:HD11	1.96	0.48
1:C:102:ASP:HB3	1:C:105:MET:HG2	1.96	0.48
1:D:60:PHE:HB3	1:D:81:ARG:HH22	1.77	0.48
1:C:64:PHE:HB2	1:C:200:LEU:HD11	1.96	0.48
1:A:335:ALA:HA	1:A:338:ILE:HG22	1.95	0.48
1:E:335:ALA:HA	1:E:338:ILE:HG22	1.95	0.48
1:E:60:PHE:HB3	1:E:81:ARG:HH22	1.77	0.48
1:D:202:GLN:C	1:D:203:PHE:HD1	2.16	0.48
1:D:278:THR:O	1:D:282:GLN:HG2	2.13	0.48
1:A:64:PHE:HB2	1:A:200:LEU:HD11	1.96	0.48
1:B:273:ILE:O	1:B:277:LEU:HG	2.13	0.48
1:C:202:GLN:C	1:C:203:PHE:HD1	2.16	0.48
1:C:277:LEU:HD11	1:D:274:THR:CG2	2.44	0.48
1:B:102:ASP:HB3	1:B:105:MET:HG2	1.96	0.48
1:B:106:LEU:HD23	1:B:132:LYS:HE2	1.95	0.47
1:B:335:ALA:HA	1:B:338:ILE:HG22	1.95	0.47
1:D:268:ARG:NH2	1:D:317:TYR:HB2	2.30	0.47
1:A:102:ASP:HB3	1:A:105:MET:HG2	1.96	0.47
1:B:64:PHE:HB2	1:B:200:LEU:HD11	1.96	0.47
1:D:106:LEU:HD21	1:D:144:TYR:CE1	2.43	0.47
1:E:106:LEU:HD21	1:E:144:TYR:CE1	2.43	0.47
1:C:320:VAL:HG13	1:C:335:ALA:HB1	1.97	0.47
1:A:320:VAL:HG13	1:A:335:ALA:HB1	1.97	0.47
1:D:106:LEU:HD23	1:D:132:LYS:HE2	1.95	0.47
1:B:268:ARG:NH2	1:B:317:TYR:HB2	2.29	0.47
1:E:268:ARG:NH2	1:E:317:TYR:HB2	2.29	0.47
1:D:335:ALA:HA	1:D:338:ILE:HG22	1.95	0.47
1:B:320:VAL:HG13	1:B:335:ALA:HB1	1.97	0.47
1:C:273:ILE:O	1:C:277:LEU:HG	2.14	0.47
1:B:56:THR:HA	1:B:185:GLU:O	2.15	0.47
1:C:268:ARG:NH2	1:C:317:TYR:HB2	2.30	0.47
1:D:320:VAL:HG13	1:D:335:ALA:HB1	1.97	0.47
1:E:320:VAL:HG13	1:E:335:ALA:HB1	1.97	0.47
1:D:64:PHE:HB2	1:D:200:LEU:HD11	1.96	0.47
1:E:335:ALA:O	1:E:338:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LEU:HD11	1:E:274:THR:CG2	2.44	0.47
1:D:56:THR:HA	1:D:185:GLU:O	2.15	0.47
1:C:280:THR:O	1:C:283:SER:OG	2.22	0.46
1:A:268:ARG:NH2	1:A:317:TYR:HB2	2.30	0.46
1:A:335:ALA:O	1:A:338:ILE:HG22	2.15	0.46
1:E:56:THR:HA	1:E:185:GLU:O	2.15	0.46
1:C:56:THR:HA	1:C:185:GLU:O	2.15	0.46
1:C:176:GLY:O	1:D:133:LEU:HD13	2.15	0.46
1:B:305:VAL:HG11	1:B:353:PHE:CZ	2.51	0.46
1:A:280:THR:O	1:A:283:SER:OG	2.22	0.46
1:C:273:ILE:HD11	1:D:271:LEU:HG	1.97	0.46
1:C:304:ALA:HB1	3:C:503:IVM:H18B	1.98	0.46
1:D:335:ALA:O	1:D:338:ILE:HG22	2.15	0.46
1:B:335:ALA:O	1:B:338:ILE:HG22	2.15	0.46
1:C:335:ALA:O	1:C:338:ILE:HG22	2.15	0.46
1:B:255:TRP:HA	1:B:258:PHE:HD2	1.81	0.46
1:C:304:ALA:HB2	3:C:503:IVM:H37	1.97	0.46
1:D:115:PHE:CE2	1:D:117:ALA:HA	2.51	0.46
1:A:56:THR:HA	1:A:185:GLU:O	2.15	0.46
1:A:220:THR:HG21	1:B:133:LEU:HD21	1.97	0.46
1:B:115:PHE:CE2	1:B:117:ALA:HA	2.51	0.46
1:C:115:PHE:CE2	1:C:117:ALA:HA	2.51	0.46
1:D:255:TRP:HA	1:D:258:PHE:HD2	1.81	0.46
1:D:304:ALA:HB2	3:D:503:IVM:H37	1.98	0.46
1:E:115:PHE:CE2	1:E:117:ALA:HA	2.51	0.45
1:C:305:VAL:HG11	1:C:353:PHE:CZ	2.51	0.45
1:E:114:LEU:HD13	1:E:184:PHE:CZ	2.52	0.45
1:D:305:VAL:HG11	1:D:353:PHE:CZ	2.51	0.45
1:E:305:VAL:HG11	1:E:353:PHE:CZ	2.51	0.45
1:D:255:TRP:HA	1:D:258:PHE:CD2	2.52	0.45
1:E:255:TRP:HA	1:E:258:PHE:CD2	2.52	0.45
1:B:287:ARG:HH12	3:B:503:IVM:H42	1.81	0.45
1:A:305:VAL:HG11	1:A:353:PHE:CZ	2.51	0.45
1:D:290:LEU:HA	1:D:290:LEU:HD23	1.77	0.45
1:B:255:TRP:HA	1:B:258:PHE:CD2	2.52	0.45
1:A:135:ARG:HG2	1:A:143:LEU:HB3	1.99	0.45
1:D:48:PHE:CE2	1:D:49:LYS:HG2	2.52	0.45
3:E:401:IVM:H38	3:E:401:IVM:O12	2.17	0.45
1:A:115:PHE:CE2	1:A:117:ALA:HA	2.51	0.45
1:A:255:TRP:HA	1:A:258:PHE:HD2	1.81	0.45
1:E:55:VAL:HG22	1:E:84:TRP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:VAL:HG22	1:B:84:TRP:HB3	1.99	0.45
1:B:304:ALA:HB2	3:B:503:IVM:H37	1.99	0.45
1:D:114:LEU:HD13	1:D:184:PHE:CZ	2.52	0.45
1:C:255:TRP:HA	1:C:258:PHE:CD2	2.52	0.45
1:B:191:ALA:HB3	1:B:211:LEU:HD21	1.98	0.45
1:E:191:ALA:HB3	1:E:211:LEU:HD21	1.98	0.45
1:D:169:ILE:HG21	1:D:229:ARG:NH1	2.32	0.45
1:A:304:ALA:HB1	3:A:503:IVM:H18B	1.99	0.45
1:D:273:ILE:HD11	1:E:271:LEU:HG	1.98	0.45
1:E:255:TRP:HA	1:E:258:PHE:HD2	1.81	0.45
3:B:503:IVM:O12	3:B:503:IVM:H38	2.17	0.45
1:D:301:ILE:HD11	1:D:357:TYR:CE1	2.52	0.45
1:A:255:TRP:HA	1:A:258:PHE:CD2	2.52	0.45
1:D:55:VAL:HG22	1:D:84:TRP:HB3	1.99	0.45
1:E:48:PHE:CE2	1:E:49:LYS:HG2	2.52	0.45
1:C:169:ILE:HG21	1:C:229:ARG:NH1	2.32	0.45
1:E:169:ILE:HG21	1:E:229:ARG:NH1	2.32	0.45
3:C:503:IVM:H38	3:C:503:IVM:O12	2.17	0.45
1:A:169:ILE:HG21	1:A:229:ARG:NH1	2.32	0.45
1:D:304:ALA:HB1	3:D:503:IVM:H18B	1.98	0.45
1:A:301:ILE:HD11	1:A:357:TYR:CE1	2.52	0.45
1:C:255:TRP:HA	1:C:258:PHE:HD2	1.81	0.45
1:C:55:VAL:HG22	1:C:84:TRP:HB3	1.99	0.45
1:D:176:GLY:O	1:E:133:LEU:HD13	2.17	0.45
1:A:114:LEU:HD13	1:A:184:PHE:CZ	2.52	0.45
1:B:301:ILE:HD11	1:B:357:TYR:CE1	2.52	0.45
1:B:135:ARG:HG2	1:B:143:LEU:HB3	1.99	0.45
1:E:273:ILE:O	1:E:276:VAL:HG12	2.18	0.44
1:E:301:ILE:HD11	1:E:357:TYR:CE1	2.52	0.44
1:C:135:ARG:HG2	1:C:143:LEU:HB3	1.99	0.44
1:C:301:ILE:HD11	1:C:357:TYR:CE1	2.52	0.44
1:A:48:PHE:CE2	1:A:49:LYS:HG2	2.52	0.44
1:B:169:ILE:HG21	1:B:229:ARG:NH1	2.32	0.44
1:C:273:ILE:O	1:C:276:VAL:HG12	2.17	0.44
1:A:191:ALA:HB3	1:A:211:LEU:HD21	1.98	0.44
1:C:114:LEU:HD13	1:C:184:PHE:CZ	2.52	0.44
1:B:74:TYR:CE1	1:B:168:CYS:HB3	2.53	0.44
1:D:273:ILE:O	1:D:276:VAL:HG12	2.18	0.44
1:D:191:ALA:HB3	1:D:211:LEU:HD21	1.98	0.44
1:E:299:ILE:O	1:E:303:MET:HG2	2.18	0.44
1:B:48:PHE:CE2	1:B:49:LYS:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ALA:HB3	1:C:211:LEU:HD21	1.98	0.44
3:D:503:IVM:H38	3:D:503:IVM:O12	2.17	0.44
1:A:287:ARG:NH2	1:B:241:ILE:HG22	2.32	0.44
3:A:503:IVM:H38	3:A:503:IVM:O12	2.17	0.44
1:A:44:ILE:HD13	1:B:26:PRO:HG2	1.99	0.44
1:E:135:ARG:HG2	1:E:143:LEU:HB3	1.99	0.44
1:C:48:PHE:CE2	1:C:49:LYS:HG2	2.52	0.44
1:A:55:VAL:HG22	1:A:84:TRP:HB3	1.99	0.44
1:D:299:ILE:O	1:D:303:MET:HG2	2.18	0.44
1:A:299:ILE:O	1:A:303:MET:HG2	2.18	0.44
1:B:114:LEU:HD13	1:B:184:PHE:CZ	2.52	0.44
1:D:135:ARG:HG2	1:D:143:LEU:HB3	1.99	0.44
1:B:44:ILE:HD13	1:C:26:PRO:HG2	1.99	0.44
1:D:106:LEU:HD11	1:D:111:LYS:HD3	2.00	0.44
1:E:290:LEU:HA	1:E:290:LEU:HD23	1.77	0.44
1:C:273:ILE:CG2	1:D:274:THR:HG21	2.48	0.44
1:A:273:ILE:O	1:A:276:VAL:HG12	2.18	0.44
1:D:283:SER:CB	3:D:503:IVM:O10	2.63	0.43
1:C:106:LEU:HD11	1:C:111:LYS:HD3	2.00	0.43
1:C:74:TYR:CE1	1:C:168:CYS:HB3	2.53	0.43
1:C:328:THR:HG22	1:C:330:LEU:H	1.83	0.43
1:A:74:TYR:CE1	1:A:168:CYS:HB3	2.53	0.43
1:B:273:ILE:O	1:B:276:VAL:HG12	2.18	0.43
1:B:106:LEU:HD11	1:B:111:LYS:HD3	2.00	0.43
1:E:74:TYR:CE1	1:E:168:CYS:HB3	2.53	0.43
1:C:290:LEU:HA	1:C:290:LEU:HD23	1.77	0.43
1:E:60:PHE:HD1	1:E:193:GLN:HB2	1.83	0.43
1:E:57:CYS:HA	1:E:81:ARG:O	2.19	0.43
1:B:299:ILE:O	1:B:303:MET:HG2	2.18	0.43
1:D:74:TYR:CE1	1:D:168:CYS:HB3	2.53	0.43
1:D:273:ILE:CG2	1:E:274:THR:HG21	2.48	0.43
1:C:299:ILE:O	1:C:303:MET:HG2	2.18	0.43
3:A:503:IVM:H10B	3:A:503:IVM:H3	1.84	0.43
1:D:57:CYS:HA	1:D:81:ARG:O	2.19	0.43
1:D:175:PHE:HZ	1:E:145:SER:HG	1.65	0.43
1:C:57:CYS:HA	1:C:81:ARG:O	2.19	0.43
1:B:328:THR:HG22	1:B:330:LEU:H	1.83	0.43
1:D:328:THR:HG22	1:D:330:LEU:H	1.83	0.43
1:C:283:SER:CB	3:C:503:IVM:O10	2.63	0.43
1:E:106:LEU:HD11	1:E:111:LYS:HD3	2.00	0.43
1:D:60:PHE:HD1	1:D:193:GLN:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:HD1	1:A:193:GLN:HB2	1.83	0.42
1:D:179:MET:SD	1:D:224:THR:HG22	2.60	0.42
1:A:179:MET:SD	1:A:224:THR:HG22	2.60	0.42
1:C:307:LEU:HD21	1:D:249:LEU:CD2	2.49	0.42
1:C:287:ARG:NH2	1:D:241:ILE:HG22	2.34	0.42
1:D:86:ASP:HA	1:D:87:PRO:HD3	1.85	0.42
1:A:328:THR:HG22	1:A:330:LEU:H	1.83	0.42
1:E:212:ARG:HH12	1:E:229:ARG:HE	1.67	0.42
1:D:212:ARG:HH12	1:D:229:ARG:HE	1.67	0.42
1:A:57:CYS:HA	1:A:81:ARG:O	2.19	0.42
1:E:212:ARG:NH1	1:E:229:ARG:HE	2.18	0.42
1:A:212:ARG:NH1	1:A:229:ARG:HE	2.18	0.42
1:C:60:PHE:HD1	1:C:193:GLN:HB2	1.83	0.42
1:A:106:LEU:HD11	1:A:111:LYS:HD3	2.00	0.42
1:B:57:CYS:HA	1:B:81:ARG:O	2.19	0.42
1:D:220:THR:HG21	1:E:133:LEU:HD21	2.02	0.42
1:C:174:SER:HB2	1:C:184:PHE:CE2	2.51	0.42
1:D:287:ARG:NH2	1:E:241:ILE:HG22	2.34	0.42
1:C:46:PRO:HB3	1:C:86:ASP:CB	2.49	0.42
1:C:179:MET:SD	1:C:224:THR:HG22	2.60	0.42
1:D:212:ARG:NH1	1:D:229:ARG:HE	2.18	0.42
1:B:179:MET:SD	1:B:224:THR:HG22	2.60	0.42
1:B:60:PHE:HD1	1:B:193:GLN:HB2	1.83	0.42
1:A:274:THR:HG21	1:E:273:ILE:CG2	2.50	0.42
1:B:212:ARG:NH1	1:B:229:ARG:HE	2.18	0.41
1:A:278:THR:HG21	1:E:277:LEU:HD22	2.01	0.41
1:C:293:VAL:O	1:D:238:TYR:HB2	2.20	0.41
1:E:328:THR:HG22	1:E:330:LEU:H	1.83	0.41
1:C:212:ARG:HH12	1:C:229:ARG:HE	1.67	0.41
1:E:179:MET:SD	1:E:224:THR:HG22	2.60	0.41
1:A:58:ASN:OD1	1:A:81:ARG:HB2	2.20	0.41
3:B:503:IVM:H3	3:B:503:IVM:H10B	1.84	0.41
1:C:253:LEU:HA	1:C:256:VAL:HG22	2.03	0.41
1:C:212:ARG:NH1	1:C:229:ARG:HE	2.18	0.41
1:D:131:ASN:C	1:D:132:LYS:HG3	2.41	0.41
1:E:131:ASN:C	1:E:132:LYS:HG3	2.41	0.41
1:A:131:ASN:C	1:A:132:LYS:HG3	2.41	0.41
1:D:342:SER:HB2	1:D:346:PHE:HE2	1.86	0.41
1:D:58:ASN:OD1	1:D:81:ARG:HB2	2.20	0.41
1:B:253:LEU:HA	1:B:256:VAL:HG22	2.03	0.41
1:C:37:VAL:O	1:C:38:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:SER:HB2	1:D:184:PHE:CE2	2.51	0.41
1:B:212:ARG:HH12	1:B:229:ARG:HE	1.67	0.41
1:B:103:PRO:O	1:B:106:LEU:HB3	2.21	0.41
1:A:103:PRO:O	1:A:106:LEU:HB3	2.21	0.41
1:A:131:ASN:ND2	1:E:115:PHE:HB3	2.36	0.41
1:D:253:LEU:HA	1:D:256:VAL:HG22	2.03	0.41
1:A:212:ARG:HH12	1:A:229:ARG:HE	1.67	0.41
1:C:131:ASN:C	1:C:132:LYS:HG3	2.41	0.41
1:A:274:THR:CG2	1:E:277:LEU:HD11	2.51	0.41
1:E:253:LEU:HA	1:E:256:VAL:HG22	2.03	0.41
1:B:124:PHE:CZ	1:C:128:THR:N	2.89	0.41
1:C:220:THR:HG21	1:D:133:LEU:HD21	2.02	0.41
1:C:103:PRO:O	1:C:106:LEU:HB3	2.21	0.41
1:B:131:ASN:C	1:B:132:LYS:HG3	2.41	0.41
1:B:58:ASN:OD1	1:B:81:ARG:HB2	2.20	0.41
1:C:102:ASP:OD2	1:C:104:SER:OG	2.31	0.41
1:E:58:ASN:OD1	1:E:81:ARG:HB2	2.20	0.41
1:D:46:PRO:HB3	1:D:86:ASP:CB	2.49	0.41
1:A:342:SER:HB2	1:A:346:PHE:HE2	1.86	0.41
1:E:103:PRO:O	1:E:106:LEU:HB3	2.21	0.41
3:E:401:IVM:H38	3:E:401:IVM:H13A	2.03	0.41
1:E:46:PRO:HB3	1:E:86:ASP:CB	2.49	0.41
1:B:277:LEU:HD11	1:C:274:THR:HG21	2.03	0.41
1:B:60:PHE:HD2	1:B:79:PHE:CD2	2.39	0.41
1:C:60:PHE:HD2	1:C:79:PHE:CD2	2.39	0.41
1:C:58:ASN:OD1	1:C:81:ARG:HB2	2.20	0.41
1:B:37:VAL:O	1:B:38:SER:HB3	2.21	0.41
1:D:37:VAL:O	1:D:38:SER:HB3	2.21	0.41
1:A:86:ASP:HA	1:A:87:PRO:HD3	1.85	0.41
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.77	0.40
3:E:401:IVM:H10B	3:E:401:IVM:H3	1.84	0.40
1:E:247:SER:O	1:E:251:VAL:HG23	2.21	0.40
3:B:503:IVM:H13A	3:B:503:IVM:H38	2.03	0.40
3:D:503:IVM:H38	3:D:503:IVM:H13A	2.03	0.40
3:A:503:IVM:H35B	3:A:503:IVM:H32	2.03	0.40
1:B:46:PRO:HB3	1:B:86:ASP:CB	2.49	0.40
1:D:307:LEU:HD21	1:E:249:LEU:CD2	2.52	0.40
1:C:247:SER:O	1:C:251:VAL:HG23	2.21	0.40
1:D:265:ALA:N	1:D:266:PRO:HD2	2.37	0.40
1:C:60:PHE:HD2	1:C:79:PHE:HD2	1.69	0.40
3:C:503:IVM:H3	3:C:503:IVM:H10B	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:SER:HB2	1:E:346:PHE:HE2	1.86	0.40
1:A:253:LEU:HA	1:A:256:VAL:HG22	2.03	0.40
1:B:247:SER:O	1:B:251:VAL:HG23	2.21	0.40
1:E:265:ALA:N	1:E:266:PRO:HD2	2.37	0.40
1:B:203:PHE:N	1:B:203:PHE:CD1	2.90	0.40
1:A:37:VAL:O	1:A:38:SER:HB3	2.21	0.40
1:C:245:ILE:HB	1:C:246:PRO:HD3	2.04	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 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	340/342 (99%)	338 (99%)	2 (1%)	0	100	100
1	B	340/342 (99%)	338 (99%)	2 (1%)	0	100	100
1	C	340/342 (99%)	338 (99%)	2 (1%)	0	100	100
1	D	340/342 (99%)	338 (99%)	2 (1%)	0	100	100
1	E	340/342 (99%)	338 (99%)	2 (1%)	0	100	100
All	All	1700/1710 (99%)	1690 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 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	284/304 (93%)	284 (100%)	0	100	100
1	B	284/304 (93%)	284 (100%)	0	100	100
1	C	284/304 (93%)	284 (100%)	0	100	100
1	D	284/304 (93%)	284 (100%)	0	100	100
1	E	284/304 (93%)	284 (100%)	0	100	100
All	All	1420/1520 (93%)	1420 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	131	ASN
1	A	235	GLN
1	B	54	ASN
1	B	131	ASN
1	B	235	GLN
1	C	54	ASN
1	C	131	ASN
1	C	202	GLN
1	C	235	GLN
1	D	54	ASN
1	D	131	ASN
1	D	235	GLN
1	E	54	ASN
1	E	131	ASN
1	E	235	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)

10 carbohydrates 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	NAG	A	501	2	14,14,15	0.45	0	15,19,21	0.70	0
2	NAG	A	502	2	14,14,15	0.28	0	15,19,21	0.34	0
2	NAG	B	501	2	14,14,15	0.45	0	15,19,21	0.70	0
2	NAG	B	502	2	14,14,15	0.28	0	15,19,21	0.34	0
2	NAG	C	501	2	14,14,15	0.46	0	15,19,21	0.70	0
2	NAG	C	502	2	14,14,15	0.29	0	15,19,21	0.34	0
2	NAG	D	501	2	14,14,15	0.46	0	15,19,21	0.70	0
2	NAG	D	502	2	14,14,15	0.29	0	15,19,21	0.34	0
2	NAG	E	402	2	14,14,15	0.46	0	15,19,21	0.70	0
2	NAG	E	403	2	14,14,15	0.30	0	15,19,21	0.34	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
2	NAG	A	501	2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	501	2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
2	NAG	C	501	2	-	0/6/23/26	0/1/1/1
2	NAG	C	502	2	-	0/6/23/26	0/1/1/1
2	NAG	D	501	2	-	0/6/23/26	0/1/1/1
2	NAG	D	502	2	-	0/6/23/26	0/1/1/1
2	NAG	E	402	2	-	0/6/23/26	0/1/1/1
2	NAG	E	403	2	-	0/6/23/26	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.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
3	IVM	A	503	-	64,68,68	0.80	1 (1%)	72,102,102	1.50	15 (20%)
3	IVM	B	503	-	64,68,68	0.80	1 (1%)	72,102,102	1.50	15 (20%)
3	IVM	C	503	-	64,68,68	0.81	1 (1%)	72,102,102	1.50	15 (20%)
3	IVM	D	503	-	64,68,68	0.80	1 (1%)	72,102,102	1.50	15 (20%)
3	IVM	E	401	-	64,68,68	0.81	1 (1%)	72,102,102	1.50	15 (20%)

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	IVM	A	503	-	-	0/43/141/141	0/5/7/7
3	IVM	B	503	-	-	0/43/141/141	0/5/7/7
3	IVM	C	503	-	-	0/43/141/141	0/5/7/7
3	IVM	D	503	-	-	0/43/141/141	0/5/7/7
3	IVM	E	401	-	-	0/43/141/141	0/5/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	IVM	O12-C46	4.90	1.45	1.34
3	D	503	IVM	O12-C46	4.90	1.45	1.34
3	B	503	IVM	O12-C46	4.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	IVM	O12-C46	4.92	1.45	1.34
3	E	401	IVM	O12-C46	4.94	1.45	1.34

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	IVM	C15-C16-C17	-3.86	120.50	127.24
3	E	401	IVM	C15-C16-C17	-3.85	120.53	127.24
3	C	503	IVM	C15-C16-C17	-3.85	120.53	127.24
3	B	503	IVM	C15-C16-C17	-3.84	120.55	127.24
3	D	503	IVM	C15-C16-C17	-3.82	120.58	127.24
3	A	503	IVM	C13-C14-C15	-3.47	108.87	113.34
3	B	503	IVM	C13-C14-C15	-3.45	108.91	113.34
3	D	503	IVM	C13-C14-C15	-3.44	108.91	113.34
3	C	503	IVM	C13-C14-C15	-3.44	108.91	113.34
3	E	401	IVM	C13-C14-C15	-3.43	108.93	113.34
3	E	401	IVM	C37-C38-C39	-3.14	121.12	130.40
3	B	503	IVM	C37-C38-C39	-3.14	121.13	130.40
3	C	503	IVM	C37-C38-C39	-3.14	121.14	130.40
3	A	503	IVM	C37-C38-C39	-3.13	121.15	130.40
3	D	503	IVM	C37-C38-C39	-3.12	121.18	130.40
3	C	503	IVM	C3-C5-C9	-2.99	110.99	116.37
3	B	503	IVM	C3-C5-C9	-2.97	111.01	116.37
3	A	503	IVM	C3-C5-C9	-2.97	111.01	116.37
3	E	401	IVM	C3-C5-C9	-2.97	111.02	116.37
3	D	503	IVM	C3-C5-C9	-2.95	111.05	116.37
3	B	503	IVM	C34-C36-C37	-2.57	120.38	126.06
3	E	401	IVM	C34-C36-C37	-2.56	120.41	126.06
3	D	503	IVM	C34-C36-C37	-2.55	120.42	126.06
3	A	503	IVM	C34-C36-C37	-2.55	120.42	126.06
3	C	503	IVM	C34-C36-C37	-2.54	120.44	126.06
3	B	503	IVM	C12-O12-C46	-2.45	114.19	117.76
3	D	503	IVM	C12-O12-C46	-2.44	114.21	117.76
3	A	503	IVM	C12-O12-C46	-2.43	114.23	117.76
3	E	401	IVM	C12-O12-C46	-2.42	114.24	117.76
3	C	503	IVM	C12-O12-C46	-2.39	114.29	117.76
3	D	503	IVM	C42-C43-C44	-2.30	119.01	121.36
3	A	503	IVM	C42-C43-C44	-2.30	119.01	121.36
3	C	503	IVM	C42-C43-C44	-2.30	119.02	121.36
3	B	503	IVM	C42-C43-C44	-2.24	119.07	121.36
3	E	401	IVM	C42-C43-C44	-2.23	119.08	121.36
3	B	503	IVM	C38-C37-C36	-2.22	118.92	124.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	IVM	C38-C37-C36	-2.19	118.97	124.06
3	E	401	IVM	C38-C37-C36	-2.19	118.97	124.06
3	C	503	IVM	C38-C37-C36	-2.19	118.99	124.06
3	D	503	IVM	C38-C37-C36	-2.19	118.99	124.06
3	D	503	IVM	O9-C40-C39	-2.09	103.63	105.66
3	A	503	IVM	O9-C40-C39	-2.07	103.66	105.66
3	C	503	IVM	O9-C40-C39	-2.06	103.66	105.66
3	B	503	IVM	C6-O1-C5	-2.06	111.30	114.42
3	E	401	IVM	C6-O1-C5	-2.05	111.30	114.42
3	A	503	IVM	C6-O1-C5	-2.05	111.31	114.42
3	C	503	IVM	C6-O1-C5	-2.05	111.31	114.42
3	B	503	IVM	O9-C40-C39	-2.05	103.68	105.66
3	E	401	IVM	O9-C40-C39	-2.03	103.70	105.66
3	D	503	IVM	C6-O1-C5	-2.03	111.34	114.42
3	C	503	IVM	O1-C6-C11	2.09	109.26	106.27
3	B	503	IVM	O1-C6-C11	2.09	109.26	106.27
3	A	503	IVM	O1-C6-C11	2.10	109.27	106.27
3	E	401	IVM	O1-C6-C11	2.11	109.28	106.27
3	D	503	IVM	C18-C17-C19	2.11	119.31	115.61
3	D	503	IVM	O1-C6-C11	2.11	109.29	106.27
3	B	503	IVM	C18-C17-C19	2.13	119.35	115.61
3	E	401	IVM	C18-C17-C19	2.13	119.36	115.61
3	A	503	IVM	C18-C17-C19	2.14	119.37	115.61
3	C	503	IVM	C18-C17-C19	2.15	119.39	115.61
3	E	401	IVM	O1-C5-C3	2.28	109.87	106.27
3	A	503	IVM	O1-C5-C3	2.29	109.88	106.27
3	B	503	IVM	O1-C5-C3	2.29	109.89	106.27
3	C	503	IVM	O1-C5-C3	2.29	109.89	106.27
3	D	503	IVM	O1-C5-C3	2.30	109.90	106.27
3	C	503	IVM	O14-C14-C15	3.65	109.29	105.87
3	B	503	IVM	O14-C14-C15	3.66	109.30	105.87
3	A	503	IVM	O14-C14-C15	3.68	109.31	105.87
3	E	401	IVM	O14-C14-C15	3.70	109.33	105.87
3	D	503	IVM	O14-C14-C15	3.70	109.34	105.87
3	B	503	IVM	O12-C46-C45	4.59	118.81	111.18
3	D	503	IVM	O12-C46-C45	4.60	118.83	111.18
3	A	503	IVM	O12-C46-C45	4.61	118.84	111.18
3	E	401	IVM	O12-C46-C45	4.61	118.84	111.18
3	C	503	IVM	O12-C46-C45	4.64	118.90	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	IVM	9	0
3	B	503	IVM	12	0
3	C	503	IVM	11	0
3	D	503	IVM	11	0
3	E	401	IVM	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.