



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 26, 2019 – 10:41 AM EST

PDB ID : 6N4B
EMDB ID: : EMD-0339
Title : Cannabinoid Receptor 1-G Protein Complex
Authors : Krishna Kumar, K.; Shalev-Benami, M.; Hu, H.; Weis, W.I.; Kobilka, B.K.;
Skiniotis, G.
Deposited on : 2018-11-18
Resolution : 3.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

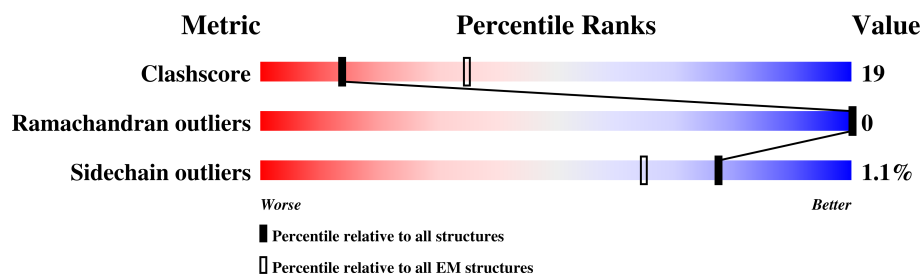
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	354	 49% 12% 38%
2	B	344	 67% 31% ..
3	C	71	 69% 11% 20%
4	R	495	 37% 19% 44%
5	S	259	 66% 22% • 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8453 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1646	1058	281	294	13		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2553	1584	459	489	21		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	57	Total	C	N	O	S	0	0
			435	273	77	82	3		

- Molecule 4 is a protein called Cannabinoid receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	276	Total	C	N	O	S	0	0
			1988	1318	343	316	11		

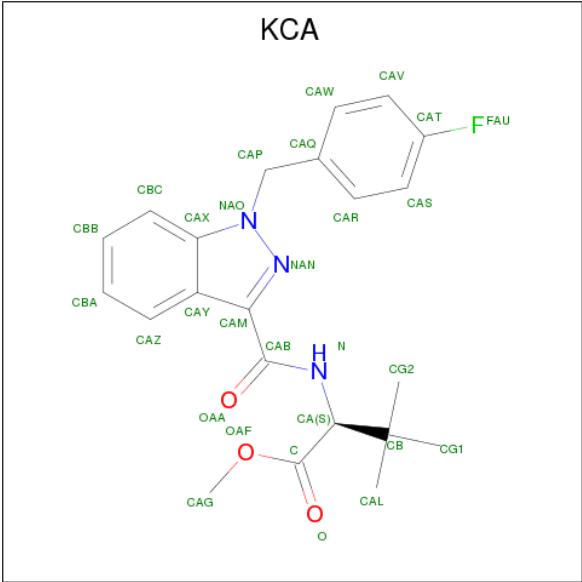
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-14	ASP	-	expression tag	UNP P21554
R	-13	TYR	-	expression tag	UNP P21554
R	-12	LYS	-	expression tag	UNP P21554
R	-11	ASP	-	expression tag	UNP P21554
R	-10	ASP	-	expression tag	UNP P21554
R	-9	ASP	-	expression tag	UNP P21554
R	-8	ASP	-	expression tag	UNP P21554
R	-7	ALA	-	expression tag	UNP P21554
R	81	GLU	-	insertion	UNP P21554
R	82	ASN	-	insertion	UNP P21554
R	83	LEU	-	insertion	UNP P21554
R	84	TYR	-	insertion	UNP P21554
R	85	PHE	-	insertion	UNP P21554
R	86	GLN	-	insertion	UNP P21554
R	87	GLY	-	insertion	UNP P21554
R	473	GLY	-	expression tag	UNP P21554
R	474	SER	-	expression tag	UNP P21554
R	475	HIS	-	expression tag	UNP P21554
R	476	HIS	-	expression tag	UNP P21554
R	477	HIS	-	expression tag	UNP P21554
R	478	HIS	-	expression tag	UNP P21554
R	479	HIS	-	expression tag	UNP P21554
R	480	HIS	-	expression tag	UNP P21554

- Molecule 5 is a protein called scFv16.

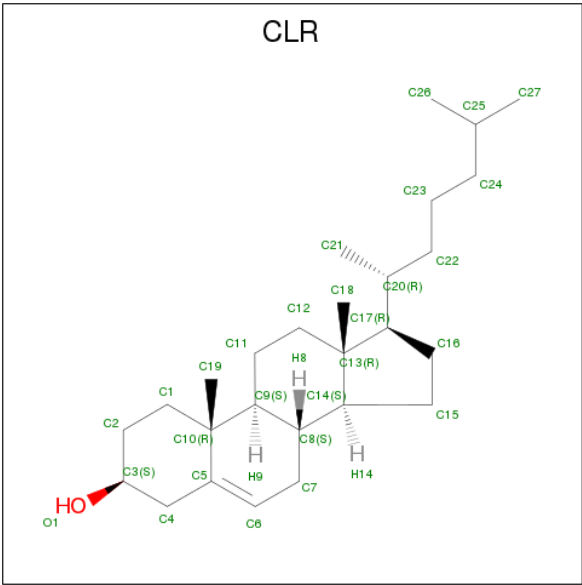
Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	232	Total	C	N	O	S	0	0
			1746	1114	294	328	10		

- Molecule 6 is methyl N-{1-[(4-fluorophenyl)methyl]-1H-indazole-3-carbonyl}-3-methyl-L-valinate (three-letter code: KCA) (formula: C₂₂H₂₄FN₃O₃).



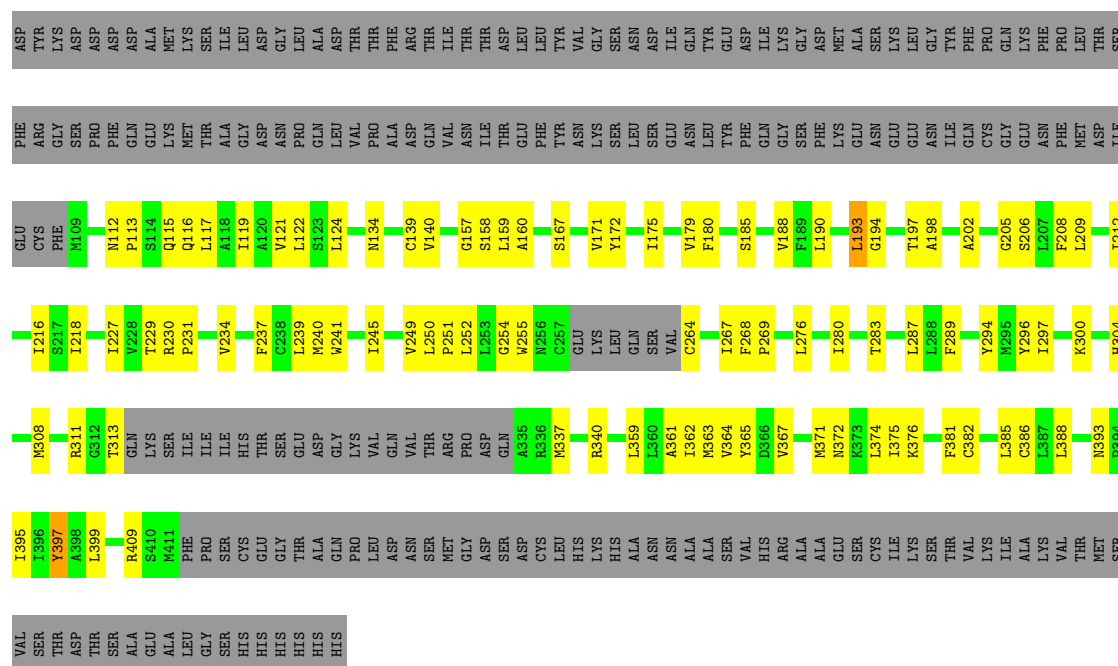
Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	F	N	O	0
			29	22	1	3	3	

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



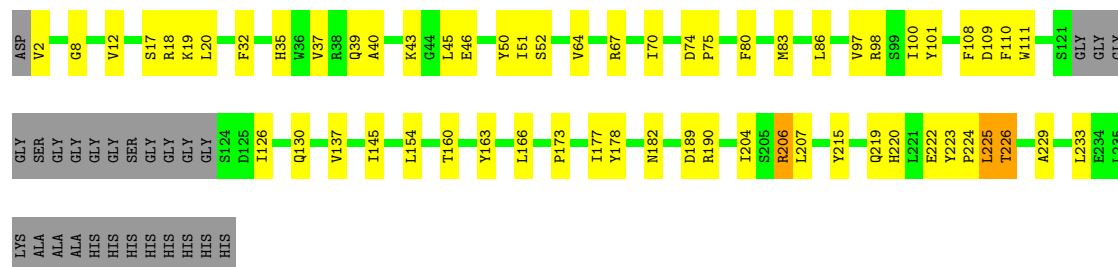
Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			56	54	2	
7	R	1	Total	C	O	0
			56	54	2	

Chain R:  37% 19% 44%



- Molecule 5: scFv16

Chain S: 66% 22% 10%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	177787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: KCA, CLR

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	0/1675	0.62	0/2261
2	B	0.58	0/2600	0.74	0/3528
3	C	0.38	0/441	0.68	0/595
4	R	0.50	0/2037	0.74	0/2789
5	S	0.61	0/1790	0.69	1/2432 (0.0%)
All	All	0.54	0/8543	0.70	1/11605 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	224	PRO	N-CA-C	5.04	125.21	112.10

There are no chirality outliers.

There are no planarity outliers.

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	1646	0	1578	33	0
2	B	2553	0	2447	82	0
3	C	435	0	445	11	0
4	R	1988	0	1857	143	0
5	S	1746	0	1667	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	29	0	0	0	0
7	R	56	0	92	30	0
All	All	8453	0	8086	315	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 (315) 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:R:371:MET:HE2	4:R:375:ILE:CB	1.37	1.53
4:R:371:MET:CE	4:R:375:ILE:CB	1.85	1.53
4:R:227:ILE:HD13	7:R:502:CLR:C26	1.09	1.52
4:R:190:LEU:CD2	4:R:252:LEU:HA	1.56	1.33
4:R:227:ILE:CD1	7:R:502:CLR:H263	1.58	1.32
4:R:227:ILE:CD1	7:R:502:CLR:C26	2.06	1.31
4:R:190:LEU:HD23	4:R:252:LEU:CA	1.63	1.26
4:R:202:ALA:HB1	4:R:241:TRP:CH2	1.74	1.22
5:S:126:ILE:HD11	5:S:222:GLU:OE2	1.37	1.21
4:R:227:ILE:HD13	7:R:502:CLR:H261	1.20	1.19
4:R:190:LEU:HD23	4:R:252:LEU:N	1.58	1.19
4:R:371:MET:HE3	4:R:375:ILE:CB	1.68	1.11
7:R:503:CLR:H211	7:R:503:CLR:H272	1.29	1.10
4:R:371:MET:HA	4:R:371:MET:HE3	1.29	1.08
4:R:227:ILE:CG2	7:R:502:CLR:H261	1.85	1.07
4:R:202:ALA:CB	4:R:241:TRP:CH2	2.40	1.05
5:S:126:ILE:CD1	5:S:222:GLU:OE2	2.08	1.02
4:R:227:ILE:HG21	7:R:502:CLR:H261	1.07	1.02
4:R:190:LEU:HD22	4:R:252:LEU:HA	1.44	0.98
4:R:227:ILE:HG21	7:R:502:CLR:C26	1.96	0.96
4:R:280:ILE:HD13	4:R:364:VAL:CG2	1.97	0.95
4:R:227:ILE:HD13	7:R:502:CLR:H262	1.49	0.93
7:R:503:CLR:H211	7:R:503:CLR:C27	1.97	0.93
4:R:240:MET:HA	7:R:503:CLR:H271	1.51	0.93
5:S:220:HIS:O	5:S:220:HIS:ND1	2.01	0.91
4:R:113:PRO:O	4:R:117:LEU:N	2.04	0.91
4:R:280:ILE:HD13	4:R:364:VAL:HG22	1.48	0.91
4:R:227:ILE:HD13	7:R:502:CLR:H263	0.90	0.89
4:R:371:MET:HA	4:R:371:MET:CE	2.01	0.89
4:R:371:MET:HB3	4:R:376:LYS:N	1.89	0.88
2:B:283:ARG:O	2:B:284:LEU:HD12	1.75	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD22	1:A:353:LEU:HD23	1.61	0.82
1:A:184:ILE:HG13	1:A:201:VAL:HG22	1.61	0.81
2:B:38:ASP:OD1	2:B:38:ASP:O	1.98	0.81
4:R:167:SER:O	4:R:171:VAL:HG23	1.80	0.81
2:B:66:ASP:O	2:B:67:SER:OG	1.96	0.81
2:B:43:ILE:HD13	2:B:284:LEU:HD21	1.63	0.80
5:S:225:LEU:H	5:S:225:LEU:HD23	1.45	0.80
4:R:283:THR:HG22	4:R:287:LEU:HD13	1.63	0.79
4:R:175:ILE:O	4:R:179:VAL:HB	1.83	0.79
4:R:239:LEU:HD23	7:R:503:CLR:H183	1.64	0.78
5:S:64:VAL:HG12	5:S:67:ARG:HH21	1.47	0.78
4:R:159:LEU:HB2	4:R:206:SER:HB3	1.65	0.78
4:R:194:GLY:O	4:R:197:THR:HG22	1.84	0.78
4:R:190:LEU:CD2	4:R:252:LEU:CA	2.35	0.78
5:S:166:LEU:HD13	5:S:215:TYR:CE1	2.19	0.78
2:B:271:CYS:HB3	2:B:290:ASP:HB3	1.67	0.77
7:R:503:CLR:H272	7:R:503:CLR:C21	2.14	0.76
4:R:240:MET:HA	7:R:503:CLR:C27	2.14	0.76
5:S:17:SER:HB2	5:S:83:MET:O	1.85	0.75
4:R:393:ASN:O	4:R:397:TYR:HB2	1.87	0.75
4:R:202:ALA:CB	4:R:241:TRP:CZ3	2.70	0.75
4:R:254:GLY:O	4:R:255:TRP:CD1	2.39	0.74
2:B:151:PHE:CE1	2:B:157:ILE:HD12	2.23	0.74
5:S:225:LEU:N	5:S:225:LEU:HD23	2.02	0.74
4:R:267:ILE:O	4:R:376:LYS:NZ	2.21	0.74
4:R:371:MET:HB3	4:R:375:ILE:CB	2.19	0.73
4:R:371:MET:CA	4:R:371:MET:HE3	2.13	0.73
4:R:239:LEU:CD2	7:R:503:CLR:H183	2.20	0.72
2:B:26:ALA:HB2	2:B:259:GLN:HE22	1.55	0.72
4:R:371:MET:HB3	4:R:375:ILE:C	2.09	0.71
5:S:64:VAL:HG12	5:S:67:ARG:NH2	2.06	0.71
4:R:254:GLY:O	4:R:255:TRP:CG	2.44	0.70
4:R:362:ILE:HA	4:R:365:TYR:HB2	1.71	0.70
1:A:216:GLU:OE2	1:A:258:TRP:HE3	1.75	0.68
4:R:158:SER:HB2	4:R:237:PHE:HE1	1.59	0.68
5:S:83:MET:HB3	5:S:86:LEU:HD21	1.75	0.68
4:R:202:ALA:HB1	4:R:241:TRP:CZ2	2.28	0.67
2:B:34:THR:HG22	2:B:34:THR:O	1.93	0.67
2:B:34:THR:HG23	2:B:37:ILE:HG21	1.76	0.67
5:S:137:VAL:HG11	5:S:207:LEU:HD21	1.75	0.67
1:A:337:ASP:OD1	4:R:311:ARG:NH1	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ASN:OD1	2:B:294:CYS:N	2.24	0.66
1:A:304:GLN:NE2	1:A:321:THR:OG1	2.28	0.66
4:R:276:LEU:O	4:R:280:ILE:CD1	2.44	0.66
5:S:32:PHE:CD2	5:S:98:ARG:HD2	2.31	0.66
7:R:503:CLR:H211	7:R:503:CLR:C24	2.27	0.65
4:R:190:LEU:HD23	4:R:251:PRO:C	2.16	0.65
2:B:68:ARG:HG2	2:B:68:ARG:O	1.96	0.64
4:R:190:LEU:N	4:R:190:LEU:HD12	2.12	0.64
4:R:283:THR:O	4:R:287:LEU:HD13	1.98	0.63
1:A:208:ARG:HD2	1:A:212:ILE:HD12	1.80	0.63
4:R:249:VAL:C	4:R:251:PRO:HD2	2.18	0.63
4:R:115:GLN:O	4:R:119:ILE:CB	2.47	0.63
4:R:193:LEU:HD23	4:R:193:LEU:O	1.99	0.63
2:B:85:TYR:HD1	3:C:61:PHE:HE1	1.47	0.62
4:R:171:VAL:O	4:R:175:ILE:HG12	2.00	0.62
4:R:239:LEU:HD23	7:R:503:CLR:C18	2.28	0.62
7:R:503:CLR:H241	7:R:503:CLR:C21	2.29	0.62
4:R:371:MET:CB	4:R:375:ILE:CB	2.78	0.62
4:R:139:CYS:SG	4:R:140:VAL:N	2.73	0.61
5:S:154:LEU:HA	5:S:160:THR:HG22	1.82	0.61
4:R:159:LEU:HB2	4:R:206:SER:CB	2.29	0.61
2:B:65:THR:CG2	2:B:107:PRO:HA	2.30	0.61
4:R:202:ALA:HB2	4:R:241:TRP:CZ3	2.34	0.61
2:B:251:ARG:HD2	2:B:260:GLU:OE2	2.00	0.61
2:B:304:ARG:HG2	2:B:305:ALA:O	1.99	0.61
2:B:308:LEU:HD11	2:B:339:TRP:CE3	2.36	0.61
5:S:98:ARG:HH11	5:S:109:ASP:CG	2.03	0.61
2:B:323:ASP:OD1	2:B:324:GLY:N	2.33	0.61
4:R:227:ILE:CD1	7:R:502:CLR:H261	2.01	0.61
2:B:34:THR:CG2	2:B:37:ILE:HG21	2.31	0.60
4:R:159:LEU:HD13	4:R:206:SER:HB2	1.83	0.60
4:R:208:PHE:O	4:R:212:ILE:HG12	2.01	0.60
4:R:179:VAL:HG12	4:R:180:PHE:N	2.16	0.60
2:B:183:HIS:ND1	2:B:203:ALA:HB2	2.17	0.59
4:R:276:LEU:O	4:R:280:ILE:HD12	2.02	0.59
2:B:260:GLU:OE2	2:B:263:THR:HG22	2.03	0.59
4:R:395:ILE:O	4:R:399:LEU:HB3	2.02	0.59
5:S:51:ILE:HD11	5:S:70:ILE:HG12	1.84	0.59
5:S:177:ILE:HG23	5:S:182:ASN:O	2.03	0.59
4:R:134:ASN:OD1	4:R:160:ALA:O	2.21	0.58
4:R:409:ARG:HD2	4:R:409:ARG:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:VAL:HG11	5:S:108:PHE:CD1	2.38	0.58
2:B:85:TYR:CD1	3:C:61:PHE:HE1	2.22	0.58
2:B:259:GLN:HE21	3:C:30:VAL:HG21	1.68	0.58
4:R:190:LEU:CD1	4:R:190:LEU:H	2.15	0.58
4:R:193:LEU:C	4:R:193:LEU:HD23	2.24	0.58
7:R:502:CLR:H121	7:R:502:CLR:H212	1.86	0.58
4:R:385:LEU:O	4:R:388:LEU:N	2.38	0.57
4:R:283:THR:CG2	4:R:287:LEU:HD13	2.33	0.57
4:R:364:VAL:O	4:R:364:VAL:HG12	2.05	0.56
7:R:502:CLR:C23	7:R:502:CLR:H162	2.35	0.56
5:S:32:PHE:CE2	5:S:98:ARG:HD2	2.40	0.56
5:S:97:VAL:HG11	5:S:108:PHE:HD1	1.71	0.56
2:B:65:THR:HG21	2:B:107:PRO:HA	1.87	0.56
2:B:164:THR:HG22	2:B:185:GLY:O	2.06	0.56
4:R:190:LEU:N	4:R:190:LEU:CD1	2.68	0.56
4:R:227:ILE:HD12	7:R:502:CLR:H263	1.77	0.56
2:B:106:ALA:HA	2:B:151:PHE:HD2	1.71	0.55
2:B:161:SER:HB2	2:B:163:ASP:OD1	2.06	0.55
1:A:271:LYS:HD2	1:A:296:TYR:OH	2.06	0.55
2:B:286:LEU:CD2	2:B:296:VAL:HG22	2.36	0.55
4:R:194:GLY:C	4:R:197:THR:HG22	2.26	0.55
4:R:158:SER:CB	4:R:237:PHE:HE1	2.20	0.55
5:S:111:TRP:CE3	5:S:173:PRO:HG2	2.42	0.55
2:B:43:ILE:CD1	2:B:284:LEU:HD21	2.36	0.55
2:B:292:PHE:N	2:B:292:PHE:CD1	2.72	0.55
7:R:503:CLR:C24	7:R:503:CLR:C21	2.85	0.55
4:R:362:ILE:CA	4:R:365:TYR:HB2	2.37	0.54
5:S:98:ARG:NH1	5:S:109:ASP:OD2	2.37	0.54
5:S:204:ILE:HG21	5:S:207:LEU:HB3	1.90	0.54
3:C:56:ALA:HB1	3:C:62:ARG:HD3	1.89	0.54
1:A:184:ILE:CG1	1:A:201:VAL:HG22	2.34	0.54
2:B:286:LEU:HD23	2:B:296:VAL:HG22	1.88	0.53
5:S:19:LYS:HE2	5:S:80:PHE:CD1	2.43	0.53
4:R:190:LEU:HB3	4:R:252:LEU:HG	1.90	0.53
4:R:218:ILE:HD12	4:R:297:ILE:HG23	1.91	0.53
1:A:184:ILE:CD1	1:A:215:PHE:HZ	2.21	0.53
2:B:235:PHE:CE1	2:B:282:GLY:HA3	2.44	0.53
3:C:56:ALA:O	3:C:62:ARG:NH1	2.41	0.53
4:R:280:ILE:HG21	4:R:364:VAL:HG21	1.90	0.53
1:A:293:SER:OG	1:A:298:GLU:OE1	2.25	0.53
2:B:62:HIS:O	2:B:71:VAL:HG12	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:239:LEU:CD2	7:R:503:CLR:C18	2.87	0.53
2:B:335:PHE:CD1	2:B:335:PHE:N	2.73	0.53
5:S:206:ARG:O	5:S:206:ARG:HD2	2.09	0.53
4:R:208:PHE:CE2	4:R:289:PHE:CD2	2.96	0.52
2:B:95:LEU:HD12	2:B:100:VAL:HG21	1.91	0.52
2:B:102:THR:HG22	2:B:103:CYS:N	2.24	0.52
5:S:130:GLN:NE2	5:S:229:ALA:O	2.42	0.52
1:A:315:ASP:OD1	1:A:316:THR:N	2.43	0.52
2:B:229:ILE:HG22	2:B:245:SER:HB3	1.91	0.52
4:R:194:GLY:O	4:R:197:THR:CG2	2.54	0.52
5:S:145:ILE:HD11	5:S:233:LEU:HD11	1.90	0.52
1:A:354:PHE:HZ	4:R:337:MET:HG3	1.75	0.51
4:R:119:ILE:CB	4:R:381:PHE:CE1	2.93	0.51
5:S:219:GLN:HE21	5:S:226:THR:H	1.59	0.51
5:S:40:ALA:CB	5:S:43:LYS:HE2	2.41	0.51
1:A:228:SER:O	1:A:277:LYS:NZ	2.30	0.51
4:R:372:ASN:C	4:R:374:LEU:N	2.62	0.51
4:R:276:LEU:O	4:R:276:LEU:HG	2.11	0.51
4:R:112:ASN:O	4:R:116:GLN:N	2.37	0.50
4:R:119:ILE:CB	4:R:381:PHE:HE1	2.23	0.50
2:B:314:ARG:HD2	2:B:332:TRP:CE2	2.46	0.50
4:R:280:ILE:HD13	4:R:364:VAL:HG23	1.85	0.50
4:R:280:ILE:CD1	4:R:364:VAL:HG22	2.31	0.50
7:R:503:CLR:H241	7:R:503:CLR:H211	1.91	0.50
2:B:51:LEU:HD22	2:B:82:TRP:CE3	2.46	0.50
2:B:102:THR:HG21	2:B:148:CYS:HA	1.94	0.50
2:B:125:ASN:HB2	2:B:136:SER:HB2	1.94	0.49
2:B:280:LYS:O	2:B:281:SER:OG	2.25	0.49
4:R:212:ILE:CD1	4:R:289:PHE:CE2	2.95	0.49
1:A:188:HIS:ND1	1:A:197:LYS:HG2	2.27	0.49
1:A:286:CYS:O	1:A:287:TYR:HD1	1.95	0.49
1:A:354:PHE:CE2	4:R:340:ARG:HD2	2.47	0.49
2:B:229:ILE:HA	2:B:245:SER:HA	1.94	0.49
4:R:208:PHE:HE2	4:R:289:PHE:CD2	2.31	0.49
4:R:372:ASN:C	4:R:374:LEU:H	2.15	0.49
5:S:109:ASP:OD1	5:S:110:PHE:N	2.45	0.49
2:B:142:HIS:CD2	2:B:146:LEU:HD11	2.47	0.49
5:S:189:ASP:O	5:S:189:ASP:OD1	2.31	0.49
1:A:8:GLU:HG3	5:S:101:TYR:HD1	1.78	0.49
2:B:269:ILE:HG21	2:B:289:TYR:CE2	2.47	0.49
4:R:171:VAL:O	4:R:175:ILE:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:230:ARG:O	4:R:234:VAL:HG23	2.12	0.49
4:R:359:LEU:O	4:R:363:MET:HB2	2.13	0.49
2:B:102:THR:OG1	2:B:147:SER:O	2.31	0.48
4:R:280:ILE:HG21	4:R:364:VAL:CG2	2.43	0.48
2:B:51:LEU:HD23	2:B:87:THR:HG23	1.96	0.48
4:R:251:PRO:O	4:R:254:GLY:N	2.43	0.48
1:A:225:VAL:HB	1:A:268:LEU:HD23	1.95	0.48
2:B:73:ALA:HB1	2:B:100:VAL:HG11	1.96	0.48
5:S:35:HIS:CE1	5:S:50:TYR:HD1	2.31	0.48
2:B:228:ASP:OD1	2:B:228:ASP:N	2.44	0.47
4:R:179:VAL:CG1	4:R:180:PHE:N	2.76	0.47
4:R:371:MET:CB	4:R:376:LYS:N	2.72	0.47
5:S:32:PHE:CE1	5:S:100:ILE:HD12	2.49	0.47
5:S:35:HIS:CE1	5:S:50:TYR:CD1	3.02	0.47
2:B:64:GLY:HA2	2:B:105:TYR:CD2	2.49	0.47
4:R:158:SER:HB2	4:R:237:PHE:CE1	2.44	0.47
4:R:296:TYR:OH	4:R:300:LYS:HD2	2.15	0.47
5:S:190:ARG:HD2	5:S:206:ARG:O	2.15	0.47
5:S:37:VAL:HG13	5:S:46:GLU:O	2.14	0.47
1:A:216:GLU:OE2	1:A:258:TRP:HA	2.14	0.47
1:A:231:ASP:OD1	1:A:232:LEU:N	2.48	0.47
2:B:211:TRP:CZ3	2:B:218:CYS:HB2	2.50	0.47
4:R:361:ALA:O	4:R:365:TYR:N	2.47	0.46
4:R:283:THR:HG22	4:R:287:LEU:CD1	2.41	0.46
5:S:39:GLN:HB2	5:S:45:LEU:HD23	1.97	0.46
2:B:124:TYR:CE1	2:B:135:VAL:HG22	2.50	0.46
5:S:32:PHE:HE1	5:S:100:ILE:HD12	1.79	0.46
2:B:193:ALA:HB1	2:B:194:PRO:HD2	1.98	0.46
2:B:150:ARG:O	2:B:157:ILE:HG13	2.15	0.46
4:R:227:ILE:CG1	7:R:502:CLR:H261	2.45	0.46
1:A:201:VAL:O	1:A:201:VAL:HG12	2.15	0.46
2:B:314:ARG:HD2	2:B:332:TRP:CZ2	2.51	0.46
4:R:212:ILE:HD11	4:R:289:PHE:CE2	2.50	0.46
5:S:51:ILE:HG22	5:S:52:SER:O	2.16	0.46
4:R:382:CYS:O	4:R:385:LEU:HG	2.17	0.45
7:R:503:CLR:H211	7:R:503:CLR:C25	2.45	0.45
2:B:112:VAL:HG12	2:B:113:ALA:N	2.32	0.45
4:R:230:ARG:N	4:R:231:PRO:HD2	2.32	0.45
5:S:74:ASP:HB2	5:S:75:PRO:HD3	1.98	0.45
2:B:197:ARG:O	2:B:198:LEU:HD23	2.17	0.45
4:R:197:THR:HG23	4:R:198:ALA:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HD11	1:A:215:PHE:HZ	1.81	0.45
4:R:113:PRO:HA	4:R:116:GLN:CB	2.47	0.45
4:R:190:LEU:HD12	4:R:190:LEU:H	1.79	0.45
5:S:12:VAL:CG2	5:S:18:ARG:HE	2.29	0.45
5:S:51:ILE:CD1	5:S:70:ILE:HG12	2.47	0.45
4:R:251:PRO:HA	4:R:255:TRP:NE1	2.32	0.45
4:R:294:TYR:HD1	4:R:294:TYR:HA	1.56	0.45
5:S:2:VAL:O	5:S:2:VAL:HG12	2.16	0.45
3:C:7:ALA:HA	3:C:11:GLN:HB3	1.99	0.45
4:R:194:GLY:CA	4:R:197:THR:HG22	2.47	0.45
4:R:208:PHE:O	4:R:208:PHE:CD1	2.71	0.45
1:A:266:LEU:HD23	1:A:321:THR:HG22	1.99	0.44
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.99	0.44
4:R:121:VAL:O	4:R:122:LEU:C	2.55	0.44
4:R:157:GLY:HA2	4:R:160:ALA:HB3	1.98	0.44
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.82	0.44
4:R:283:THR:CG2	4:R:287:LEU:CD1	2.95	0.44
7:R:502:CLR:C23	7:R:502:CLR:C16	2.95	0.44
4:R:208:PHE:CG	4:R:208:PHE:O	2.70	0.44
2:B:61:MET:SD	2:B:70:LEU:HD21	2.58	0.44
1:A:269:ASN:HA	1:A:324:THR:O	2.18	0.44
2:B:78:LYS:HA	2:B:93:ILE:O	2.17	0.43
2:B:121:CYS:HB3	2:B:139:LEU:HB2	2.01	0.43
5:S:163:TYR:CE2	5:S:178:TYR:O	2.71	0.43
1:A:40:GLY:HA3	1:A:46:LYS:HD3	2.00	0.43
2:B:233:CYS:O	2:B:241:PHE:HB2	2.19	0.43
4:R:216:ILE:HG21	4:R:227:ILE:HD11	2.00	0.43
4:R:304:HIS:O	4:R:308:MET:HG2	2.17	0.43
2:B:180:PHE:HE1	2:B:216:GLY:HA2	1.83	0.43
4:R:194:GLY:HA2	4:R:197:THR:HG22	2.00	0.43
2:B:298:ASP:O	2:B:301:LYS:O	2.37	0.43
2:B:339:TRP:CD1	2:B:339:TRP:N	2.87	0.43
4:R:283:THR:O	4:R:287:LEU:CD1	2.66	0.43
2:B:313:ASN:ND2	2:B:332:TRP:HB2	2.34	0.43
1:A:348:LEU:HD11	4:R:218:ILE:HD11	2.01	0.43
2:B:42:ARG:HD3	2:B:44:GLN:NE2	2.34	0.42
4:R:268:PHE:HB3	4:R:269:PRO:HD2	2.01	0.42
4:R:121:VAL:O	4:R:124:LEU:N	2.52	0.42
4:R:250:LEU:N	4:R:251:PRO:HD2	2.33	0.42
5:S:223:TYR:N	5:S:223:TYR:CD1	2.85	0.42
2:B:183:HIS:CE1	2:B:203:ALA:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLY:O	2:B:95:LEU:HG	2.18	0.42
2:B:48:ARG:HB3	3:C:61:PHE:HB3	2.02	0.42
3:C:62:ARG:O	3:C:63:GLU:HB2	2.19	0.42
4:R:230:ARG:N	4:R:231:PRO:CD	2.82	0.42
2:B:254:ASP:OD2	2:B:261:LEU:HD21	2.19	0.42
4:R:113:PRO:O	4:R:116:GLN:N	2.52	0.42
1:A:212:ILE:HD11	1:A:259:PHE:HE2	1.85	0.42
2:B:271:CYS:SG	2:B:291:ASP:HB3	2.60	0.42
4:R:172:TYR:HA	4:R:175:ILE:HG12	2.01	0.42
1:A:185:VAL:HG12	1:A:186:GLU:N	2.35	0.42
4:R:185:SER:H	4:R:188:VAL:HB	1.85	0.42
4:R:385:LEU:HD12	4:R:386:CYS:N	2.34	0.42
2:B:259:GLN:NE2	3:C:30:VAL:HG21	2.32	0.41
2:B:235:PHE:CE2	3:C:37:LEU:HD22	2.55	0.41
4:R:313:THR:HG22	4:R:313:THR:O	2.20	0.41
2:B:42:ARG:HD3	2:B:44:GLN:HE21	1.85	0.41
2:B:157:ILE:HG23	2:B:169:TRP:HB2	2.02	0.41
2:B:151:PHE:HE1	2:B:157:ILE:HD12	1.78	0.41
2:B:100:VAL:HG13	2:B:114:CYS:SG	2.61	0.41
2:B:112:VAL:HG23	2:B:126:LEU:HD11	2.02	0.41
4:R:205:GLY:O	4:R:209:LEU:HG	2.21	0.41
4:R:212:ILE:HD13	4:R:289:PHE:CE2	2.56	0.41
5:S:8:GLY:HA3	5:S:20:LEU:HD23	2.01	0.41
2:B:81:ILE:HD12	2:B:91:HIS:HB2	2.02	0.41
4:R:190:LEU:HG	4:R:251:PRO:HB2	2.03	0.41
4:R:229:THR:CB	4:R:231:PRO:HD2	2.51	0.41
5:S:51:ILE:HG21	5:S:51:ILE:HD13	1.89	0.41
4:R:241:TRP:O	4:R:245:ILE:HG13	2.20	0.41
4:R:367:VAL:CB	4:R:371:MET:SD	3.09	0.41
1:A:320:TYR:HD1	4:R:313:THR:HG21	1.85	0.40
7:R:503:CLR:C27	7:R:503:CLR:C21	2.85	0.40
2:B:283:ARG:O	2:B:283:ARG:CG	2.70	0.40
2:B:48:ARG:HD2	3:C:61:PHE:O	2.21	0.40
5:S:50:TYR:CG	5:S:51:ILE:N	2.90	0.40
1:A:36:LEU:HD13	1:A:222:ILE:HD11	2.04	0.40
1:A:8:GLU:HG3	5:S:101:TYR:CD1	2.55	0.40
1:A:334:PHE:HE1	4:R:313:THR:OG1	2.04	0.40
2:B:104:ALA:O	2:B:112:VAL:HG13	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	212/354 (60%)	211 (100%)	1 (0%)	0	100	100
2	B	336/344 (98%)	326 (97%)	10 (3%)	0	100	100
3	C	55/71 (78%)	53 (96%)	2 (4%)	0	100	100
4	R	270/495 (54%)	259 (96%)	11 (4%)	0	100	100
5	S	228/259 (88%)	222 (97%)	6 (3%)	0	100	100
All	All	1101/1523 (72%)	1071 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	164/305 (54%)	164 (100%)	0	100	100
2	B	267/285 (94%)	264 (99%)	3 (1%)	76	92
3	C	45/58 (78%)	45 (100%)	0	100	100
4	R	173/437 (40%)	170 (98%)	3 (2%)	63	88
5	S	184/209 (88%)	181 (98%)	3 (2%)	65	89
All	All	833/1294 (64%)	824 (99%)	9 (1%)	77	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	154	ASP
2	B	292	PHE
2	B	335	PHE
4	R	193	LEU
4	R	264	CYS
4	R	397	TYR
5	S	206	ARG
5	S	225	LEU
5	S	226	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	244	HIS
1	A	304	GLN
1	A	306	GLN
1	A	311	ASN
2	B	62	HIS
2	B	259	GLN
4	R	143	HIS
4	R	154	HIS
4	R	178	HIS
5	S	219	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$
6	KCA	R	501	-	28,31,31	3.38	8 (28%)	33,45,45	2.35	11 (33%)
7	CLR	R	502	-	31,31,31	0.69	0	48,48,48	1.14	5 (10%)
7	CLR	R	503	-	31,31,31	0.77	0	48,48,48	1.56	9 (18%)

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	KCA	R	501	-	-	0/20/24/24	0/3/3/3
7	CLR	R	502	-	-	0/10/68/68	0/4/4/4
7	CLR	R	503	-	-	0/10/68/68	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	KCA	FAU-CAT	-10.83	1.10	1.36
6	R	501	KCA	CAM-CAB	-10.28	1.35	1.50
6	R	501	KCA	CAP-CAQ	-4.99	1.40	1.51
6	R	501	KCA	CAZ-CAY	-4.44	1.33	1.42
6	R	501	KCA	CBC-CAX	-3.74	1.33	1.41
6	R	501	KCA	NAN-NAO	-3.51	1.33	1.37
6	R	501	KCA	CAM-NAN	-2.47	1.33	1.35
6	R	501	KCA	CA-C	2.14	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	KCA	O-C-CA	-4.19	116.84	124.18
7	R	503	CLR	C13-C17-C20	-3.56	113.75	119.47
7	R	502	CLR	C13-C17-C20	-3.22	114.29	119.47
7	R	503	CLR	C8-C7-C6	-2.93	108.39	112.73
7	R	503	CLR	C13-C14-C8	-2.78	110.18	114.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	KCA	CAW-CAV-CAT	-2.70	115.51	118.35
6	R	501	KCA	CAQ-CAP-NAO	-2.68	108.56	112.48
7	R	503	CLR	C7-C6-C5	-2.55	120.20	125.06
7	R	502	CLR	C11-C12-C13	-2.54	108.40	112.79
7	R	503	CLR	C2-C3-C4	-2.52	106.84	110.28
6	R	501	KCA	CB-CA-N	-2.47	108.65	111.74
7	R	502	CLR	C13-C14-C8	-2.44	110.69	114.38
7	R	503	CLR	C11-C12-C13	-2.38	108.66	112.79
6	R	501	KCA	CAG-OAF-C	-2.05	111.25	115.97
7	R	503	CLR	C10-C5-C6	-2.01	119.73	122.92
6	R	501	KCA	OAA-CAB-CAM	2.11	123.81	120.56
7	R	502	CLR	C4-C5-C10	2.14	119.33	116.41
7	R	502	CLR	C17-C13-C14	2.23	102.72	100.07
7	R	503	CLR	C1-C10-C5	2.56	113.56	108.76
6	R	501	KCA	CAP-CAQ-CAR	3.05	126.04	120.41
6	R	501	KCA	CAL-CB-CA	3.21	116.39	109.73
7	R	503	CLR	C4-C5-C10	4.02	121.90	116.41
6	R	501	KCA	CAV-CAW-CAQ	4.39	127.08	121.02
6	R	501	KCA	CAP-NAO-NAN	5.50	129.53	118.10
6	R	501	KCA	OAF-C-CA	6.47	120.48	111.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	502	CLR	15	0
7	R	503	CLR	15	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.