



Full wwPDB Geometry-Only Validation Report ⓘ

Jun 26, 2019 – 02:28 PM EDT

PDB ID : 6I2X
Title : Structure of Complement C5 in Complex with small molecule inhibitor and CVF
Authors : Srinivas, H.
Deposited on : 2018-11-02
Resolution : 3.35 Å(reported)

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (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) : 2.3.2

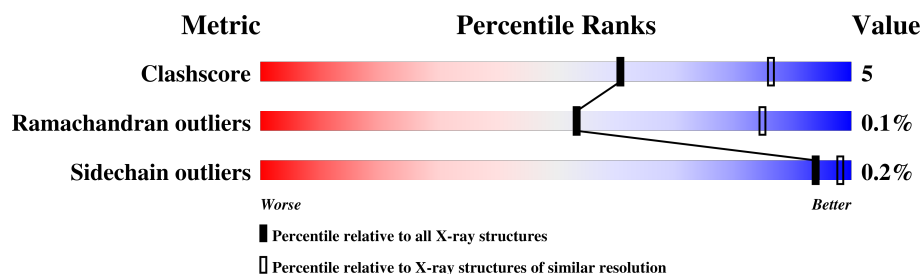
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1380 (3.42-3.30)
Ramachandran outliers	120053	1359 (3.42-3.30)
Sidechain outliers	120020	1358 (3.42-3.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	657	
2	A	999	
3	B	1642	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19109 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	648	Total	C	N	O	S	0	0	0
			5123	3286	820	1004	13			

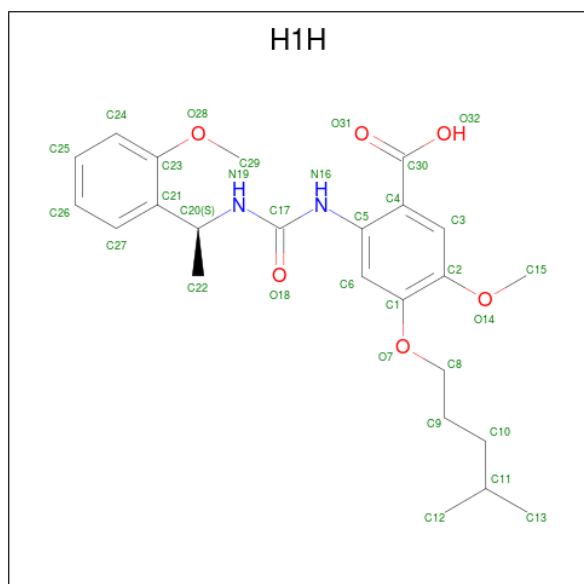
- Molecule 2 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	815	Total	C	N	O	S	0	0	0
			6454	4128	1089	1207	30			

- Molecule 3 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	951	Total	C	N	O	S	0	0	0
			7499	4803	1256	1408	32			

- Molecule 4 is 5-methoxy-2-[[[(1 {S})-1-(2-methoxyphenyl)ethyl]carbamoylamino]-4-(4-methylpentoxy)benzoic acid (three-letter code: H1H) (formula: C₂₄H₃₂N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	24	2	6		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

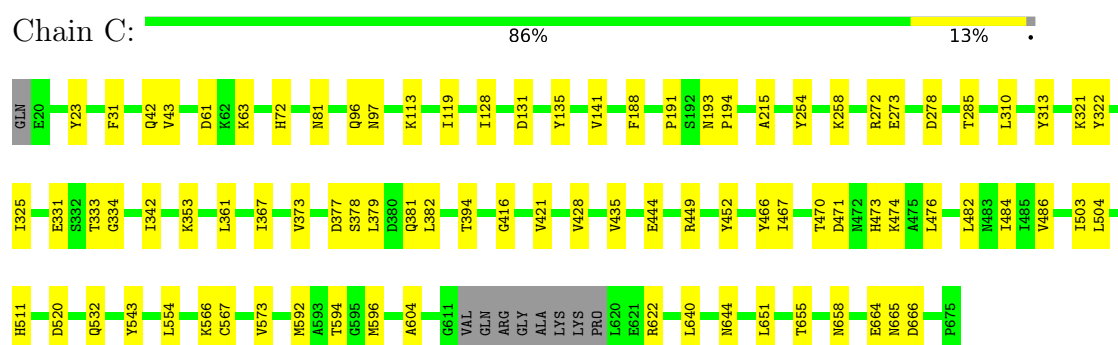
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

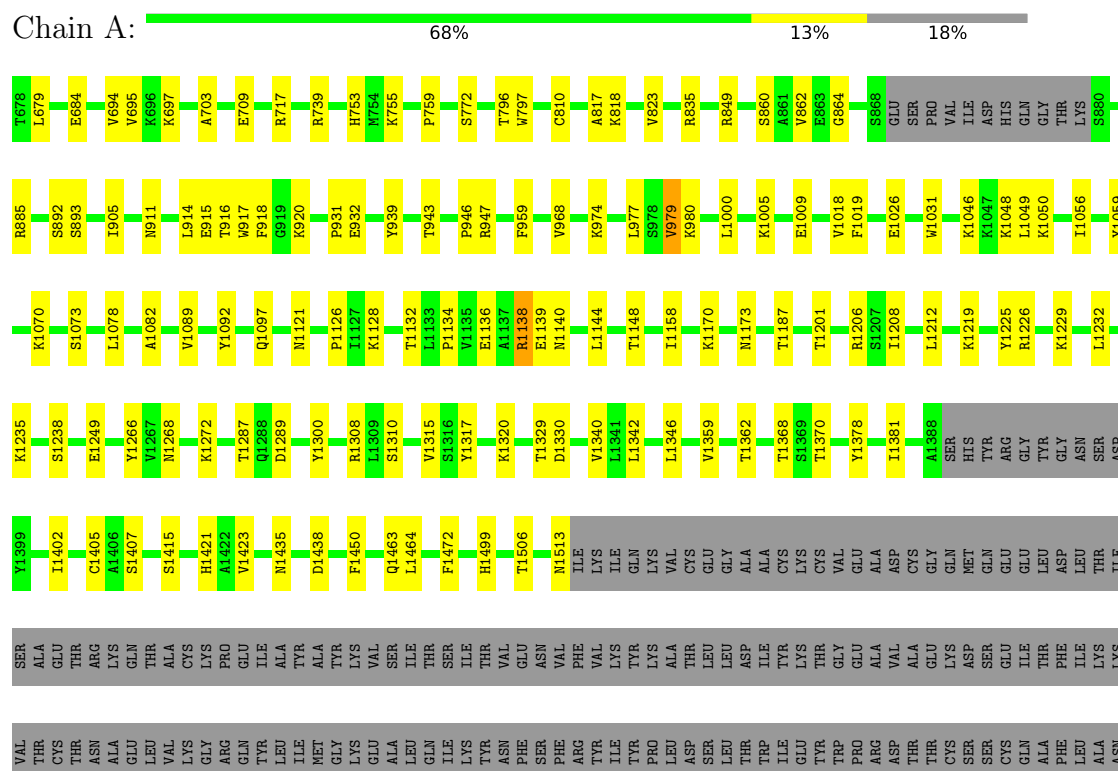
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Complement C5



• Molecule 2: Complement C5



Chain B: 51% 7% 42%



4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H1H, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.41	0/5242	0.56	0/7131
2	A	0.34	0/6588	0.53	0/8923
3	B	0.40	0/7664	0.57	1/10408 (0.0%)
All	All	0.39	0/19494	0.56	1/26462 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	144	LEU	CA-CB-CG	5.81	128.67	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	679	LEU	Peptide
1	C	310	LEU	Peptide

4.2 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	C	5123	0	5029	51	0
2	A	6454	0	6505	77	0
3	B	7499	0	7519	69	0
4	A	32	0	0	0	0
5	B	1	0	0	0	0
All	All	19109	0	19053	188	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 5.

All (188) 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:C:394:THR:HG23	1:C:428:VAL:HG23	1.77	0.66
3:B:414:ARG:HH12	3:B:416:ASN:HD22	1.45	0.65
3:B:222:PRO:HD2	3:B:583:ALA:HB1	1.82	0.62
3:B:857:CYS:HB3	3:B:885:VAL:HG13	1.81	0.62
1:C:476:LEU:HD11	1:C:482:LEU:HD13	1.82	0.61
1:C:373:VAL:HG11	1:C:435:VAL:HG11	1.82	0.61
3:B:137:TYR:HB2	3:B:216:VAL:HG12	1.83	0.60
3:B:166:GLN:OE1	3:B:198:ARG:NH1	2.35	0.60
1:C:467:ILE:HB	1:C:484:ILE:HD11	1.83	0.59
1:C:61:ASP:HB2	1:C:63:LYS:HD3	1.86	0.58
1:C:520:ASP:OD1	1:C:520:ASP:N	2.37	0.58
1:C:353:LYS:HE2	1:C:378:SER:HA	1.86	0.57
2:A:1128:LYS:NZ	2:A:1415:SER:OG	2.37	0.57
3:B:1405:ASP:N	3:B:1405:ASP:OD1	2.37	0.57
3:B:485:ASN:ND2	3:B:517:SER:O	2.38	0.56
1:C:532:GLN:NE2	1:C:566:LYS:O	2.36	0.55
1:C:640:LEU:H	1:C:644:ASN:HD22	1.54	0.55
1:C:325:ILE:HD12	1:C:342:ILE:HD12	1.87	0.55
1:C:141:VAL:HB	1:C:188:PHE:HB3	1.87	0.55
2:A:959:PHE:HB2	2:A:1346:LEU:HB2	1.88	0.54
3:B:1397:LEU:HD21	3:B:1408:ILE:HG21	1.89	0.54
2:A:892:SER:OG	2:A:893:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:748:ARG:HB3	3:B:782:ASP:HB3	1.89	0.54
1:C:131:ASP:OD1	1:C:131:ASP:N	2.38	0.54
3:B:124:GLN:NE2	3:B:125:SER:O	2.41	0.54
2:A:916:THR:HG23	2:A:918:PHE:H	1.74	0.53
2:A:1340:VAL:HG21	2:A:1346:LEU:HD11	1.90	0.53
3:B:1473:HIS:HB2	3:B:1479:GLY:HA2	1.91	0.53
2:A:939:TYR:HD1	2:A:1362:THR:HG22	1.72	0.53
3:B:1384:ILE:HG12	3:B:1456:VAL:HG22	1.91	0.53
2:A:1026:GLU:OE2	2:A:1031:TRP:NE1	2.38	0.53
2:A:684:GLU:HA	2:A:753:HIS:HE1	1.73	0.53
2:A:1005:LYS:O	2:A:1463:GLN:NE2	2.42	0.53
2:A:1317:TYR:HB2	2:A:1320:LYS:HB3	1.90	0.52
3:B:61:PHE:HB2	3:B:103:TYR:HB2	1.90	0.52
2:A:697:LYS:HD3	2:A:759:PRO:HD3	1.91	0.52
1:C:96:GLN:NE2	1:C:97:ASN:OD1	2.42	0.52
2:A:835:ARG:NH2	2:A:932:GLU:OE2	2.42	0.52
2:A:1056:ILE:HG13	2:A:1059:TYR:HB2	1.92	0.52
2:A:1329:THR:OG1	2:A:1330:ASP:N	2.42	0.52
2:A:1000:LEU:HD13	2:A:1287:THR:HG22	1.91	0.52
1:C:655:THR:OG1	1:C:658:ASN:O	2.28	0.51
2:A:1201:THR:HA	2:A:1206:ARG:HH12	1.75	0.51
2:A:797:TRP:HB2	2:A:817:ALA:HB3	1.93	0.51
1:C:471:ASP:OD2	1:C:474:LYS:NZ	2.44	0.51
2:A:1046:LYS:NZ	2:A:1092:TYR:O	2.43	0.50
2:A:1136:GLU:OE2	2:A:1140:ASN:ND2	2.44	0.50
3:B:788:VAL:HG22	3:B:807:GLU:HG2	1.92	0.50
1:C:31:PHE:HB2	1:C:119:ILE:HG22	1.93	0.50
3:B:1378:THR:O	3:B:1460:SER:OG	2.29	0.50
1:C:573:VAL:HG12	1:C:592:MET:HG2	1.93	0.50
2:A:703:ALA:O	2:A:739:ARG:NH2	2.42	0.50
3:B:238:ASP:OD1	3:B:238:ASP:N	2.44	0.50
2:A:1078:LEU:O	2:A:1082:ALA:N	2.44	0.50
2:A:1423:VAL:HG22	2:A:1463:GLN:HG2	1.94	0.50
3:B:261:ALA:HA	3:B:320:VAL:HA	1.93	0.50
2:A:946:PRO:HB2	2:A:947:ARG:HH21	1.77	0.50
2:A:1126:PRO:O	2:A:1499:HIS:ND1	2.36	0.50
2:A:1320:LYS:HG2	2:A:1342:LEU:HD22	1.94	0.49
3:B:566:LYS:NZ	3:B:773:SER:OG	2.39	0.49
2:A:943:THR:OG1	2:A:1272:LYS:NZ	2.45	0.49
3:B:847:ARG:HE	3:B:869:GLN:HE21	1.60	0.49
3:B:275:SER:OG	3:B:276:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASN:HD21	2:A:1070:LYS:HD3	1.77	0.49
2:A:1226:ARG:NH1	2:A:1266:TYR:O	2.45	0.49
1:C:191:PRO:HD2	1:C:194:PRO:HB3	1.93	0.49
2:A:1132:THR:HG23	2:A:1134:PRO:HD2	1.94	0.49
3:B:362:LEU:HD23	3:B:398:LEU:HD12	1.93	0.49
3:B:379:VAL:HA	3:B:415:THR:HA	1.93	0.49
3:B:840:VAL:HG12	3:B:842:GLU:H	1.76	0.49
1:C:554:LEU:HD11	1:C:655:THR:HG21	1.94	0.49
3:B:858:SER:HB3	3:B:884:ILE:HG12	1.95	0.48
2:A:1405:CYS:HB3	2:A:1472:PHE:HB3	1.94	0.48
1:C:131:ASP:OD1	1:C:135:TYR:OH	2.29	0.48
3:B:270:ASP:OD1	3:B:270:ASP:N	2.43	0.48
2:A:979:VAL:HG12	2:A:1359:VAL:HG22	1.95	0.48
2:A:905:ILE:HD13	2:A:931:PRO:HG3	1.95	0.48
3:B:422:ARG:NH1	3:B:422:ARG:O	2.39	0.48
2:A:1018:VAL:HG11	2:A:1048:LYS:HB2	1.96	0.48
2:A:1370:THR:HG21	2:A:1506:THR:HB	1.96	0.48
2:A:1134:PRO:O	2:A:1138:ARG:NE	2.43	0.48
3:B:44:GLU:OE1	3:B:523:TYR:OH	2.31	0.48
2:A:1170:LYS:HA	2:A:1173:ASN:HB2	1.96	0.47
2:A:1219:LYS:HB2	2:A:1225:TYR:HB2	1.96	0.47
1:C:604:ALA:O	2:A:772:SER:OG	2.30	0.47
1:C:72:HIS:H	1:C:81:ASN:HD22	1.62	0.47
3:B:164:GLU:OE1	3:B:202:LYS:NZ	2.48	0.47
1:C:503:ILE:HB	1:C:511:HIS:HB2	1.97	0.47
1:C:421:VAL:HG11	3:B:505:THR:HG23	1.97	0.47
3:B:393:ASP:OD2	3:B:393:ASP:N	2.44	0.47
3:B:379:VAL:HG12	3:B:415:THR:HG22	1.96	0.47
2:A:849:ARG:HH12	3:B:555:LEU:HD13	1.80	0.47
3:B:1484:ILE:HG12	3:B:1493:ALA:HB2	1.98	0.46
3:B:71:THR:OG1	3:B:72:ARG:N	2.49	0.46
1:C:377:ASP:OD1	1:C:381:GLN:N	2.45	0.46
2:A:1208:ILE:O	2:A:1212:LEU:N	2.45	0.46
3:B:370:ASP:N	3:B:370:ASP:OD1	2.48	0.46
2:A:849:ARG:NH2	3:B:556:ILE:O	2.44	0.46
2:A:1229:LYS:NZ	2:A:1238:SER:O	2.45	0.46
2:A:980:LYS:HD3	2:A:980:LYS:HA	1.75	0.46
1:C:473:HIS:NE2	3:B:452:THR:O	2.42	0.46
3:B:1444:LYS:HE3	3:B:1447:GLU:HG2	1.98	0.45
3:B:552:GLY:O	3:B:554:ASN:ND2	2.49	0.45
1:C:272:ARG:HB3	1:C:322:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:347:PHE:O	3:B:349:LYS:N	2.49	0.45
1:C:272:ARG:HH21	1:C:278:ASP:HA	1.81	0.45
2:A:1268:ASN:OD1	2:A:1300:TYR:OH	2.27	0.45
1:C:42:GLN:OE1	1:C:543:TYR:OH	2.32	0.45
2:A:1049:LEU:HD22	2:A:1089:VAL:HG13	1.98	0.45
3:B:520:PHE:HB3	3:B:536:VAL:HG12	1.97	0.45
2:A:1139:GLU:HG3	2:A:1187:THR:HG21	1.99	0.45
3:B:282:ARG:NH1	3:B:1379:MET:SD	2.89	0.45
3:B:118:VAL:HG13	3:B:638:GLN:HE22	1.81	0.45
1:C:594:THR:OG1	1:C:596:MET:O	2.29	0.45
3:B:133:ASP:OD1	3:B:133:ASP:N	2.43	0.45
2:A:885:ARG:NH2	3:B:903:ALA:O	2.47	0.45
1:C:128:ILE:HB	1:C:215:ALA:HB2	1.99	0.45
2:A:1232:LEU:H	2:A:1235:LYS:HE2	1.81	0.45
2:A:1378:TYR:HB2	2:A:1407:SER:HB3	1.99	0.45
1:C:353:LYS:HB2	1:C:353:LYS:HE3	1.80	0.45
3:B:1401:SER:HB3	3:B:1408:ILE:HG12	1.98	0.44
3:B:618:LEU:HD21	3:B:634:LEU:HG	1.99	0.44
1:C:333:THR:OG1	1:C:334:GLY:N	2.50	0.44
2:A:1050:LYS:HB3	2:A:1050:LYS:HE2	1.81	0.44
2:A:1073:SER:OG	2:A:1121:ASN:ND2	2.50	0.44
3:B:360:TYR:HD2	3:B:400:LEU:HD23	1.82	0.44
2:A:974:LYS:HB3	2:A:974:LYS:HE2	1.79	0.44
3:B:548:LEU:HD22	3:B:793:SER:HB3	2.00	0.44
2:A:1144:LEU:O	2:A:1148:THR:OG1	2.32	0.44
3:B:24:LEU:HB3	3:B:46:HIS:HB2	2.00	0.44
3:B:784:ILE:HG23	3:B:811:MET:HA	1.99	0.44
3:B:1387:LEU:HB3	3:B:1451:ILE:HD11	2.01	0.43
1:C:254:TYR:HB2	1:C:258:LYS:HB2	1.99	0.43
3:B:610:THR:OG1	3:B:611:ALA:N	2.52	0.43
1:C:254:TYR:N	1:C:258:LYS:O	2.48	0.43
3:B:56:ILE:HG13	3:B:108:VAL:HG13	2.00	0.43
2:A:1513:ASN:N	2:A:1513:ASN:OD1	2.51	0.43
2:A:755:LYS:HB3	2:A:755:LYS:HE3	1.72	0.43
3:B:1382:ILE:HB	3:B:1425:ILE:HB	2.00	0.43
1:C:273:GLU:OE1	1:C:321:LYS:NZ	2.47	0.43
2:A:862:VAL:HG13	2:A:864:GLY:H	1.84	0.43
1:C:470:THR:HG23	3:B:450:THR:HB	2.00	0.43
2:A:1009:GLU:OE2	2:A:1287:THR:OG1	2.33	0.42
3:B:41:ILE:HG13	3:B:85:PRO:HD2	1.99	0.42
2:A:915:GLU:HB3	2:A:920:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:796:THR:HB	2:A:818:LYS:HG3	2.02	0.42
2:A:1170:LYS:HE3	2:A:1170:LYS:HB2	1.79	0.42
2:A:1450:PHE:HD1	2:A:1464:LEU:HB2	1.84	0.42
3:B:1473:HIS:CD2	3:B:1474:PRO:HD2	2.55	0.42
1:C:23:TYR:HB3	1:C:43:VAL:HG12	2.02	0.42
1:C:664:GLU:H	1:C:664:GLU:HG2	1.67	0.42
2:A:1019:PHE:HB2	2:A:1049:LEU:HD21	2.02	0.42
1:C:444:GLU:O	1:C:449:ARG:NH2	2.53	0.42
2:A:709:GLU:OE1	2:A:717:ARG:NH1	2.39	0.41
2:A:823:VAL:HG12	2:A:914:LEU:HD21	2.02	0.41
3:B:43:VAL:HG11	3:B:54:LEU:HD11	2.01	0.41
3:B:471:ASN:N	3:B:471:ASN:OD1	2.44	0.41
3:B:1383:ASP:HB3	3:B:1457:LYS:HB2	2.02	0.41
2:A:1005:LYS:HE2	2:A:1005:LYS:HB3	1.80	0.41
1:C:254:TYR:OH	1:C:331:GLU:OE2	2.33	0.41
1:C:567:CYS:HB2	2:A:810:CYS:HB2	1.86	0.41
2:A:1097:GLN:HE22	2:A:1158:ILE:HG22	1.84	0.41
3:B:25:TYR:OH	3:B:48:ASP:OD2	2.39	0.41
2:A:1381:ILE:HD11	2:A:1402:ILE:HD11	2.02	0.41
3:B:159:LYS:HB3	3:B:203:TYR:HD2	1.86	0.41
3:B:459:ASN:HB3	3:B:507:ASN:HD22	1.84	0.41
1:C:379:LEU:HA	1:C:379:LEU:HD23	1.81	0.41
2:A:1249:GLU:HB2	2:A:1289:ASP:HB3	2.03	0.41
3:B:104:VAL:HG23	3:B:121:LEU:HD21	2.02	0.41
3:B:164:GLU:HB2	3:B:200:VAL:HG23	2.02	0.41
2:A:1308:ARG:HH11	2:A:1310:SER:HB3	1.84	0.41
2:A:694:VAL:HG13	2:A:695:VAL:HG13	2.02	0.41
3:B:92:LYS:HB3	3:B:92:LYS:HE3	1.91	0.41
1:C:113:LYS:HB3	1:C:113:LYS:HE3	1.92	0.41
2:A:977:LEU:HD21	2:A:1315:VAL:HG21	2.02	0.41
2:A:968:VAL:HG12	2:A:1368:THR:HG23	2.02	0.40
3:B:333:GLN:NE2	3:B:334:SER:O	2.54	0.40
1:C:367:ILE:HD13	1:C:466:TYR:HB2	2.01	0.40
1:C:665:ASN:OD1	1:C:665:ASN:N	2.54	0.40
2:A:860:SER:HB3	2:A:911:ASN:H	1.85	0.40
3:B:616:ASN:N	3:B:616:ASN:OD1	2.53	0.40
1:C:504:LEU:HD21	1:C:651:LEU:HG	2.03	0.40
2:A:1421:HIS:NE2	2:A:1463:GLN:OE1	2.53	0.40
1:C:382:LEU:HB3	1:C:416:GLY:HA3	2.04	0.40
2:A:1435:ASN:ND2	2:A:1438:ASP:OD1	2.55	0.40
2:A:916:THR:OG1	2:A:917:TRP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LEU:HD21	1:C:452:TYR:HB3	2.03	0.40
1:C:467:ILE:HG22	1:C:486:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	644/657 (98%)	596 (92%)	47 (7%)	1 (0%)	49	81
2	A	809/999 (81%)	750 (93%)	59 (7%)	0	100	100
3	B	943/1642 (57%)	893 (95%)	49 (5%)	1 (0%)	53	85
All	All	2396/3298 (73%)	2239 (93%)	155 (6%)	2 (0%)	53	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	348	THR
1	C	313	TYR

4.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	575/582 (99%)	572 (100%)	3 (0%)	90	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	726/886 (82%)	724 (100%)	2 (0%)	93	97
3	B	843/1435 (59%)	843 (100%)	0	100	100
All	All	2144/2903 (74%)	2139 (100%)	5 (0%)	94	98

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

Mol	Chain	Res	Type
1	C	285	THR
1	C	622	ARG
1	C	666	ASP
2	A	979	VAL
2	A	1138	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	80	GLN
1	C	96	GLN
1	C	289	ASN
1	C	399	GLN
1	C	500	ASN
1	C	533	ASN
1	C	642	ASN
1	C	644	ASN
1	C	656	ASN
1	C	658	ASN
2	A	753	HIS
2	A	1096	ASN
2	A	1097	GLN
2	A	1121	ASN
2	A	1178	ASN
3	B	181	ASN
3	B	305	ASN
3	B	333	GLN
3	B	405	ASN
3	B	416	ASN
3	B	465	ASN
3	B	485	ASN
3	B	507	ASN
3	B	554	ASN

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Mol	Chain	Res	Type
3	B	557	GLN
3	B	638	GLN
3	B	869	GLN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

4.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
4	H1H	A	1701	-	31,33,33	1.16	2 (6%)	37,44,44	1.83	9 (24%)

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
4	H1H	A	1701	-	-	9/23/27/27	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1701	H1H	C4-C30	4.30	1.51	1.47
4	A	1701	H1H	C21-C20	2.48	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	H1H	O28-C23-C21	5.63	121.25	115.82
4	A	1701	H1H	N16-C17-N19	3.33	118.45	113.76
4	A	1701	H1H	C23-C21-C20	3.19	125.95	120.62
4	A	1701	H1H	O28-C23-C24	-2.86	119.49	124.36
4	A	1701	H1H	C29-O28-C23	2.76	121.62	117.53
4	A	1701	H1H	O18-C17-N19	-2.75	117.64	122.60
4	A	1701	H1H	C15-O14-C2	2.71	121.55	117.53
4	A	1701	H1H	O14-C2-C1	2.66	119.11	115.41
4	A	1701	H1H	C27-C21-C20	-2.30	115.04	120.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

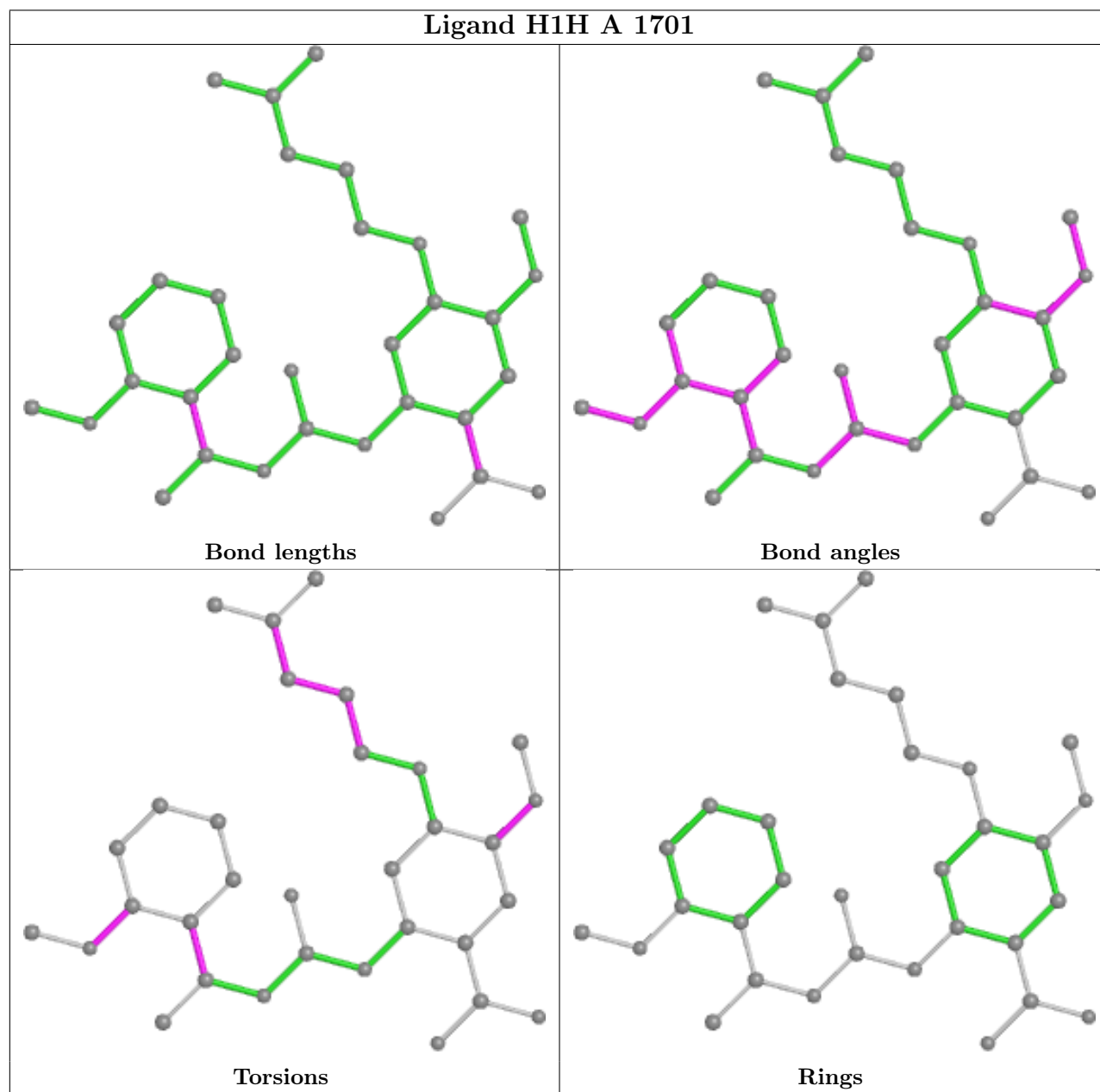
Mol	Chain	Res	Type	Atoms
4	A	1701	H1H	C24-C23-O28-C29
4	A	1701	H1H	C21-C23-O28-C29
4	A	1701	H1H	C11-C10-C9-C8
4	A	1701	H1H	N19-C20-C21-C27
4	A	1701	H1H	C1-C2-O14-C15
4	A	1701	H1H	C9-C10-C11-C12
4	A	1701	H1H	C9-C10-C11-C13
4	A	1701	H1H	O7-C8-C9-C10
4	A	1701	H1H	C3-C2-O14-C15

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.