



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 1G4K / pdb_00001g4k
Title : X-ray Structure of a Novel Matrix Metalloproteinase Inhibitor Complexed to Stromelysin
Authors : Dunten, P.; Kammlott, U.; Crowther, R.; Levin, W.; Foley, L.H.; Wang, P.; Palermo, R.
Deposited on : 2000-10-27
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

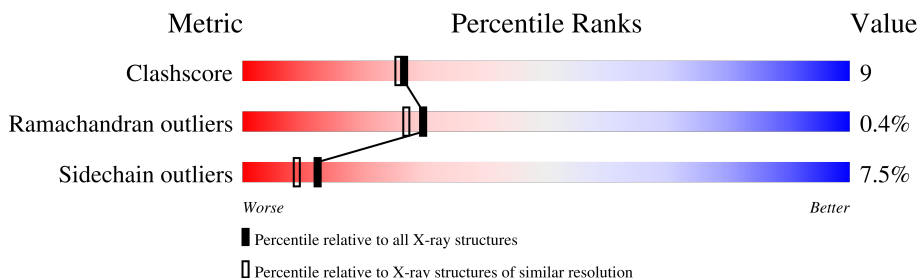
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	
1	B	168	
1	C	168	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4294 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 STROMELYSIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1339	861	223	253	2			
1	B	168	Total	C	N	O	S	0	0	0
			1339	861	223	253	2			
1	C	168	Total	C	N	O	S	0	0	0
			1339	861	223	253	2			

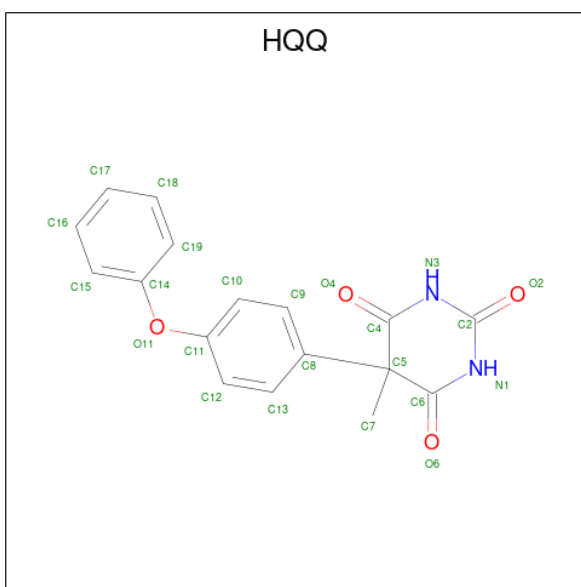
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		
3	C	3	Total	Ca	0	0
			3	3		

- Molecule 4 is 5-METHYL-5-(4-PHENOXY-PHENYL)-PYRIMIDINE-2,4,6-TRIONE (CCD ID: HQQ) (formula: C₁₇H₁₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	17	2	4		
4	B	1	Total	C	N	O	0	0
			23	17	2	4		
4	C	1	Total	C	N	O	0	0
			23	17	2	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total 71	O 71	0	0
6	B	91	Total 91	O 91	0	0
6	C	25	Total 25	O 25	0	0

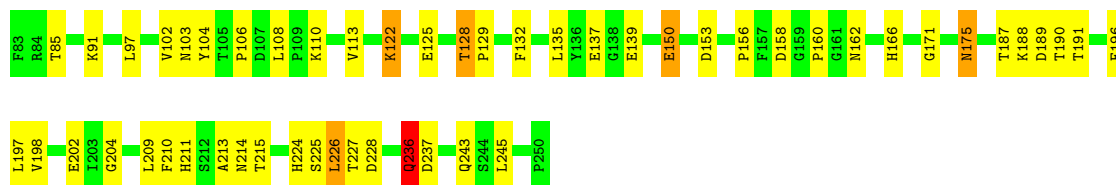
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

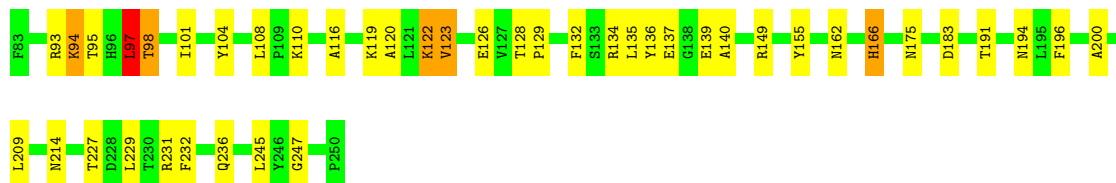
• Molecule 1: STROMELYSIN-1

Chain A: 



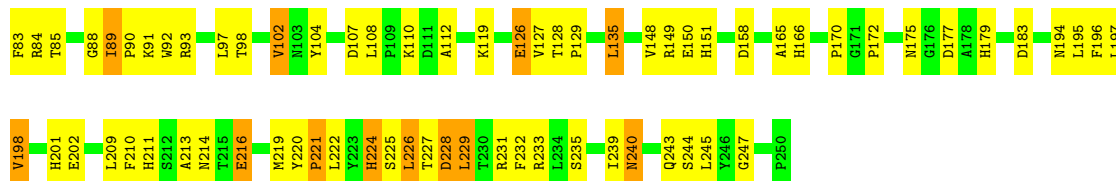
• Molecule 1: STROMELYSIN-1

Chain B: 



• Molecule 1: STROMELYSIN-1

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.80Å 103.80Å 147.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.9 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.244 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4294	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HQQ, ZN, GOL, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.97	0/1383	1.74	26/1888 (1.4%)
1	B	1.01	0/1383	1.78	29/1888 (1.5%)
1	C	0.69	0/1383	1.60	14/1888 (0.7%)
All	All	0.90	0/4149	1.71	69/5664 (1.2%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ARG	CD-NE-CZ	11.31	140.24	124.40
1	B	123	VAL	N-CA-CB	-8.83	100.71	110.51
1	C	102	VAL	CA-C-O	-8.57	111.22	120.47
1	A	243	GLN	OE1-CD-NE2	8.37	130.97	122.60
1	B	175	ASN	CA-CB-CG	-7.85	104.75	112.60
1	B	214	ASN	OD1-CG-ND2	7.79	130.39	122.60
1	A	236	GLN	CB-CG-CD	7.23	124.89	112.60
1	C	166	HIS	CA-CB-CG	7.17	120.97	113.80
1	B	236	GLN	OE1-CD-NE2	-6.97	115.63	122.60
1	C	195	LEU	CA-C-O	-6.96	113.51	120.82
1	B	166	HIS	CA-CB-CG	6.68	120.48	113.80
1	C	226	LEU	N-CA-C	6.58	120.34	107.98
1	B	231	ARG	CD-NE-CZ	6.55	133.57	124.40
1	A	85	THR	CA-CB-OG1	-6.54	99.80	109.60
1	C	151	HIS	N-CA-C	6.43	120.73	113.02
1	A	158	ASP	N-CA-CB	-6.40	101.68	111.66
1	A	85	THR	CA-C-O	-6.37	113.14	121.73
1	C	183	ASP	CA-CB-CG	6.36	118.95	112.60
1	B	183	ASP	N-CA-C	-6.27	105.66	113.38
1	B	149	ARG	NE-CZ-NH2	-6.24	113.59	119.20
1	B	247	GLY	CA-C-N	6.24	126.81	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	GLY	C-N-CA	6.24	126.81	120.38
1	B	137	GLU	CA-C-O	-6.18	114.62	121.23
1	A	226	LEU	N-CA-C	6.15	119.15	108.76
1	A	103	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	A	175	ASN	CA-CB-CG	-5.94	106.66	112.60
1	A	150	GLU	CB-CG-CD	5.93	122.68	112.60
1	B	123	VAL	CB-CA-C	5.92	119.46	111.88
1	A	162	ASN	CB-CA-C	-5.80	109.86	116.54
1	A	204	GLY	N-CA-C	-5.71	105.88	112.50
1	A	166	HIS	N-CA-CB	5.71	120.41	111.56
1	B	136	TYR	CA-C-O	5.68	126.08	119.32
1	B	140	ALA	CA-C-N	-5.67	113.07	120.44
1	B	140	ALA	C-N-CA	-5.67	113.07	120.44
1	A	160	PRO	CA-C-O	-5.63	115.00	121.36
1	A	162	ASN	CA-CB-CG	-5.62	106.97	112.60
1	B	95	THR	CA-C-N	-5.61	115.31	122.77
1	B	95	THR	C-N-CA	-5.61	115.31	122.77
1	A	214	ASN	N-CA-C	5.61	117.36	108.67
1	C	213	ALA	N-CA-C	-5.48	106.95	113.97
1	B	191	THR	CA-C-O	-5.47	115.27	121.72
1	C	112	ALA	CA-C-O	-5.45	114.77	120.55
1	B	162	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	98	THR	CA-C-O	-5.41	115.05	121.16
1	A	156	PRO	CA-C-O	-5.40	115.38	121.43
1	B	116	ALA	CA-C-N	5.39	127.46	120.56
1	B	116	ALA	C-N-CA	5.39	127.46	120.56
1	C	112	ALA	O-C-N	5.37	127.81	122.12
1	C	90	PRO	CA-C-O	-5.34	115.52	121.23
1	C	177	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	213	ALA	N-CA-C	-5.33	106.82	113.38
1	B	94	LYS	CA-C-O	-5.33	115.58	121.33
1	A	91	LYS	CA-C-O	-5.31	115.59	121.33
1	B	227	THR	CA-C-N	-5.26	115.14	123.23
1	B	227	THR	C-N-CA	-5.26	115.14	123.23
1	C	158	ASP	N-CA-C	5.24	119.15	109.24
1	C	240	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	196	PHE	CA-C-O	5.16	126.42	120.90
1	B	97	LEU	CA-C-O	-5.15	115.29	121.11
1	A	215	THR	N-CA-CB	5.13	118.12	110.22
1	B	101	ILE	CB-CG1-CD1	5.12	124.55	113.80
1	A	102	VAL	N-CA-C	5.11	115.88	110.72
1	B	236	GLN	CG-CD-NE2	5.09	124.04	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	VAL	N-CA-C	-5.07	105.45	110.62
1	A	106	PRO	CB-CA-C	-5.06	104.29	111.68
1	C	198	VAL	N-CA-CB	5.04	116.11	110.51
1	A	128	THR	CA-C-N	5.03	125.48	120.04
1	A	128	THR	C-N-CA	5.03	125.48	120.04
1	A	175	ASN	OD1-CG-ND2	-5.01	117.59	122.60

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	1339	0	1266	19	0
1	B	1339	0	1266	12	0
1	C	1339	0	1266	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	23	0	13	3	0
4	B	23	0	13	0	0
4	C	23	0	13	2	0
5	B	6	0	8	1	0
6	A	71	0	0	3	0
6	B	91	0	0	0	0
6	C	25	0	0	0	0
All	All	4294	0	3845	74	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 9.

All (74) 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:126:GLU:HG2	1:C:127:VAL:HG13	1.61	0.80
1:C:197:LEU:HD11	1:C:226:LEU:HG	1.66	0.78
1:C:89:ILE:HD11	1:C:245:LEU:HD11	1.72	0.72
1:C:88:GLY:O	1:C:89:ILE:HG22	1.90	0.71
1:B:98:THR:HB	1:B:135:LEU:HD13	1.78	0.64
1:C:98:THR:HB	1:C:135:LEU:HD22	1.81	0.63
1:C:149:ARG:O	1:C:150:GLU:C	2.41	0.63
1:C:226:LEU:HD13	1:C:229:LEU:HB3	1.81	0.62
1:B:98:THR:HB	1:B:135:LEU:CD1	2.30	0.62
1:C:91:LYS:HA	1:C:170:PRO:HG2	1.81	0.61
4:A:306:HQQ:H12	4:A:306:HQQ:C19	2.31	0.60
1:A:150:GLU:HG3	6:A:352:HOH:O	2.00	0.60
1:C:211:HIS:HB3	1:C:221:PRO:HD3	1.84	0.60
1:C:92:TRP:CE2	1:C:170:PRO:HB3	2.39	0.58
1:C:235:SER:O	1:C:239:ILE:HG13	2.03	0.58
1:A:187:THR:OG1	1:A:188:LYS:N	2.36	0.58
1:C:128:THR:HB	1:C:129:PRO:CD	2.37	0.55
1:A:189:ASP:OD1	1:A:191:THR:N	2.41	0.53
1:C:197:LEU:HD11	1:C:226:LEU:CG	2.36	0.53
1:C:214:ASN:ND2	1:C:216:GLU:OE1	2.41	0.53
1:C:85:THR:CB	1:C:89:ILE:HD13	2.39	0.53
1:A:128:THR:HB	1:A:129:PRO:CD	2.40	0.52
1:C:226:LEU:O	1:C:228:ASP:N	2.43	0.52
1:B:232:PHE:CE1	5:B:307:GOL:H11	2.45	0.51
1:A:122:LYS:HB2	1:A:122:LYS:NZ	2.25	0.51
1:C:228:ASP:OD2	1:C:231:ARG:HB3	2.11	0.51
1:A:153:ASP:HB2	6:A:354:HOH:O	2.11	0.50
1:B:155:TYR:O	1:B:166:HIS:HE1	1.93	0.50
1:C:198:VAL:O	1:C:202:GLU:HG2	2.11	0.50
1:C:85:THR:HG21	1:C:245:LEU:HD11	1.93	0.50
4:A:306:HQQ:C19	4:A:306:HQQ:C12	2.88	0.49
1:A:236:GLN:HG3	6:A:341:HOH:O	2.13	0.49
1:B:104:TYR:CG	1:B:110:LYS:HD3	2.48	0.48
1:B:128:THR:HB	1:B:129:PRO:CD	2.44	0.48
1:C:165:ALA:HB1	1:C:179:HIS:O	2.13	0.48
1:C:85:THR:HB	1:C:89:ILE:HD13	1.95	0.47
1:C:226:LEU:HD22	1:C:228:ASP:O	2.15	0.47
1:A:125:GLU:HG3	1:A:132:PHE:CD2	2.49	0.47
1:C:224:HIS:O	1:C:225:SER:HB3	2.13	0.47
1:C:201:HIS:O	1:C:219:MET:HE1	2.15	0.47
1:C:172:PRO:O	1:C:175:ASN:HB2	2.16	0.46
1:A:104:TYR:CD2	1:A:110:LYS:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:HIS:ND1	1:A:225:SER:O	2.49	0.46
1:C:104:TYR:CD1	1:C:110:LYS:HD3	2.52	0.45
1:C:224:HIS:ND1	4:C:306:HQQ:H16	2.31	0.45
4:C:306:HQQ:H9	4:C:306:HQQ:N1	2.31	0.45
1:C:214:ASN:O	1:C:220:TYR:HB2	2.17	0.45
1:C:220:TYR:HA	1:C:221:PRO:HD2	1.83	0.45
1:B:122:LYS:O	1:B:126:GLU:HG3	2.16	0.45
1:A:227:THR:O	1:A:228:ASP:HB3	2.17	0.45
1:C:194:ASN:OD1	1:C:197:LEU:HG	2.17	0.44
1:A:224:HIS:HB2	1:C:93:ARG:NH1	2.33	0.44
1:A:171:GLY:C	1:A:175:ASN:HB2	2.42	0.44
1:A:226:LEU:O	1:A:228:ASP:N	2.51	0.44
1:C:88:GLY:O	1:C:89:ILE:CG2	2.64	0.44
1:A:198:VAL:O	1:A:202:GLU:HG2	2.17	0.43
1:C:119:LYS:HG2	1:C:196:PHE:CE2	2.52	0.43
1:B:97:LEU:O	1:B:132:PHE:HA	2.18	0.43
1:B:194:ASN:HD21	1:B:229:LEU:HD11	1.82	0.43
1:C:240:ASN:O	1:C:244:SER:HB3	2.19	0.43
1:A:128:THR:HB	1:A:129:PRO:HD2	2.02	0.42
1:C:89:ILE:HD11	1:C:245:LEU:CD1	2.46	0.42
1:A:224:HIS:O	4:A:306:HQQ:H16	2.20	0.41
1:C:85:THR:HG21	1:C:89:ILE:HD13	2.02	0.41
1:C:83:PHE:O	1:C:84:ARG:HD3	2.20	0.41
1:A:236:GLN:CD	1:A:237:ASP:N	2.79	0.41
1:B:120:ALA:HB1	1:B:200:ALA:HA	2.03	0.41
1:C:210:PHE:CG	1:C:211:HIS:N	2.89	0.41
1:C:232:PHE:O	1:C:233:ARG:NH1	2.41	0.41
1:B:119:LYS:HG2	1:B:196:PHE:CE2	2.56	0.41
1:C:148:VAL:O	1:C:149:ARG:C	2.64	0.41
1:C:243:GLN:HG2	1:C:247:GLY:O	2.21	0.41
1:A:210:PHE:CG	1:A:211:HIS:N	2.88	0.40
1:B:134:ARG:C	1:B:135:LEU:HD12	2.46	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 X-ray entries followed by that with respect to entries

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/168 (99%)	154 (93%)	12 (7%)	0	100	100
1	B	166/168 (99%)	159 (96%)	7 (4%)	0	100	100
1	C	166/168 (99%)	152 (92%)	12 (7%)	2 (1%)	10	6
All	All	498/504 (99%)	465 (93%)	31 (6%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	PRO
1	C	227	THR

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/142 (100%)	131 (92%)	11 (8%)	12	8
1	B	142/142 (100%)	134 (94%)	8 (6%)	19	16
1	C	142/142 (100%)	129 (91%)	13 (9%)	8	5
All	All	426/426 (100%)	394 (92%)	32 (8%)	12	9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	A	108	LEU
1	A	122	LYS
1	A	135	LEU
1	A	137	GLU
1	A	139	GLU
1	A	190	THR

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Mol	Chain	Res	Type
1	A	197	LEU
1	A	209	LEU
1	A	236	GLN
1	A	245	LEU
1	B	94	LYS
1	B	97	LEU
1	B	108	LEU
1	B	122	LYS
1	B	123	VAL
1	B	139	GLU
1	B	209	LEU
1	B	245	LEU
1	C	89	ILE
1	C	97	LEU
1	C	102	VAL
1	C	107	ASP
1	C	108	LEU
1	C	126	GLU
1	C	135	LEU
1	C	209	LEU
1	C	216	GLU
1	C	222	LEU
1	C	224	HIS
1	C	228	ASP
1	C	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	236	GLN
1	B	236	GLN
1	C	162	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 15 are monoatomic - leaving 4 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	$\# Z > 2$
5	GOL	B	307	-	5,5,5	0.97	0	5,5,5	0.80	0
4	HQQ	B	306	2	23,25,25	1.89	9 (39%)	33,36,36	1.77	8 (24%)
4	HQQ	C	306	2	23,25,25	2.04	9 (39%)	33,36,36	1.60	6 (18%)
4	HQQ	A	306	2	23,25,25	2.18	10 (43%)	33,36,36	1.94	6 (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
5	GOL	B	307	-	-	2/4/4/4	-
4	HQQ	B	306	2	-	1/10/30/30	0/3/3/3
4	HQQ	C	306	2	-	0/10/30/30	0/3/3/3
4	HQQ	A	306	2	-	0/10/30/30	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	306	HQQ	C9-C8	4.22	1.46	1.39
4	C	306	HQQ	C9-C8	3.98	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	306	HQQ	C12-C11	3.63	1.45	1.38
4	C	306	HQQ	C19-C14	3.55	1.45	1.38
4	A	306	HQQ	C12-C11	3.28	1.44	1.38
4	A	306	HQQ	C19-C14	3.27	1.44	1.38
4	B	306	HQQ	C18-C19	3.24	1.44	1.38
4	B	306	HQQ	C12-C11	3.11	1.44	1.38
4	B	306	HQQ	C19-C14	3.09	1.44	1.38
4	B	306	HQQ	C13-C8	3.06	1.44	1.39
4	A	306	HQQ	C16-C15	3.01	1.44	1.38
4	C	306	HQQ	C15-C14	2.98	1.44	1.38
4	B	306	HQQ	C9-C8	2.72	1.43	1.39
4	A	306	HQQ	C13-C8	2.69	1.43	1.39
4	C	306	HQQ	C17-C16	2.63	1.44	1.38
4	B	306	HQQ	C15-C14	2.60	1.43	1.38
4	A	306	HQQ	C15-C14	2.59	1.43	1.38
4	C	306	HQQ	C13-C8	2.58	1.43	1.39
4	A	306	HQQ	C18-C19	2.54	1.43	1.38
4	A	306	HQQ	C5-C8	2.54	1.59	1.54
4	A	306	HQQ	C17-C16	2.53	1.43	1.38
4	A	306	HQQ	C13-C12	2.42	1.42	1.38
4	B	306	HQQ	C16-C15	2.37	1.43	1.38
4	C	306	HQQ	C18-C19	2.21	1.42	1.38
4	C	306	HQQ	C5-C8	2.20	1.58	1.54
4	B	306	HQQ	C17-C16	2.19	1.43	1.38
4	B	306	HQQ	O11-C14	2.14	1.44	1.39
4	C	306	HQQ	C10-C9	2.13	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	306	HQQ	O6-C6-C5	-5.26	117.42	121.77
4	A	306	HQQ	O6-C6-C5	-5.09	117.56	121.77
4	A	306	HQQ	O4-C4-N3	-5.03	112.44	120.59
4	C	306	HQQ	O6-C6-C5	-4.89	117.73	121.77
4	A	306	HQQ	C8-C5-C4	-4.22	97.38	107.53
4	B	306	HQQ	C8-C5-C4	-4.01	97.88	107.53
4	A	306	HQQ	O2-C2-N3	-3.74	115.22	121.86
4	B	306	HQQ	C10-C9-C8	-3.35	116.54	121.17
4	C	306	HQQ	C8-C5-C4	-2.89	100.58	107.53
4	A	306	HQQ	C18-C17-C16	2.73	123.61	119.87
4	C	306	HQQ	O4-C4-C5	-2.64	119.58	121.77
4	B	306	HQQ	C13-C8-C9	2.60	121.91	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	306	HQQ	C13-C12-C11	-2.59	116.77	119.73
4	A	306	HQQ	C4-N3-C2	-2.52	122.28	126.04
4	C	306	HQQ	O2-C2-N3	-2.49	117.43	121.86
4	C	306	HQQ	O4-C4-N3	-2.46	116.60	120.59
4	B	306	HQQ	C13-C8-C5	-2.18	117.44	121.22
4	B	306	HQQ	C17-C18-C19	-2.07	117.68	120.24
4	C	306	HQQ	O2-C2-N1	-2.02	118.27	121.86
4	B	306	HQQ	C5-C6-N1	2.00	120.40	118.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

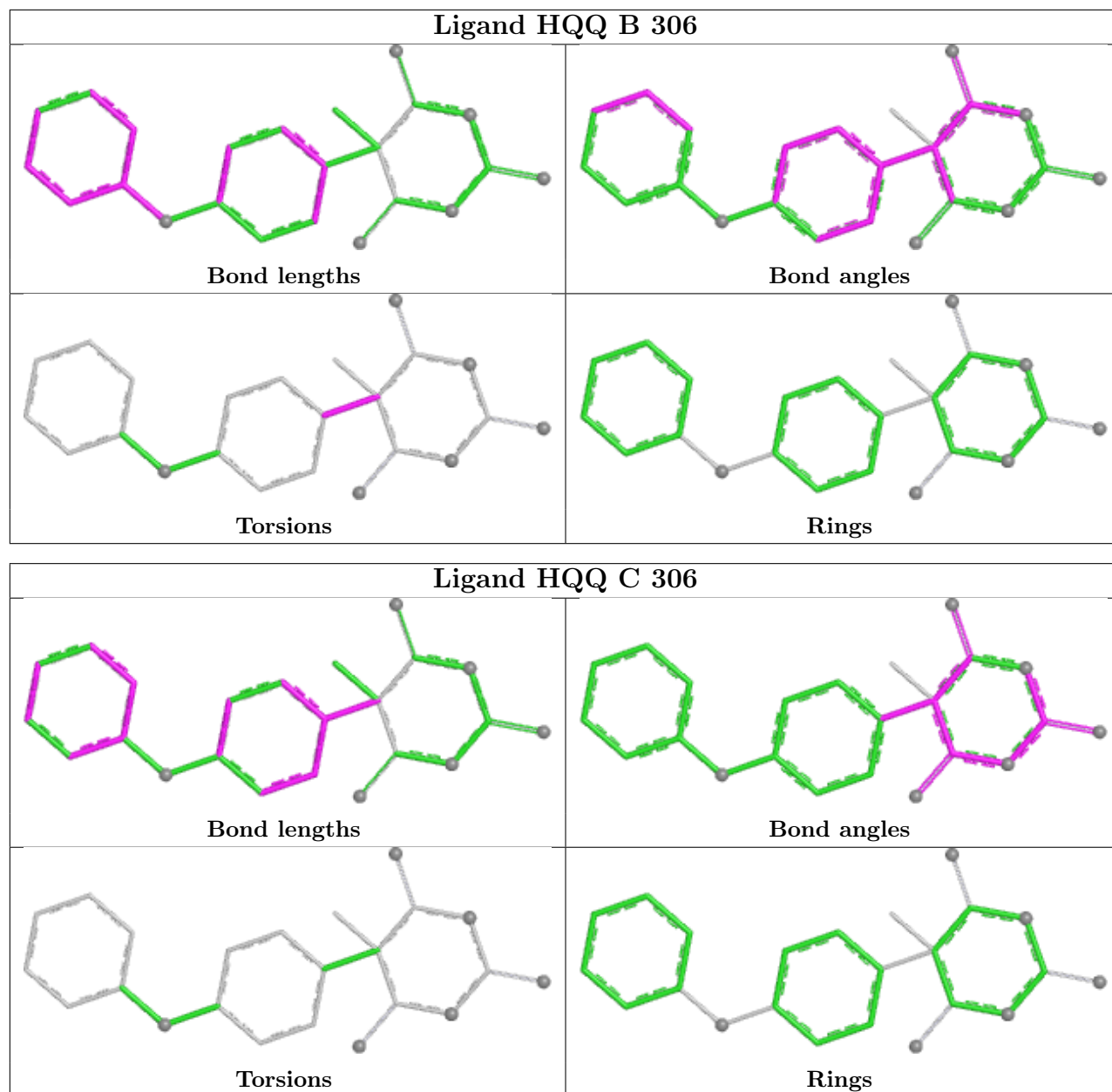
Mol	Chain	Res	Type	Atoms
5	B	307	GOL	O1-C1-C2-C3
5	B	307	GOL	O1-C1-C2-O2
4	B	306	HQQ	C7-C5-C8-C9

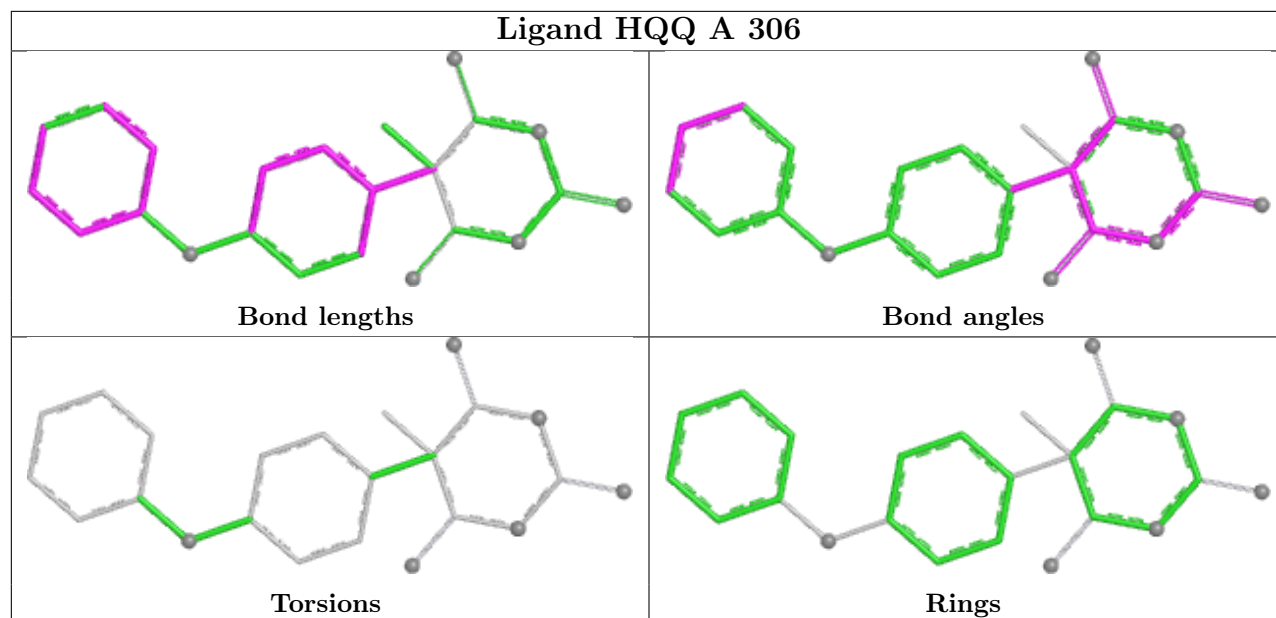
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	307	GOL	1	0
4	C	306	HQQ	2	0
4	A	306	HQQ	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.