



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 PM UTC

PDB ID : 1Y0L / pdb_00001y0l
Title : Catalytic elimination antibody 34E4 in complex with hapten
Authors : Debler, E.W.; Ito, S.; Heine, A.; Wilson, I.A.
Deposited on : 2004-11-15
Resolution : 2.50 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

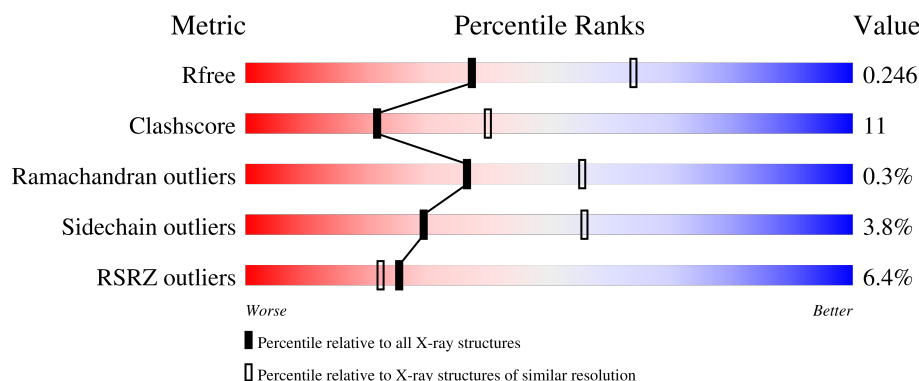
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



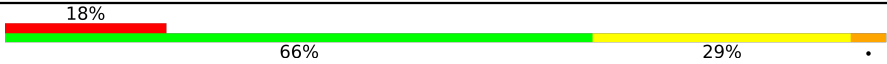
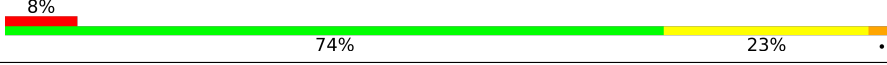
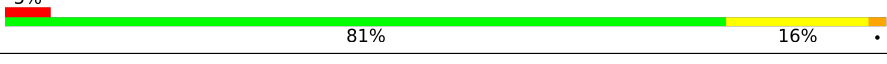
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	2% 78% 20% .
1	C	216	12% 72% 24% .
1	E	216	% 78% 21% .
1	L	216	78% 19% .
2	B	226	5% 77% 19% ..

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Mol	Chain	Length	Quality of chain
2	D	226	
2	F	226	
2	H	226	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13966 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.

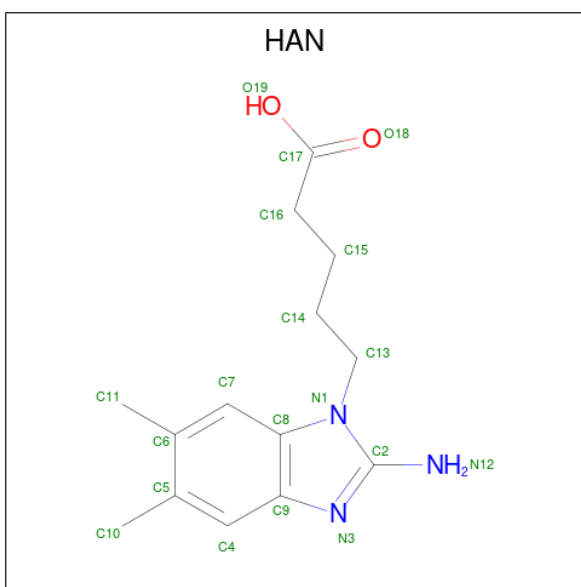
- Molecule 1 is a protein called Catalytic Antibody Fab 34E4 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1635	1019	278	333	5			
1	A	216	Total	C	N	O	S	0	0	0
			1635	1019	278	333	5			
1	C	216	Total	C	N	O	S	0	0	0
			1635	1019	278	333	5			
1	E	216	Total	C	N	O	S	0	0	0
			1635	1019	278	333	5			

- Molecule 2 is a protein called Catalytic Antibody Fab 34E4 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1731	1099	290	335	7			
2	B	226	Total	C	N	O	S	0	0	0
			1731	1099	290	335	7			
2	D	226	Total	C	N	O	S	0	0	0
			1731	1099	290	335	7			
2	F	226	Total	C	N	O	S	0	0	0
			1731	1099	290	335	7			

- Molecule 3 is 2-AMINO-5,6-DIMETHYL-BENZIMIDAZOLE-1-PENTANOIC ACID (CCD ID: HAN) (formula: C₁₄H₁₉N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			19	14	3	2		
3	A	1	Total	C	N	O	0	0
			19	14	3	2		
3	D	1	Total	C	N	O	0	0
			19	14	3	2		
3	F	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	65	Total	O	0	0
			65	65		
5	H	57	Total	O	0	0
			57	57		
5	A	55	Total	O	0	0
			55	55		
5	B	55	Total	O	0	0
			55	55		

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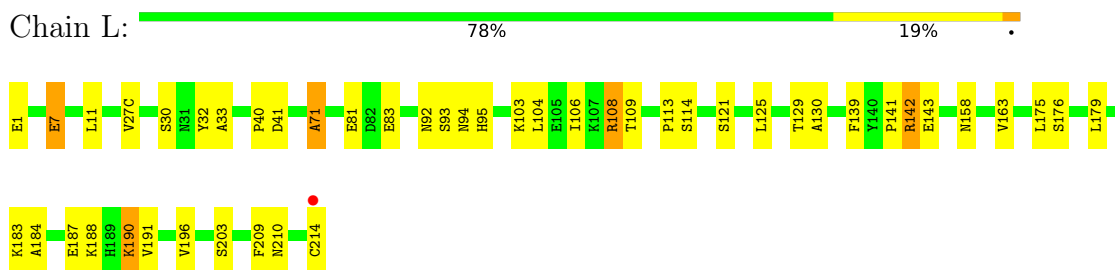
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	23	Total 23	O 23	0	0
5	D	22	Total 22	O 22	0	0
5	E	83	Total 83	O 83	0	0
5	F	65	Total 65	O 65	0	0

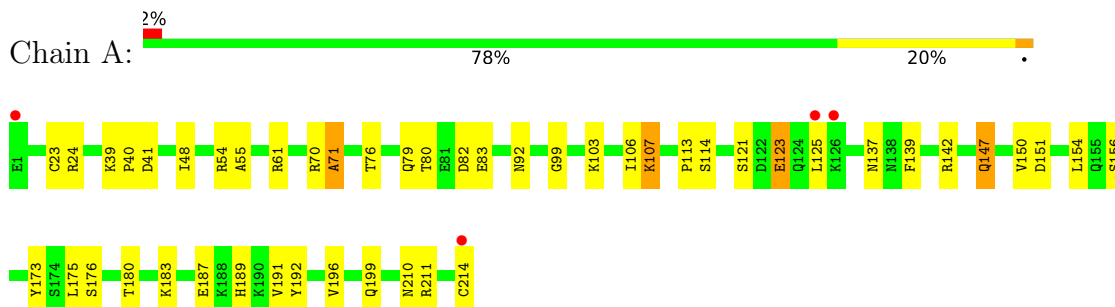
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

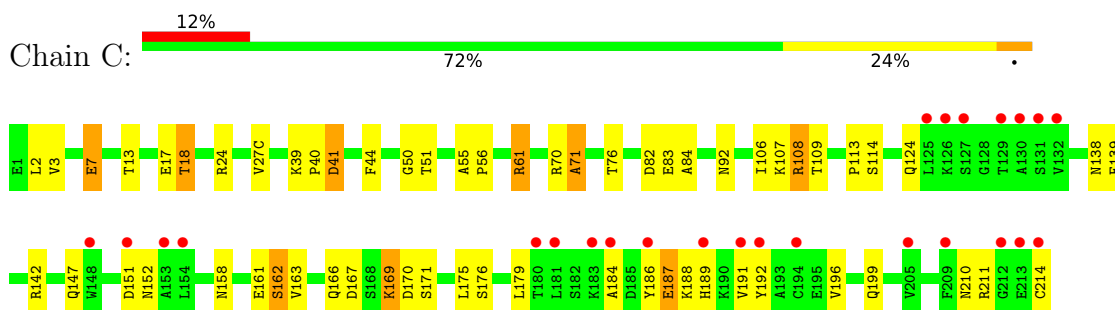
- Molecule 1: Catalytic Antibody Fab 34E4 Light chain



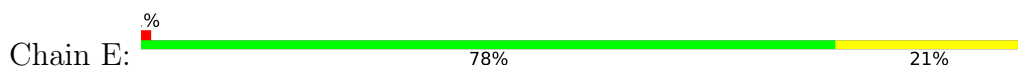
- Molecule 1: Catalytic Antibody Fab 34E4 Light chain

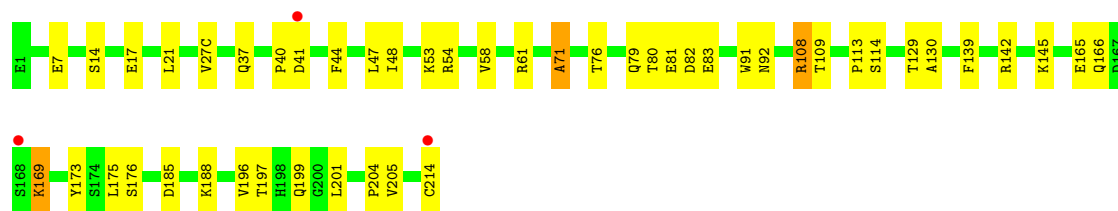


- Molecule 1: Catalytic Antibody Fab 34E4 Light chain

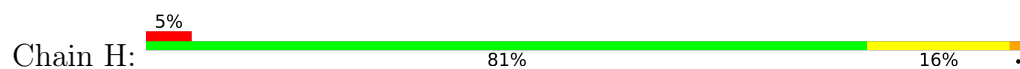


- Molecule 1: Catalytic Antibody Fab 34E4 Light chain

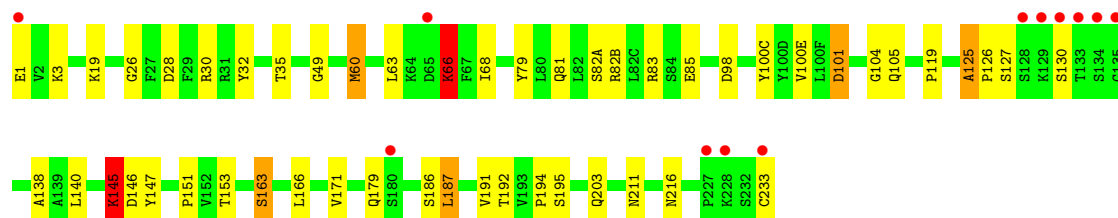
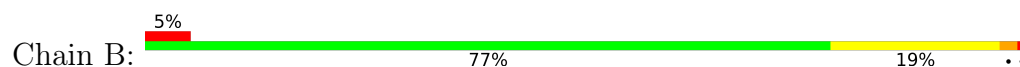




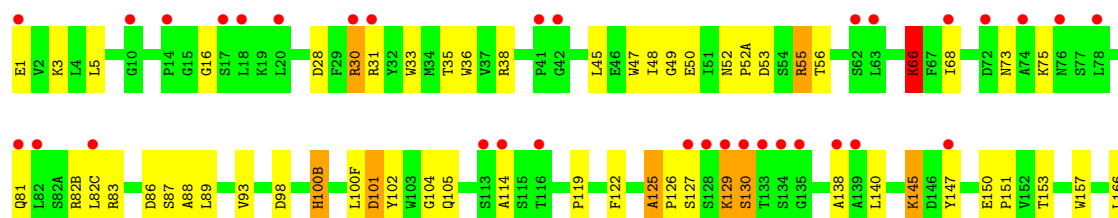
● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain



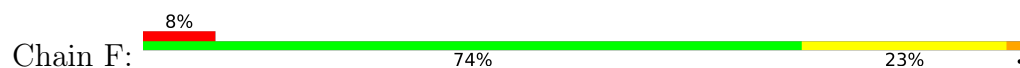
● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain

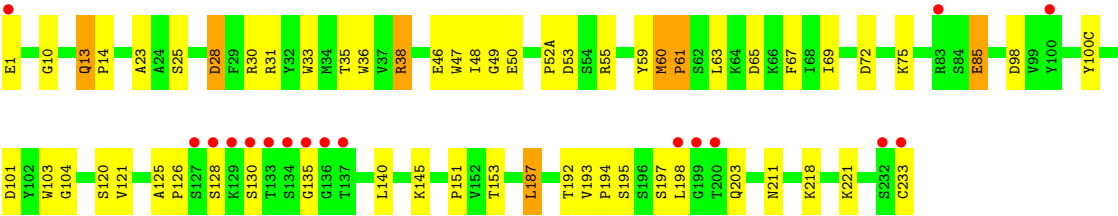


● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain



● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.20Å 165.20Å 152.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.50) 92.2 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.239 0.209 , 0.246	Depositor DCC
R_{free} test set	3926 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13966	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.56	2/1667 (0.1%)	0.92	5/2266 (0.2%)
1	C	0.47	2/1667 (0.1%)	0.87	3/2266 (0.1%)
1	E	0.52	2/1667 (0.1%)	0.93	3/2266 (0.1%)
1	L	0.53	3/1667 (0.2%)	0.91	5/2266 (0.2%)
2	B	0.50	2/1775 (0.1%)	0.94	6/2413 (0.2%)
2	D	0.52	4/1775 (0.2%)	0.91	8/2413 (0.3%)
2	F	0.51	2/1775 (0.1%)	0.95	7/2413 (0.3%)
2	H	0.49	2/1775 (0.1%)	0.95	9/2413 (0.4%)
All	All	0.51	19/13768 (0.1%)	0.92	46/18716 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	GLN	CD-OE1	5.51	1.34	1.23
1	A	199	GLN	CD-OE1	5.42	1.33	1.23
2	B	216	ASN	CG-OD1	5.42	1.33	1.23
2	D	105	GLN	CD-OE1	5.33	1.33	1.23
1	E	199	GLN	CD-OE1	5.32	1.33	1.23
1	C	199	GLN	CD-OE1	5.29	1.33	1.23
1	E	92	ASN	CG-OD1	5.28	1.33	1.23
2	D	100(B)	HIS	ND1-CE1	5.26	1.37	1.32
1	A	92	ASN	CG-OD1	5.25	1.33	1.23
2	D	216	ASN	CG-OD1	5.25	1.33	1.23
2	F	203	GLN	CD-OE1	5.23	1.33	1.23
1	L	95	HIS	ND1-CE1	5.22	1.37	1.32
2	H	100(B)	HIS	ND1-CE1	5.13	1.37	1.32
2	D	211	ASN	CG-OD1	5.13	1.33	1.23
2	H	76	ASN	CG-OD1	5.11	1.33	1.23
1	L	94	ASN	CG-OD1	5.08	1.33	1.23
1	C	92	ASN	CG-OD1	5.07	1.33	1.23
1	L	92	ASN	CG-OD1	5.06	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	13	GLN	CD-OE1	5.05	1.33	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	101	ASP	N-CA-C	9.21	121.09	111.14
2	B	66	LYS	N-CA-C	-8.85	101.71	111.36
2	H	101	ASP	N-CA-C	8.84	120.84	111.03
2	F	60	MET	N-CA-C	-6.91	99.35	109.50
2	H	60	MET	N-CA-C	-6.86	99.41	109.50
2	D	100(B)	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	L	95	HIS	CB-CG-CD2	-6.54	122.69	131.20
2	F	120	SER	N-CA-C	-6.40	98.76	109.07
2	H	100(B)	HIS	CB-CG-CD2	-6.39	122.89	131.20
2	F	145	LYS	N-CA-C	6.37	119.40	109.52
2	H	145	LYS	N-CA-C	6.34	119.35	109.52
2	B	145	LYS	N-CA-C	6.26	119.22	109.52
2	H	125	ALA	N-CA-C	6.08	117.36	109.64
2	D	125	ALA	N-CA-C	6.05	117.33	109.64
1	E	196	VAL	N-CA-C	6.02	116.59	108.17
2	F	125	ALA	N-CA-C	6.00	117.26	109.64
2	B	125	ALA	N-CA-C	5.83	117.05	109.64
1	L	114	SER	N-CA-C	-5.81	99.72	108.96
1	C	114	SER	N-CA-C	-5.77	99.78	108.96
1	E	71	ALA	N-CA-C	-5.76	100.89	110.17
1	E	114	SER	N-CA-C	-5.73	99.84	108.96
2	F	104	GLY	N-CA-C	-5.73	103.38	112.66
1	A	196	VAL	N-CA-C	5.73	116.19	108.17
1	L	71	ALA	N-CA-C	-5.72	100.95	110.17
1	C	196	VAL	N-CA-C	5.68	116.06	108.11
1	C	71	ALA	N-CA-C	-5.66	101.05	110.17
2	D	33	TRP	N-CA-C	-5.66	102.10	110.48
2	H	104	GLY	N-CA-C	-5.66	103.49	112.66
2	D	203	GLN	N-CA-C	5.58	118.19	108.76
2	B	104	GLY	N-CA-C	-5.57	103.63	112.66
1	L	95	HIS	CB-CG-ND1	5.57	131.06	122.70
2	D	66	LYS	N-CA-C	-5.56	105.31	111.71
1	A	99	GLY	N-CA-C	-5.53	104.14	112.60
1	L	196	VAL	N-CA-C	5.52	115.90	108.17
2	D	104	GLY	N-CA-C	-5.50	103.75	112.66
2	D	100(B)	HIS	CB-CG-ND1	5.50	130.95	122.70
2	H	100(B)	HIS	CB-CG-ND1	5.40	130.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ALA	N-CA-C	-5.38	101.52	110.17
1	A	114	SER	N-CA-C	-5.33	100.49	108.96
2	H	33	TRP	N-CA-C	-5.29	102.65	110.48
2	B	100(E)	VAL	N-CA-C	5.16	116.14	108.46
1	A	137	ASN	N-CA-C	5.13	118.18	109.76
2	B	32	TYR	N-CA-C	5.09	117.86	109.72
2	D	145	LYS	N-CA-C	5.07	117.83	109.72
2	F	33	TRP	N-CA-C	-5.06	103.00	110.48
2	H	66	LYS	N-CA-C	-5.01	107.21	113.72

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	1635	0	1594	29	0
1	C	1635	0	1594	46	0
1	E	1635	0	1594	34	0
1	L	1635	0	1594	30	0
2	B	1731	0	1702	35	0
2	D	1731	0	1702	55	0
2	F	1731	0	1702	49	0
2	H	1731	0	1702	36	0
3	A	19	0	18	1	0
3	D	19	0	18	0	0
3	F	19	0	18	1	0
3	H	19	0	18	0	0
4	E	1	0	0	0	0
5	A	55	0	0	2	0
5	B	55	0	0	1	0
5	C	23	0	0	0	0
5	D	22	0	0	2	0
5	E	83	0	0	3	0
5	F	65	0	0	2	0
5	H	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	65	0	0	1	0
All	All	13966	0	13256	289	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 11.

All (289) 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)
2:B:126:PRO:HG3	2:B:140:LEU:HB3	1.55	0.88
2:D:126:PRO:HG3	2:D:140:LEU:HB3	1.56	0.85
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.59	0.84
2:D:100(B):HIS:HD2	5:D:715:HOH:O	1.62	0.83
1:A:123:GLU:CD	1:A:123:GLU:H	1.85	0.82
1:C:142:ARG:HG2	1:C:142:ARG:HH11	1.45	0.82
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.60	0.82
2:H:3:LYS:HE2	2:B:192:THR:O	1.80	0.82
2:F:193:VAL:HB	2:F:194:PRO:HD2	1.63	0.81
2:H:63:LEU:HD13	2:H:67:PHE:CE2	2.16	0.80
1:A:121:SER:HB2	1:A:123:GLU:OE2	1.81	0.80
1:L:121:SER:HA	2:H:228:LYS:NZ	1.97	0.79
2:D:83:ARG:HG2	2:D:86:ASP:OD1	1.82	0.78
1:E:80:THR:O	1:E:83:GLU:HG2	1.85	0.77
2:D:53:ASP:OD1	2:D:55:ARG:HB2	1.86	0.76
1:E:197:THR:HG22	1:E:204:PRO:HB3	1.66	0.76
2:H:192:THR:OG1	2:B:3:LYS:HE3	1.88	0.73
1:C:142:ARG:HG2	1:C:142:ARG:NH1	2.03	0.73
2:D:38:ARG:HD3	2:D:48:ILE:HD11	1.70	0.73
2:B:127:SER:HB3	2:B:130:SER:HB2	1.70	0.72
2:H:205:THR:HG23	2:H:222:LYS:HD2	1.72	0.71
2:D:30:ARG:HA	2:D:73:ASN:OD1	1.92	0.70
2:H:63:LEU:HD22	2:H:66:LYS:HD3	1.74	0.70
1:L:121:SER:HA	2:H:228:LYS:HZ1	1.55	0.70
2:H:60:MET:SD	2:H:63:LEU:HG	2.31	0.70
2:F:60:MET:SD	2:F:61:PRO:HD2	2.32	0.70
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.56	0.69
2:F:153:THR:OG1	2:F:211:ASN:HB3	1.93	0.69
1:A:125:LEU:O	1:A:183:LYS:HE3	1.92	0.68
1:C:167:ASP:OD2	1:C:169:LYS:HG2	1.94	0.68
1:E:201:LEU:HD13	1:E:205:VAL:HG23	1.75	0.67
1:E:166:GLN:HG3	1:E:173:TYR:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:LYS:O	2:D:66:LYS:HD3	1.95	0.66
1:L:143:GLU:CD	1:L:143:GLU:H	2.04	0.66
2:F:13:GLN:HG3	2:F:14:PRO:HD2	1.78	0.66
2:D:138:ALA:HB2	2:D:195:SER:HB3	1.76	0.65
1:A:175:LEU:HD23	1:A:176:SER:N	2.12	0.65
1:C:175:LEU:HD23	1:C:176:SER:N	2.12	0.65
1:A:79:GLN:HG2	5:A:649:HOH:O	1.96	0.65
2:D:212:HIS:CD2	2:D:214:PRO:HD2	2.33	0.64
1:L:125:LEU:O	1:L:183:LYS:HE2	1.97	0.64
1:C:169:LYS:HD3	1:C:169:LYS:N	2.12	0.64
1:E:40:PRO:O	1:E:41:ASP:HB2	1.98	0.63
1:C:187:GLU:O	1:C:211:ARG:NH1	2.31	0.63
2:F:55:ARG:HG2	2:F:55:ARG:HH11	1.63	0.63
1:A:142:ARG:HG2	1:A:142:ARG:NH1	2.12	0.63
1:C:158:ASN:ND2	1:C:179:LEU:HD11	2.13	0.62
1:C:184:ALA:O	1:C:188:LYS:HG2	1.99	0.62
2:B:82(B):ARG:O	2:B:82(B):ARG:HG2	1.99	0.62
1:L:40:PRO:O	1:L:41:ASP:HB2	1.98	0.62
1:C:83:GLU:HG3	1:C:106:ILE:HG12	1.82	0.61
2:D:28:ASP:OD1	2:D:30:ARG:HG2	2.01	0.61
1:A:40:PRO:O	1:A:41:ASP:HB2	2.02	0.60
1:C:61:ARG:HG3	1:C:76:THR:O	2.02	0.60
1:C:187:GLU:OE1	1:C:211:ARG:HD2	2.02	0.60
2:B:145:LYS:HD3	2:B:146:ASP:OD2	2.01	0.59
1:C:214:CYS:C	2:D:233:CYS:SG	2.86	0.59
1:C:108:ARG:HD3	1:C:109:THR:O	2.03	0.59
1:E:54:ARG:HD2	1:E:58:VAL:O	2.01	0.59
2:F:72:ASP:OD2	2:F:75:LYS:HE2	2.03	0.59
1:L:108:ARG:HD3	1:L:109:THR:O	2.04	0.58
1:A:80:THR:O	1:A:83:GLU:HG3	2.04	0.58
2:B:66:LYS:HE3	2:B:82(A):SER:O	2.04	0.57
2:H:66:LYS:O	2:H:67:PHE:HD1	1.87	0.57
2:B:187:LEU:HD12	2:B:187:LEU:C	2.29	0.57
2:F:63:LEU:HD13	2:F:67:PHE:CE2	2.39	0.57
2:F:187:LEU:C	2:F:187:LEU:HD12	2.30	0.57
2:F:59:TYR:HE1	2:F:69:ILE:HG13	1.70	0.57
2:D:187:LEU:C	2:D:187:LEU:HD12	2.29	0.57
1:C:142:ARG:HH21	1:C:163:VAL:HG11	1.69	0.57
1:L:190:LYS:HD3	1:L:210:ASN:HB3	1.85	0.57
2:D:47:TRP:CZ2	2:D:50:GLU:HG2	2.40	0.56
2:F:126:PRO:HG3	2:F:140:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:ND2	2:F:1:GLU:HB2	2.20	0.56
2:D:31:ARG:HG2	2:D:31:ARG:HH11	1.70	0.56
1:E:169:LYS:HE3	1:E:169:LYS:HA	1.87	0.56
1:C:124:GLN:HG3	2:D:122:PHE:CE2	2.41	0.56
1:C:142:ARG:NH2	1:C:163:VAL:HG11	2.20	0.56
1:C:175:LEU:HD23	1:C:175:LEU:C	2.31	0.56
1:A:76:THR:HG23	5:A:648:HOH:O	2.06	0.55
1:C:107:LYS:HD3	1:C:107:LYS:C	2.32	0.55
1:E:145:LYS:HB3	1:E:197:THR:OG1	2.07	0.55
2:D:153:THR:OG1	2:D:211:ASN:HB3	2.06	0.55
2:H:98:ASP:HB3	2:H:100(C):TYR:HB3	1.88	0.55
2:B:83:ARG:HH21	2:B:85:GLU:HG2	1.71	0.55
2:B:19:LYS:HE2	2:B:79:TYR:HB3	1.89	0.55
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.89	0.54
1:E:108:ARG:HD3	1:E:109:THR:O	2.06	0.54
2:H:66:LYS:C	2:H:67:PHE:HD1	2.15	0.54
1:E:214:CYS:O	2:F:233:CYS:HB3	2.07	0.54
1:A:175:LEU:HD23	1:A:175:LEU:C	2.33	0.54
2:H:25:SER:HB3	2:B:194:PRO:HA	1.89	0.53
1:A:48:ILE:HD13	1:A:54:ARG:HA	1.90	0.53
1:L:121:SER:HA	2:H:228:LYS:HZ3	1.73	0.53
1:L:183:LYS:O	1:L:187:GLU:HG2	2.08	0.53
1:L:1:GLU:OE1	1:L:1:GLU:HA	2.09	0.53
2:B:140:LEU:C	2:B:140:LEU:HD12	2.34	0.53
1:E:214:CYS:C	2:F:233:CYS:SG	2.92	0.53
1:C:138:ASN:HD22	2:F:1:GLU:HB2	1.71	0.52
2:B:85:GLU:CD	2:B:85:GLU:H	2.18	0.52
2:F:194:PRO:HG2	2:F:197:SER:HB2	1.90	0.52
1:L:108:ARG:CD	1:L:109:THR:O	2.58	0.52
1:E:197:THR:HG23	5:E:978:HOH:O	2.10	0.51
1:C:186:TYR:O	1:C:192:TYR:OH	2.28	0.51
1:L:1:GLU:N	5:L:276:HOH:O	2.44	0.51
2:D:98:ASP:C	2:D:98:ASP:OD1	2.53	0.51
1:L:27(C):VAL:HG11	1:L:71:ALA:HB2	1.92	0.51
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.91	0.51
1:E:175:LEU:C	1:E:175:LEU:HD23	2.36	0.51
1:C:162:SER:OG	2:D:175:PRO:HG2	2.11	0.51
1:C:40:PRO:O	1:C:41:ASP:CB	2.59	0.50
1:C:169:LYS:N	1:C:169:LYS:CD	2.73	0.50
2:F:38:ARG:HD2	2:F:46:GLU:OE1	2.11	0.50
2:F:63:LEU:HD13	2:F:67:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:194:PRO:HG2	2:F:197:SER:CB	2.41	0.50
2:H:48:ILE:HA	2:H:60:MET:HE3	1.93	0.50
2:D:150:GLU:HG2	2:D:185:TYR:CE2	2.46	0.50
2:F:53:ASP:OD1	2:F:55:ARG:HB2	2.12	0.50
2:F:193:VAL:HB	2:F:194:PRO:CD	2.39	0.50
1:E:27(C):VAL:HG11	1:E:71:ALA:HB2	1.93	0.50
1:C:83:GLU:OE2	1:C:171:SER:HB3	2.12	0.50
2:D:178:LEU:HD13	2:D:185:TYR:CE1	2.46	0.50
1:E:185:ASP:HA	1:E:188:LYS:HD3	1.92	0.50
1:L:191:VAL:HG22	1:L:210:ASN:OD1	2.11	0.50
2:H:129:LYS:C	2:H:133:THR:H	2.20	0.50
2:F:47:TRP:CZ2	2:F:50:GLU:HG2	2.47	0.50
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.94	0.49
1:A:214:CYS:C	2:B:233:CYS:SG	2.95	0.49
1:C:24:ARG:HB3	1:C:70:ARG:HG2	1.93	0.49
2:H:163:SER:HA	2:B:163:SER:OG	2.11	0.49
1:E:79:GLN:NE2	1:E:81:GLU:OE1	2.45	0.49
1:E:61:ARG:NH2	1:E:82:ASP:OD2	2.44	0.49
2:B:153:THR:OG1	2:B:211:ASN:HB3	2.12	0.49
2:H:187:LEU:C	2:H:187:LEU:HD12	2.37	0.49
2:B:68:ILE:HB	2:B:81:GLN:HB3	1.93	0.49
2:D:127:SER:OG	2:D:129:LYS:HG3	2.12	0.49
2:B:66:LYS:HD3	2:B:66:LYS:C	2.38	0.49
2:D:3:LYS:HE2	2:F:192:THR:OG1	2.12	0.49
1:C:39:LYS:HE3	1:C:84:ALA:HB2	1.95	0.49
1:A:147:GLN:OE1	1:A:154:LEU:HD23	2.12	0.48
1:L:214:CYS:C	2:H:233:CYS:SG	2.96	0.48
2:F:28:ASP:HB3	2:F:31:ARG:HG2	1.94	0.48
2:F:38:ARG:HG2	2:F:48:ILE:HD11	1.95	0.48
1:C:50:GLY:O	1:C:51:THR:HB	2.12	0.48
1:E:53:LYS:HD3	5:E:932:HOH:O	2.12	0.48
1:L:143:GLU:CD	1:L:143:GLU:N	2.69	0.48
2:D:101:ASP:HB3	2:D:102:TYR:CD2	2.48	0.48
2:F:47:TRP:HZ2	2:F:50:GLU:HG2	1.78	0.48
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.46	0.48
1:E:61:ARG:NH2	1:E:82:ASP:OD1	2.46	0.48
2:D:75:LYS:HG3	2:F:135:GLY:HA3	1.96	0.47
2:D:82(B):ARG:HG3	2:D:82(B):ARG:HH11	1.79	0.47
1:E:165:GLU:OE1	1:E:165:GLU:HA	2.14	0.47
2:D:47:TRP:HZ2	2:D:50:GLU:HG2	1.78	0.47
2:D:93:VAL:HG11	2:D:100(F):LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:LEU:HD23	1:L:176:SER:N	2.30	0.47
2:F:140:LEU:C	2:F:140:LEU:HD12	2.39	0.47
1:L:141:PRO:HB2	1:L:143:GLU:OE1	2.14	0.47
1:L:175:LEU:HD23	1:L:175:LEU:C	2.39	0.47
2:F:130:SER:HA	2:F:195:SER:O	2.14	0.47
2:F:59:TYR:CE1	2:F:69:ILE:HG13	2.48	0.47
2:H:66:LYS:HG3	2:H:67:PHE:CD1	2.50	0.47
2:B:119:PRO:CB	2:B:147:TYR:HB3	2.38	0.47
1:A:183:LYS:O	1:A:187:GLU:HG3	2.15	0.47
2:D:31:ARG:HG2	2:D:31:ARG:NH1	2.30	0.47
2:F:55:ARG:HG2	2:F:55:ARG:NH1	2.27	0.47
2:D:1:GLU:HG3	2:D:1:GLU:O	2.14	0.47
1:E:91:TRP:CE2	3:F:801:HAN:H131	2.50	0.47
1:E:113:PRO:HB3	1:E:139:PHE:HB3	1.96	0.47
1:A:191:VAL:HG22	1:A:210:ASN:OD1	2.15	0.46
1:C:166:GLN:NE2	1:C:171:SER:HB2	2.30	0.46
2:D:1:GLU:O	2:D:3:LYS:HG3	2.15	0.46
2:D:212:HIS:HD2	2:D:214:PRO:HD2	1.80	0.46
1:A:83:GLU:HG2	1:A:106:ILE:HG12	1.98	0.46
1:C:7:GLU:CD	1:C:7:GLU:H	2.24	0.46
2:D:125:ALA:HA	2:D:126:PRO:HD3	1.81	0.46
2:F:55:ARG:NH2	5:F:812:HOH:O	2.48	0.46
1:L:83:GLU:HG2	1:L:106:ILE:HG12	1.98	0.46
1:C:214:CYS:O	2:D:233:CYS:HB3	2.16	0.46
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.97	0.46
2:H:147:TYR:CE1	2:H:152:VAL:HG13	2.51	0.46
2:D:66:LYS:HD3	2:D:66:LYS:C	2.41	0.46
2:D:140:LEU:C	2:D:140:LEU:HD12	2.41	0.46
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.31	0.46
2:F:35:THR:HG23	2:F:49:GLY:O	2.15	0.46
1:A:154:LEU:HD12	1:A:154:LEU:N	2.31	0.46
1:E:175:LEU:HD23	1:E:176:SER:N	2.31	0.45
1:E:129:THR:HG22	1:E:130:ALA:N	2.32	0.45
2:F:10:GLY:HA2	5:F:859:HOH:O	2.16	0.45
2:F:35:THR:HG22	2:F:36:TRP:N	2.31	0.45
1:L:158:ASN:ND2	1:L:179:LEU:HD11	2.31	0.45
2:B:179:GLN:NE2	2:B:186:SER:HB2	2.30	0.45
2:D:195:SER:HA	2:D:198:LEU:HG	1.99	0.45
3:A:601:HAN:H161	5:B:254:HOH:O	2.16	0.45
1:C:61:ARG:NH1	1:C:82:ASP:OD2	2.47	0.45
2:H:129:LYS:C	2:H:133:THR:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:THR:HG23	2:D:49:GLY:O	2.17	0.45
2:D:87:SER:O	2:D:88:ALA:HB2	2.17	0.45
1:E:14:SER:O	1:E:17:GLU:HB2	2.16	0.45
1:E:76:THR:HG23	5:E:954:HOH:O	2.16	0.45
1:A:113:PRO:HB3	1:A:139:PHE:HB3	1.99	0.44
2:B:119:PRO:HB3	2:B:147:TYR:CB	2.41	0.44
1:C:2:LEU:HD12	1:C:3:VAL:N	2.32	0.44
1:C:151:ASP:OD2	1:C:189:HIS:HB3	2.17	0.44
2:D:157:TRP:CH2	2:D:208:CYS:HB3	2.52	0.44
1:E:21:LEU:HD12	1:E:21:LEU:N	2.33	0.44
2:H:137:THR:CG2	2:H:192:THR:HB	2.47	0.44
1:E:197:THR:CG2	1:E:204:PRO:HB3	2.42	0.44
1:A:142:ARG:HB2	1:A:173:TYR:CE2	2.52	0.44
1:C:44:PHE:CE2	2:D:45:LEU:HD21	2.52	0.44
1:E:44:PHE:HB2	2:F:103:TRP:CG	2.52	0.44
2:H:30:ARG:HE	2:H:30:ARG:HB3	1.58	0.44
2:H:205:THR:HG22	2:H:207:ILE:HG13	1.99	0.44
2:B:138:ALA:HB2	2:B:195:SER:HB2	2.00	0.44
2:D:5:LEU:HD13	2:F:194:PRO:HD3	2.00	0.44
1:C:167:ASP:HB3	1:C:170:ASP:OD1	2.18	0.44
2:D:197:SER:HB3	2:F:23:ALA:CB	2.48	0.44
2:F:53:ASP:OD1	2:F:53:ASP:C	2.61	0.43
2:H:126:PRO:HD2	2:H:227:PRO:HA	1.99	0.43
2:D:56:THR:HA	5:D:720:HOH:O	2.16	0.43
2:H:1:GLU:O	2:H:1:GLU:HG2	2.18	0.43
2:H:121:VAL:O	2:H:221:LYS:HE3	2.18	0.43
2:D:166:LEU:HD21	2:D:191:VAL:HG21	1.99	0.43
2:H:63:LEU:HA	2:H:66:LYS:HG2	1.99	0.43
1:L:142:ARG:CZ	1:L:163:VAL:HG11	2.48	0.43
1:L:7:GLU:HG3	1:L:11:LEU:HD11	2.00	0.43
1:L:129:THR:HG22	1:L:130:ALA:N	2.33	0.43
2:H:125:ALA:HA	2:H:126:PRO:HD3	1.88	0.43
2:H:145:LYS:HD3	2:H:146:ASP:OD2	2.19	0.43
1:A:55:ALA:HA	2:B:100(C):TYR:OH	2.19	0.43
1:C:17:GLU:HG3	1:C:18:THR:H	1.83	0.43
2:B:35:THR:HG23	2:B:49:GLY:O	2.19	0.43
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.19	0.43
1:C:107:LYS:HD3	1:C:108:ARG:N	2.34	0.43
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.84	0.43
2:B:82(B):ARG:O	2:B:82(B):ARG:CG	2.64	0.43
1:C:191:VAL:HG22	1:C:210:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HB3	1:A:70:ARG:HG2	2.01	0.42
1:E:54:ARG:CG	1:E:58:VAL:HB	2.48	0.42
2:B:166:LEU:HD21	2:B:191:VAL:HG21	2.01	0.42
2:D:16:GLY:O	2:D:82(C):LEU:HG	2.19	0.42
2:F:126:PRO:C	2:F:128:SER:H	2.26	0.42
2:B:63:LEU:CD2	2:B:82(B):ARG:HH12	2.33	0.42
1:C:27(C):VAL:HG11	1:C:71:ALA:HB2	2.00	0.42
1:C:83:GLU:HG2	1:C:166:GLN:OE1	2.19	0.42
2:F:85:GLU:CD	2:F:85:GLU:H	2.26	0.42
2:F:98:ASP:HB3	2:F:100(C):TYR:HB3	2.01	0.42
2:B:98:ASP:OD1	2:B:98:ASP:C	2.62	0.42
1:C:40:PRO:O	1:C:41:ASP:HB3	2.19	0.42
2:D:127:SER:HB3	2:D:130:SER:OG	2.18	0.42
1:L:1:GLU:OE1	1:L:1:GLU:CA	2.68	0.42
2:H:66:LYS:C	2:H:67:PHE:CD1	2.97	0.42
1:A:23:CYS:HB3	1:A:71:ALA:HB3	2.02	0.42
2:F:121:VAL:O	2:F:221:LYS:HE3	2.20	0.42
2:H:63:LEU:HD13	2:H:67:PHE:CD2	2.55	0.42
2:B:28:ASP:OD1	2:B:30:ARG:HG2	2.20	0.42
2:B:125:ALA:HA	2:B:126:PRO:HD3	1.80	0.42
1:E:48:ILE:HD13	1:E:54:ARG:HA	2.02	0.42
2:D:52:ASN:HB2	2:D:52(A):PRO:CD	2.50	0.41
2:D:145:LYS:HG3	2:D:186:SER:OG	2.19	0.41
1:E:61:ARG:NH2	1:E:82:ASP:CG	2.78	0.41
2:D:194:PRO:HA	2:F:25:SER:HB3	2.02	0.41
2:D:194:PRO:HB3	2:F:25:SER:HB3	2.02	0.41
2:F:28:ASP:HB3	2:F:31:ARG:CG	2.50	0.41
1:A:123:GLU:CD	1:A:123:GLU:N	2.63	0.41
1:C:167:ASP:O	1:C:171:SER:HA	2.20	0.41
2:D:52:ASN:HB2	2:D:52(A):PRO:HD2	2.02	0.41
1:A:150:VAL:HG13	1:A:192:TYR:CE1	2.55	0.41
2:D:205:THR:HG23	2:D:222:LYS:HE3	2.01	0.41
2:H:140:LEU:HD12	2:H:140:LEU:C	2.46	0.41
2:F:194:PRO:HG2	2:F:197:SER:OG	2.19	0.41
2:B:1:GLU:O	2:B:26:GLY:HA3	2.20	0.41
2:B:171:VAL:HG22	2:B:191:VAL:HB	2.03	0.41
1:L:184:ALA:O	1:L:188:LYS:HG3	2.21	0.41
2:B:60:MET:O	2:B:60:MET:HG3	2.20	0.41
2:D:68:ILE:HB	2:D:81:GLN:HB2	2.02	0.41
1:E:54:ARG:HG2	1:E:58:VAL:HB	2.03	0.41
1:C:83:GLU:HG3	1:C:106:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:LEU:HB3	2:F:67:PHE:CD2	2.56	0.41
1:L:103:LYS:HD2	1:L:104:LEU:N	2.37	0.40
1:L:209:PHE:CD1	1:L:209:PHE:C	3.00	0.40
2:H:66:LYS:HE2	2:H:67:PHE:CE1	2.56	0.40
1:C:55:ALA:HB1	1:C:56:PRO:HD2	2.03	0.40
2:D:35:THR:HG22	2:D:36:TRP:N	2.35	0.40
1:L:32:TYR:O	1:L:33:ALA:C	2.64	0.40
2:H:87:SER:O	2:H:88:ALA:HB2	2.21	0.40
2:F:30:ARG:O	2:F:52(A):PRO:HB3	2.21	0.40
2:F:218:LYS:HE3	2:F:218:LYS:HB2	1.88	0.40
2:B:85:GLU:CD	2:B:85:GLU:N	2.80	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	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
1	C	214/216 (99%)	204 (95%)	9 (4%)	1 (0%)	24	43
1	E	214/216 (99%)	204 (95%)	10 (5%)	0	100	100
1	L	214/216 (99%)	204 (95%)	10 (5%)	0	100	100
2	B	224/226 (99%)	208 (93%)	15 (7%)	1 (0%)	30	49
2	D	224/226 (99%)	209 (93%)	12 (5%)	3 (1%)	9	18
2	F	224/226 (99%)	211 (94%)	12 (5%)	1 (0%)	30	49
2	H	224/226 (99%)	211 (94%)	13 (6%)	0	100	100
All	All	1752/1768 (99%)	1654 (94%)	92 (5%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	101	ASP
2	D	130	SER
2	D	101	ASP
2	D	114	ALA
2	F	198	LEU
1	C	41	ASP

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	183/183 (100%)	176 (96%)	7 (4%)	29	56
1	C	183/183 (100%)	172 (94%)	11 (6%)	17	36
1	E	183/183 (100%)	179 (98%)	4 (2%)	45	73
1	L	183/183 (100%)	175 (96%)	8 (4%)	25	50
2	B	195/195 (100%)	187 (96%)	8 (4%)	27	53
2	D	195/195 (100%)	188 (96%)	7 (4%)	31	58
2	F	195/195 (100%)	188 (96%)	7 (4%)	31	58
2	H	195/195 (100%)	189 (97%)	6 (3%)	35	62
All	All	1512/1512 (100%)	1454 (96%)	58 (4%)	29	56

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	GLU
1	L	30	SER
1	L	81	GLU
1	L	93	SER
1	L	108	ARG
1	L	142	ARG
1	L	190	LYS
1	L	203	SER
2	H	3	LYS
2	H	60	MET

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Mol	Chain	Res	Type
2	H	65	ASP
2	H	89	LEU
2	H	151	PRO
2	H	187	LEU
1	A	39	LYS
1	A	103	LYS
1	A	107	LYS
1	A	123	GLU
1	A	147	GLN
1	A	156	SER
1	A	180	THR
2	B	60	MET
2	B	66	LYS
2	B	101	ASP
2	B	145	LYS
2	B	151	PRO
2	B	163	SER
2	B	187	LEU
2	B	203	GLN
1	C	7	GLU
1	C	13	THR
1	C	18	THR
1	C	61	ARG
1	C	108	ARG
1	C	147	GLN
1	C	152	ASN
1	C	161	GLU
1	C	162	SER
1	C	169	LYS
1	C	187	GLU
2	D	30	ARG
2	D	55	ARG
2	D	66	LYS
2	D	89	LEU
2	D	129	LYS
2	D	151	PRO
2	D	187	LEU
1	E	7	GLU
1	E	108	ARG
1	E	142	ARG
1	E	169	LYS
2	F	28	ASP

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Mol	Chain	Res	Type
2	F	38	ARG
2	F	61	PRO
2	F	65	ASP
2	F	85	GLU
2	F	151	PRO
2	F	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	42	HIS
1	A	137	ASN
1	A	138	ASN
2	B	39	GLN
2	B	100(A)	ASN
2	B	211	ASN
2	D	39	GLN
1	E	42	HIS
1	E	166	GLN
1	E	189	HIS
2	F	100(B)	HIS
2	F	172	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	HAN	F	801	-	20,20,20	2.31	9 (45%)	25,28,28	1.49	3 (12%)
3	HAN	D	701	-	20,20,20	2.40	7 (35%)	25,28,28	1.66	4 (16%)
3	HAN	A	601	-	20,20,20	2.26	9 (45%)	25,28,28	1.52	3 (12%)
3	HAN	H	501	-	20,20,20	2.24	10 (50%)	25,28,28	1.56	3 (12%)

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	HAN	F	801	-	-	3/7/7/7	0/2/2/2
3	HAN	D	701	-	-	3/7/7/7	0/2/2/2
3	HAN	A	601	-	-	3/7/7/7	0/2/2/2
3	HAN	H	501	-	-	4/7/7/7	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	701	HAN	C2-N1	5.54	1.47	1.37
3	F	801	HAN	C2-N1	5.05	1.46	1.37
3	F	801	HAN	C2-N12	4.89	1.42	1.34
3	A	601	HAN	C2-N1	4.80	1.45	1.37
3	A	601	HAN	C2-N12	4.73	1.42	1.34
3	D	701	HAN	C2-N12	4.66	1.42	1.34
3	H	501	HAN	C2-N1	4.51	1.45	1.37
3	H	501	HAN	C2-N12	4.29	1.41	1.34
3	H	501	HAN	C4-C9	3.27	1.44	1.40
3	A	601	HAN	C7-C8	3.10	1.44	1.39
3	D	701	HAN	C7-C8	3.00	1.44	1.39
3	D	701	HAN	C7-C6	2.92	1.43	1.39
3	A	601	HAN	C4-C9	2.85	1.44	1.40
3	A	601	HAN	C4-C5	2.79	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	HAN	C4-C5	2.77	1.43	1.39
3	H	501	HAN	C7-C8	2.76	1.44	1.39
3	D	701	HAN	C4-C5	2.75	1.43	1.39
3	F	801	HAN	C4-C5	2.69	1.43	1.39
3	F	801	HAN	C2-N3	-2.69	1.28	1.32
3	F	801	HAN	C7-C8	2.61	1.43	1.39
3	H	501	HAN	C2-N3	-2.60	1.28	1.32
3	F	801	HAN	C4-C9	2.59	1.43	1.40
3	F	801	HAN	C7-C6	2.59	1.43	1.39
3	D	701	HAN	C4-C9	2.56	1.43	1.40
3	D	701	HAN	C2-N3	-2.39	1.29	1.32
3	A	601	HAN	C10-C5	2.38	1.55	1.51
3	H	501	HAN	C6-C5	2.35	1.46	1.40
3	F	801	HAN	C6-C5	2.35	1.46	1.40
3	A	601	HAN	C2-N3	-2.27	1.29	1.32
3	A	601	HAN	C6-C5	2.20	1.46	1.40
3	H	501	HAN	C7-C6	2.19	1.42	1.39
3	F	801	HAN	C10-C5	2.15	1.55	1.51
3	A	601	HAN	C7-C6	2.08	1.42	1.39
3	H	501	HAN	C11-C6	2.05	1.54	1.51
3	H	501	HAN	C10-C5	2.00	1.54	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	HAN	N12-C2-N3	-5.14	120.32	124.78
3	A	601	HAN	N12-C2-N3	-4.29	121.06	124.78
3	F	801	HAN	N12-C2-N3	-4.26	121.09	124.78
3	H	501	HAN	N12-C2-N3	-4.20	121.14	124.78
3	D	701	HAN	C9-C8-N1	3.77	108.53	105.55
3	A	601	HAN	C9-C8-N1	3.54	108.35	105.55
3	H	501	HAN	C9-C8-N1	3.47	108.30	105.55
3	F	801	HAN	C9-C8-N1	3.27	108.14	105.55
3	H	501	HAN	C13-N1-C8	2.81	130.16	124.51
3	F	801	HAN	C13-N1-C8	2.63	129.79	124.51
3	D	701	HAN	C13-N1-C8	2.60	129.74	124.51
3	A	601	HAN	C13-N1-C8	2.55	129.65	124.51
3	D	701	HAN	C13-N1-C2	2.09	130.36	125.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

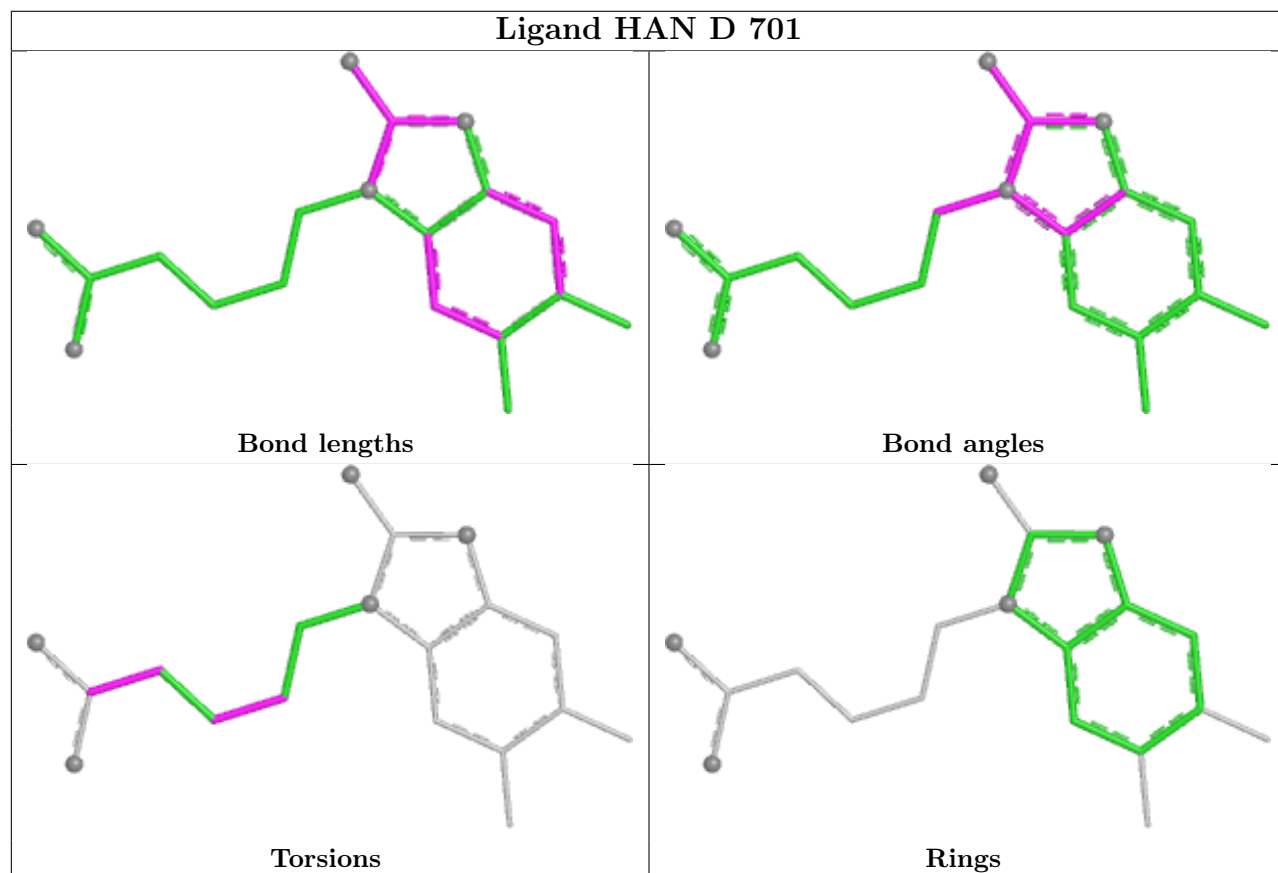
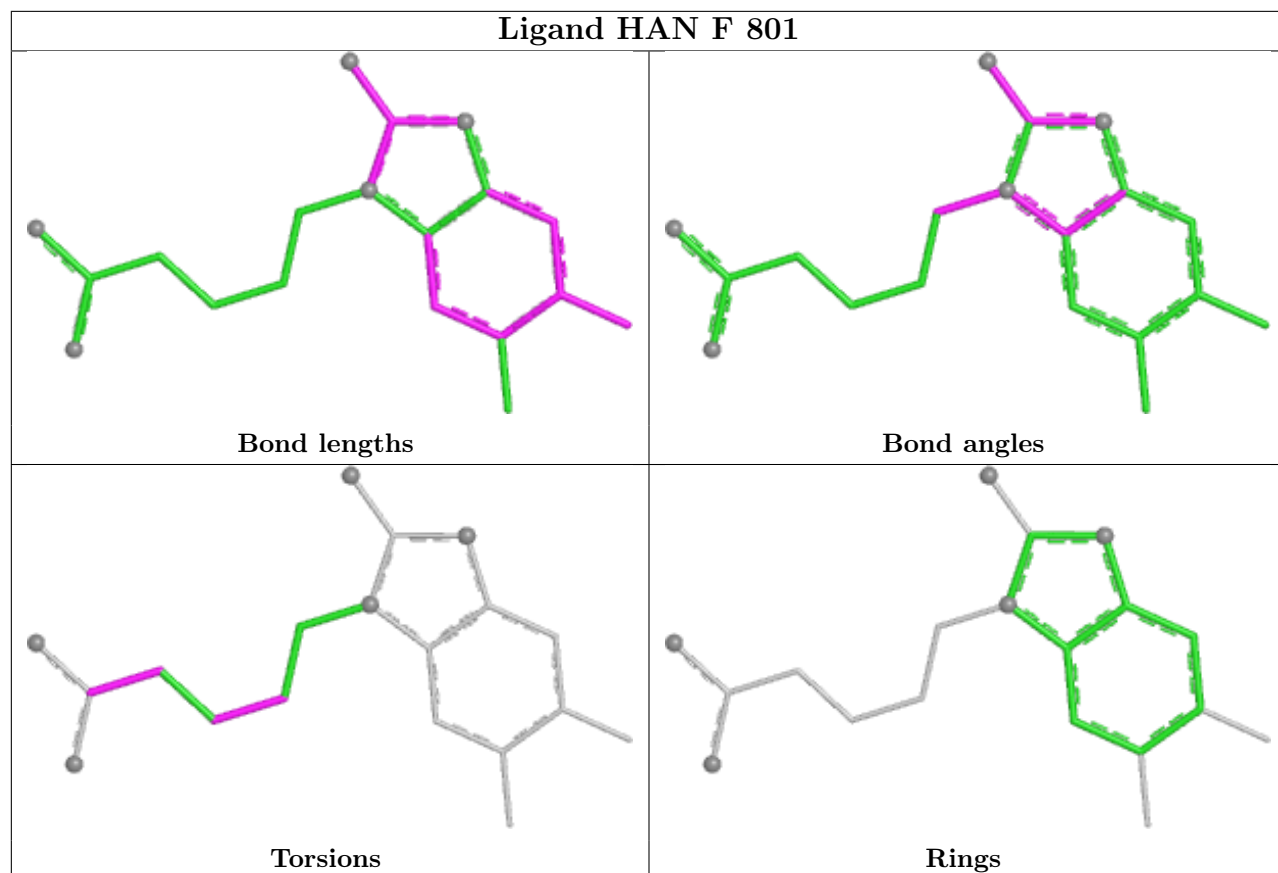
Mol	Chain	Res	Type	Atoms
3	H	501	HAN	N1-C13-C14-C15
3	H	501	HAN	C14-C15-C16-C17
3	F	801	HAN	C13-C14-C15-C16
3	A	601	HAN	C13-C14-C15-C16
3	D	701	HAN	C13-C14-C15-C16
3	F	801	HAN	C15-C16-C17-O19
3	F	801	HAN	C15-C16-C17-O18
3	A	601	HAN	C15-C16-C17-O19
3	D	701	HAN	C15-C16-C17-O19
3	A	601	HAN	C15-C16-C17-O18
3	D	701	HAN	C15-C16-C17-O18
3	H	501	HAN	C15-C16-C17-O18
3	H	501	HAN	C15-C16-C17-O19

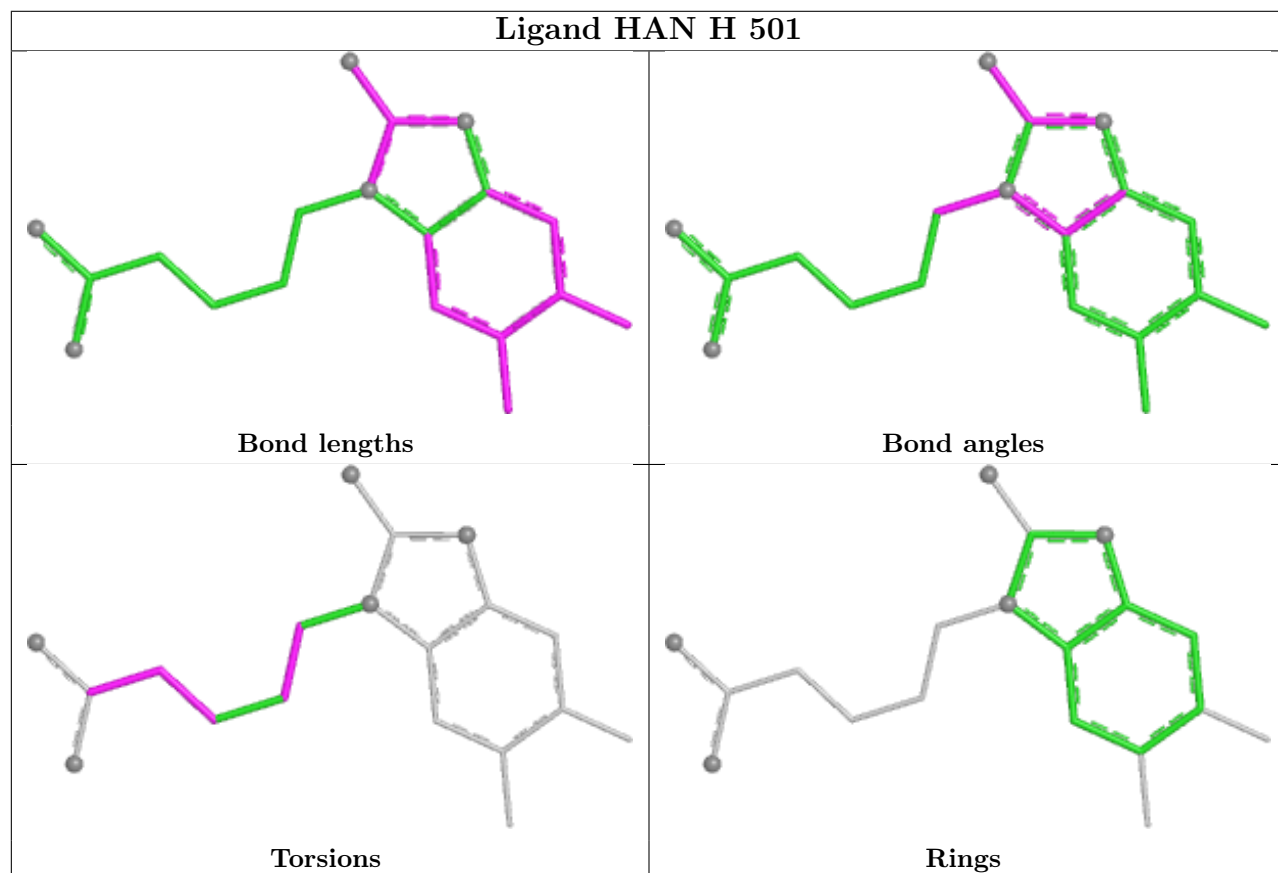
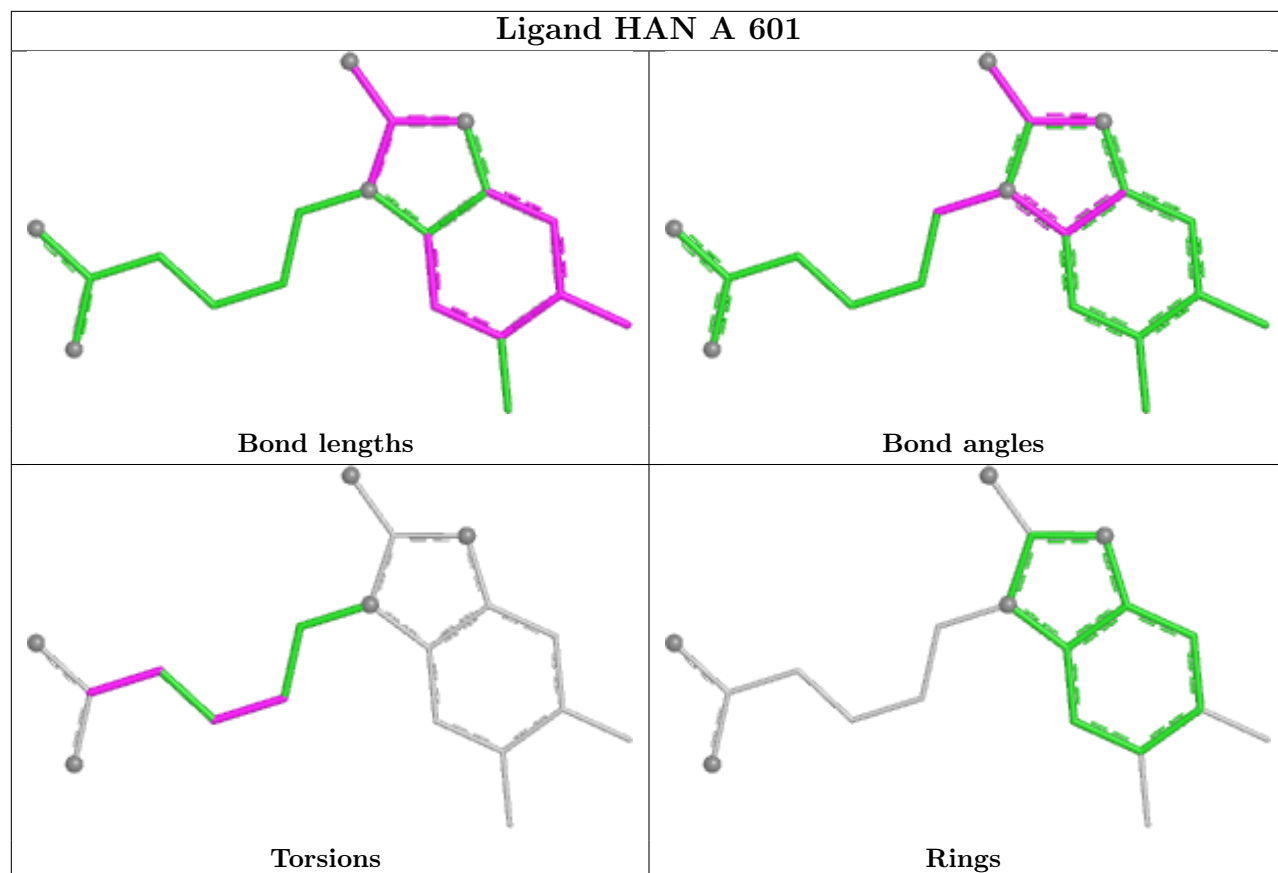
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	HAN	1	0
3	A	601	HAN	1	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/216 (100%)	0.25	4 (1%) 66 62	22, 43, 68, 101	0
1	C	216/216 (100%)	0.78	25 (11%) 9 8	27, 52, 93, 114	0
1	E	216/216 (100%)	-0.24	3 (1%) 73 70	17, 30, 46, 84	0
1	L	216/216 (100%)	-0.17	1 (0%) 87 85	16, 35, 65, 104	0
2	B	226/226 (100%)	0.25	12 (5%) 32 28	22, 44, 76, 105	0
2	D	226/226 (100%)	1.12	40 (17%) 4 3	28, 62, 92, 116	0
2	F	226/226 (100%)	0.03	17 (7%) 20 18	17, 32, 68, 87	0
2	H	226/226 (100%)	-0.04	12 (5%) 32 28	16, 36, 64, 103	0
All	All	1768/1768 (100%)	0.25	114 (6%) 25 22	16, 40, 82, 116	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	214	CYS	5.8
1	C	194	CYS	4.6
2	D	133	THR	4.4
2	D	130	SER	4.3
2	D	134	SER	4.2
2	F	128	SER	4.0
2	B	133	THR	4.0
2	F	134	SER	3.9
2	D	135	GLY	3.8
2	F	133	THR	3.6
2	D	116	THR	3.5
2	H	63	LEU	3.4
1	A	214	CYS	3.4
2	D	232	SER	3.3
2	H	134	SER	3.2
2	B	134	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	82	LEU	3.2
2	D	128	SER	3.1
2	F	130	SER	3.1
2	F	135	GLY	3.1
2	D	18	LEU	3.0
2	F	127	SER	3.0
2	D	78	LEU	3.0
2	D	81	GLN	3.0
2	D	114	ALA	2.9
2	H	227	PRO	2.9
1	C	126	LYS	2.9
2	F	136	GLY	2.9
2	D	10	GLY	2.9
2	F	1	GLU	2.9
1	C	181	LEU	2.9
2	B	130	SER	2.9
2	B	1	GLU	2.9
2	B	228	LYS	2.8
1	L	214	CYS	2.8
2	D	1	GLU	2.8
1	C	212	GLY	2.8
1	C	214	CYS	2.8
1	A	1	GLU	2.8
2	D	17	SER	2.7
1	C	127	SER	2.7
2	H	228	LYS	2.7
2	F	233	CYS	2.7
2	B	227	PRO	2.7
2	D	41	PRO	2.7
2	D	82(C)	LEU	2.7
2	D	129	LYS	2.6
1	C	213	GLU	2.6
2	H	128	SER	2.6
2	H	60	MET	2.6
1	C	184	ALA	2.6
1	C	125	LEU	2.6
2	D	62	SER	2.6
2	D	113	SER	2.6
1	C	183	LYS	2.6
2	F	129	LYS	2.6
2	F	83	ARG	2.5
2	D	63	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	199	GLY	2.5
1	C	154	LEU	2.5
2	D	138	ALA	2.5
1	C	131	SER	2.5
2	H	233	CYS	2.5
2	D	233	CYS	2.5
2	H	129	LYS	2.5
2	D	42	GLY	2.5
2	F	100	TYR	2.5
2	D	72	ASP	2.4
1	C	129	THR	2.4
1	C	209	PHE	2.4
2	F	137	THR	2.4
1	A	126	LYS	2.4
2	B	180	SER	2.3
2	H	1	GLU	2.3
2	B	129	LYS	2.3
2	B	65	ASP	2.3
2	D	68	ILE	2.3
2	D	227	PRO	2.3
2	D	228	LYS	2.2
2	F	200	THR	2.2
1	C	151	ASP	2.2
1	C	189	HIS	2.2
2	D	127	SER	2.2
1	C	132	VAL	2.2
2	D	139	ALA	2.2
2	D	223	VAL	2.1
1	E	41	ASP	2.1
2	F	232	SER	2.1
1	C	205	VAL	2.1
1	C	180	THR	2.1
2	D	14	PRO	2.1
1	C	153	ALA	2.1
2	D	20	LEU	2.1
2	D	30	ARG	2.1
2	H	133	THR	2.1
1	C	191	VAL	2.0
2	D	31	ARG	2.0
2	D	74	ALA	2.0
1	A	125	LEU	2.0
2	D	76	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	198	LEU	2.0
1	C	148	TRP	2.0
2	B	135	GLY	2.0
1	C	186	TYR	2.0
2	H	65	ASP	2.0
2	B	128	SER	2.0
2	B	233	CYS	2.0
2	D	179	GLN	2.0
1	C	130	ALA	2.0
2	D	184	LEU	2.0
2	H	135	GLY	2.0
1	C	192	TYR	2.0
1	E	168	SER	2.0
2	D	147	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

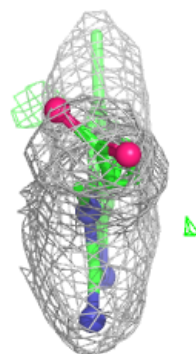
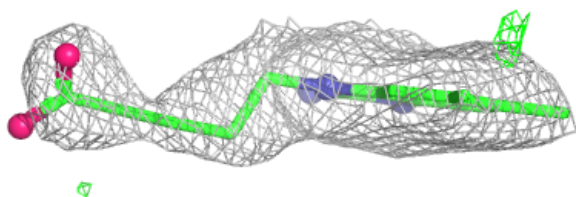
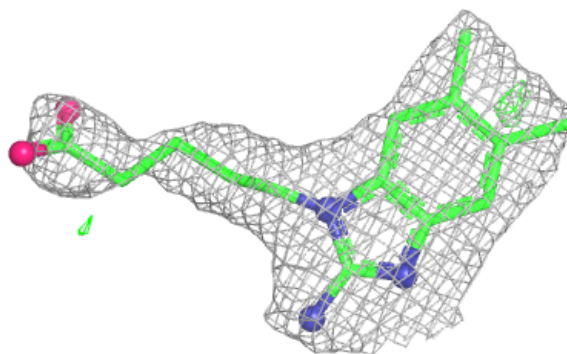
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HAN	D	701	19/19	0.92	0.12	32,36,60,60	0
3	HAN	F	801	19/19	0.93	0.10	29,35,57,57	0
3	HAN	H	501	19/19	0.95	0.09	14,20,48,49	0
3	HAN	A	601	19/19	0.95	0.09	25,27,58,59	0
4	CL	E	901	1/1	0.99	0.06	30,30,30,30	0

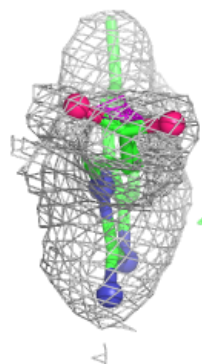
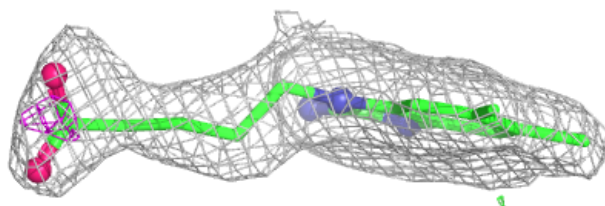
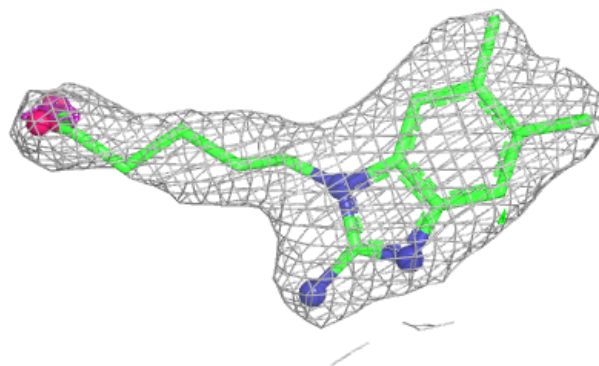
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HAN D 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

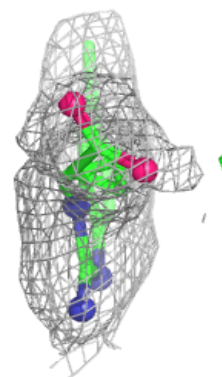
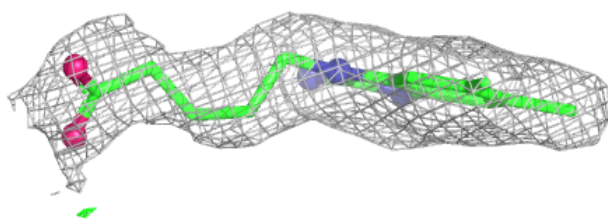
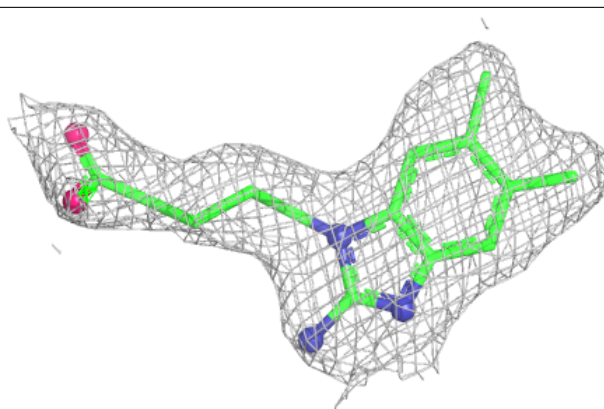
**Electron density around HAN F 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

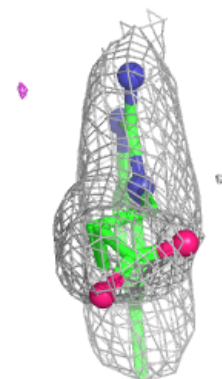
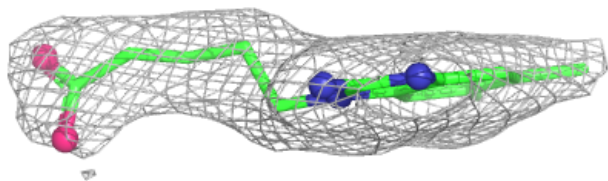
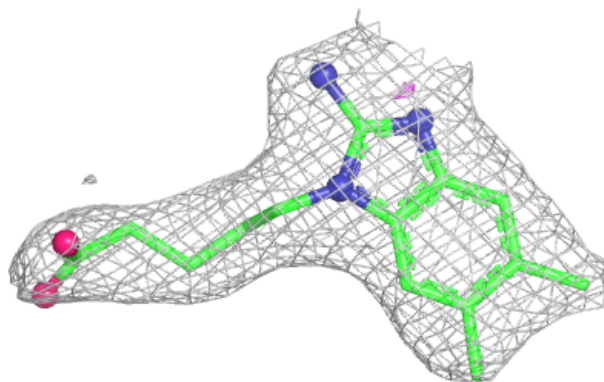


Electron density around HAN H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HAN A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.