



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 10:59 AM EDT

PDB ID : 1Y0L
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

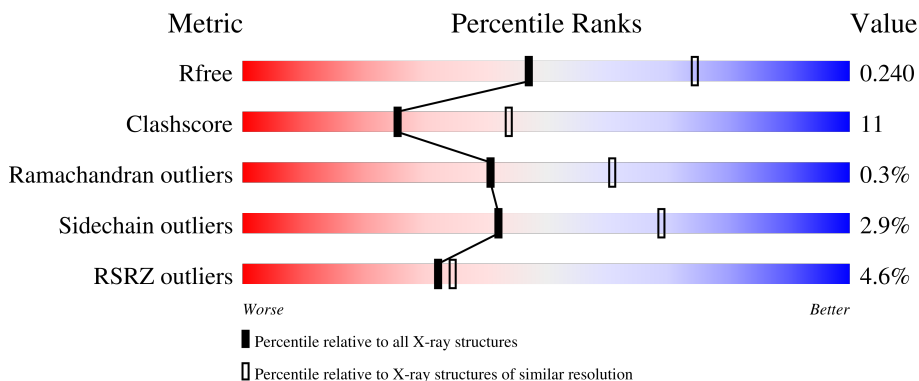
1 Overall quality at a glance i

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.



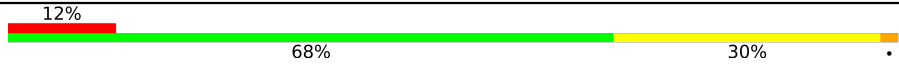

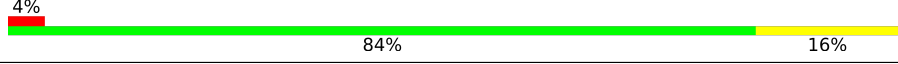
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">81% 18% .</p>
1	C	216	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">9% 73% 25% .</p>
1	E	216	<div style="display: flex; align-items: center;"> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">80% 19% .</p>
1	L	216	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">82% 16% .</p>
2	B	226	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">4% 80% 18% .</p>

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

2 Entry composition [i](#)

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.

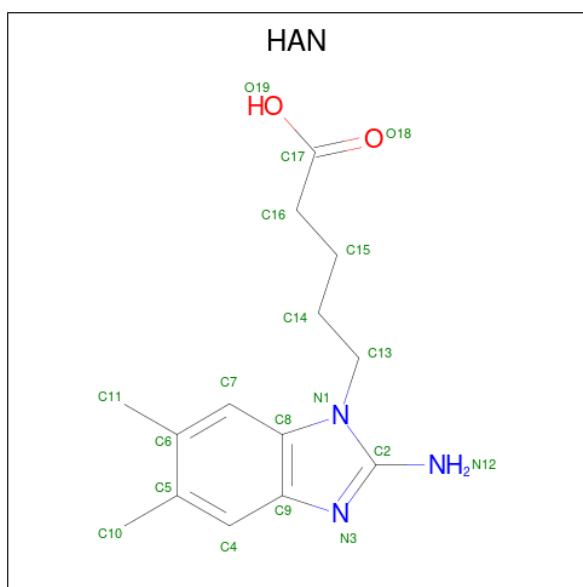
- Molecule 1 is a protein called Catalytic Antibody Fab 34E4 Light chain.

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

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

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

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



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

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

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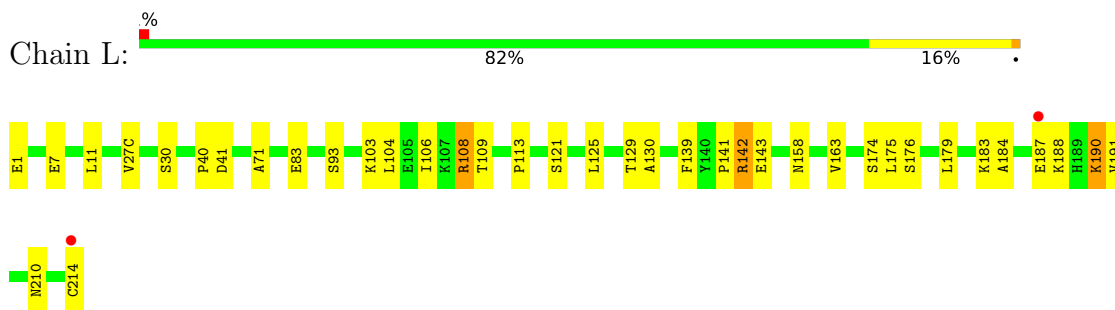
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	23	Total 23	O 23	0	0
5	D	22	Total 22	O 22	0	0
5	E	83	Total 83	O 83	0	0
5	F	65	Total 65	O 65	0	0

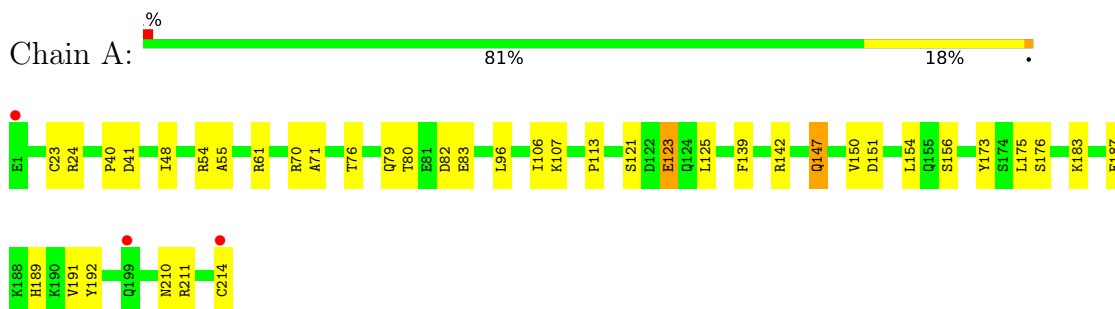
3 Residue-property plots [i](#)

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.

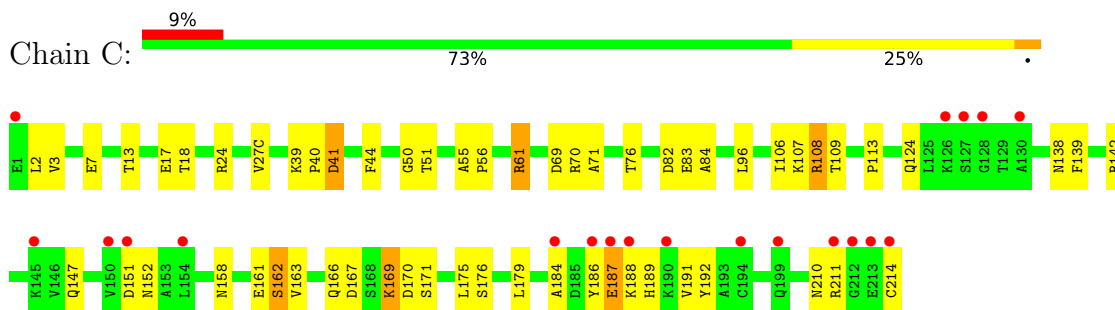
- Molecule 1: Catalytic Antibody Fab 34E4 Light chain



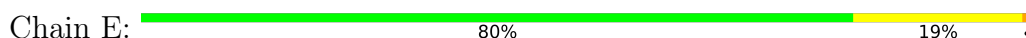
- Molecule 1: Catalytic Antibody Fab 34E4 Light chain

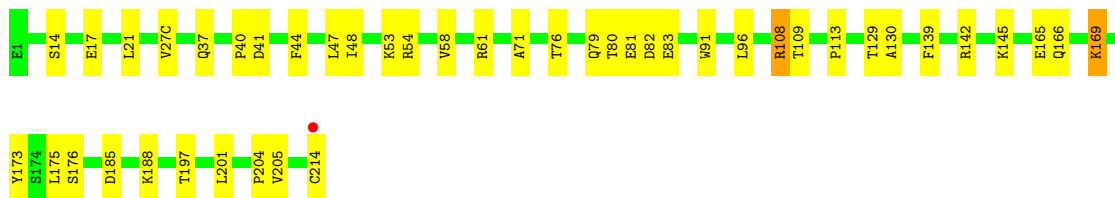


- Molecule 1: Catalytic Antibody Fab 34E4 Light chain

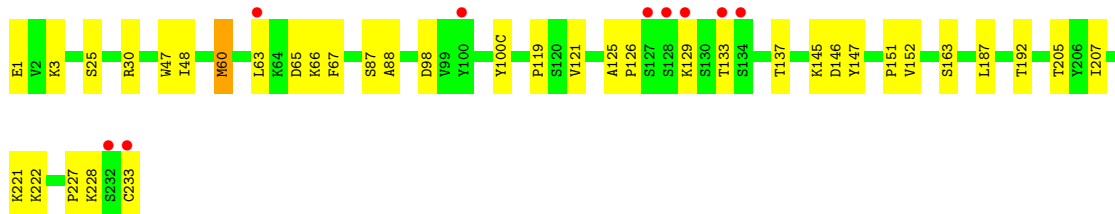
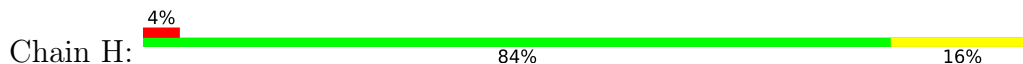


- Molecule 1: Catalytic Antibody Fab 34E4 Light chain

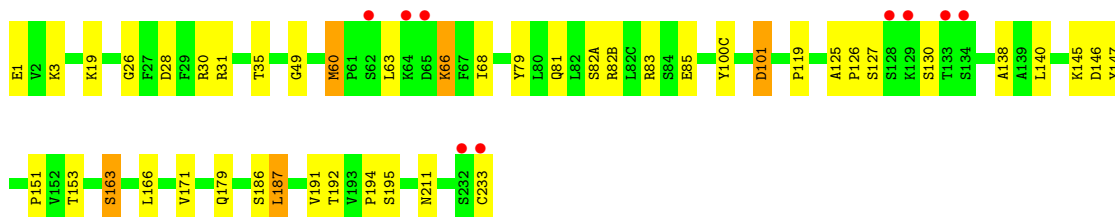
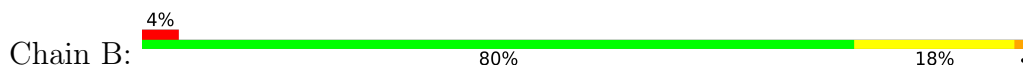




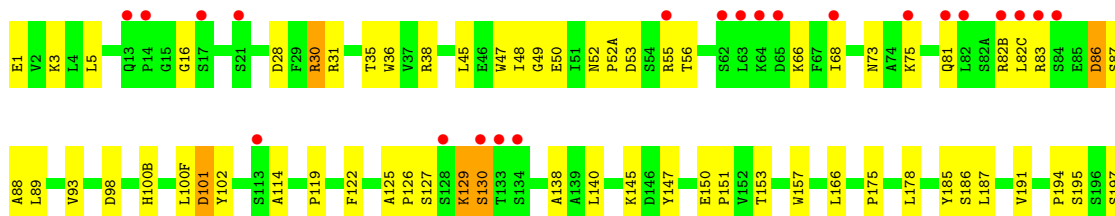
● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain



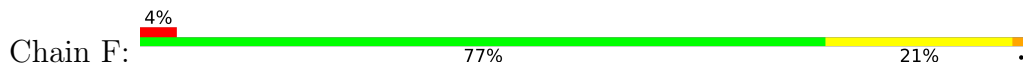
● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain

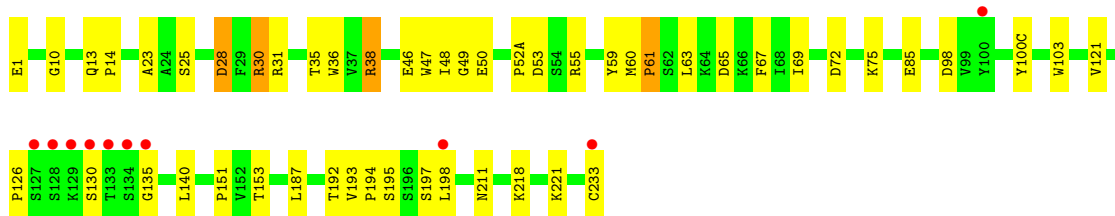


● Molecule 2: Catalytic Antibody Fab 34E4 Heavy chain



● 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 34.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.50) 92.2 (34.82-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.239 0.203 , 0.240	Depositor DCC
R_{free} test set	3926 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.282	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/1667	0.68	0/2266
1	C	0.41	0/1667	0.64	0/2266
1	E	0.45	0/1667	0.69	0/2266
1	L	0.44	0/1667	0.66	0/2266
2	B	0.45	0/1775	0.67	0/2413
2	D	0.44	0/1775	0.64	0/2413
2	F	0.45	0/1775	0.68	0/2413
2	H	0.42	0/1775	0.67	0/2413
All	All	0.44	0/13768	0.67	0/18716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	47	0
1	E	1635	0	1594	34	0
1	L	1635	0	1594	28	0
2	B	1731	0	1702	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1731	0	1702	55	0
2	F	1731	0	1702	46	0
2	H	1731	0	1702	36	0
3	A	19	0	18	2	0
3	D	19	0	18	1	0
3	F	19	0	18	2	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
5	L	65	0	0	1	0
All	All	13966	0	13256	283	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 (283) 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: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:A:123:GLU:CD	1:A:123:GLU:H	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:66:LYS:O	2:D:66:LYS:HD3	1.95	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:L:143:GLU:CD	1:L:143:GLU:H	2.04	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:HD22	3:D:701:HAN:H102	1.85	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:F:63:LEU:HD13	2:F:67:PHE:CE2	2.39	0.57
2:F:59:TYR:HE1	2:F:69:ILE:HG13	1.70	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
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:A:96:LEU:HD22	3:A:601:HAN:H102	1.88	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:A:76:THR:HG23	5:A:648:HOH:O	2.06	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
1:C:214:CYS:C	2:D:233:CYS:SG	2.86	0.54
1:E:214:CYS:O	2:F:233:CYS:HB3	2.07	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:187:LEU:HD12	2:B:187:LEU:C	2.29	0.53
2:F:187:LEU:C	2:F:187:LEU:HD12	2.30	0.53
1:C:138:ASN:HD22	2:F:1:GLU:HB2	1.71	0.52
2:D:187:LEU:C	2:D:187:LEU:HD12	2.29	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:L:27(C):VAL:HG11	1:L:71:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.91	0.51
1:C:175:LEU:HD23	1:C:175:LEU:C	2.31	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
2:F:194:PRO:HG2	2:F:197:SER:CB	2.41	0.50
2:D:150:GLU:HG2	2:D:185:TYR:CE2	2.46	0.50
1:C:107:LYS:HD3	1:C:107:LYS:C	2.32	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:F:47:TRP:CZ2	2:F:50:GLU:HG2	2.47	0.50
1:C:50:GLY:O	1:C:51:THR:HB	2.12	0.50
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.94	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:66:LYS:C	2:H:67:PHE:HD1	2.15	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: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
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:A:175:LEU:HD23	1:A:175:LEU:C	2.33	0.48
2:B:140:LEU:C	2:B:140:LEU:HD12	2.34	0.48
1:E:53:LYS:HD3	5:E:932:HOH:O	2.12	0.48
2:D:101:ASP:HB3	2:D:102:TYR:CD2	2.48	0.48
1:C:186:TYR:O	1:C:192:TYR:OH	2.28	0.48
2:F:47:TRP:HZ2	2:F:50:GLU:HG2	1.78	0.48
2:H:48:ILE:HA	2:H:60:MET:HE3	1.96	0.48
1:E:214:CYS:C	2:F:233:CYS:SG	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:85:GLU:CD	2:B:85:GLU:H	2.18	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
1:L:175:LEU:HD23	1:L:176:SER:N	2.30	0.47
1:L:141:PRO:HB2	1:L:143:GLU:OE1	2.14	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:H:192:THR:HG1	2:B:3:LYS:HE3	1.77	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
2:D:98:ASP:C	2:D:98:ASP:OD1	2.53	0.46
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
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
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:L:1:GLU:N	5:L:276:HOH:O	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:ASN:ND2	1:L:179:LEU:HD11	2.31	0.45
2:H:129:LYS:C	2:H:133:THR:H	2.20	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:E:175:LEU:HD23	1:E:175:LEU:C	2.36	0.45
1:A:214:CYS:C	2:B:233:CYS:SG	2.95	0.45
1:C:61:ARG:NH1	1:C:82:ASP:OD2	2.47	0.45
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
2:H:187:LEU:C	2:H:187:LEU:HD12	2.37	0.44
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
2:B:66:LYS:HD3	2:B:66:LYS:C	2.38	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:L:143:GLU:CD	1:L:143:GLU:N	2.69	0.44
1:L:214:CYS:C	2:H:233:CYS:SG	2.96	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
1:E:96:LEU:HD22	3:F:801:HAN:H102	1.98	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:47:TRP:O	2:H:60:MET:HE2	2.19	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
2:F:140:LEU:C	2:F:140:LEU:HD12	2.39	0.43
2:H:129:LYS:C	2:H:133:THR:N	2.72	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
1:L:175:LEU:HD23	1:L:175:LEU:C	2.39	0.42
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: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:98:ASP:HB3	2:F:100(C):TYR:HB3	2.01	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
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:C:7:GLU:CD	1:C:7:GLU:H	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:66:LYS:HD3	2:D:66:LYS:C	2.41	0.41
2:D:140:LEU:HD12	2:D:140:LEU:C	2.41	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
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
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
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

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%)	29 48
1	E	214/216 (99%)	204 (95%)	10 (5%)	0	100 100
1	L	214/216 (99%)	204 (95%)	10 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	224/226 (99%)	208 (93%)	15 (7%)	1 (0%)	34	54
2	D	224/226 (99%)	209 (93%)	12 (5%)	3 (1%)	12	21
2	F	224/226 (99%)	211 (94%)	12 (5%)	1 (0%)	34	54
2	H	224/226 (99%)	211 (94%)	13 (6%)	0	100	100
All	All	1752/1768 (99%)	1654 (94%)	92 (5%)	6 (0%)	41	61

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 [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	A	183/183 (100%)	180 (98%)	3 (2%)	62	84
1	C	183/183 (100%)	173 (94%)	10 (6%)	21	41
1	E	183/183 (100%)	180 (98%)	3 (2%)	62	84
1	L	183/183 (100%)	177 (97%)	6 (3%)	38	64
2	B	195/195 (100%)	188 (96%)	7 (4%)	35	61
2	D	195/195 (100%)	190 (97%)	5 (3%)	46	72
2	F	195/195 (100%)	188 (96%)	7 (4%)	35	61
2	H	195/195 (100%)	192 (98%)	3 (2%)	65	85
All	All	1512/1512 (100%)	1468 (97%)	44 (3%)	42	69

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	30	SER
1	L	93	SER
1	L	108	ARG
1	L	142	ARG
1	L	174	SER
1	L	190	LYS
2	H	60	MET
2	H	65	ASP
2	H	151	PRO
1	A	123	GLU
1	A	147	GLN
1	A	156	SER
2	B	31	ARG
2	B	60	MET
2	B	66	LYS
2	B	101	ASP
2	B	151	PRO
2	B	163	SER
2	B	187	LEU
1	C	13	THR
1	C	61	ARG
1	C	69	ASP
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	86	ASP
2	D	89	LEU
2	D	129	LYS
2	D	151	PRO
1	E	108	ARG
1	E	142	ARG
1	E	169	LYS
2	F	28	ASP
2	F	30	ARG
2	F	38	ARG
2	F	61	PRO
2	F	65	ASP
2	F	85	GLU

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Mol	Chain	Res	Type
2	F	151	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
2	B	179	GLN
2	B	211	ASN

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 monosaccharides 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	A	601	-	17,20,20	1.97	5 (29%)	21,28,28	1.07	1 (4%)
3	HAN	H	501	-	17,20,20	1.98	5 (29%)	21,28,28	1.11	1 (4%)
3	HAN	F	801	-	17,20,20	2.02	5 (29%)	21,28,28	1.06	1 (4%)
3	HAN	D	701	-	17,20,20	1.99	4 (23%)	21,28,28	1.12	2 (9%)

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	A	601	-	-	3/7/7/7	0/2/2/2
3	HAN	H	501	-	-	4/7/7/7	0/2/2/2
3	HAN	F	801	-	-	5/7/7/7	0/2/2/2
3	HAN	D	701	-	-	3/7/7/7	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	801	HAN	C2-N12	4.38	1.42	1.33
3	A	601	HAN	C2-N12	4.24	1.42	1.33
3	F	801	HAN	C2-N3	-4.19	1.28	1.35
3	D	701	HAN	C2-N12	4.18	1.42	1.33
3	H	501	HAN	C2-N3	-4.12	1.28	1.35
3	D	701	HAN	C2-N3	-3.94	1.29	1.35
3	H	501	HAN	C2-N12	3.86	1.41	1.33
3	A	601	HAN	C2-N3	-3.84	1.29	1.35
3	D	701	HAN	C7-C6	2.31	1.43	1.37
3	H	501	HAN	C6-C5	2.29	1.46	1.40
3	F	801	HAN	C6-C5	2.29	1.46	1.40
3	A	601	HAN	C4-C5	2.24	1.43	1.37
3	H	501	HAN	C4-C5	2.23	1.43	1.37
3	D	701	HAN	C4-C5	2.22	1.43	1.37
3	A	601	HAN	C10-C5	2.22	1.55	1.51
3	F	801	HAN	C4-C5	2.19	1.43	1.37
3	A	601	HAN	C6-C5	2.14	1.46	1.40
3	F	801	HAN	C7-C6	2.13	1.43	1.37
3	H	501	HAN	C4-C9	2.00	1.44	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	HAN	C13-N1-C2	2.95	130.36	125.34
3	A	601	HAN	C13-N1-C2	2.52	129.63	125.34
3	F	801	HAN	C13-N1-C2	2.45	129.51	125.34
3	H	501	HAN	C13-N1-C2	2.43	129.47	125.34
3	D	701	HAN	N12-C2-N3	-2.28	120.32	123.28

There are no chirality outliers.

All (15) torsion outliers are listed below:

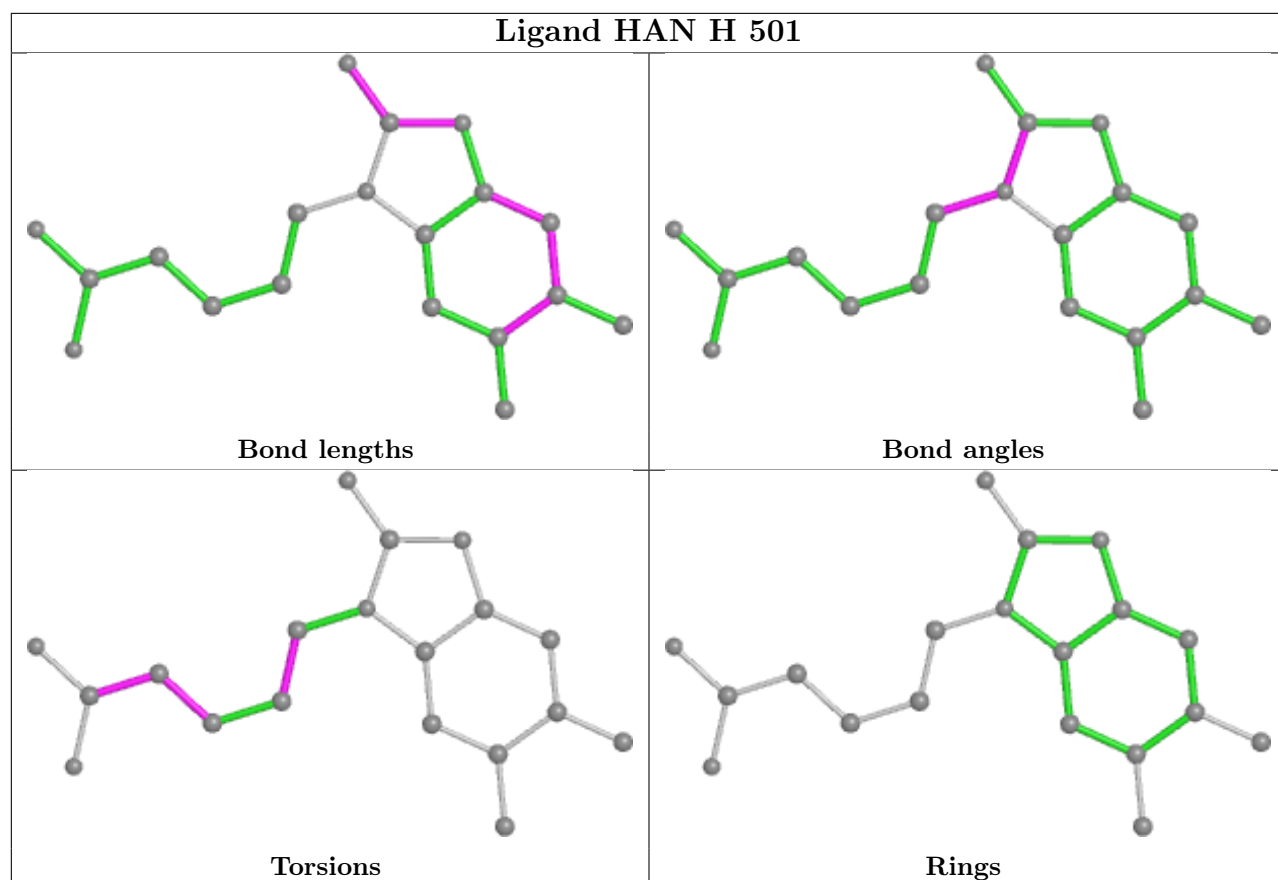
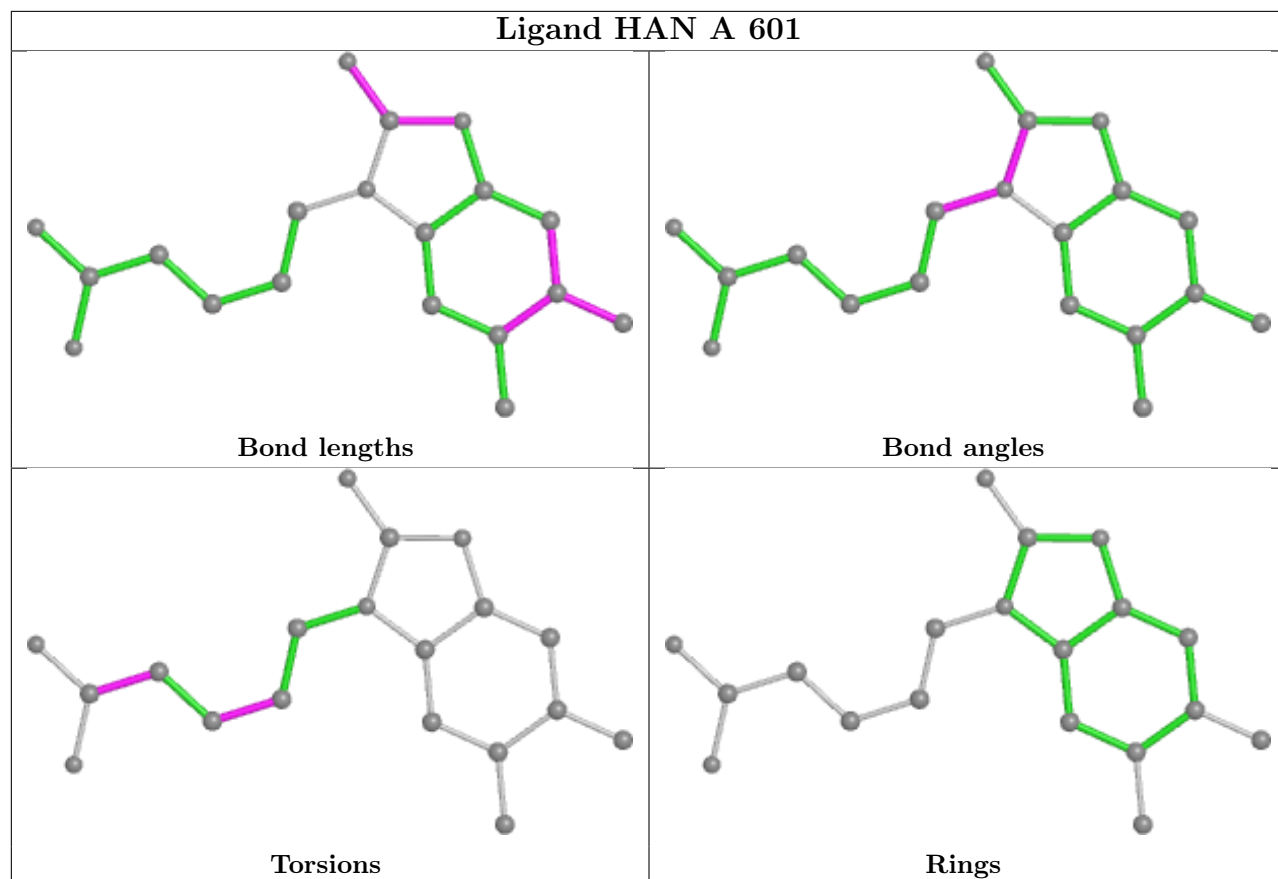
Mol	Chain	Res	Type	Atoms
3	H	501	HAN	N1-C13-C14-C15
3	H	501	HAN	C14-C15-C16-C17
3	F	801	HAN	C13-C14-C15-C16
3	A	601	HAN	C13-C14-C15-C16
3	F	801	HAN	C14-C13-N1-C2
3	D	701	HAN	C13-C14-C15-C16
3	F	801	HAN	C14-C13-N1-C8
3	F	801	HAN	C15-C16-C17-O19
3	F	801	HAN	C15-C16-C17-O18
3	A	601	HAN	C15-C16-C17-O19
3	A	601	HAN	C15-C16-C17-O18
3	D	701	HAN	C15-C16-C17-O19
3	H	501	HAN	C15-C16-C17-O18
3	D	701	HAN	C15-C16-C17-O18
3	H	501	HAN	C15-C16-C17-O19

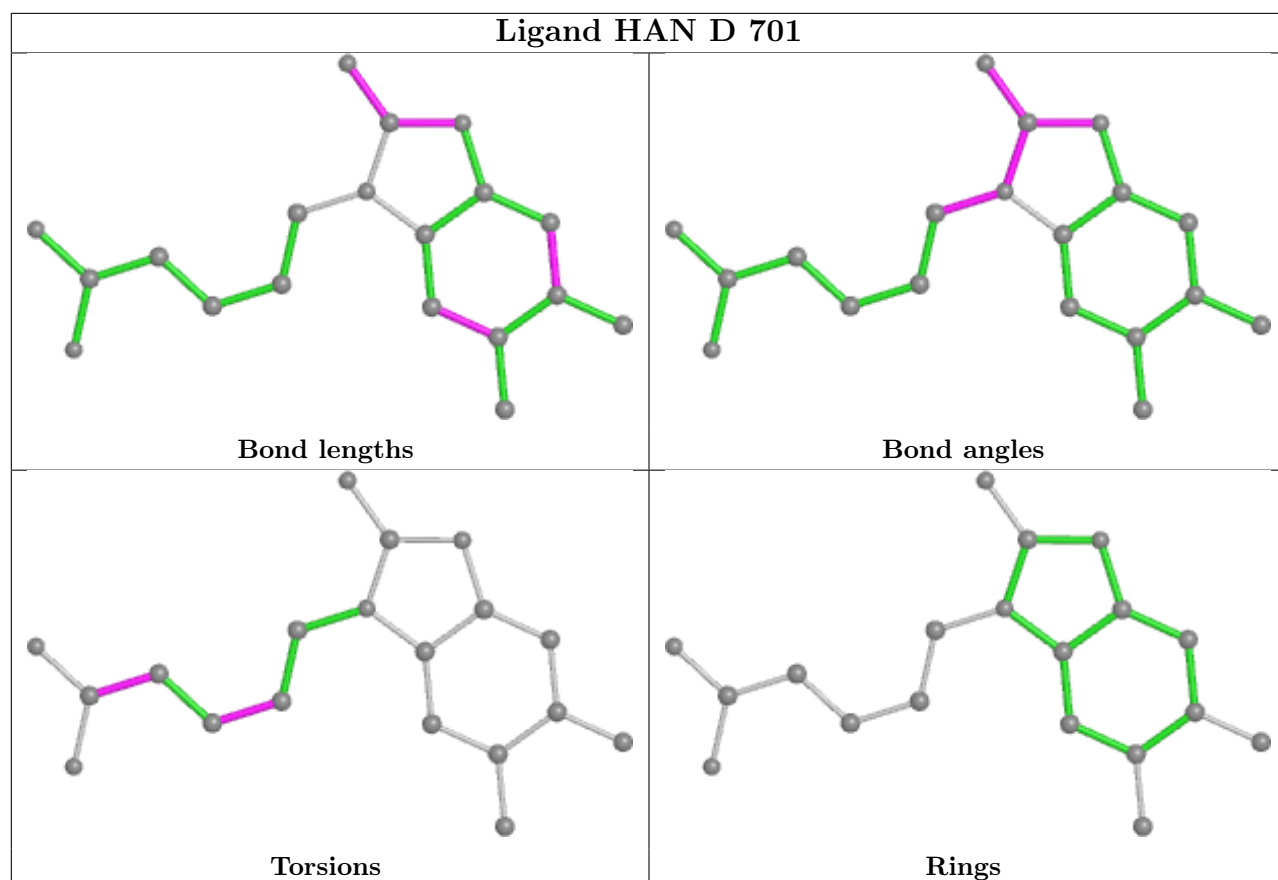
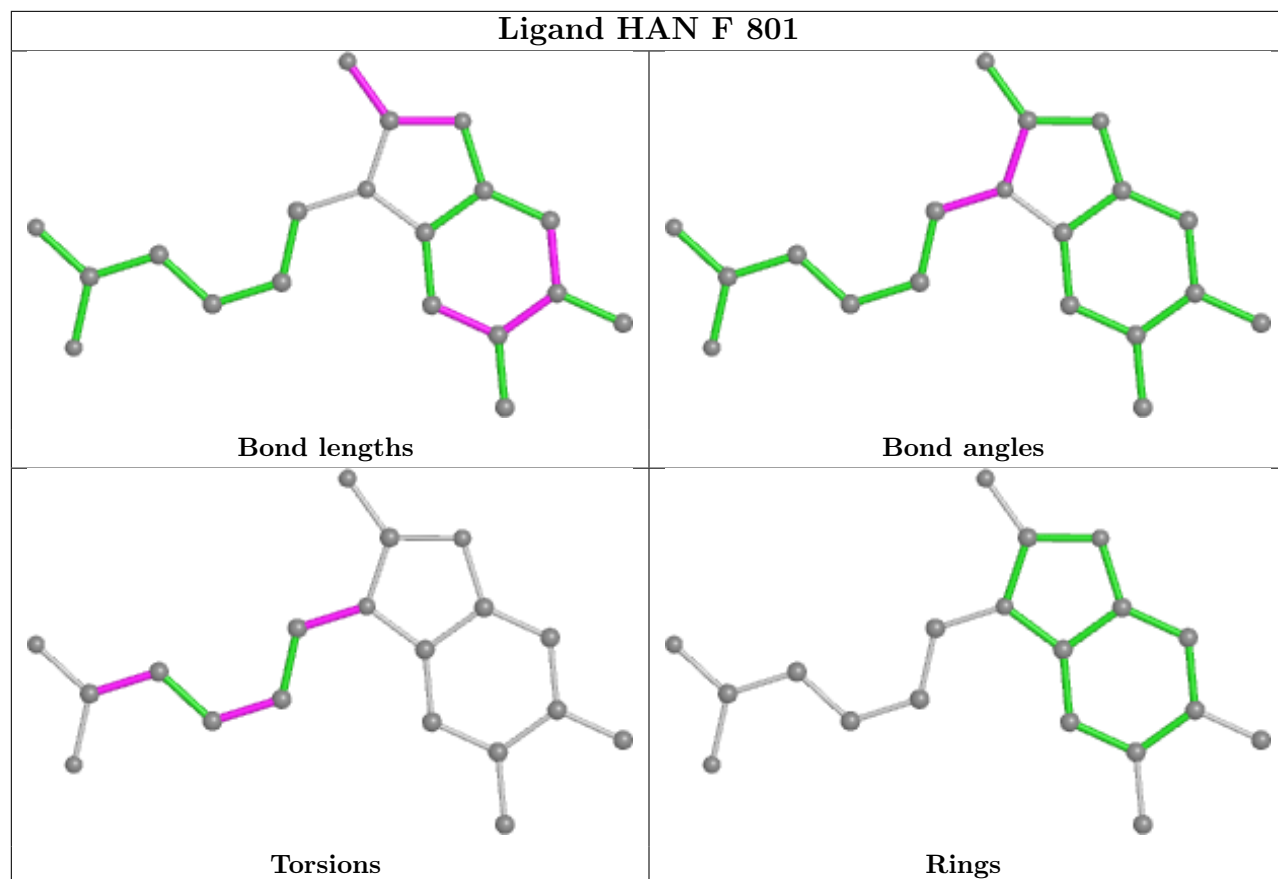
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HAN	2	0
3	F	801	HAN	2	0
3	D	701	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%)	0.17	3 (1%) 75 77	22, 43, 68, 101	0
1	C	216/216 (100%)	0.54	20 (9%) 8 8	27, 52, 93, 114	0
1	E	216/216 (100%)	-0.28	1 (0%) 91 91	17, 30, 46, 84	0
1	L	216/216 (100%)	-0.23	2 (0%) 84 86	16, 35, 65, 104	0
2	B	226/226 (100%)	0.03	9 (3%) 38 41	22, 44, 76, 105	0
2	D	226/226 (100%)	0.79	27 (11%) 4 4	28, 62, 92, 116	0
2	F	226/226 (100%)	-0.03	10 (4%) 34 37	17, 32, 68, 87	0
2	H	226/226 (100%)	-0.10	9 (3%) 38 41	16, 36, 64, 103	0
All	All	1768/1768 (100%)	0.11	81 (4%) 32 34	16, 40, 82, 116	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	233	CYS	9.7
1	E	214	CYS	9.5
1	L	214	CYS	8.2
2	H	233	CYS	8.0
2	F	134	SER	7.2
1	A	214	CYS	7.1
2	F	233	CYS	6.9
2	F	133	THR	5.6
2	D	63	LEU	5.3
2	D	232	SER	5.1
1	C	214	CYS	5.1
2	D	113	SER	5.0
2	F	100	TYR	4.8
2	D	130	SER	4.7
2	D	133	THR	4.6
2	F	128	SER	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	135	GLY	4.6
2	F	129	LYS	4.4
2	F	130	SER	4.4
2	B	65	ASP	4.3
2	B	233	CYS	4.3
2	D	228	LYS	4.2
1	C	126	LYS	4.2
2	H	129	LYS	4.2
2	D	128	SER	4.1
2	H	134	SER	4.0
2	D	62	SER	4.0
2	D	65	ASP	3.9
2	B	232	SER	3.9
2	D	82	LEU	3.7
2	H	128	SER	3.6
2	F	127	SER	3.5
2	D	64	LYS	3.5
1	C	188	LYS	3.3
1	C	212	GLY	3.3
1	C	127	SER	3.3
1	C	1	GLU	3.2
2	D	83	ARG	3.2
2	H	133	THR	3.2
1	A	1	GLU	3.2
2	B	128	SER	3.2
1	C	128	GLY	3.2
2	H	63	LEU	3.1
1	C	190	LYS	3.0
1	C	150	VAL	3.0
2	D	134	SER	2.9
1	C	194	CYS	2.9
2	D	82(B)	ARG	2.9
1	C	151	ASP	2.8
2	H	100	TYR	2.8
2	B	62	SER	2.8
2	D	81	GLN	2.8
1	C	184	ALA	2.7
2	D	13	GLN	2.7
1	C	186	TYR	2.6
2	B	134	SER	2.6
2	D	68	ILE	2.6
2	B	133	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	84	SER	2.5
1	L	187	GLU	2.5
1	C	154	LEU	2.5
1	C	213	GLU	2.5
1	C	187	GLU	2.4
1	C	130	ALA	2.4
1	C	145	LYS	2.4
2	D	75	LYS	2.4
1	A	199	GLN	2.4
1	C	199	GLN	2.4
2	D	226	GLU	2.3
2	D	82(C)	LEU	2.3
2	B	64	LYS	2.2
2	D	55	ARG	2.2
1	C	211	ARG	2.2
2	H	232	SER	2.2
2	D	14	PRO	2.2
2	H	127	SER	2.2
2	D	21	SER	2.2
2	F	198	LEU	2.1
2	D	17	SER	2.1
2	D	222	LYS	2.1
2	B	129	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

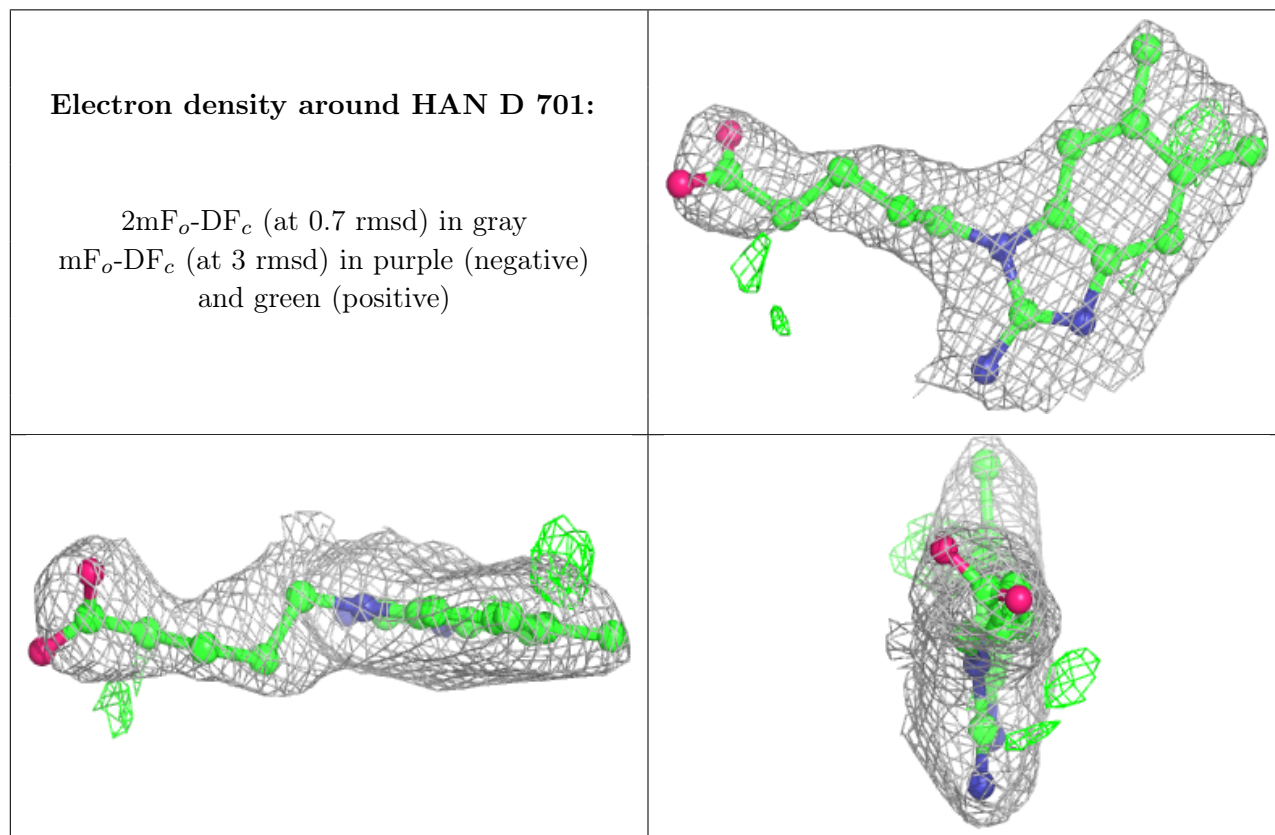
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

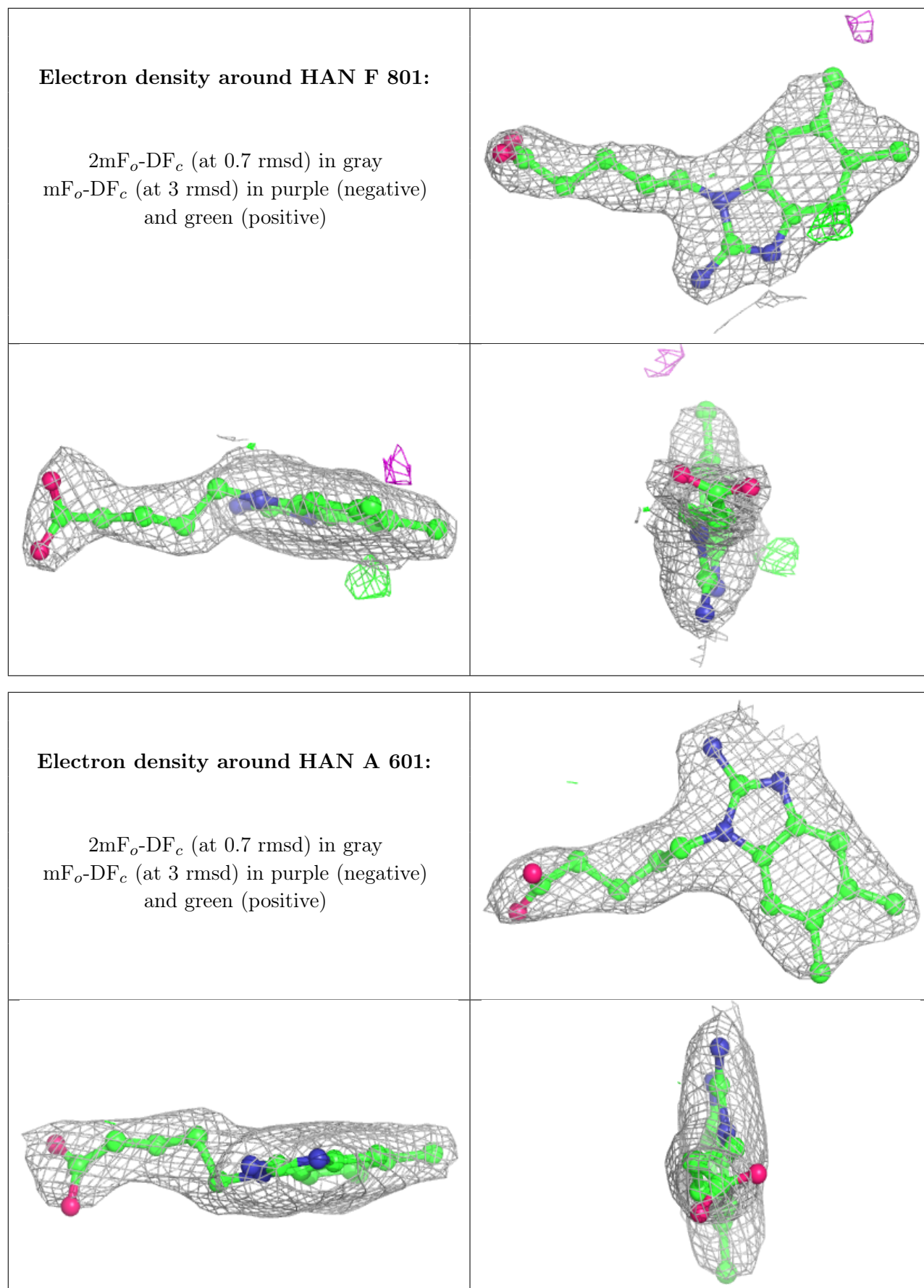
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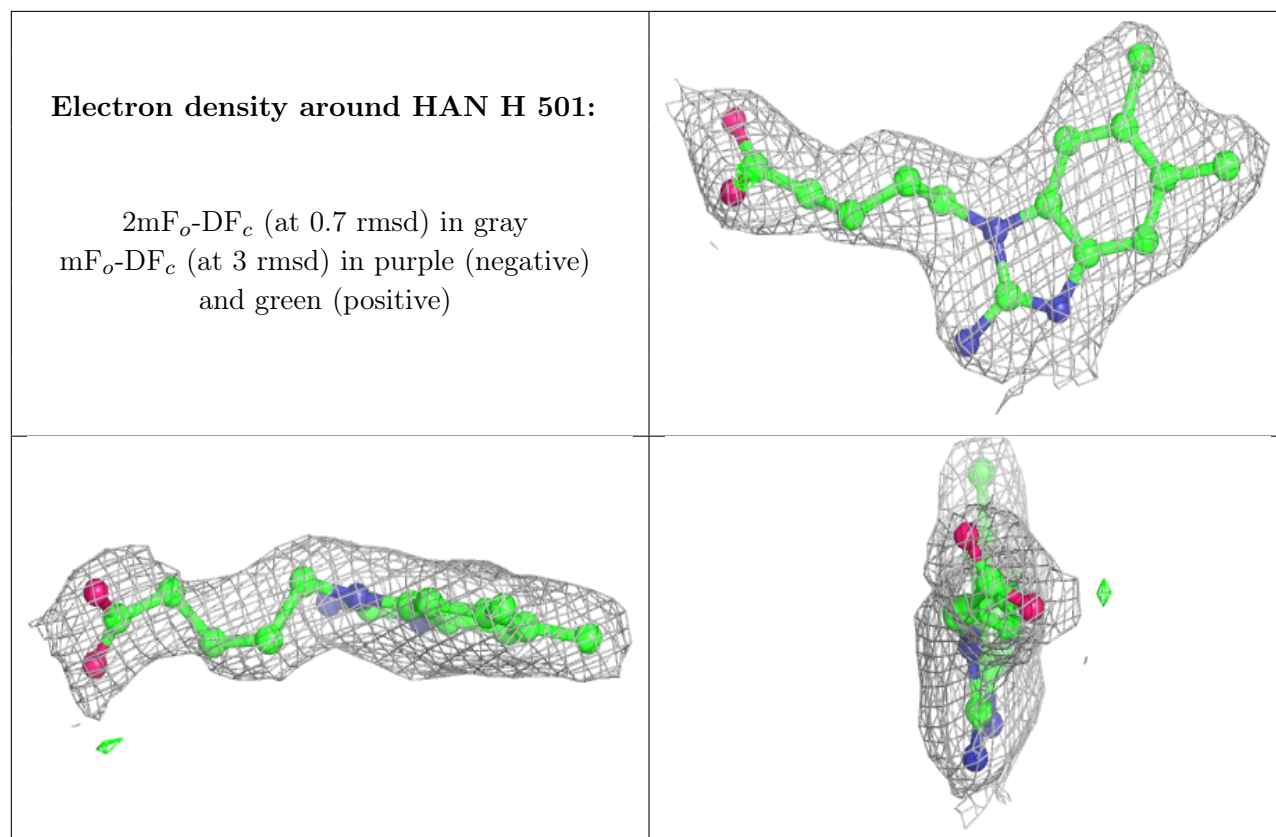
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HAN	D	701	19/19	0.91	0.20	32,36,60,60	0
3	HAN	F	801	19/19	0.93	0.18	29,35,57,57	0
3	HAN	A	601	19/19	0.94	0.18	25,27,58,59	0
3	HAN	H	501	19/19	0.95	0.17	14,20,48,49	0
4	CL	E	901	1/1	0.99	0.07	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.







6.5 Other polymers [i](#)

There are no such residues in this entry.