



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:37 AM UTC

PDB ID : 6B0T / pdb_00006b0t
Title : Structural Insights into the Induced-fit Inhibition of Fascin by a Small Molecule
Authors : Dey, R.; Huang, X.Y.
Deposited on : 2017-09-15
Resolution : 2.80 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:

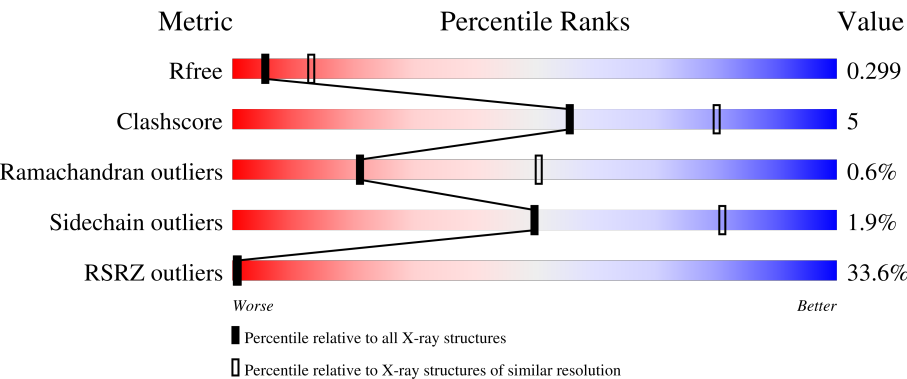
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	487	44% 87% 13%
1	B	487	14% 90% 10%
1	C	487	17% 92% 8%
1	D	487	45% 86% 13% .
1	E	487	43% 88% 11% .

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Mol	Chain	Length	Quality of chain
1	F	487	39% 88% 11%

2 Entry composition [i](#)

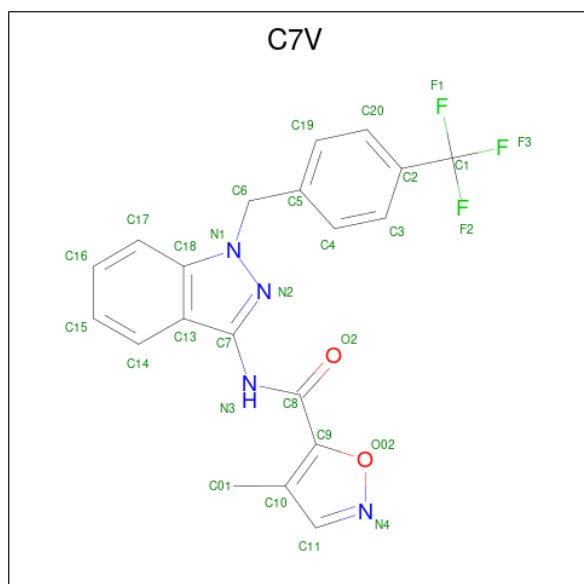
There are 3 unique types of molecules in this entry. The entry contains 45507 atoms, of which 22171 are hydrogens and 0 are deuteriums.

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 Fascin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	B	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	C	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	D	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			
1	E	487	Total	C	H	N	O	S	0	0	0
			7474	2376	3671	680	733	14			
1	F	487	Total	C	H	N	O	S	0	0	0
			7485	2376	3682	680	733	14			

- Molecule 2 is 4-methyl-N-(1-{[4-(trifluoromethyl)phenyl]methyl}-1H-indazol-3-yl)-1,2-oxazole-5-carboxamide (CCD ID: C7V) (formula: C₂₀H₁₅F₃N₄O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			44	20	3	15	4	2		
2	B	1	Total	C	F	H	N	O	0	0
			44	20	3	15	4	2		
2	C	1	Total	C	F	H	N	O	0	0
			44	20	3	15	4	2		
2	D	1	Total	C	F	H	N	O	0	0
			44	20	3	15	4	2		
2	E	1	Total	C	F	H	N	O	0	0
			44	20	3	15	4	2		
2	F	1	Total	C	F	H	N	O	0	0
			44	20	3	15	4	2		

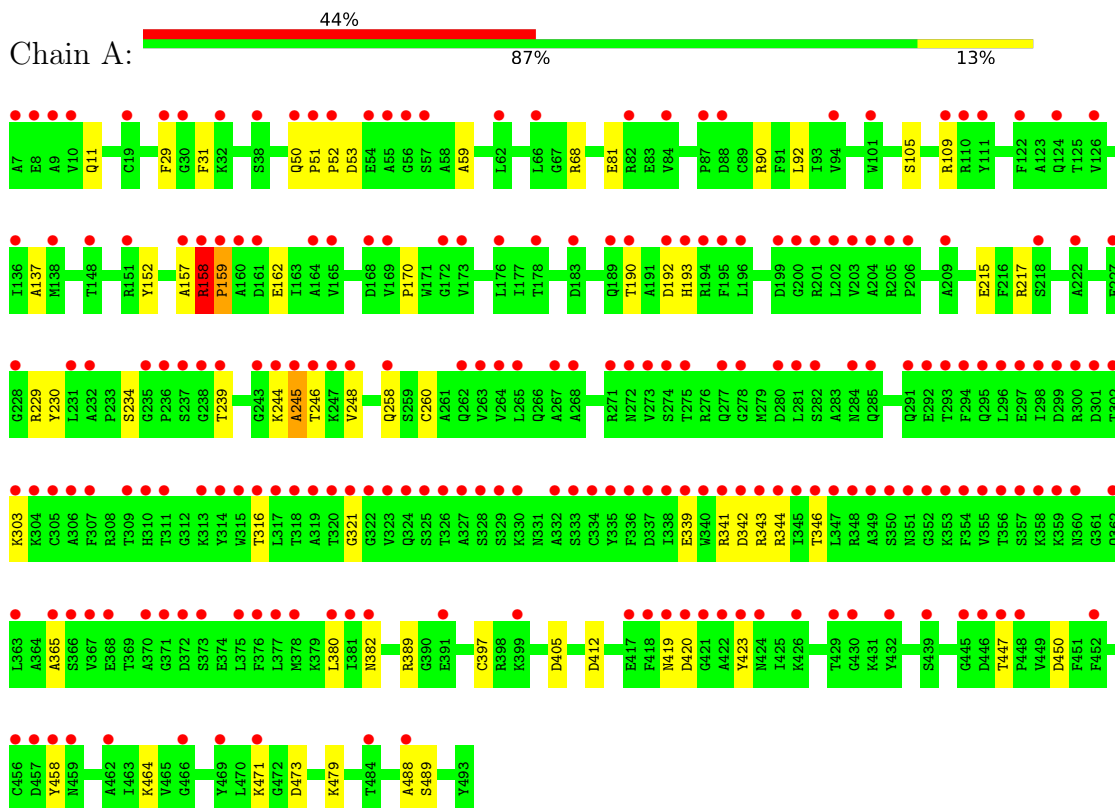
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	78	Total	O	0	0
			78	78		
3	C	89	Total	O	0	0
			89	89		
3	D	40	Total	O	0	0
			40	40		
3	E	58	Total	O	0	0
			58	58		
3	F	47	Total	O	0	0
			47	47		

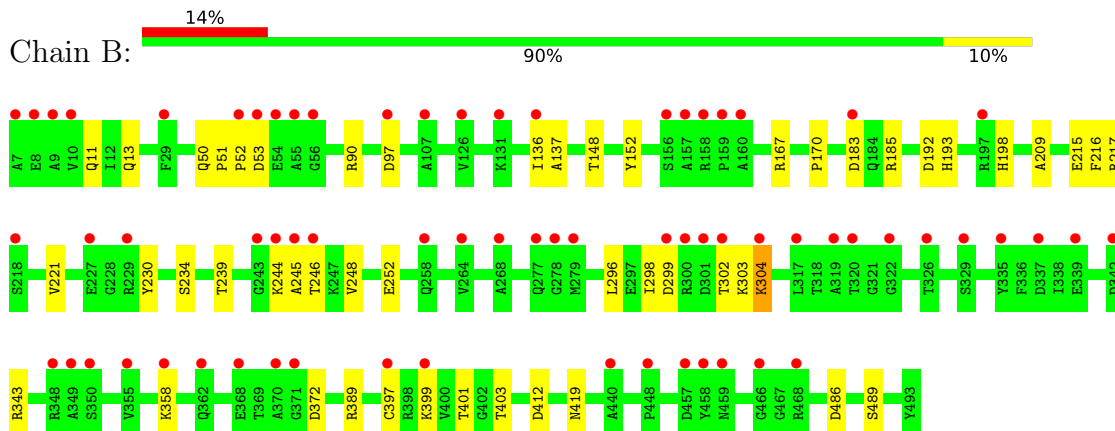
3 Residue-property plots

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 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.

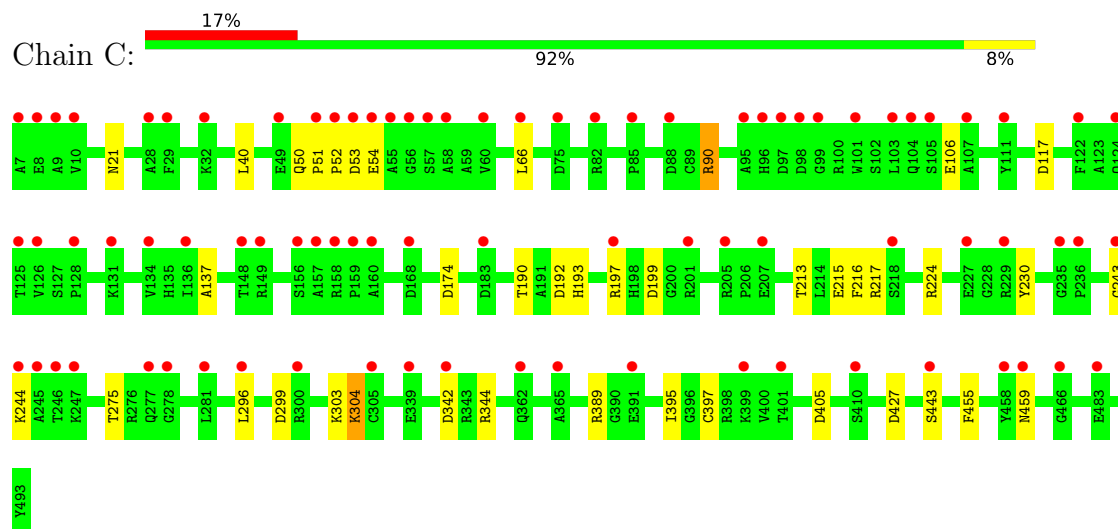
• Molecule 1: Fascin



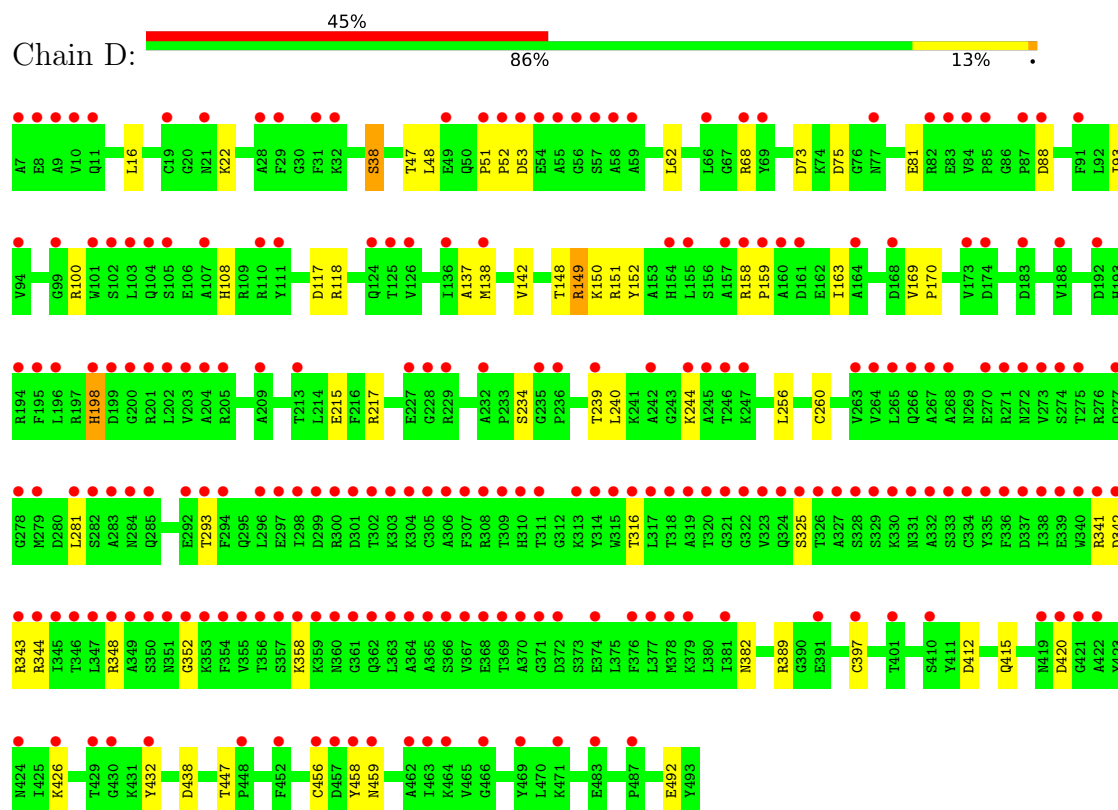
• Molecule 1: Fascin



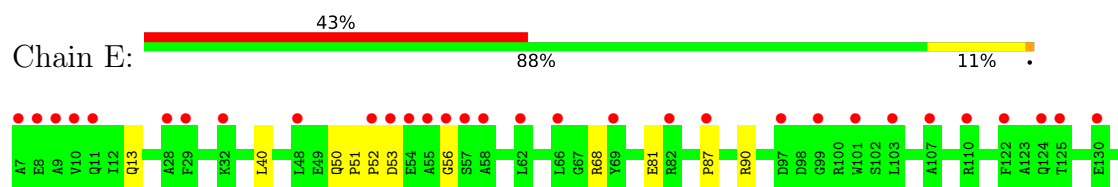
- Molecule 1: Fascin

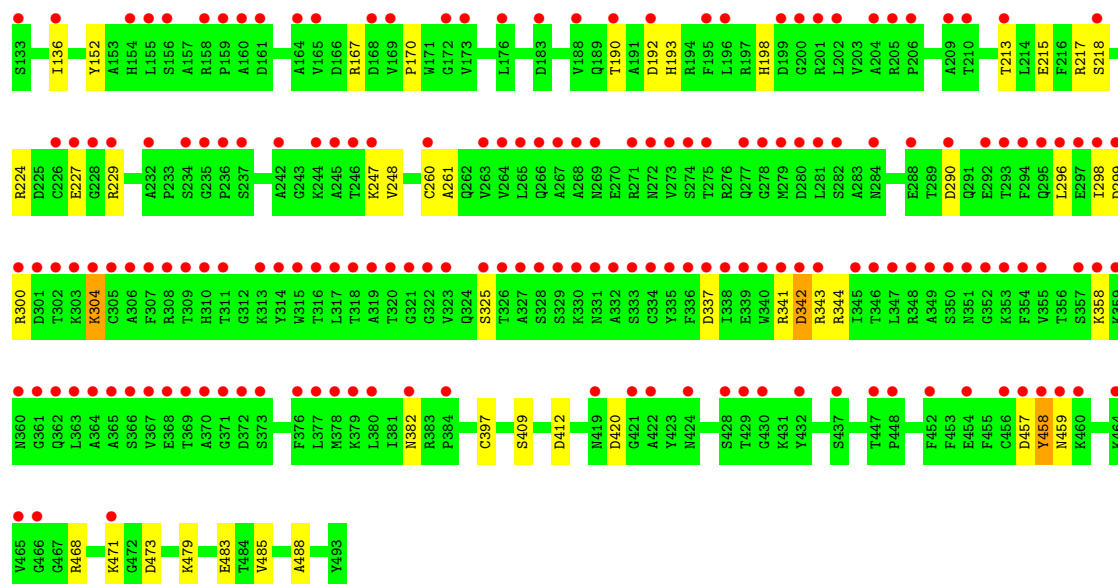


- Molecule 1: Fascin

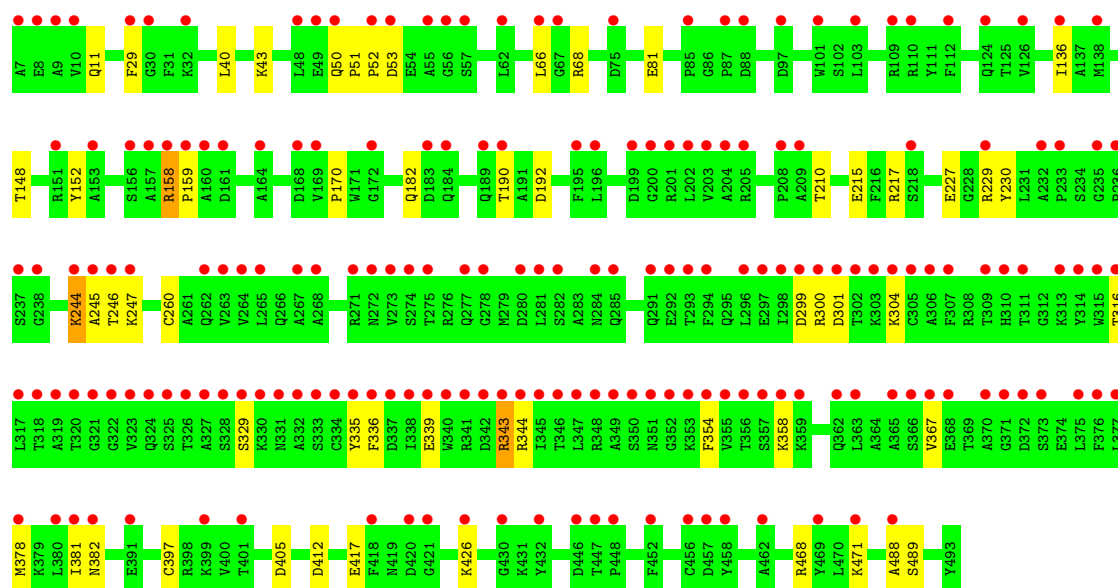
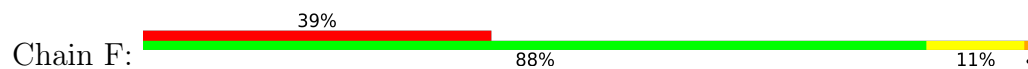


- Molecule 1: Fascin





• Molecule 1: Fascin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.58Å 59.26Å 293.65Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	45.44 – 2.80 45.44 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.44-2.80) 98.8 (45.44-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.265 , 0.303 0.267 , 0.299	Depositor DCC
R_{free} test set	10489 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	45507	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6790e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: C7V

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	0.22	1/3884 (0.0%)	0.40	3/5252 (0.1%)
1	B	0.16	0/3884	0.34	1/5252 (0.0%)
1	C	0.21	1/3884 (0.0%)	0.35	1/5252 (0.0%)
1	D	0.22	2/3884 (0.1%)	0.37	1/5252 (0.0%)
1	E	0.16	0/3884	0.32	1/5252 (0.0%)
1	F	0.22	0/3884	0.38	2/5252 (0.0%)
All	All	0.20	4/23304 (0.0%)	0.36	9/31512 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLU	C-N	-8.37	1.23	1.33
1	D	149	ARG	CA-C	6.65	1.61	1.52
1	C	244	LYS	CA-C	5.86	1.60	1.52
1	D	244	LYS	CA-C	5.13	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ARG	CA-C-O	8.47	130.06	119.05
1	F	244	LYS	N-CA-C	-7.06	103.19	111.03
1	B	244	LYS	N-CA-C	-5.76	104.69	110.97
1	A	158	ARG	CA-C-N	5.49	126.70	119.84
1	A	158	ARG	C-N-CA	5.49	126.70	119.84
1	A	303	LYS	CB-CA-C	-5.39	110.38	116.63
1	F	343	ARG	N-CA-C	5.24	119.38	113.15
1	C	243	GLY	CA-C-O	-5.09	116.34	121.64
1	E	342	ASP	CB-CA-C	-5.06	110.72	116.54

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	3803	3682	3682	40	0
1	B	3803	3682	3682	33	0
1	C	3803	3682	3682	22	0
1	D	3803	3682	3682	42	0
1	E	3803	3671	3682	35	0
1	F	3803	3682	3682	37	0
2	A	29	15	0	3	0
2	B	29	15	0	4	0
2	C	29	15	0	3	0
2	D	29	15	0	2	0
2	E	29	15	0	5	0
2	F	29	15	0	2	0
3	A	32	0	0	2	0
3	B	78	0	0	3	0
3	C	89	0	0	2	0
3	D	40	0	0	4	0
3	E	58	0	0	3	0
3	F	47	0	0	10	0
All	All	23336	22171	22092	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (211) 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:A:50:GLN:HG2	2:A:501:C7V:N4	1.74	1.02
1:A:157:ALA:O	1:A:158:ARG:O	1.85	0.93
1:F:152:TYR:CE2	1:F:170:PRO:HD3	2.03	0.92
1:D:215:GLU:OE2	1:D:217:ARG:NH2	2.02	0.92
1:F:215:GLU:OE2	1:F:217:ARG:NH2	2.02	0.92
1:A:215:GLU:OE2	1:A:217:ARG:NH2	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:OG1	1:F:468:ARG:HG2	1.78	0.83
1:A:343:ARG:NH2	1:A:450:ASP:OD2	2.12	0.83
1:A:152:TYR:CE2	1:A:170:PRO:HD3	2.15	0.81
1:E:50:GLN:HG2	2:E:501:C7V:N4	1.96	0.79
1:A:50:GLN:CG	2:A:501:C7V:N4	2.46	0.77
1:D:456:CYS:SG	3:D:638:HOH:O	2.43	0.77
1:B:51:PRO:O	1:B:53:ASP:N	2.18	0.76
1:C:137:ALA:O	1:C:389:ARG:NH2	2.18	0.76
1:A:471:LYS:HG3	1:A:488:ALA:O	1.86	0.76
1:E:260:CYS:O	1:E:382:ASN:ND2	2.19	0.75
1:A:419:ASN:ND2	3:A:602:HOH:O	2.21	0.73
1:F:210:THR:O	3:F:601:HOH:O	2.06	0.73
1:B:217:ARG:HA	2:B:501:C7V:C01	2.19	0.72
1:E:87:PRO:O	3:E:601:HOH:O	2.08	0.71
1:C:51:PRO:O	1:C:53:ASP:N	2.24	0.70
1:F:43:LYS:NZ	3:F:606:HOH:O	2.24	0.70
1:A:51:PRO:O	1:A:53:ASP:N	2.24	0.70
1:B:152:TYR:CE1	1:B:170:PRO:HD3	2.27	0.70
1:F:51:PRO:O	1:F:53:ASP:N	2.25	0.69
1:D:438:ASP:OD2	3:D:601:HOH:O	2.11	0.69
1:A:405:ASP:OD1	3:A:601:HOH:O	2.12	0.68
1:A:157:ALA:C	1:A:158:ARG:O	2.35	0.68
1:B:230:TYR:HD1	1:B:245:ALA:O	1.77	0.68
1:E:51:PRO:O	1:E:53:ASP:N	2.27	0.67
1:D:51:PRO:O	1:D:53:ASP:N	2.27	0.67
1:B:372:ASP:OD1	3:B:601:HOH:O	2.12	0.66
1:E:152:TYR:CE1	1:E:170:PRO:HD3	2.31	0.66
1:E:409:SER:O	3:E:602:HOH:O	2.13	0.65
1:B:245:ALA:O	1:B:246:THR:C	2.40	0.65
1:F:227:GLU:OE1	1:F:229:ARG:NH2	2.31	0.64
1:A:380:LEU:HD12	1:A:423:TYR:CE1	2.32	0.64
1:E:50:GLN:CG	2:E:501:C7V:N4	2.61	0.64
1:E:299:ASP:OD1	1:E:300:ARG:N	2.32	0.63
1:E:53:ASP:OD2	1:E:90:ARG:NH2	2.32	0.63
1:F:246:THR:HG22	1:F:247:LYS:N	2.14	0.62
1:E:397:CYS:N	1:E:412:ASP:OD2	2.32	0.62
1:D:22:LYS:NZ	1:D:38:SER:OG	2.34	0.61
1:D:348:ARG:NH1	1:D:352:GLY:O	2.33	0.61
1:C:53:ASP:OD1	1:C:54:GLU:N	2.36	0.59
1:B:198:HIS:ND1	1:B:209:ALA:HB1	2.16	0.59
1:B:230:TYR:HB2	1:B:245:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:THR:HG22	1:F:247:LYS:H	1.67	0.59
1:E:213:THR:OG1	1:E:224:ARG:HB3	2.02	0.59
1:D:152:TYR:CE1	1:D:170:PRO:HD3	2.37	0.59
1:E:298:ILE:O	1:E:458:TYR:CE1	2.55	0.58
1:F:190:THR:OG1	1:F:192:ASP:OD1	2.21	0.58
1:E:457:ASP:O	1:E:459:ASN:N	2.37	0.58
1:D:344:ARG:NH1	1:D:420:ASP:OD1	2.33	0.57
1:F:50:GLN:HG2	2:F:501:C7V:N4	2.19	0.57
1:C:397:CYS:SG	1:C:443:SER:OG	2.60	0.57
1:A:190:THR:OG1	1:A:192:ASP:OD1	2.20	0.57
1:A:260:CYS:O	1:A:382:ASN:ND2	2.37	0.57
1:D:293:THR:O	3:D:602:HOH:O	2.17	0.57
2:F:501:C7V:O2	2:F:501:C7V:C14	2.53	0.56
1:C:224:ARG:NH1	1:C:230:TYR:OH	2.39	0.56
2:D:501:C7V:O2	2:D:501:C7V:C14	2.53	0.56
2:A:501:C7V:O2	2:A:501:C7V:C14	2.53	0.56
2:B:501:C7V:O2	2:B:501:C7V:C14	2.53	0.56
2:C:501:C7V:O2	2:C:501:C7V:C14	2.54	0.56
1:E:218:SER:H	2:E:501:C7V:C01	2.18	0.56
1:B:403:THR:OG1	1:D:118:ARG:NH1	2.39	0.56
1:E:215:GLU:OE2	1:E:217:ARG:NH2	2.39	0.56
1:B:230:TYR:HB2	1:B:245:ALA:CB	2.35	0.56
1:B:397:CYS:N	1:B:412:ASP:OD2	2.39	0.56
2:E:501:C7V:O2	2:E:501:C7V:C14	2.53	0.56
1:C:90:ARG:NH1	1:C:106:GLU:OE1	2.39	0.55
1:F:152:TYR:CZ	1:F:170:PRO:HD3	2.41	0.55
1:B:234:SER:O	1:B:239:THR:N	2.40	0.55
1:A:246:THR:OG1	1:F:468:ARG:CG	2.53	0.55
1:E:217:ARG:HA	2:E:501:C7V:C01	2.36	0.55
1:E:227:GLU:OE1	1:E:229:ARG:NH2	2.40	0.55
1:A:471:LYS:HD2	1:A:488:ALA:CB	2.37	0.54
1:D:343:ARG:O	1:D:344:ARG:NH1	2.34	0.54
1:E:68:ARG:NH1	1:E:81:GLU:O	2.38	0.54
1:D:415:GLN:OE1	1:D:426:LYS:HE3	2.09	0.53
1:A:343:ARG:NH1	1:A:419:ASN:O	2.41	0.53
1:C:190:THR:OG1	1:C:192:ASP:OD1	2.21	0.53
1:B:167:ARG:NH1	3:B:611:HOH:O	2.41	0.53
1:C:197:ARG:HG2	1:C:199:ASP:OD1	2.08	0.53
1:C:296:LEU:HD21	1:C:455:PHE:CG	2.43	0.53
1:D:100:ARG:N	3:D:605:HOH:O	2.40	0.53
1:C:217:ARG:NH1	3:C:605:HOH:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ARG:HB2	1:D:420:ASP:O	2.08	0.53
1:F:343:ARG:O	1:F:344:ARG:HD3	2.08	0.53
1:A:397:CYS:N	1:A:412:ASP:OD2	2.41	0.52
1:D:149:ARG:O	1:D:151:ARG:HG2	2.09	0.52
1:B:215:GLU:OE2	1:B:217:ARG:NH2	2.42	0.52
1:B:230:TYR:CD1	1:B:245:ALA:O	2.60	0.52
1:F:304:LYS:HD3	1:F:335:TYR:HB3	1.91	0.52
1:E:190:THR:OG1	1:E:192:ASP:OD1	2.23	0.52
1:A:473:ASP:OD2	1:A:479:LYS:NZ	2.36	0.52
1:F:182:GLN:CG	3:F:615:HOH:O	2.58	0.52
1:F:182:GLN:HG2	3:F:615:HOH:O	2.10	0.52
1:B:97:ASP:O	1:B:185:ARG:NH2	2.40	0.52
1:A:229:ARG:HG3	1:A:244:LYS:O	2.10	0.52
1:E:344:ARG:NH2	1:E:420:ASP:OD1	2.37	0.52
1:D:138:MET:HE1	1:D:256:LEU:CB	2.40	0.51
1:A:53:ASP:OD2	1:A:90:ARG:NH1	2.42	0.51
1:E:298:ILE:O	1:E:458:TYR:CD1	2.63	0.51
1:A:68:ARG:NH1	1:A:81:GLU:O	2.39	0.51
1:A:152:TYR:CZ	1:A:170:PRO:HD3	2.45	0.51
1:B:299:ASP:O	1:B:303:LYS:HA	2.10	0.51
1:C:215:GLU:OE2	1:C:217:ARG:NH2	2.44	0.51
1:D:198:HIS:C	1:D:198:HIS:ND1	2.69	0.51
1:E:304:LYS:HG2	1:E:337:ASP:OD1	2.10	0.51
1:F:304:LYS:HB3	1:F:336:PHE:O	2.11	0.51
1:E:341:ARG:O	1:E:342:ASP:C	2.54	0.50
1:F:301:ASP:O	3:F:602:HOH:O	2.20	0.50
1:F:417:GLU:OE2	1:F:426:LYS:NZ	2.43	0.50
1:B:53:ASP:OD2	1:B:90:ARG:NH2	2.44	0.50
1:B:192:ASP:O	1:B:193:HIS:HB2	2.11	0.49
1:D:260:CYS:O	1:D:382:ASN:ND2	2.46	0.49
1:D:341:ARG:O	1:D:342:ASP:C	2.54	0.49
1:F:471:LYS:HG3	1:F:488:ALA:O	2.12	0.49
1:D:68:ARG:NH1	1:D:81:GLU:O	2.46	0.49
1:E:56:GLY:O	3:E:603:HOH:O	2.20	0.49
1:A:50:GLN:NE2	1:A:59:ALA:O	2.38	0.49
1:E:261:ALA:O	1:E:296:LEU:N	2.44	0.49
1:F:260:CYS:O	1:F:382:ASN:ND2	2.46	0.49
1:F:358:LYS:NZ	3:F:609:HOH:O	2.44	0.49
1:D:426:LYS:HB3	1:D:432:TYR:CD1	2.48	0.49
1:F:68:ARG:NH1	1:F:81:GLU:O	2.43	0.49
1:A:341:ARG:O	1:A:342:ASP:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ILE:HG21	1:D:240:LEU:HD23	1.95	0.48
1:D:426:LYS:HB3	1:D:432:TYR:CE1	2.48	0.48
1:F:158:ARG:CB	1:F:159:PRO:CD	2.92	0.48
1:E:152:TYR:CZ	1:E:170:PRO:HD3	2.49	0.47
1:F:230:TYR:CE1	1:F:246:THR:O	2.67	0.47
1:F:354:PHE:N	1:F:367:VAL:O	2.31	0.47
1:E:217:ARG:NH1	1:E:248:VAL:HB	2.30	0.47
1:C:216:PHE:O	2:C:501:C7V:N3	2.48	0.47
1:A:471:LYS:HD2	1:A:488:ALA:HB1	1.96	0.47
1:D:198:HIS:C	1:D:198:HIS:HD1	2.22	0.46
1:D:138:MET:HE3	1:D:142:VAL:HG11	1.97	0.46
1:D:73:ASP:OD1	1:D:75:ASP:N	2.49	0.46
1:A:217:ARG:NH1	1:A:248:VAL:HB	2.30	0.46
1:A:234:SER:O	1:A:239:THR:N	2.49	0.46
1:C:296:LEU:HD21	1:C:455:PHE:CB	2.45	0.46
1:D:459:ASN:O	1:D:492:GLU:HA	2.15	0.46
1:C:117:ASP:OD2	3:C:601:HOH:O	2.20	0.46
1:C:427:ASP:OD2	1:C:443:SER:HB2	2.16	0.45
1:D:148:THR:HG23	1:D:149:ARG:N	2.31	0.45
1:F:405:ASP:OD1	3:F:603:HOH:O	2.21	0.45
1:F:329:SER:OG	3:F:604:HOH:O	2.21	0.45
1:A:29:PHE:N	1:A:29:PHE:CD1	2.84	0.45
1:B:245:ALA:HB1	1:B:252:GLU:HG2	1.99	0.45
1:B:50:GLN:OE1	2:B:501:C7V:N4	2.50	0.45
1:A:230:TYR:HD2	1:A:245:ALA:O	2.00	0.45
1:B:152:TYR:CZ	1:B:170:PRO:HD3	2.52	0.45
1:E:473:ASP:OD2	1:E:479:LYS:NZ	2.42	0.45
1:A:344:ARG:NH2	1:A:420:ASP:OD1	2.45	0.44
1:D:138:MET:HE1	1:D:256:LEU:HB2	1.99	0.44
1:F:230:TYR:CD1	1:F:246:THR:O	2.71	0.44
1:A:321:GLY:O	1:A:365:ALA:N	2.50	0.44
1:B:217:ARG:NH1	1:B:248:VAL:HB	2.33	0.44
1:D:138:MET:HE1	1:D:256:LEU:HB3	2.00	0.44
1:D:137:ALA:O	1:D:389:ARG:NH2	2.44	0.44
1:E:167:ARG:NH2	1:E:290:ASP:OD1	2.46	0.44
1:B:343:ARG:NH1	1:B:419:ASN:O	2.51	0.43
1:E:343:ARG:HB3	1:E:420:ASP:O	2.17	0.43
1:A:471:LYS:HG3	1:A:488:ALA:HB1	1.99	0.43
1:B:401:THR:HG21	1:D:117:ASP:OD2	2.19	0.43
1:A:339:GLU:OE2	1:A:346:THR:OG1	2.28	0.43
1:B:216:PHE:O	2:B:501:C7V:N3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PHE:HB3	1:A:81:GLU:HB3	2.01	0.43
1:C:342:ASP:O	1:C:344:ARG:N	2.52	0.43
1:D:281:LEU:HD21	1:D:325:SER:OG	2.18	0.43
1:F:299:ASP:OD1	1:F:300:ARG:N	2.52	0.43
1:E:13:GLN:O	1:E:136:ILE:HD12	2.18	0.42
1:F:397:CYS:N	1:F:412:ASP:OD2	2.51	0.42
1:B:137:ALA:O	1:B:389:ARG:NH2	2.42	0.42
1:B:486:ASP:N	1:B:489:SER:OG	2.49	0.42
1:F:29:PHE:CD1	1:F:29:PHE:N	2.86	0.42
1:F:158:ARG:HB3	1:F:159:PRO:CD	2.48	0.42
1:A:92:LEU:CD1	1:A:109:ARG:NH1	2.83	0.42
1:C:395:ILE:HA	1:C:405:ASP:O	2.20	0.42
1:E:468:ARG:NH1	1:E:483:GLU:CG	2.83	0.42
1:E:468:ARG:NH1	1:E:483:GLU:HG2	2.35	0.42
1:B:298:ILE:N	1:B:298:ILE:HD12	2.34	0.42
1:C:299:ASP:HB3	1:C:303:LYS:O	2.20	0.42
1:C:296:LEU:CD2	1:C:455:PHE:CG	3.02	0.42
1:A:105:SER:O	1:A:109:ARG:N	2.45	0.42
1:D:158:ARG:N	1:D:159:PRO:CD	2.82	0.42
1:E:471:LYS:HE3	1:E:488:ALA:CB	2.50	0.42
1:D:16:LEU:HD21	2:D:501:C7V:F1	2.10	0.41
1:D:397:CYS:N	1:D:412:ASP:OD2	2.53	0.41
1:D:415:GLN:HB2	1:D:426:LYS:HG3	2.02	0.41
1:D:234:SER:O	1:D:239:THR:N	2.54	0.41
1:F:244:LYS:O	1:F:246:THR:N	2.53	0.41
1:B:13:GLN:O	1:B:136:ILE:HD12	2.21	0.41
1:F:378:MET:HG2	3:F:620:HOH:O	2.20	0.41
1:A:471:LYS:HD2	1:A:488:ALA:HB3	2.02	0.41
1:A:137:ALA:O	1:A:389:ARG:NH2	2.47	0.41
1:B:183:ASP:O	3:B:602:HOH:O	2.21	0.41
1:C:303:LYS:O	1:C:304:LYS:O	2.38	0.41
1:D:149:ARG:O	1:D:150:LYS:C	2.64	0.41
1:D:152:TYR:CZ	1:D:170:PRO:HD3	2.56	0.41
1:E:198:HIS:ND1	1:E:198:HIS:C	2.79	0.41
1:C:50:GLN:NE2	2:C:501:C7V:N4	2.69	0.41
1:B:302:THR:HG22	1:B:304:LYS:HG3	2.02	0.41
1:C:174:ASP:OD1	1:C:174:ASP:N	2.53	0.40
1:D:88:ASP:OD1	1:D:108:HIS:NE2	2.46	0.40
1:F:182:GLN:HG3	3:F:615:HOH:O	2.21	0.40
1:B:230:TYR:H	1:B:245:ALA:HB3	1.86	0.40
1:D:48:LEU:HD21	1:D:93:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	485/487 (100%)	439 (90%)	41 (8%)	5 (1%)	12	38
1	B	485/487 (100%)	443 (91%)	39 (8%)	3 (1%)	21	51
1	C	485/487 (100%)	445 (92%)	38 (8%)	2 (0%)	30	60
1	D	485/487 (100%)	440 (91%)	44 (9%)	1 (0%)	43	72
1	E	485/487 (100%)	447 (92%)	35 (7%)	3 (1%)	21	51
1	F	485/487 (100%)	442 (91%)	40 (8%)	3 (1%)	21	51
All	All	2910/2922 (100%)	2656 (91%)	237 (8%)	17 (1%)	21	51

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	159	PRO
1	A	458	TYR
1	B	304	LYS
1	E	458	TYR
1	F	245	ALA
1	F	158	ARG
1	C	52	PRO
1	C	304	LYS
1	E	304	LYS
1	F	52	PRO
1	A	52	PRO
1	A	245	ALA
1	D	52	PRO
1	E	52	PRO
1	B	399	LYS
1	B	52	PRO

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	400/400 (100%)	392 (98%)	8 (2%)	48	80
1	B	400/400 (100%)	395 (99%)	5 (1%)	61	86
1	C	400/400 (100%)	392 (98%)	8 (2%)	48	80
1	D	400/400 (100%)	391 (98%)	9 (2%)	44	78
1	E	400/400 (100%)	394 (98%)	6 (2%)	57	84
1	F	400/400 (100%)	391 (98%)	9 (2%)	44	78
All	All	2400/2400 (100%)	2355 (98%)	45 (2%)	50	81

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	159	PRO
1	A	193	HIS
1	A	258	GLN
1	A	316	THR
1	A	447	THR
1	A	464	LYS
1	A	489	SER
1	B	11	GLN
1	B	148	THR
1	B	221	VAL
1	B	296	LEU
1	B	358	LYS
1	C	21	ASN
1	C	40	LEU
1	C	66	LEU
1	C	90	ARG
1	C	193	HIS
1	C	213	THR
1	C	275	THR
1	C	459	ASN
1	D	38	SER

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Mol	Chain	Res	Type
1	D	47	THR
1	D	62	LEU
1	D	169	VAL
1	D	198	HIS
1	D	316	THR
1	D	358	LYS
1	D	447	THR
1	D	458	TYR
1	E	40	LEU
1	E	193	HIS
1	E	247	LYS
1	E	325	SER
1	E	358	LYS
1	E	485	VAL
1	F	11	GLN
1	F	40	LEU
1	F	66	LEU
1	F	136	ILE
1	F	148	THR
1	F	316	THR
1	F	339	GLU
1	F	381	ILE
1	F	489	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	182	GLN
1	B	143	ASN
1	B	193	HIS
1	B	291	GLN
1	C	11	GLN
1	C	184	GLN
1	C	193	HIS
1	C	262	GLN
1	D	193	HIS
1	D	459	ASN
1	E	182	GLN
1	E	198	HIS
1	E	277	GLN
1	E	392	HIS

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Mol	Chain	Res	Type
1	F	415	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	C7V	A	501	-	32,32,32	2.23	7 (21%)	39,47,47	3.14	13 (33%)
2	C7V	E	501	-	32,32,32	2.24	7 (21%)	39,47,47	3.16	13 (33%)
2	C7V	D	501	-	32,32,32	2.23	6 (18%)	39,47,47	3.15	13 (33%)
2	C7V	C	501	-	32,32,32	2.25	6 (18%)	39,47,47	3.15	13 (33%)
2	C7V	F	501	-	32,32,32	2.23	7 (21%)	39,47,47	3.13	13 (33%)
2	C7V	B	501	-	32,32,32	2.24	6 (18%)	39,47,47	3.15	13 (33%)

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
2	C7V	A	501	-	-	3/18/18/18	0/4/4/4
2	C7V	E	501	-	-	3/18/18/18	0/4/4/4
2	C7V	D	501	-	-	3/18/18/18	0/4/4/4
2	C7V	C	501	-	-	3/18/18/18	0/4/4/4
2	C7V	F	501	-	-	3/18/18/18	0/4/4/4
2	C7V	B	501	-	-	3/18/18/18	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	C7V	O02-N4	-7.82	1.33	1.42
2	F	501	C7V	O02-N4	-7.82	1.33	1.42
2	E	501	C7V	O02-N4	-7.81	1.33	1.42
2	A	501	C7V	O02-N4	-7.77	1.33	1.42
2	B	501	C7V	O02-N4	-7.76	1.33	1.42
2	D	501	C7V	O02-N4	-7.74	1.33	1.42
2	D	501	C7V	C11-C10	5.21	1.45	1.40
2	C	501	C7V	C11-C10	5.15	1.45	1.40
2	E	501	C7V	C11-C10	5.15	1.45	1.40
2	B	501	C7V	C11-C10	5.14	1.45	1.40
2	A	501	C7V	C11-C10	5.14	1.45	1.40
2	C	501	C7V	C11-N4	5.14	1.35	1.30
2	D	501	C7V	C11-N4	5.10	1.35	1.30
2	F	501	C7V	C11-C10	5.09	1.45	1.40
2	E	501	C7V	C11-N4	5.08	1.35	1.30
2	B	501	C7V	C11-N4	5.08	1.35	1.30
2	F	501	C7V	C11-N4	5.04	1.35	1.30
2	A	501	C7V	C11-N4	5.03	1.35	1.30
2	F	501	C7V	C7-N2	3.80	1.37	1.31
2	A	501	C7V	C7-N2	3.80	1.37	1.31
2	C	501	C7V	C7-N2	3.79	1.37	1.31
2	D	501	C7V	C7-N2	3.79	1.37	1.31
2	B	501	C7V	C7-N2	3.78	1.37	1.31
2	E	501	C7V	C7-N2	3.76	1.37	1.31
2	C	501	C7V	C13-C7	-3.19	1.42	1.47
2	B	501	C7V	C13-C7	-3.18	1.42	1.47
2	A	501	C7V	C13-C7	-3.16	1.42	1.47
2	E	501	C7V	C13-C7	-3.13	1.42	1.47
2	F	501	C7V	C13-C7	-3.13	1.42	1.47
2	D	501	C7V	C13-C7	-3.08	1.43	1.47
2	E	501	C7V	O02-C9	2.09	1.38	1.35
2	B	501	C7V	O02-C9	2.07	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	C7V	O02-C9	2.06	1.38	1.35
2	C	501	C7V	O02-C9	2.05	1.38	1.35
2	A	501	C7V	O02-C9	2.04	1.38	1.35
2	D	501	C7V	O02-C9	2.03	1.38	1.35
2	F	501	C7V	C6-C5	-2.03	1.47	1.51
2	E	501	C7V	C6-C5	-2.02	1.47	1.51
2	A	501	C7V	C6-C5	-2.00	1.47	1.51

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	C7V	O02-N4-C11	10.38	108.93	104.91
2	E	501	C7V	O02-N4-C11	10.38	108.93	104.91
2	A	501	C7V	O02-N4-C11	10.28	108.89	104.91
2	B	501	C7V	O02-N4-C11	10.28	108.89	104.91
2	C	501	C7V	O02-N4-C11	10.23	108.88	104.91
2	F	501	C7V	O02-N4-C11	10.18	108.86	104.91
2	B	501	C7V	C6-N1-N2	7.38	125.70	119.98
2	F	501	C7V	C6-N1-N2	7.38	125.70	119.98
2	E	501	C7V	C6-N1-N2	7.37	125.69	119.98
2	D	501	C7V	C6-N1-N2	7.36	125.68	119.98
2	A	501	C7V	C6-N1-N2	7.34	125.67	119.98
2	C	501	C7V	C6-N1-N2	7.30	125.63	119.98
2	C	501	C7V	C5-C6-N1	-7.18	102.19	112.51
2	E	501	C7V	C5-C6-N1	-7.18	102.20	112.51
2	A	501	C7V	C5-C6-N1	-7.16	102.22	112.51
2	B	501	C7V	C5-C6-N1	-7.16	102.22	112.51
2	F	501	C7V	C5-C6-N1	-7.15	102.24	112.51
2	D	501	C7V	C5-C6-N1	-7.12	102.28	112.51
2	E	501	C7V	C10-C11-N4	-7.03	108.31	113.45
2	D	501	C7V	C10-C11-N4	-7.01	108.33	113.45
2	C	501	C7V	C10-C11-N4	-6.96	108.36	113.45
2	B	501	C7V	C10-C11-N4	-6.95	108.37	113.45
2	A	501	C7V	C10-C11-N4	-6.94	108.38	113.45
2	F	501	C7V	C10-C11-N4	-6.91	108.40	113.45
2	B	501	C7V	C6-N1-C18	-6.32	120.50	128.71
2	F	501	C7V	C6-N1-C18	-6.31	120.50	128.71
2	C	501	C7V	C6-N1-C18	-6.31	120.51	128.71
2	A	501	C7V	C6-N1-C18	-6.28	120.54	128.71
2	E	501	C7V	C6-N1-C18	-6.28	120.55	128.71
2	D	501	C7V	C6-N1-C18	-6.27	120.56	128.71
2	C	501	C7V	C18-N1-N2	4.62	113.83	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	C7V	C18-N1-N2	4.49	113.78	111.71
2	F	501	C7V	C18-N1-N2	4.48	113.77	111.71
2	A	501	C7V	C18-N1-N2	4.46	113.76	111.71
2	E	501	C7V	C18-N1-N2	4.41	113.74	111.71
2	D	501	C7V	C18-N1-N2	4.39	113.73	111.71
2	D	501	C7V	C01-C10-C11	-2.78	122.40	127.88
2	E	501	C7V	C01-C10-C11	-2.78	122.41	127.88
2	C	501	C7V	C01-C10-C11	-2.76	122.43	127.88
2	A	501	C7V	C01-C10-C11	-2.76	122.44	127.88
2	F	501	C7V	C01-C10-C11	-2.76	122.44	127.88
2	B	501	C7V	C01-C10-C11	-2.76	122.45	127.88
2	C	501	C7V	C13-C18-N1	-2.56	105.59	106.76
2	C	501	C7V	C17-C18-C13	2.49	124.73	121.95
2	E	501	C7V	C17-C18-C13	2.47	124.71	121.95
2	B	501	C7V	C13-C18-N1	-2.46	105.63	106.76
2	A	501	C7V	C17-C18-C13	2.46	124.69	121.95
2	D	501	C7V	C17-C18-C13	2.45	124.68	121.95
2	B	501	C7V	C17-C18-C13	2.43	124.66	121.95
2	F	501	C7V	C17-C18-C13	2.43	124.66	121.95
2	A	501	C7V	C13-C18-N1	-2.42	105.65	106.76
2	F	501	C7V	C13-C18-N1	-2.41	105.66	106.76
2	E	501	C7V	C13-C18-N1	-2.40	105.66	106.76
2	D	501	C7V	C16-C15-C14	2.36	123.15	120.24
2	C	501	C7V	C16-C15-C14	2.36	123.15	120.24
2	E	501	C7V	C16-C15-C14	2.35	123.14	120.24
2	A	501	C7V	C16-C15-C14	2.35	123.13	120.24
2	C	501	C7V	C14-C13-C7	2.34	135.50	131.38
2	B	501	C7V	C16-C15-C14	2.34	123.12	120.24
2	F	501	C7V	C16-C15-C14	2.33	123.12	120.24
2	E	501	C7V	C14-C13-C7	2.33	135.48	131.38
2	A	501	C7V	C14-C13-C7	2.32	135.46	131.38
2	B	501	C7V	C14-C13-C7	2.31	135.45	131.38
2	F	501	C7V	C14-C13-C7	2.30	135.43	131.38
2	D	501	C7V	C14-C13-C7	2.28	135.40	131.38
2	D	501	C7V	C13-C18-N1	-2.28	105.72	106.76
2	D	501	C7V	C17-C18-N1	-2.16	129.60	132.88
2	E	501	C7V	C17-C18-N1	-2.14	129.63	132.88
2	A	501	C7V	C17-C18-N1	-2.12	129.66	132.88
2	F	501	C7V	C17-C18-N1	-2.11	129.68	132.88
2	C	501	C7V	C17-C18-N1	-2.11	129.69	132.88
2	C	501	C7V	C20-C2-C3	2.10	121.17	118.03
2	B	501	C7V	C17-C18-N1	-2.09	129.70	132.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	C7V	C20-C2-C3	2.09	121.15	118.03
2	B	501	C7V	C20-C2-C3	2.09	121.14	118.03
2	A	501	C7V	C20-C2-C3	2.08	121.13	118.03
2	E	501	C7V	C20-C2-C3	2.07	121.12	118.03
2	F	501	C7V	C20-C2-C3	2.07	121.11	118.03

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	C7V	O2-C8-C9-O02
2	B	501	C7V	O2-C8-C9-O02
2	C	501	C7V	O2-C8-C9-O02
2	D	501	C7V	O2-C8-C9-O02
2	E	501	C7V	O2-C8-C9-O02
2	F	501	C7V	O2-C8-C9-O02
2	A	501	C7V	N2-C7-N3-C8
2	B	501	C7V	N2-C7-N3-C8
2	C	501	C7V	N2-C7-N3-C8
2	D	501	C7V	N2-C7-N3-C8
2	E	501	C7V	N2-C7-N3-C8
2	F	501	C7V	N2-C7-N3-C8
2	A	501	C7V	C13-C7-N3-C8
2	B	501	C7V	C13-C7-N3-C8
2	C	501	C7V	C13-C7-N3-C8
2	D	501	C7V	C13-C7-N3-C8
2	E	501	C7V	C13-C7-N3-C8
2	F	501	C7V	C13-C7-N3-C8

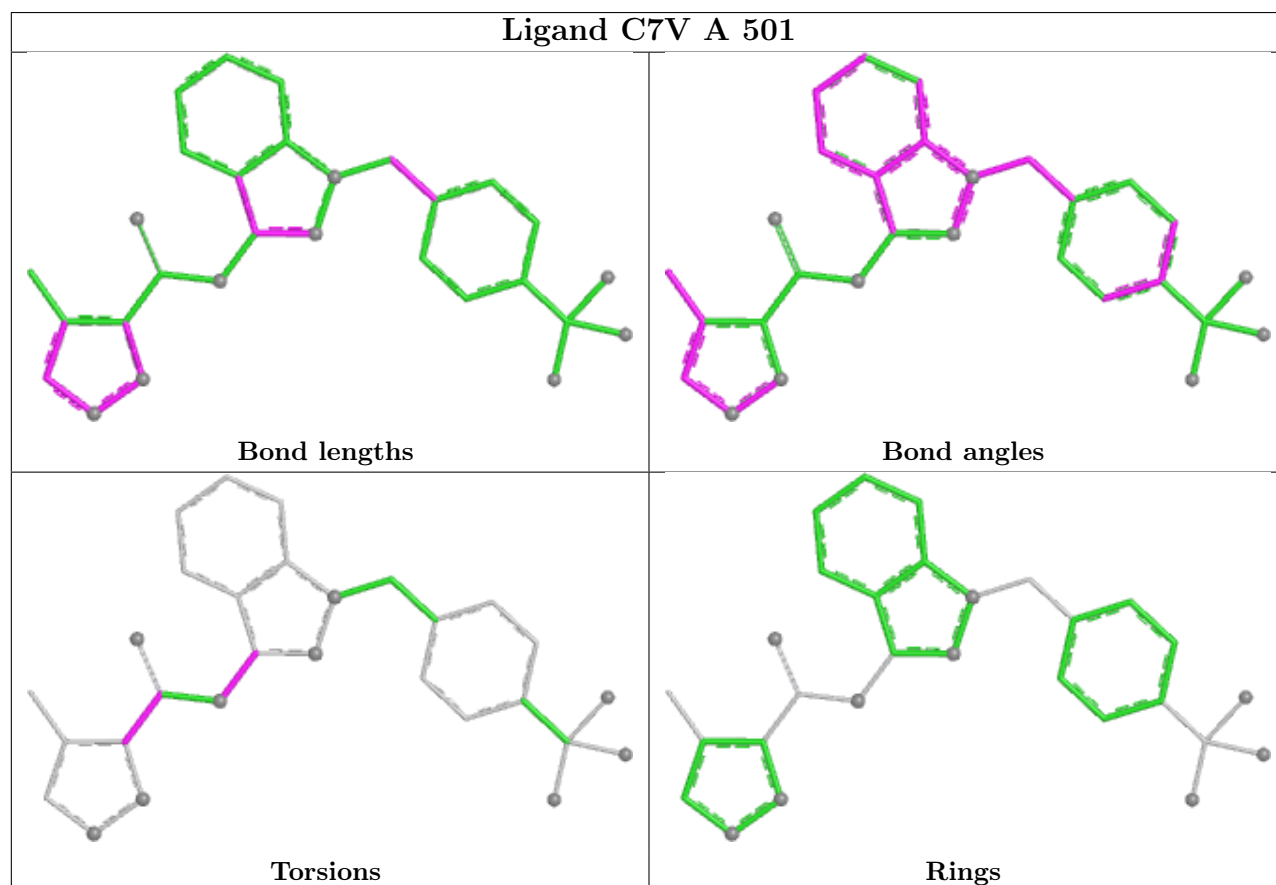
There are no ring outliers.

6 monomers are involved in 19 short contacts:

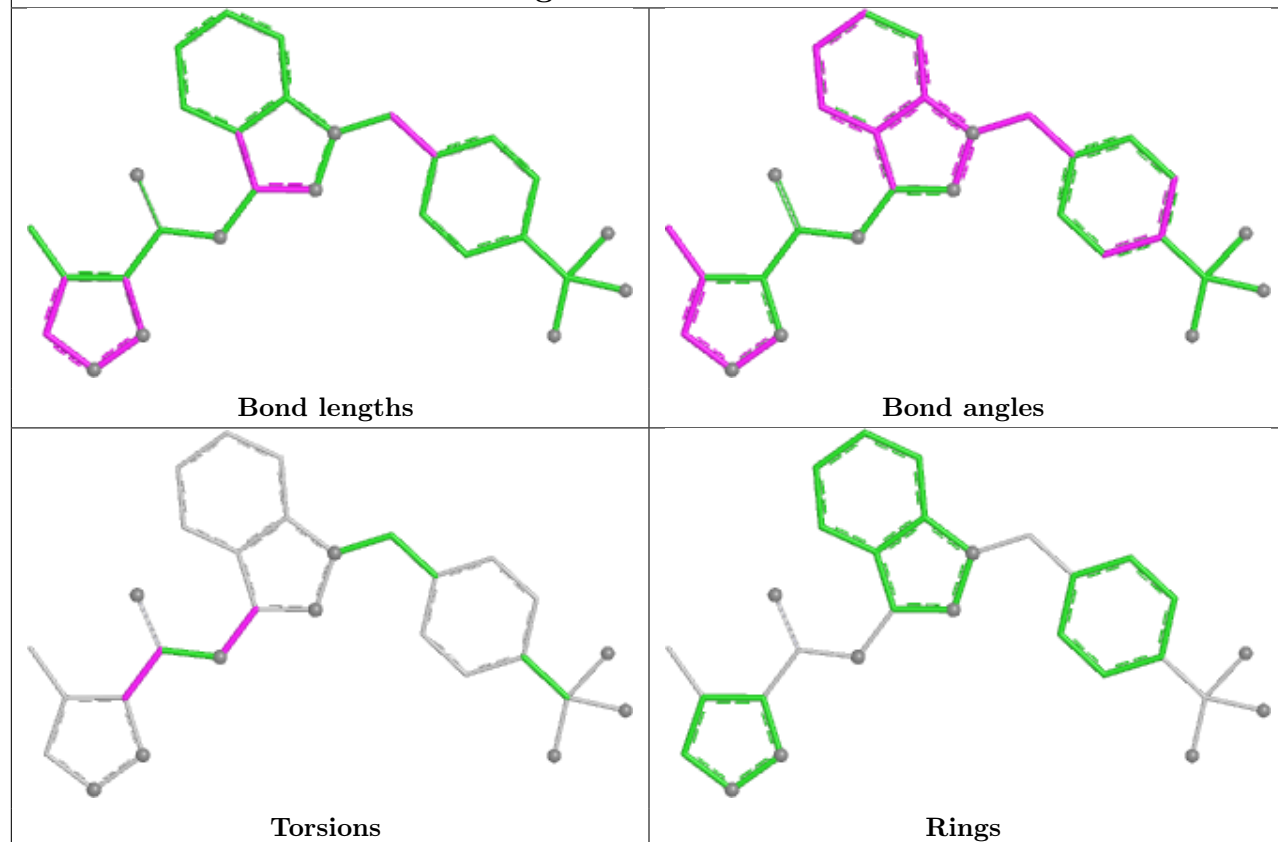
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	C7V	3	0
2	E	501	C7V	5	0
2	D	501	C7V	2	0
2	C	501	C7V	3	0
2	F	501	C7V	2	0
2	B	501	C7V	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

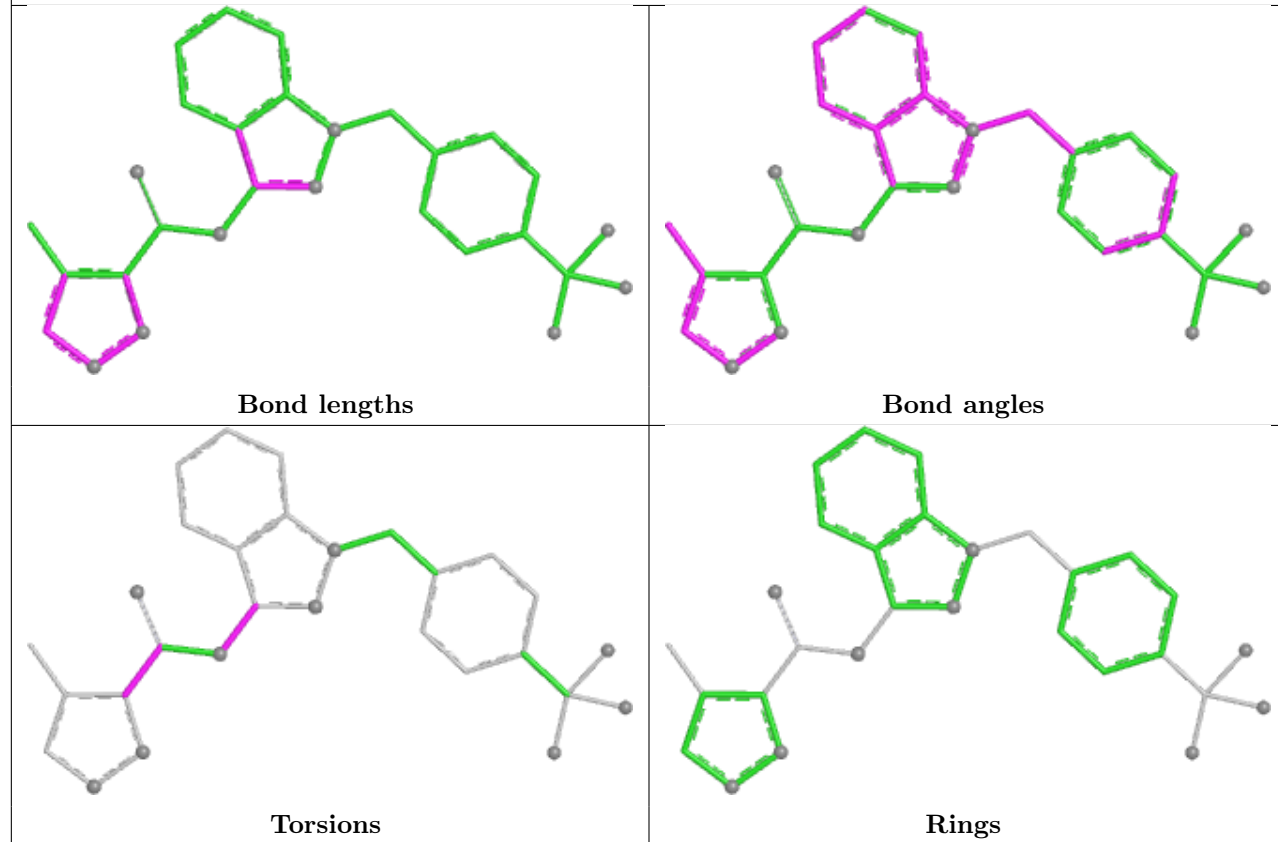
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



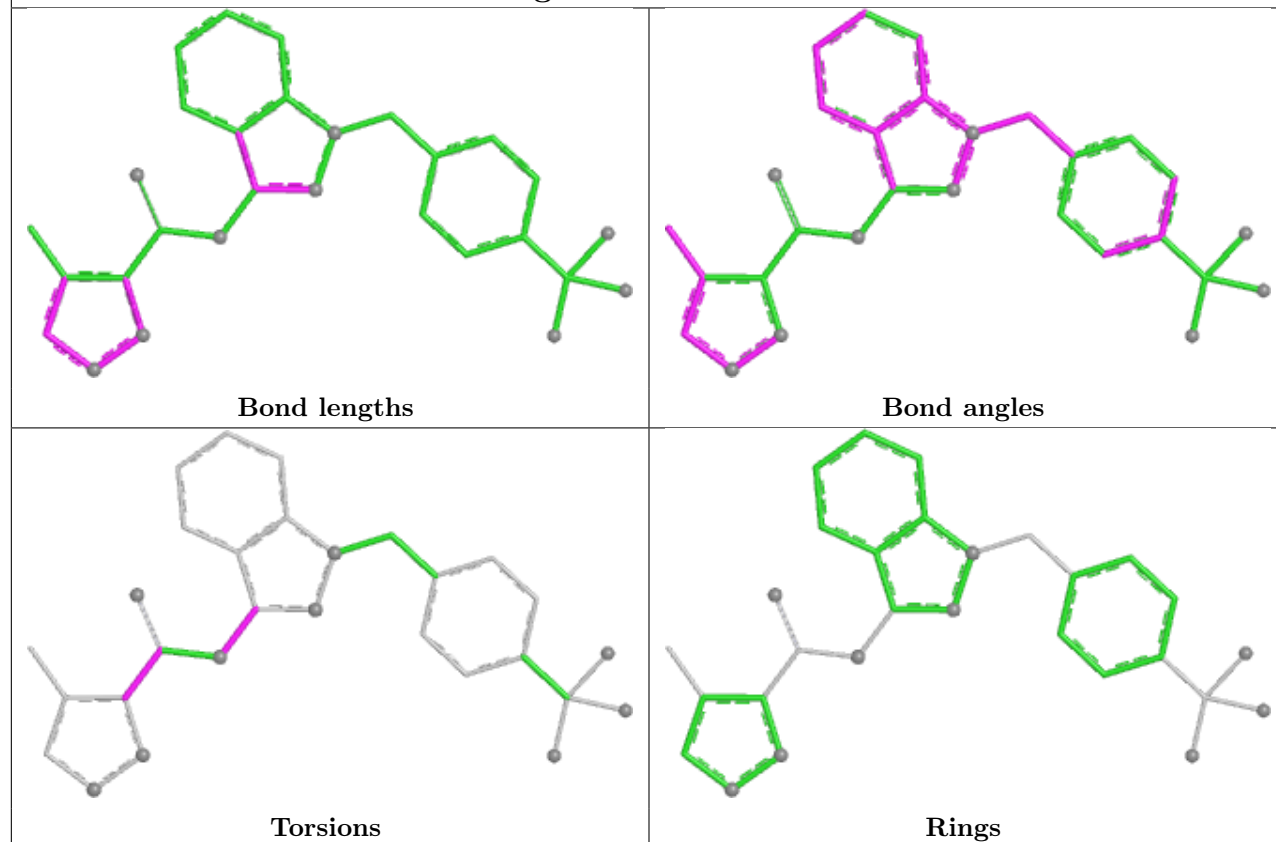
Ligand C7V E 501



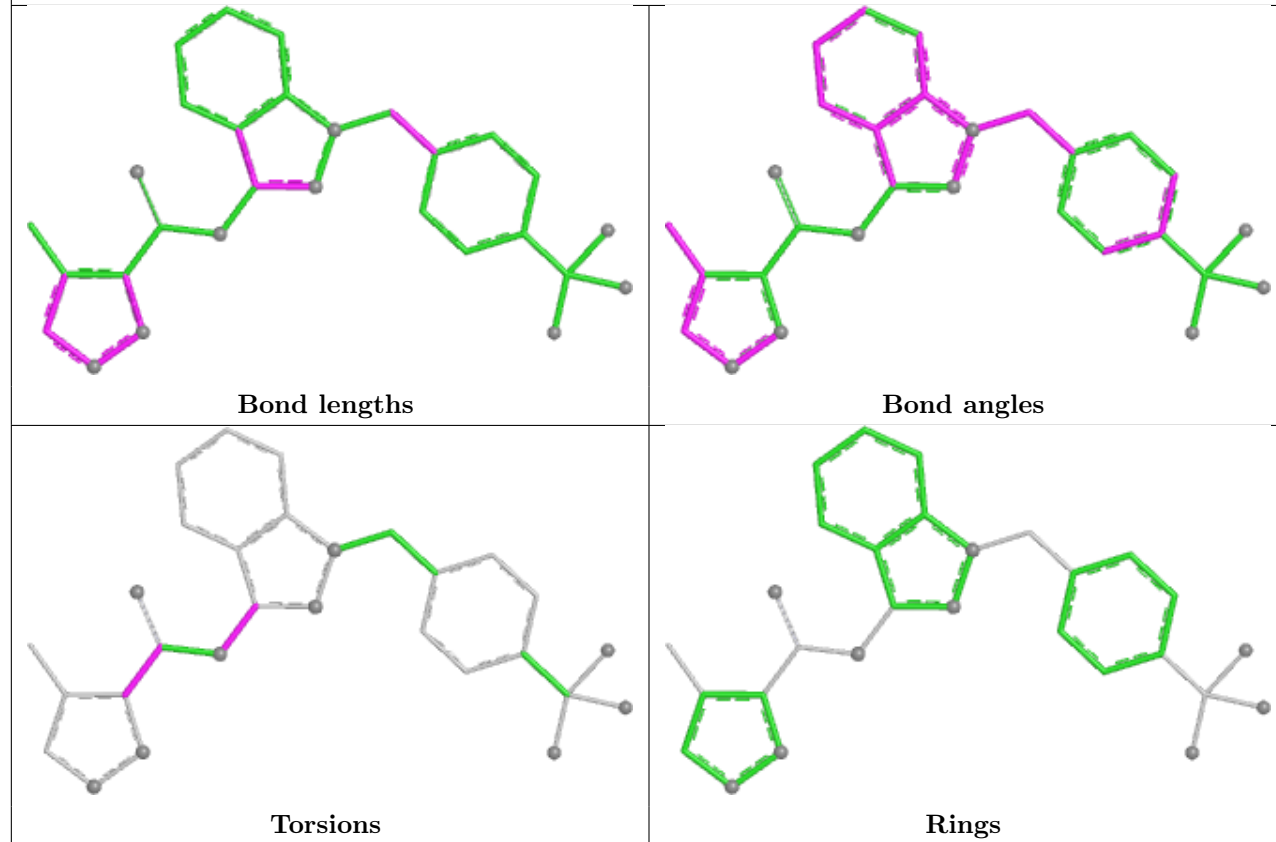
Ligand C7V D 501

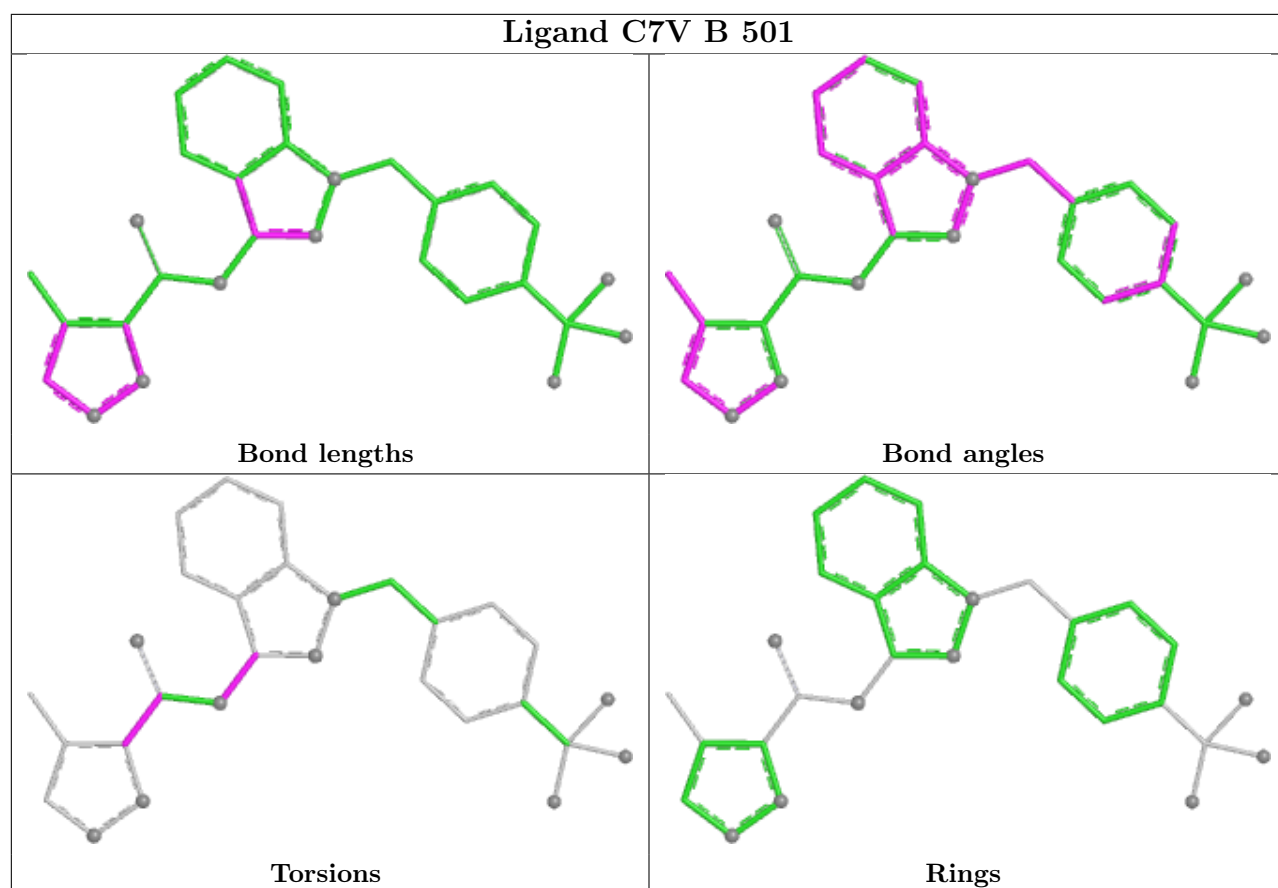


Ligand C7V C 501



Ligand C7V F 501





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	487/487 (100%)	2.08	214 (43%)	0 0	22, 64, 105, 143	2 (0%)
1	B	487/487 (100%)	0.97	68 (13%)	6 5	20, 43, 74, 132	2 (0%)
1	C	487/487 (100%)	1.02	83 (17%)	4 3	19, 44, 75, 162	2 (0%)
1	D	487/487 (100%)	2.04	218 (44%)	0 0	24, 64, 109, 154	2 (0%)
1	E	487/487 (100%)	1.98	207 (42%)	0 0	21, 63, 108, 162	2 (0%)
1	F	487/487 (100%)	1.86	192 (39%)	1 0	23, 62, 105, 138	2 (0%)
All	All	2922/2922 (100%)	1.66	982 (33%)	1 1	19, 56, 103, 162	12 (0%)

All (982) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	LYS	8.7
1	E	350	SER	8.7
1	D	350	SER	8.3
1	E	347	LEU	7.9
1	A	347	LEU	7.6
1	E	349	ALA	7.5
1	E	362	GLN	7.5
1	D	302	THR	7.3
1	D	362	GLN	7.2
1	E	458	TYR	7.1
1	F	347	LEU	7.0
1	A	350	SER	6.9
1	A	66	LEU	6.9
1	A	458	TYR	6.8
1	D	338	ILE	6.7
1	A	246	THR	6.7
1	D	349	ALA	6.6
1	E	335	TYR	6.6
1	A	355	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	347	LEU	6.6
1	A	335	TYR	6.5
1	F	355	VAL	6.4
1	D	458	TYR	6.4
1	A	349	ALA	6.4
1	E	338	ILE	6.3
1	A	333	SER	6.3
1	E	302	THR	6.3
1	D	315	TRP	6.3
1	A	337	ASP	6.2
1	A	363	LEU	6.2
1	A	264	VAL	6.2
1	D	99	GLY	6.2
1	E	305	CYS	6.2
1	A	263	VAL	6.0
1	D	337	ASP	6.0
1	A	456	CYS	6.0
1	B	245	ALA	6.0
1	F	349	ALA	6.0
1	E	263	VAL	6.0
1	B	458	TYR	5.9
1	D	335	TYR	5.9
1	D	209	ALA	5.9
1	E	355	VAL	5.8
1	D	55	ALA	5.8
1	F	236	PRO	5.8
1	E	246	THR	5.8
1	F	317	LEU	5.8
1	F	333	SER	5.8
1	D	305	CYS	5.7
1	A	273	VAL	5.7
1	E	9	ALA	5.7
1	F	371	GLY	5.7
1	B	278	GLY	5.7
1	B	9	ALA	5.7
1	A	380	LEU	5.6
1	E	456	CYS	5.6
1	D	263	VAL	5.6
1	A	336	PHE	5.6
1	F	352	GLY	5.5
1	A	275	THR	5.5
1	F	370	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	244	LYS	5.5
1	E	293	THR	5.5
1	C	54	GLU	5.4
1	B	243	GLY	5.4
1	D	355	VAL	5.4
1	D	365	ALA	5.4
1	C	53	ASP	5.4
1	F	366	SER	5.4
1	D	273	VAL	5.4
1	D	352	GLY	5.4
1	F	275	THR	5.4
1	E	306	ALA	5.4
1	D	314	TYR	5.4
1	C	244	LYS	5.4
1	F	273	VAL	5.3
1	A	305	CYS	5.3
1	F	305	CYS	5.3
1	F	362	GLN	5.3
1	C	9	ALA	5.3
1	A	317	LEU	5.3
1	E	337	ASP	5.3
1	F	350	SER	5.3
1	C	7	ALA	5.2
1	B	246	THR	5.2
1	E	315	TRP	5.2
1	A	366	SER	5.2
1	F	336	PHE	5.2
1	F	335	TYR	5.2
1	A	202	LEU	5.2
1	A	245	ALA	5.2
1	A	293	THR	5.1
1	D	343	ARG	5.1
1	E	160	ALA	5.1
1	D	318	THR	5.1
1	F	246	THR	5.1
1	A	124	GLN	5.1
1	F	245	ALA	5.0
1	F	471	LYS	5.0
1	D	245	ALA	5.0
1	F	337	ASP	5.0
1	F	293	THR	5.0
1	A	448	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	52	PRO	5.0
1	E	360	ASN	5.0
1	E	459	ASN	5.0
1	D	199	ASP	5.0
1	D	341	ARG	4.9
1	E	267	ALA	4.9
1	A	199	ASP	4.9
1	B	159	PRO	4.9
1	B	157	ALA	4.9
1	F	263	VAL	4.9
1	E	32	LYS	4.9
1	E	159	PRO	4.9
1	E	314	TYR	4.9
1	F	299	ASP	4.9
1	F	365	ALA	4.8
1	C	99	GLY	4.8
1	D	159	PRO	4.8
1	E	264	VAL	4.8
1	A	338	ILE	4.8
1	A	301	ASP	4.7
1	F	199	ASP	4.7
1	D	366	SER	4.7
1	F	237	SER	4.7
1	A	371	GLY	4.7
1	D	246	THR	4.7
1	F	264	VAL	4.7
1	F	367	VAL	4.7
1	A	354	PHE	4.7
1	A	370	ALA	4.7
1	E	7	ALA	4.7
1	A	471	LYS	4.7
1	E	275	THR	4.6
1	A	307	PHE	4.6
1	E	199	ASP	4.6
1	F	307	PHE	4.6
1	A	159	PRO	4.6
1	D	264	VAL	4.6
1	B	29	PHE	4.6
1	D	336	PHE	4.6
1	A	445	GLY	4.6
1	E	348	ARG	4.6
1	F	448	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	382	ASN	4.6
1	E	53	ASP	4.6
1	E	56	GLY	4.6
1	F	159	PRO	4.6
1	F	124	GLN	4.6
1	A	340	TRP	4.6
1	E	54	GLU	4.6
1	A	314	TYR	4.5
1	A	346	THR	4.5
1	F	136	ILE	4.5
1	D	330	LYS	4.5
1	D	333	SER	4.5
1	D	275	THR	4.5
1	A	300	ARG	4.5
1	A	367	VAL	4.5
1	F	291	GLN	4.5
1	D	348	ARG	4.5
1	F	315	TRP	4.5
1	D	293	THR	4.5
1	F	338	ILE	4.5
1	F	304	LYS	4.5
1	D	7	ALA	4.5
1	E	55	ALA	4.5
1	E	365	ALA	4.5
1	C	243	GLY	4.5
1	F	301	ASP	4.5
1	E	452	PHE	4.5
1	E	336	PHE	4.4
1	F	314	TYR	4.4
1	A	183	ASP	4.4
1	A	218	SER	4.4
1	A	318	THR	4.4
1	A	319	ALA	4.4
1	A	432	TYR	4.4
1	E	339	GLU	4.4
1	A	168	ASP	4.4
1	A	278	GLY	4.4
1	E	421	GLY	4.4
1	E	66	LEU	4.4
1	A	32	LYS	4.4
1	A	87	PRO	4.4
1	D	157	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	273	VAL	4.3
1	D	340	TRP	4.3
1	D	303	LYS	4.3
1	E	471	LYS	4.3
1	F	303	LYS	4.3
1	D	310	HIS	4.3
1	D	306	ALA	4.3
1	A	158	ARG	4.3
1	C	278	GLY	4.3
1	A	244	LYS	4.3
1	A	296	LEU	4.3
1	A	316	THR	4.3
1	E	358	LYS	4.3
1	F	458	TYR	4.3
1	E	136	ILE	4.3
1	A	299	ASP	4.3
1	A	348	ARG	4.3
1	E	429	THR	4.2
1	D	53	ASP	4.2
1	E	297	GLU	4.2
1	D	359	LYS	4.2
1	F	302	THR	4.2
1	D	307	PHE	4.2
1	E	164	ALA	4.2
1	B	56	GLY	4.2
1	E	328	SER	4.2
1	A	421	GLY	4.2
1	A	430	GLY	4.2
1	E	368	GLU	4.2
1	F	183	ASP	4.2
1	D	354	PHE	4.2
1	E	330	LYS	4.1
1	E	367	VAL	4.1
1	F	354	PHE	4.1
1	D	274	SER	4.1
1	E	303	LYS	4.1
1	D	342	ASP	4.1
1	E	318	THR	4.1
1	F	363	LEU	4.1
1	C	159	PRO	4.1
1	A	342	ASP	4.0
1	E	301	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	296	LEU	4.0
1	F	372	ASP	4.0
1	A	323	VAL	4.0
1	A	268	ALA	4.0
1	D	422	ALA	4.0
1	A	57	SER	4.0
1	B	350	SER	4.0
1	E	310	HIS	4.0
1	D	426	LYS	4.0
1	E	304	LYS	4.0
1	C	466	GLY	4.0
1	A	195	PHE	4.0
1	A	281	LEU	4.0
1	A	362	GLN	4.0
1	F	346	THR	4.0
1	D	304	LYS	4.0
1	D	353	LYS	4.0
1	A	315	TRP	4.0
1	E	158	ARG	4.0
1	D	57	SER	4.0
1	E	282	SER	4.0
1	C	277	GLN	4.0
1	F	157	ALA	4.0
1	E	352	GLY	4.0
1	F	281	LEU	4.0
1	D	358	LYS	4.0
1	E	428	SER	4.0
1	A	365	ALA	3.9
1	A	161	ASP	3.9
1	B	54	GLU	3.9
1	D	297	GLU	3.9
1	E	340	TRP	3.9
1	A	291	GLN	3.9
1	C	305	CYS	3.9
1	D	268	ALA	3.9
1	F	348	ARG	3.9
1	E	307	PHE	3.9
1	D	320	THR	3.9
1	E	361	GLY	3.9
1	E	354	PHE	3.9
1	C	124	GLN	3.9
1	D	456	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	301	ASP	3.9
1	C	339	GLU	3.9
1	D	29	PHE	3.9
1	F	359	LYS	3.9
1	B	158	ARG	3.9
1	E	300	ARG	3.9
1	D	9	ALA	3.9
1	D	125	THR	3.9
1	A	321	GLY	3.8
1	E	342	ASP	3.8
1	F	319	ALA	3.8
1	F	218	SER	3.8
1	D	368	GLU	3.8
1	F	292	GLU	3.8
1	F	161	ASP	3.8
1	E	52	PRO	3.8
1	A	7	ALA	3.8
1	C	160	ALA	3.8
1	F	278	GLY	3.8
1	E	57	SER	3.8
1	E	274	SER	3.8
1	D	334	CYS	3.8
1	B	468	ARG	3.8
1	F	341	ARG	3.8
1	E	244	LYS	3.8
1	A	352	GLY	3.8
1	E	346	THR	3.8
1	A	452	PHE	3.8
1	F	156	SER	3.8
1	D	192	ASP	3.8
1	E	245	ALA	3.8
1	A	265	LEU	3.8
1	E	309	THR	3.8
1	F	294	PHE	3.8
1	A	292	GLU	3.7
1	D	227	GLU	3.7
1	D	471	LYS	3.7
1	D	87	PRO	3.7
1	A	422	ALA	3.7
1	B	7	ALA	3.7
1	A	294	PHE	3.7
1	A	356	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	201	ARG	3.7
1	D	298	ILE	3.7
1	C	29	PHE	3.7
1	D	244	LYS	3.7
1	D	367	VAL	3.7
1	E	448	PRO	3.7
1	A	310	HIS	3.7
1	F	9	ALA	3.7
1	F	340	TRP	3.7
1	D	421	GLY	3.7
1	F	297	GLU	3.7
1	E	323	VAL	3.7
1	A	306	ALA	3.7
1	A	345	ILE	3.7
1	A	236	PRO	3.6
1	A	375	LEU	3.6
1	E	192	ASP	3.6
1	A	358	LYS	3.6
1	B	304	LYS	3.6
1	D	351	ASN	3.6
1	E	363	LEU	3.6
1	F	377	LEU	3.6
1	A	328	SER	3.6
1	E	209	ALA	3.6
1	C	56	GLY	3.6
1	E	227	GLU	3.6
1	D	10	VAL	3.6
1	F	160	ALA	3.6
1	C	105	SER	3.6
1	D	357	SER	3.6
1	F	342	ASP	3.6
1	A	169	VAL	3.6
1	F	202	LEU	3.6
1	F	380	LEU	3.6
1	A	303	LYS	3.6
1	D	328	SER	3.6
1	D	452	PHE	3.6
1	E	333	SER	3.6
1	F	325	SER	3.6
1	E	278	GLY	3.6
1	F	56	GLY	3.6
1	D	202	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	429	THR	3.6
1	F	265	LEU	3.6
1	D	32	LYS	3.5
1	F	300	ARG	3.5
1	A	243	GLY	3.5
1	E	372	ASP	3.5
1	C	458	TYR	3.5
1	F	334	CYS	3.5
1	D	277	GLN	3.5
1	D	200	GLY	3.5
1	D	278	GLY	3.5
1	F	323	VAL	3.5
1	E	97	ASP	3.5
1	D	459	ASN	3.5
1	E	280	ASP	3.5
1	A	341	ARG	3.5
1	D	309	THR	3.5
1	E	296	LEU	3.5
1	B	342	ASP	3.5
1	F	280	ASP	3.5
1	A	326	THR	3.5
1	E	316	THR	3.5
1	A	334	CYS	3.4
1	A	378	MET	3.4
1	D	321	GLY	3.4
1	D	103	LEU	3.4
1	E	359	LYS	3.4
1	F	358	LYS	3.4
1	A	237	SER	3.4
1	A	280	ASP	3.4
1	D	232	ALA	3.4
1	F	7	ALA	3.4
1	D	285	GLN	3.4
1	D	363	LEU	3.4
1	F	339	GLU	3.4
1	F	271	ARG	3.4
1	A	157	ALA	3.4
1	D	299	ASP	3.4
1	C	459	ASN	3.4
1	D	317	LEU	3.4
1	D	361	GLY	3.4
1	C	51	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	85	PRO	3.4
1	A	325	SER	3.4
1	D	267	ALA	3.4
1	D	301	ASP	3.4
1	E	8	GLU	3.4
1	A	373	SER	3.4
1	E	366	SER	3.4
1	F	201	ARG	3.3
1	F	343	ARG	3.3
1	F	456	CYS	3.3
1	F	318	THR	3.3
1	F	357	SER	3.3
1	C	111	TYR	3.3
1	D	420	ASP	3.3
1	C	300	ARG	3.3
1	F	421	GLY	3.3
1	A	9	ALA	3.3
1	D	296	LEU	3.3
1	D	173	VAL	3.3
1	F	158	ARG	3.3
1	F	205	ARG	3.3
1	E	200	GLY	3.3
1	E	351	ASN	3.3
1	F	55	ALA	3.3
1	A	377	LEU	3.3
1	D	281	LEU	3.3
1	E	447	THR	3.3
1	D	282	SER	3.3
1	E	325	SER	3.3
1	A	247	LYS	3.3
1	D	52	PRO	3.3
1	D	204	ALA	3.3
1	D	66	LEU	3.3
1	D	265	LEU	3.3
1	D	158	ARG	3.3
1	C	60	VAL	3.3
1	F	138	MET	3.2
1	D	327	ALA	3.2
1	A	376	PHE	3.2
1	A	10	VAL	3.2
1	D	323	VAL	3.2
1	C	8	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	57	SER	3.2
1	D	377	LEU	3.2
1	F	327	ALA	3.2
1	E	294	PHE	3.2
1	C	10	VAL	3.2
1	A	302	THR	3.2
1	A	309	THR	3.2
1	B	466	GLY	3.2
1	E	236	PRO	3.2
1	E	357	SER	3.2
1	B	53	ASP	3.2
1	E	299	ASP	3.2
1	A	459	ASN	3.2
1	D	331	ASN	3.2
1	D	300	ARG	3.2
1	E	332	ALA	3.2
1	E	343	ARG	3.2
1	F	399	LYS	3.2
1	F	309	THR	3.2
1	B	457	ASP	3.2
1	C	183	ASP	3.2
1	D	229	ARG	3.2
1	D	247	LYS	3.2
1	E	173	VAL	3.2
1	E	277	GLN	3.2
1	A	297	GLU	3.2
1	B	136	ILE	3.2
1	D	271	ARG	3.1
1	F	328	SER	3.1
1	D	332	ALA	3.1
1	E	279	MET	3.1
1	F	326	THR	3.1
1	D	345	ILE	3.1
1	C	101	TRP	3.1
1	C	158	ARG	3.1
1	E	265	LEU	3.1
1	E	317	LEU	3.1
1	A	55	ALA	3.1
1	A	359	LYS	3.1
1	F	310	HIS	3.1
1	F	313	LYS	3.1
1	F	168	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	29	PHE	3.1
1	F	351	ASN	3.1
1	A	200	GLY	3.1
1	F	238	GLY	3.1
1	A	381	ILE	3.1
1	D	8	GLU	3.1
1	D	448	PRO	3.1
1	E	320	THR	3.1
1	A	176	LEU	3.1
1	A	343	ARG	3.1
1	F	373	SER	3.1
1	F	382	ASN	3.1
1	C	362	GLN	3.1
1	E	11	GLN	3.1
1	E	235	GLY	3.1
1	B	339	GLU	3.1
1	D	54	GLU	3.1
1	A	447	THR	3.1
1	E	377	LEU	3.1
1	F	66	LEU	3.1
1	E	422	ALA	3.1
1	A	357	SER	3.1
1	D	279	MET	3.1
1	A	201	ARG	3.1
1	D	110	ARG	3.1
1	C	52	PRO	3.1
1	E	48	LEU	3.1
1	A	267	ALA	3.0
1	B	107	ALA	3.0
1	D	160	ALA	3.0
1	D	164	ALA	3.0
1	A	173	VAL	3.0
1	D	138	MET	3.0
1	E	371	GLY	3.0
1	E	82	ARG	3.0
1	E	229	ARG	3.0
1	C	128	PRO	3.0
1	D	292	GLU	3.0
1	D	326	THR	3.0
1	C	55	ALA	3.0
1	F	268	ALA	3.0
1	A	418	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	195	PHE	3.0
1	F	195	PHE	3.0
1	C	57	SER	3.0
1	A	285	GLN	3.0
1	D	371	GLY	3.0
1	A	313	LYS	3.0
1	D	401	THR	3.0
1	C	245	ALA	3.0
1	D	58	ALA	3.0
1	A	151	ARG	3.0
1	E	460	LYS	3.0
1	A	272	ASN	3.0
1	A	329	SER	3.0
1	B	258	GLN	3.0
1	D	124	GLN	3.0
1	C	95	ALA	3.0
1	D	107	ALA	3.0
1	F	10	VAL	3.0
1	D	266	GLN	3.0
1	E	419	ASN	3.0
1	E	292	GLU	3.0
1	F	209	ALA	3.0
1	A	304	LYS	2.9
1	C	201	ARG	2.9
1	C	296	LEU	2.9
1	D	432	TYR	2.9
1	B	448	PRO	2.9
1	F	368	GLU	2.9
1	A	203	VAL	2.9
1	E	154	HIS	2.9
1	C	247	LYS	2.9
1	B	362	GLN	2.9
1	D	360	ASN	2.9
1	D	372	ASP	2.9
1	F	420	ASP	2.9
1	C	107	ALA	2.9
1	D	283	ALA	2.9
1	F	306	ALA	2.9
1	E	341	ARG	2.9
1	F	375	LEU	2.9
1	D	235	GLY	2.9
1	A	351	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	373	SER	2.9
1	D	84	VAL	2.9
1	E	188	VAL	2.9
1	F	267	ALA	2.9
1	F	345	ILE	2.9
1	A	30	GLY	2.9
1	E	432	TYR	2.9
1	A	339	GLU	2.9
1	A	330	LYS	2.9
1	D	77	ASN	2.9
1	B	55	ALA	2.9
1	E	213	THR	2.9
1	F	316	THR	2.9
1	D	466	GLY	2.8
1	A	138	MET	2.8
1	B	279	MET	2.8
1	E	101	TRP	2.8
1	A	327	ALA	2.8
1	C	229	ARG	2.8
1	F	452	PHE	2.8
1	C	342	ASP	2.8
1	C	125	THR	2.8
1	D	311	THR	2.8
1	A	50	GLN	2.8
1	F	50	GLN	2.8
1	E	122	PHE	2.8
1	B	299	ASP	2.8
1	E	196	LEU	2.8
1	E	457	ASP	2.8
1	E	247	LYS	2.8
1	A	164	ALA	2.8
1	A	332	ALA	2.8
1	C	58	ALA	2.8
1	F	282	SER	2.8
1	A	56	GLY	2.8
1	A	52	PRO	2.8
1	B	300	ARG	2.8
1	D	94	VAL	2.8
1	D	203	VAL	2.8
1	D	198	HIS	2.8
1	B	459	ASN	2.8
1	F	321	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	368	GLU	2.7
1	D	83	GLU	2.7
1	F	344	ARG	2.7
1	F	164	ALA	2.7
1	D	419	ASN	2.7
1	D	183	ASP	2.7
1	A	282	SER	2.7
1	D	325	SER	2.7
1	A	262	GLN	2.7
1	C	103	LEU	2.7
1	F	462	ALA	2.7
1	C	136	ILE	2.7
1	F	330	LYS	2.7
1	A	320	THR	2.7
1	B	183	ASP	2.7
1	B	337	ASP	2.7
1	E	290	ASP	2.7
1	F	52	PRO	2.7
1	F	277	GLN	2.7
1	C	227	GLU	2.7
1	B	370	ALA	2.7
1	A	399	LYS	2.7
1	D	469	TYR	2.7
1	E	378	MET	2.7
1	A	424	ASN	2.7
1	A	110	ARG	2.7
1	A	148	THR	2.7
1	B	302	THR	2.7
1	C	246	THR	2.7
1	D	21	ASN	2.7
1	E	201	ARG	2.7
1	A	420	ASP	2.7
1	A	439	SER	2.7
1	C	49	GLU	2.7
1	C	156	SER	2.7
1	E	266	GLN	2.7
1	D	188	VAL	2.7
1	F	391	GLU	2.7
1	E	28	ALA	2.7
1	E	298	ILE	2.7
1	A	353	LYS	2.7
1	A	19	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	397	CYS	2.7
1	C	401	THR	2.7
1	E	326	THR	2.7
1	F	356	THR	2.7
1	D	161	ASP	2.7
1	B	131	LYS	2.6
1	A	111	TYR	2.6
1	A	344	ARG	2.6
1	B	197	ARG	2.6
1	C	82	ARG	2.6
1	D	56	GLY	2.6
1	D	322	GLY	2.6
1	B	277	GLN	2.6
1	D	168	ASP	2.6
1	E	10	VAL	2.6
1	E	168	ASP	2.6
1	F	203	VAL	2.6
1	C	218	SER	2.6
1	E	156	SER	2.6
1	E	195	PHE	2.6
1	F	378	MET	2.6
1	E	260	CYS	2.6
1	C	236	PRO	2.6
1	E	87	PRO	2.6
1	E	125	THR	2.6
1	E	269	ASN	2.6
1	F	353	LYS	2.6
1	E	437	SER	2.6
1	D	430	GLY	2.6
1	A	239	THR	2.6
1	E	369	THR	2.6
1	F	331	ASN	2.6
1	B	329	SER	2.6
1	C	205	ARG	2.6
1	E	464	LYS	2.6
1	A	238	GLY	2.6
1	E	321	GLY	2.6
1	A	62	LEU	2.6
1	D	155	LEU	2.6
1	D	213	THR	2.6
1	D	316	THR	2.6
1	F	311	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	2.6
1	C	104	GLN	2.6
1	E	288	GLU	2.6
1	E	183	ASP	2.6
1	E	271	ARG	2.5
1	A	274	SER	2.5
1	E	329	SER	2.5
1	F	274	SER	2.5
1	E	99	GLY	2.5
1	E	384	PRO	2.5
1	F	103	LEU	2.5
1	C	391	GLU	2.5
1	E	190	THR	2.5
1	E	327	ALA	2.5
1	F	488	ALA	2.5
1	E	272	ASN	2.5
1	A	271	ARG	2.5
1	C	98	ASP	2.5
1	D	205	ARG	2.5
1	E	205	ARG	2.5
1	F	110	ARG	2.5
1	E	353	LYS	2.5
1	D	51	PRO	2.5
1	A	322	GLY	2.5
1	F	235	GLY	2.5
1	F	298	ILE	2.5
1	D	49	GLU	2.5
1	A	189	GLN	2.5
1	A	429	THR	2.5
1	D	294	PHE	2.5
1	A	194	ARG	2.5
1	A	419	ASN	2.5
1	C	149	ARG	2.5
1	E	379	LYS	2.5
1	F	53	ASP	2.5
1	A	196	LEU	2.5
1	D	236	PRO	2.5
1	E	176	LEU	2.5
1	F	87	PRO	2.5
1	F	101	TRP	2.5
1	D	111	TYR	2.5
1	D	270	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	339	GLU	2.5
1	D	324	GLN	2.5
1	F	29	PHE	2.5
1	D	370	ALA	2.5
1	D	308	ARG	2.5
1	C	88	ASP	2.5
1	E	202	LEU	2.5
1	D	126	VAL	2.5
1	B	368	GLU	2.5
1	A	488	ALA	2.5
1	E	370	ALA	2.5
1	F	153	ALA	2.5
1	C	131	LYS	2.5
1	F	247	LYS	2.5
1	E	345	ILE	2.4
1	E	234	SER	2.4
1	F	169	VAL	2.4
1	C	122	PHE	2.4
1	C	207	GLU	2.4
1	A	209	ALA	2.4
1	A	426	LYS	2.4
1	B	358	LYS	2.4
1	D	11	GLN	2.4
1	C	148	THR	2.4
1	D	356	THR	2.4
1	D	272	ASN	2.4
1	F	272	ASN	2.4
1	A	446	ASP	2.4
1	D	85	PRO	2.4
1	A	94	VAL	2.4
1	F	329	SER	2.4
1	B	8	GLU	2.4
1	B	268	ALA	2.4
1	E	232	ALA	2.4
1	A	311	THR	2.4
1	E	331	ASN	2.4
1	A	206	PRO	2.4
1	F	85	PRO	2.4
1	B	371	GLY	2.4
1	E	165	VAL	2.4
1	F	88	ASP	2.4
1	E	376	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	440	ALA	2.4
1	D	319	ALA	2.4
1	F	232	ALA	2.4
1	F	332	ALA	2.4
1	A	190	THR	2.4
1	E	382	ASN	2.4
1	A	126	VAL	2.4
1	A	172	GLY	2.4
1	B	126	VAL	2.4
1	F	75	ASP	2.4
1	A	391	GLU	2.4
1	C	28	ALA	2.4
1	E	268	ALA	2.4
1	D	329	SER	2.4
1	E	124	GLN	2.4
1	F	285	GLN	2.4
1	A	178	THR	2.4
1	D	69	TYR	2.4
1	F	401	THR	2.4
1	C	96	HIS	2.4
1	E	103	LEU	2.4
1	F	62	LEU	2.4
1	D	136	ILE	2.4
1	A	248	VAL	2.3
1	C	134	VAL	2.3
1	D	464	LYS	2.3
1	A	235	GLY	2.3
1	D	228	GLY	2.3
1	D	91	PHE	2.3
1	D	242	ALA	2.3
1	A	101	TRP	2.3
1	E	237	SER	2.3
1	A	469	TYR	2.3
1	F	190	THR	2.3
1	A	136	ILE	2.3
1	A	51	PRO	2.3
1	C	399	LYS	2.3
1	A	205	ARG	2.3
1	E	430	GLY	2.3
1	F	284	ASN	2.3
1	E	58	ALA	2.3
1	E	107	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	242	ALA	2.3
1	D	378	MET	2.3
1	F	324	GLN	2.3
1	E	155	LEU	2.3
1	A	423	TYR	2.3
1	D	346	THR	2.3
1	F	151	ARG	2.3
1	E	465	VAL	2.3
1	C	365	ALA	2.3
1	D	28	ALA	2.3
1	D	462	ALA	2.3
1	E	130	GLU	2.3
1	C	75	ASP	2.3
1	F	446	ASP	2.3
1	D	19	CYS	2.3
1	E	281	LEU	2.3
1	F	381	ILE	2.3
1	D	369	THR	2.3
1	D	344	ARG	2.3
1	F	229	ARG	2.3
1	B	264	VAL	2.3
1	E	169	VAL	2.3
1	A	466	GLY	2.3
1	B	322	GLY	2.3
1	A	227	GLU	2.3
1	C	157	ALA	2.3
1	F	204	ALA	2.3
1	A	324	GLN	2.3
1	F	184	GLN	2.3
1	B	399	LYS	2.3
1	A	298	ILE	2.3
1	D	154	HIS	2.3
1	A	484	THR	2.3
1	D	194	ARG	2.3
1	F	320	THR	2.3
1	D	487	PRO	2.3
1	F	469	TYR	2.3
1	C	483	GLU	2.2
1	E	424	ASN	2.2
1	A	258	GLN	2.2
1	A	372	ASP	2.2
1	F	97	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	308	ARG	2.2
1	D	101	TRP	2.2
1	E	228	GLY	2.2
1	E	29	PHE	2.2
1	D	59	ALA	2.2
1	D	364	ALA	2.2
1	E	62	LEU	2.2
1	F	32	LYS	2.2
1	F	189	GLN	2.2
1	A	193	HIS	2.2
1	D	457	ASP	2.2
1	F	457	ASP	2.2
1	E	210	THR	2.2
1	E	226	CYS	2.2
1	E	334	CYS	2.2
1	B	218	SER	2.2
1	E	172	GLY	2.2
1	A	231	LEU	2.2
1	E	380	LEU	2.2
1	E	454	GLU	2.2
1	E	284	ASN	2.2
1	D	381	ILE	2.2
1	D	174	ASP	2.2
1	E	161	ASP	2.2
1	F	447	THR	2.2
1	B	156	SER	2.2
1	D	410	SER	2.2
1	E	133	SER	2.2
1	E	322	GLY	2.2
1	F	172	GLY	2.2
1	F	322	GLY	2.2
1	D	376	PHE	2.2
1	F	112	PHE	2.2
1	D	391	GLU	2.2
1	A	284	ASN	2.2
1	A	360	ASN	2.2
1	D	313	LYS	2.2
1	F	67	GLY	2.2
1	F	426	LYS	2.2
1	A	38	SER	2.2
1	E	218	SER	2.2
1	F	376	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	160	ALA	2.2
1	A	204	ALA	2.2
1	A	462	ALA	2.2
1	F	49	GLU	2.2
1	A	109	ARG	2.1
1	C	197	ARG	2.1
1	E	110	ARG	2.1
1	A	277	GLN	2.1
1	F	262	GLN	2.1
1	B	355	VAL	2.1
1	B	320	THR	2.1
1	B	326	THR	2.1
1	E	313	LYS	2.1
1	F	30	GLY	2.1
1	E	319	ALA	2.1
1	A	417	GLU	2.1
1	B	229	ARG	2.1
1	A	295	GLN	2.1
1	B	10	VAL	2.1
1	C	32	LYS	2.1
1	D	379	LYS	2.1
1	A	228	GLY	2.1
1	C	66	LEU	2.1
1	B	348	ARG	2.1
1	B	349	ALA	2.1
1	D	102	SER	2.1
1	D	105	SER	2.1
1	D	397	CYS	2.1
1	D	483	GLU	2.1
1	A	457	ASP	2.1
1	B	97	ASP	2.1
1	C	97	ASP	2.1
1	C	281	LEU	2.1
1	D	196	LEU	2.1
1	E	466	GLY	2.1
1	F	48	LEU	2.1
1	F	430	GLY	2.1
1	A	82	ARG	2.1
1	E	364	ALA	2.1
1	B	335	TYR	2.1
1	E	69	TYR	2.1
1	F	8	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	432	TYR	2.1
1	D	104	GLN	2.1
1	F	208	PRO	2.1
1	B	317	LEU	2.1
1	F	196	LEU	2.1
1	A	122	PHE	2.1
1	C	235	GLY	2.1
1	F	200	GLY	2.1
1	A	88	ASP	2.1
1	B	227	GLU	2.1
1	A	84	VAL	2.0
1	D	424	ASN	2.0
1	F	418	PHE	2.0
1	E	311	THR	2.0
1	A	222	ALA	2.0
1	A	232	ALA	2.0
1	B	160	ALA	2.0
1	D	88	ASP	2.0
1	E	204	ALA	2.0
1	A	8	GLU	2.0
1	A	165	VAL	2.0
1	C	410	SER	2.0
1	C	443	SER	2.0
1	E	295	GLN	2.0
1	F	126	VAL	2.0
1	E	206	PRO	2.0
1	F	233	PRO	2.0
1	D	68	ARG	2.0
1	D	82	ARG	2.0
1	D	284	ASN	2.0
1	F	109	ARG	2.0
1	D	31	PHE	2.0
1	D	463	ILE	2.0
1	B	319	ALA	2.0
1	D	239	THR	2.0
1	A	192	ASP	2.0
1	C	168	ASP	2.0
1	D	374	GLU	2.0
1	C	126	VAL	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](#)

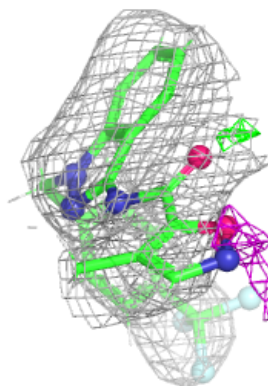
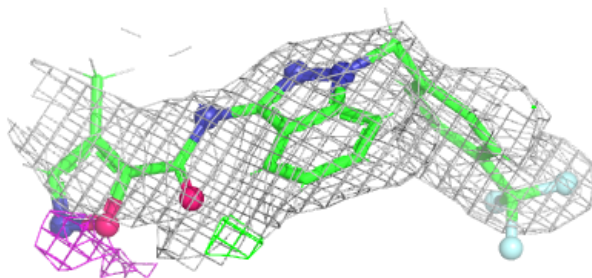
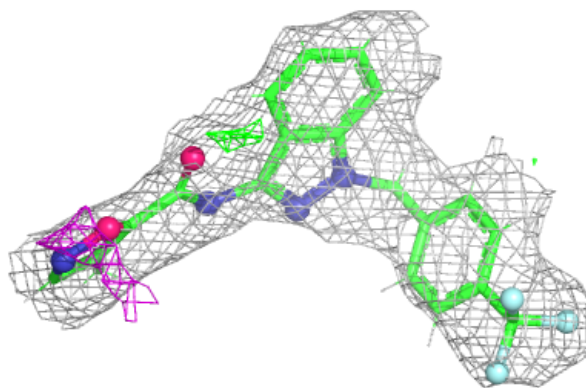
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	C7V	C	501	29/29	0.82	0.24	58,71,105,192	0
2	C7V	A	501	29/29	0.83	0.23	60,73,105,192	0
2	C7V	E	501	29/29	0.83	0.24	58,70,105,192	0
2	C7V	D	501	29/29	0.85	0.24	59,71,105,192	0
2	C7V	B	501	29/29	0.86	0.23	51,66,105,192	0
2	C7V	F	501	29/29	0.87	0.20	57,69,105,192	0

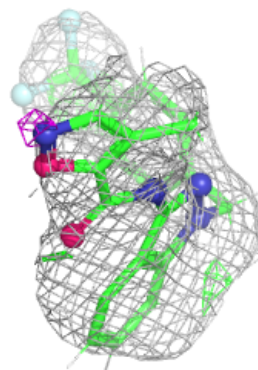
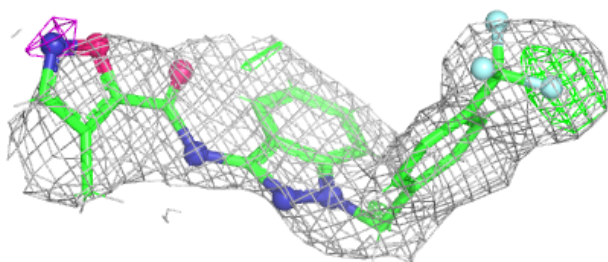
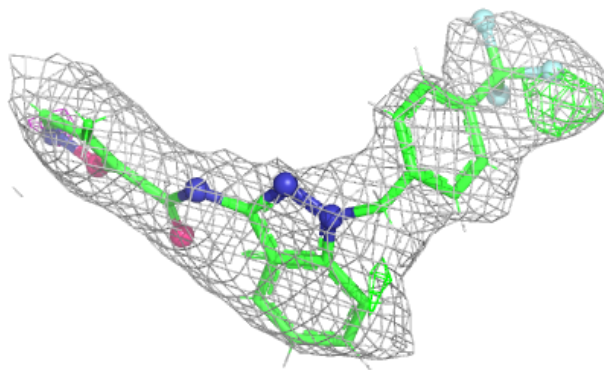
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C7V C 501:

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

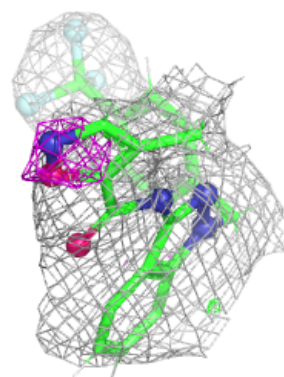
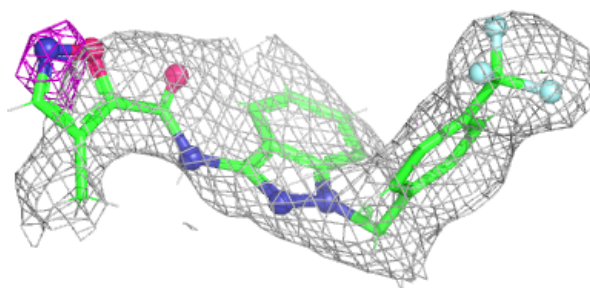
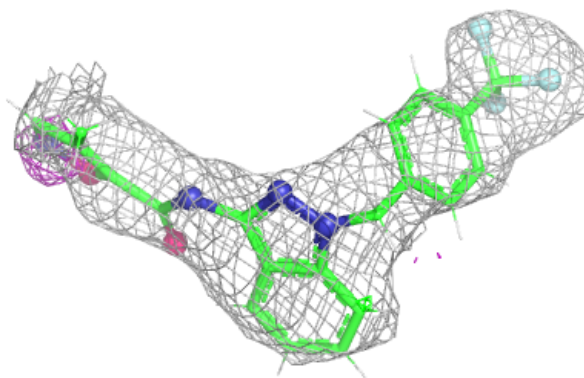
**Electron density around C7V A 501:**

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

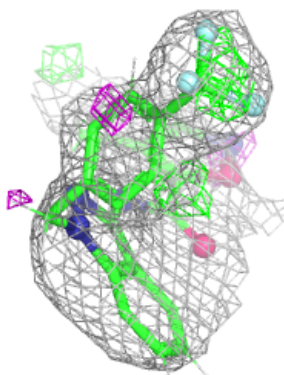
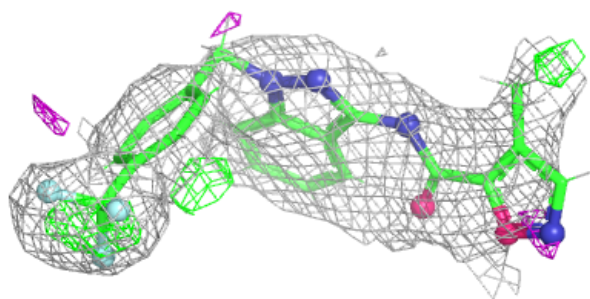
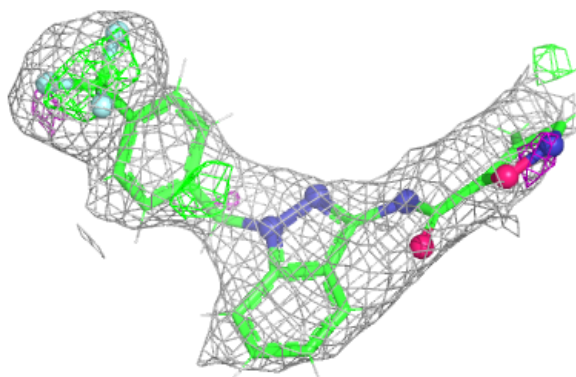


Electron density around C7V E 501:

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

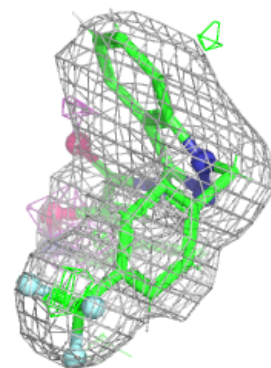
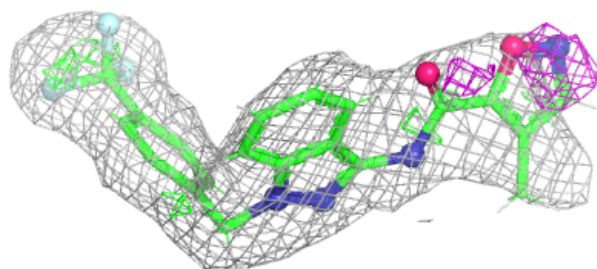
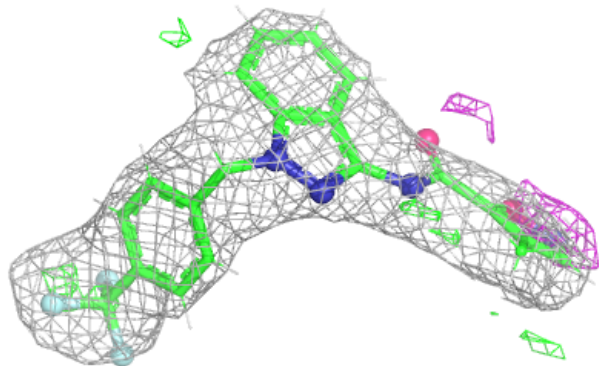
**Electron density around C7V D 501:**

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

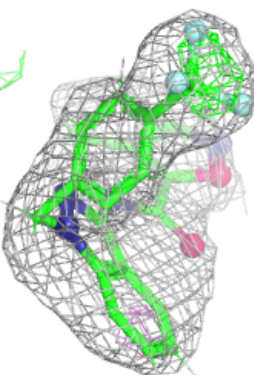
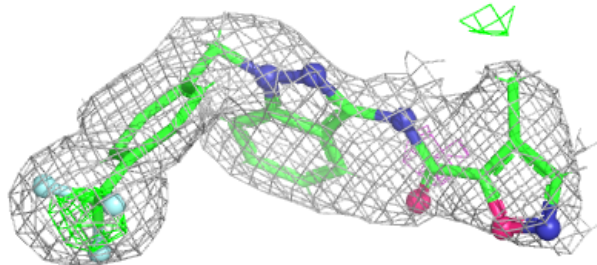
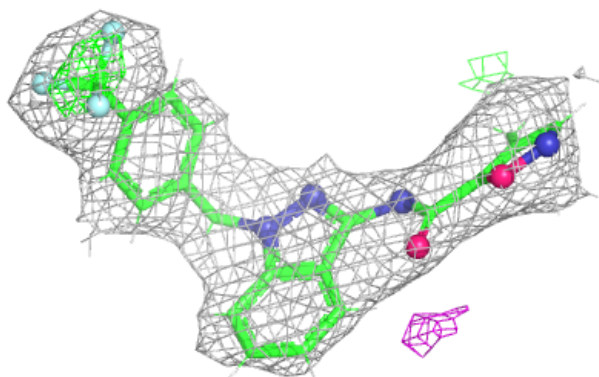


Electron density around C7V B 501:

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

**Electron density around C7V F 501:**

$2mF_o-DF_c$ (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.