



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:42 PM UTC

PDB ID : 5EY8 / pdb_00005ey8
Title : Structure of FadD32 from Mycobacterium smegmatis complexed to AMPC20
Authors : Guillet, V.; Maveyraud, L.; Mourey, L.
Deposited on : 2015-11-24
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

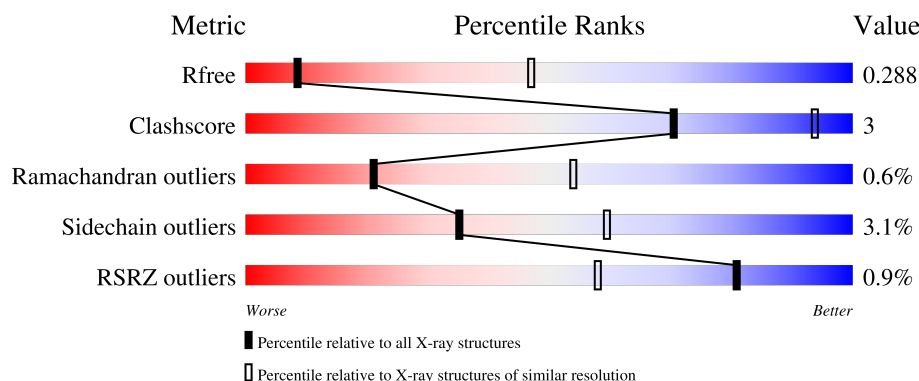
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	630	83% 11% • 5%
1	B	630	87% 7% 6%
1	C	630	89% 7% • •
1	D	630	87% 8% • •
1	E	630	85% 8% • 6%

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Mol	Chain	Length	Quality of chain	
1	F	630	86% 9% • •	
1	G	630	87% 7% • 5%	
1	H	630	87% 7% 6%	

2 Entry composition

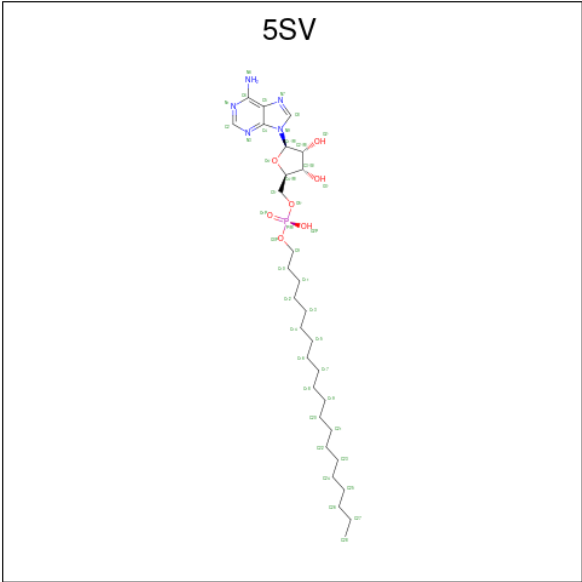
There are 3 unique types of molecules in this entry. The entry contains 33378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acyl-CoA synthase.

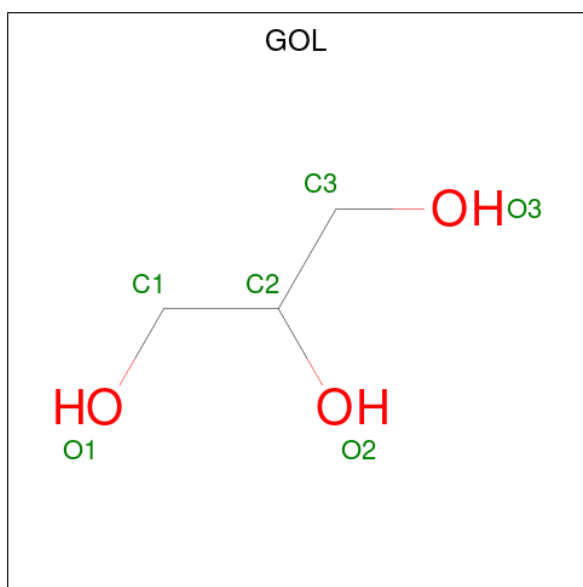
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4279	2719	744	809	7			
1	B	594	Total	C	N	O	S	0	0	0
			4129	2614	725	783	7			
1	C	605	Total	C	N	O	S	0	0	0
			4153	2626	726	794	7			
1	D	603	Total	C	N	O	S	0	0	0
			4194	2659	727	801	7			
1	E	592	Total	C	N	O	S	0	0	0
			4095	2598	714	776	7			
1	F	606	Total	C	N	O	S	0	0	0
			4303	2712	769	815	7			
1	G	597	Total	C	N	O	S	0	0	0
			4057	2572	697	781	7			
1	H	595	Total	C	N	O	S	0	0	0
			3871	2427	687	751	6			

- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl icosyl hydrogen phosphate (CCD ID: 5SV) (formula: C₃₀H₅₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	23	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			35	22	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			36	23	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			39	26	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			36	23	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			34	21	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			34	21	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			35	22	5	7	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

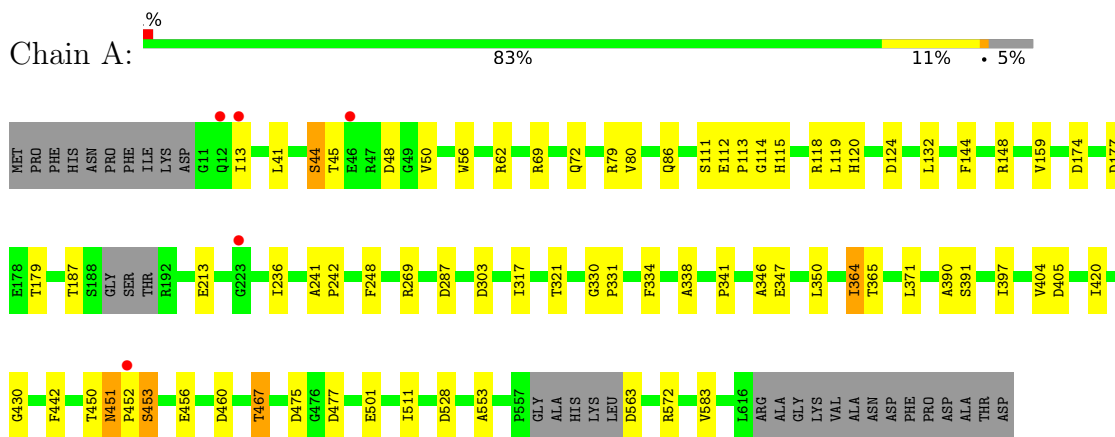


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

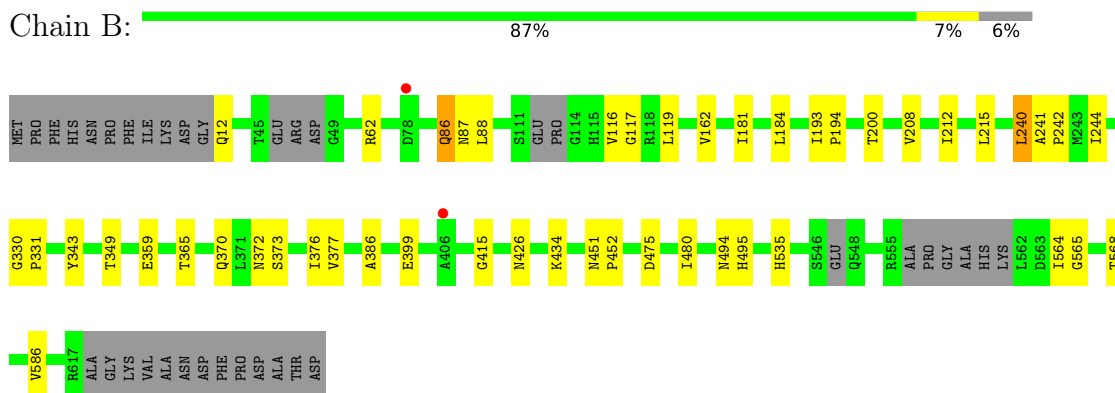
3 Residue-property plots

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.

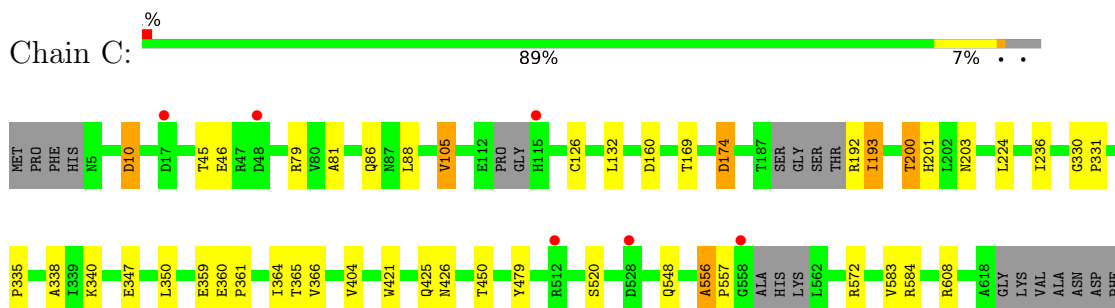
• Molecule 1: Acyl-CoA synthase



• Molecule 1: Acyl-CoA synthase



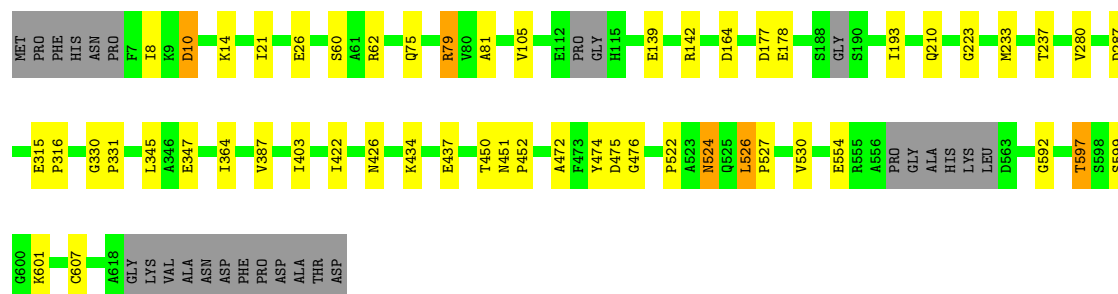
• Molecule 1: Acyl-CoA synthase



PRO
ASP
ALA
THR
ASP

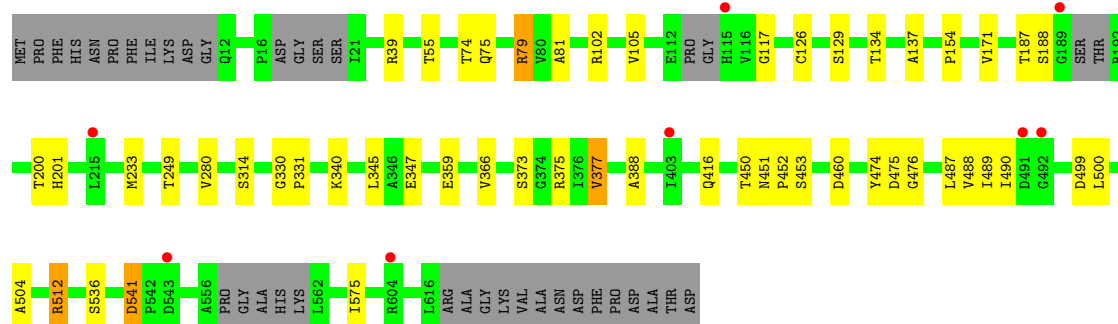
• Molecule 1: Acyl-CoA synthase

Chain D: 87% 8% . .



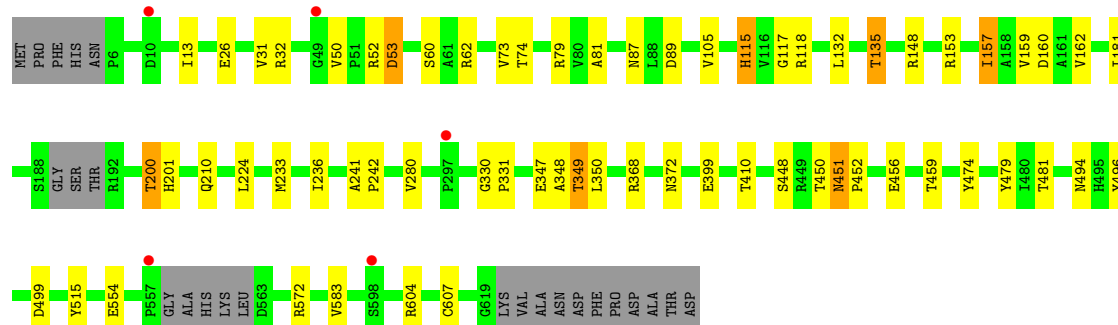
• Molecule 1: Acyl-CoA synthase

Chain E: 85% 8% . 6%



• Molecule 1: Acyl-CoA synthase

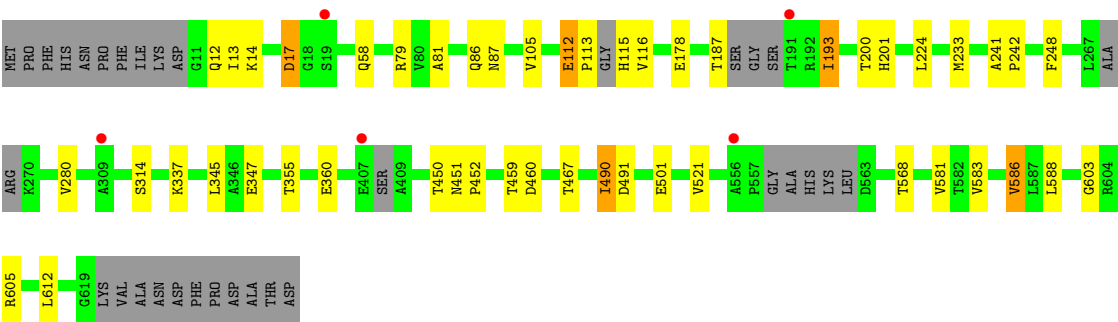
Chain F: 86% 9% . .



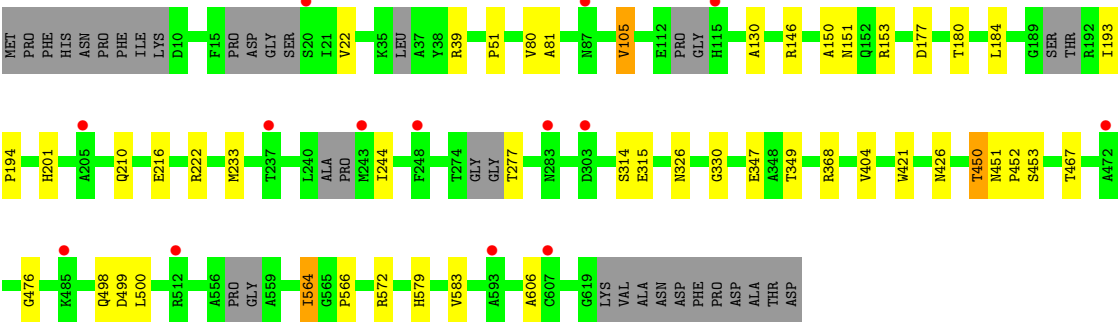
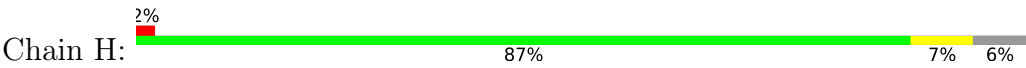
• Molecule 1: Acyl-CoA synthase

Chain G: 87% 7% . 5%





● Molecule 1: Acyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	164.04Å 164.04Å 231.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 3.50 49.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.44-3.50) 93.5 (49.44-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.286 0.228 , 0.288	Depositor DCC
R_{free} test set	3632 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.075 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	33378	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5SV, GOL

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	0.43	0/4384	0.83	4/6025 (0.1%)
1	B	0.41	0/4228	0.79	2/5814 (0.0%)
1	C	0.42	0/4259	0.79	3/5867 (0.1%)
1	D	0.41	0/4298	0.80	5/5913 (0.1%)
1	E	0.42	0/4194	0.82	1/5770 (0.0%)
1	F	0.42	0/4409	0.80	0/6054
1	G	0.41	0/4160	0.80	2/5736 (0.0%)
1	H	0.40	0/3957	0.78	2/5452 (0.0%)
All	All	0.42	0/33889	0.80	19/46631 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	2
1	G	0	1
All	All	0	4

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	VAL	CA-C-N	-8.44	110.19	119.98
1	A	50	VAL	C-N-CA	-8.44	110.19	119.98
1	G	193	ILE	CA-C-N	-8.15	111.62	119.85
1	G	193	ILE	C-N-CA	-8.15	111.62	119.85
1	A	451	ASN	CA-C-N	-7.92	109.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	ASN	C-N-CA	-7.92	109.94	119.84
1	D	524	ASN	N-CA-C	-7.55	103.33	112.54
1	H	476	GLY	N-CA-C	-6.80	105.69	115.27
1	C	556	ALA	CA-C-N	-6.25	112.04	118.85
1	C	556	ALA	C-N-CA	-6.25	112.04	118.85
1	B	565	GLY	CA-C-N	6.21	125.62	118.85
1	B	565	GLY	C-N-CA	6.21	125.62	118.85
1	C	88	LEU	N-CA-C	-5.46	105.34	112.23
1	D	607	CYS	N-CA-C	5.46	117.31	111.36
1	D	10	ASP	N-CA-C	5.20	117.00	110.24
1	D	526	LEU	CA-C-N	-5.13	114.70	120.14
1	D	526	LEU	C-N-CA	-5.13	114.70	120.14
1	E	117	GLY	N-CA-C	-5.13	106.17	113.86
1	H	606	ALA	N-CA-C	-5.06	105.46	111.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	SER	Peptide
1	E	373	SER	Peptide
1	E	512	ARG	Peptide
1	G	116	VAL	Peptide

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	4279	0	3939	37	0
1	B	4129	0	3651	26	0
1	C	4153	0	3555	25	0
1	D	4194	0	3660	28	0
1	E	4095	0	3589	27	0
1	F	4303	0	3861	31	0
1	G	4057	0	3423	21	0
1	H	3871	0	3107	20	0
2	A	36	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	35	0	34	0	0
2	C	36	0	36	1	0
2	D	39	0	42	1	0
2	E	36	0	36	0	0
2	F	34	0	32	0	0
2	G	34	0	32	0	0
2	H	35	0	34	0	0
3	E	6	0	8	1	0
3	F	6	0	8	0	0
All	All	33378	0	29083	215	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 3.

All (215) 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:F:572:ARG:NH1	1:F:583:VAL:O	2.04	0.91
1:H:572:ARG:NH1	1:H:583:VAL:O	2.09	0.85
1:A:572:ARG:NH1	1:A:583:VAL:O	2.16	0.79
1:A:269:ARG:NH1	1:A:303:ASP:OD2	2.17	0.78
1:C:520:SER:O	1:C:608:ARG:NH1	2.17	0.78
1:D:223:GLY:HA3	2:D:701:5SV:H45	1.68	0.75
1:E:388:ALA:H	3:E:702:GOL:H11	1.50	0.74
1:H:450:THR:O	1:H:453:SER:OG	2.07	0.72
1:A:62:ARG:NH2	1:A:159:VAL:O	2.23	0.72
1:C:572:ARG:NH1	1:C:583:VAL:O	2.25	0.69
1:C:347:GLU:OE1	1:C:347:GLU:N	2.26	0.67
1:D:597:THR:OG1	1:D:601:LYS:O	2.12	0.67
1:D:139:GLU:OE1	1:D:142:ARG:NH1	2.28	0.66
1:E:74:THR:O	1:E:102:ARG:NH2	2.29	0.64
1:C:556:ALA:HB3	1:C:557:PRO:HD3	1.79	0.64
1:D:347:GLU:N	1:D:347:GLU:OE2	2.32	0.63
1:B:399:GLU:OE2	1:B:426:ASN:ND2	2.32	0.62
1:H:564:ILE:C	1:H:566:PRO:HD2	2.25	0.61
1:H:347:GLU:OE1	1:H:347:GLU:N	2.32	0.61
1:D:554:GLU:OE1	1:D:592:GLY:N	2.33	0.61
1:E:347:GLU:N	1:E:347:GLU:OE1	2.33	0.60
1:F:368:ARG:NH1	1:F:499:ASP:OD2	2.34	0.60
1:F:347:GLU:OE1	1:F:347:GLU:N	2.34	0.60
1:B:372:ASN:ND2	1:B:494:ASN:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:GLN:NE2	1:H:426:ASN:OD1	2.36	0.59
1:H:81:ALA:HA	1:H:105:VAL:HG13	1.86	0.58
1:G:347:GLU:N	1:G:347:GLU:OE1	2.37	0.58
1:C:340:LYS:NZ	1:C:359:GLU:O	2.37	0.57
1:G:490:ILE:HG23	1:G:491:ASP:H	1.68	0.57
1:A:347:GLU:OE1	1:A:347:GLU:N	2.38	0.57
1:F:115:HIS:NE2	1:F:118:ARG:HG3	2.21	0.56
1:G:112:GLU:CB	1:G:115:HIS:HA	2.37	0.54
1:B:87:ASN:OD1	1:B:88:LEU:N	2.40	0.54
1:A:177:ASP:OD1	1:A:179:THR:OG1	2.24	0.54
1:D:451:ASN:HB3	1:D:452:PRO:HD3	1.90	0.54
1:F:348:ALA:O	1:F:349:THR:HG22	2.08	0.54
1:D:81:ALA:HA	1:D:105:VAL:HG13	1.89	0.54
1:G:451:ASN:CB	1:G:452:PRO:HD3	2.38	0.54
1:F:53:ASP:OD1	1:F:53:ASP:N	2.41	0.53
1:D:10:ASP:OD1	1:D:10:ASP:N	2.40	0.53
1:E:81:ALA:HA	1:E:105:VAL:HG13	1.90	0.53
1:F:31:VAL:HG13	1:F:32:ARG:HG2	1.91	0.53
1:B:194:PRO:O	1:B:434:LYS:NZ	2.26	0.53
1:F:372:ASN:ND2	1:F:494:ASN:O	2.43	0.52
1:C:364:ILE:HG22	1:C:365:THR:H	1.74	0.52
1:A:317:ILE:HG13	1:A:390:ALA:HB3	1.91	0.52
1:F:236:ILE:HD12	1:F:350:LEU:HB2	1.91	0.52
1:A:124:ASP:OD1	1:A:148:ARG:NH2	2.43	0.52
1:B:86:GLN:O	1:B:87:ASN:CG	2.52	0.52
1:D:434:LYS:NZ	1:D:437:GLU:OE1	2.41	0.52
1:G:233:MET:SD	1:G:314:SER:HB3	2.50	0.52
1:A:563:ASP:N	1:A:563:ASP:OD1	2.43	0.51
1:A:120:HIS:CE1	1:A:144:PHE:CE1	2.98	0.51
1:A:453:SER:HB3	1:A:456:GLU:HG2	1.93	0.51
1:G:112:GLU:CB	1:G:113:PRO:CD	2.89	0.51
1:H:368:ARG:NH1	1:H:499:ASP:OD2	2.44	0.51
1:C:200:THR:OG1	1:C:201:HIS:N	2.43	0.51
1:C:330:GLY:N	1:C:331:PRO:HD2	2.25	0.51
1:A:80:VAL:CG1	1:A:132:LEU:HD13	2.41	0.50
1:F:62:ARG:NH2	1:F:159:VAL:O	2.43	0.50
1:F:330:GLY:N	1:F:331:PRO:HD2	2.26	0.50
1:E:39:ARG:HB3	1:E:249:THR:HG22	1.94	0.50
1:H:233:MET:SD	1:H:314:SER:OG	2.67	0.50
1:F:50:VAL:O	1:F:52:ARG:N	2.45	0.50
1:D:522:PRO:C	1:D:524:ASN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:701:5SV:H2	2:C:701:5SV:H19	1.93	0.49
1:E:79:ARG:HD2	1:E:126:CYS:HB2	1.94	0.49
1:B:241:ALA:N	1:B:242:PRO:HD2	2.26	0.49
1:G:81:ALA:HA	1:G:105:VAL:HG13	1.93	0.49
1:G:112:GLU:CB	1:G:113:PRO:HD2	2.42	0.49
1:E:233:MET:HE3	1:E:280:VAL:HG22	1.94	0.49
1:A:44:SER:OG	1:A:45:THR:N	2.46	0.49
1:E:79:ARG:NE	1:E:126:CYS:O	2.45	0.49
1:F:451:ASN:HB2	1:F:452:PRO:HD3	1.94	0.49
1:E:102:ARG:N	1:E:102:ARG:HD2	2.27	0.48
1:B:212:ILE:CD1	1:B:244:ILE:HD11	2.44	0.48
1:C:364:ILE:HG22	1:C:365:THR:N	2.29	0.48
1:G:17:ASP:OD1	1:G:17:ASP:N	2.45	0.48
1:D:330:GLY:N	1:D:331:PRO:HD2	2.28	0.48
1:F:148:ARG:O	1:F:153:ARG:NH1	2.47	0.47
1:H:150:ALA:HA	1:H:153:ARG:HD2	1.96	0.47
1:C:81:ALA:HA	1:C:105:VAL:HG13	1.95	0.47
1:E:187:THR:HG22	1:E:188:SER:N	2.29	0.47
1:E:541:ASP:OD1	1:E:541:ASP:N	2.47	0.47
1:H:404:VAL:HG21	1:H:421:TRP:CE2	2.49	0.47
1:D:62:ARG:NH1	1:D:164:ASP:OD1	2.47	0.47
1:E:129:SER:C	1:E:154:PRO:HB3	2.39	0.47
1:A:317:ILE:CD1	1:A:341:PRO:HB3	2.45	0.47
1:B:86:GLN:CG	1:B:87:ASN:H	2.28	0.47
1:C:192:ARG:O	1:C:193:ILE:HG22	2.14	0.47
1:E:451:ASN:CB	1:E:452:PRO:HD3	2.45	0.47
1:D:8:ILE:CB	1:D:14:LYS:H	2.27	0.47
1:C:556:ALA:CB	1:C:557:PRO:HD3	2.44	0.47
1:F:73:VAL:HG23	1:F:74:THR:HG23	1.96	0.47
1:B:376:ILE:N	1:B:415:GLY:O	2.39	0.46
1:C:174:ASP:OD1	1:C:174:ASP:N	2.43	0.46
1:C:556:ALA:HB3	1:C:557:PRO:CD	2.45	0.46
1:D:26:GLU:OE1	1:D:60:SER:OG	2.28	0.46
1:A:451:ASN:HB3	1:A:452:PRO:HD3	1.96	0.46
1:B:343:TYR:CD1	1:B:480:ILE:CD1	2.99	0.46
1:F:200:THR:OG1	1:F:201:HIS:N	2.49	0.46
1:B:451:ASN:CB	1:B:452:PRO:HD3	2.46	0.46
1:A:330:GLY:N	1:A:331:PRO:CD	2.79	0.45
1:B:349:THR:OG1	1:B:426:ASN:O	2.31	0.45
1:E:200:THR:HG22	1:E:201:HIS:H	1.81	0.45
1:F:181:ILE:HA	1:F:200:THR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:PRO:HG2	1:D:530:VAL:HG23	1.97	0.45
1:H:500:LEU:HD23	1:H:579:HIS:CD2	2.51	0.45
1:E:187:THR:HG22	1:E:188:SER:H	1.82	0.45
1:F:132:LEU:HD23	1:F:157:ILE:CD1	2.47	0.45
1:C:236:ILE:HB	1:C:350:LEU:HD22	1.98	0.45
1:G:241:ALA:N	1:G:242:PRO:HD2	2.32	0.45
1:G:568:THR:HG23	1:G:586:VAL:CG1	2.47	0.45
1:C:364:ILE:HD11	1:C:479:TYR:OH	2.16	0.45
1:G:521:VAL:HG11	1:G:612:LEU:HD21	1.98	0.45
1:A:430:GLY:HA2	1:A:442:PHE:CD1	2.51	0.45
1:B:343:TYR:CG	1:B:480:ILE:CD1	3.00	0.45
1:C:45:THR:HG23	1:C:46:GLU:H	1.81	0.45
1:B:116:VAL:O	1:B:119:LEU:N	2.49	0.44
1:B:330:GLY:N	1:B:331:PRO:HD2	2.31	0.44
1:C:404:VAL:HG11	1:C:421:TRP:CE2	2.52	0.44
1:B:181:ILE:HD11	1:B:184:LEU:HD13	1.98	0.44
1:H:146:ARG:HA	1:H:153:ARG:HH21	1.82	0.44
1:F:233:MET:HE2	1:F:280:VAL:CG2	2.48	0.44
1:A:112:GLU:O	1:A:114:GLY:N	2.50	0.44
1:B:208:VAL:HG13	1:B:240:LEU:HD12	1.98	0.44
1:E:488:VAL:HG12	1:E:488:VAL:O	2.18	0.44
1:H:451:ASN:CB	1:H:452:PRO:HD3	2.48	0.44
1:F:410:THR:HG22	1:F:448:SER:HB3	2.00	0.44
1:A:213:GLU:CB	1:A:397:ILE:HD12	2.48	0.44
1:A:364:ILE:HG23	1:A:365:THR:N	2.32	0.44
1:A:80:VAL:HG13	1:A:132:LEU:CD1	2.48	0.44
1:F:241:ALA:HB3	1:F:242:PRO:HD3	2.00	0.44
1:H:177:ASP:HB3	1:H:180:THR:HG23	2.00	0.44
1:E:504:ALA:HB2	1:E:575:ILE:HD11	2.00	0.43
1:F:115:HIS:C	1:F:117:GLY:H	2.25	0.43
1:F:604:ARG:O	1:F:607:CYS:N	2.51	0.43
1:A:80:VAL:CG1	1:A:132:LEU:CD1	2.96	0.43
1:G:200:THR:HG22	1:G:201:HIS:H	1.84	0.43
1:B:343:TYR:CG	1:B:480:ILE:HD11	2.54	0.43
1:G:241:ALA:CB	1:G:248:PHE:HB2	2.48	0.43
1:A:334:PHE:CZ	1:A:338:ALA:HB3	2.53	0.43
1:G:233:MET:HE3	1:G:280:VAL:HG22	1.99	0.43
1:E:499:ASP:OD1	1:E:500:LEU:N	2.51	0.43
1:B:116:VAL:HG13	1:B:117:GLY:N	2.33	0.43
1:B:494:ASN:O	1:B:495:HIS:ND1	2.52	0.43
1:E:474:TYR:O	1:E:476:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:HB2	1:A:248:PHE:HB2	2.01	0.43
1:F:135:THR:OG1	1:F:160:ASP:OD2	2.37	0.43
1:G:345:LEU:HD11	1:G:467:THR:HB	2.00	0.43
1:B:86:GLN:HG3	1:B:87:ASN:H	1.84	0.42
1:F:515:TYR:CB	1:F:554:GLU:HB2	2.49	0.42
1:H:193:ILE:HG13	1:H:194:PRO:HD2	2.01	0.42
1:A:391:SER:HB2	1:A:477:ASP:HB3	2.00	0.42
1:B:365:THR:CG2	1:B:386:ALA:HB1	2.49	0.42
1:D:315:GLU:HB2	1:D:316:PRO:HD2	2.00	0.42
1:D:233:MET:O	1:D:237:THR:OG1	2.27	0.42
1:E:233:MET:SD	1:E:314:SER:HB3	2.60	0.42
1:G:178:GLU:O	1:G:200:THR:HG21	2.20	0.42
1:G:603:GLY:C	1:G:605:ARG:H	2.28	0.42
1:A:452:PRO:O	1:A:453:SER:C	2.62	0.42
1:B:370:GLN:HG2	1:B:377:VAL:HG22	2.02	0.42
1:C:132:LEU:HD12	1:C:132:LEU:N	2.35	0.42
1:D:233:MET:HE2	1:D:280:VAL:CG2	2.50	0.42
1:D:233:MET:HE2	1:D:280:VAL:HG22	2.02	0.42
1:G:490:ILE:HG21	1:G:581:VAL:HG11	2.02	0.42
1:A:187:THR:HG21	1:A:346:ALA:CB	2.50	0.42
1:C:548:GLN:HB3	1:C:584:ARG:HG3	2.00	0.42
1:F:81:ALA:HA	1:F:105:VAL:HG13	2.01	0.42
1:D:403:ILE:HG21	1:D:472:ALA:HA	2.02	0.42
1:F:26:GLU:OE1	1:F:60:SER:OG	2.36	0.42
1:G:12:GLN:CB	1:G:14:LYS:H	2.33	0.42
1:C:203:ASN:ND2	1:C:425:GLN:O	2.53	0.42
1:B:181:ILE:HA	1:B:200:THR:HA	2.02	0.41
1:C:79:ARG:HD2	1:C:126:CYS:HB2	2.02	0.41
1:E:200:THR:HG22	1:E:201:HIS:N	2.35	0.41
1:H:222:ARG:HG2	1:H:277:THR:HG22	2.01	0.41
1:A:56:TRP:CH2	1:A:242:PRO:HA	2.55	0.41
1:A:287:ASP:OD2	1:A:321:THR:OG1	2.32	0.41
1:A:404:VAL:HG12	1:A:405:ASP:N	2.35	0.41
1:A:236:ILE:HD12	1:A:350:LEU:HB2	2.02	0.41
1:D:210:GLN:OE1	1:D:426:ASN:ND2	2.53	0.41
1:E:340:LYS:NZ	1:E:359:GLU:O	2.53	0.41
1:F:474:TYR:HB3	1:F:479:TYR:CE1	2.55	0.41
1:A:69:ARG:O	1:A:72:GLN:HG2	2.21	0.41
1:C:160:ASP:OD1	1:C:160:ASP:N	2.54	0.41
1:D:75:GLN:HA	1:H:151:ASN:HB3	2.03	0.41
1:D:79:ARG:HH11	1:D:79:ARG:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:VAL:O	1:E:489:ILE:C	2.64	0.41
1:F:87:ASN:OD1	1:F:89:ASP:N	2.53	0.41
1:A:420:ILE:HB	1:A:467:THR:HG21	2.02	0.41
1:C:360:GLU:HG2	1:C:361:PRO:HD2	2.03	0.41
1:D:474:TYR:O	1:D:476:GLY:N	2.53	0.41
1:E:375:ARG:HA	1:E:416:GLN:HA	2.02	0.41
1:A:317:ILE:CG1	1:A:390:ALA:HB3	2.50	0.41
1:C:335:PRO:HG2	1:C:338:ALA:HB2	2.03	0.41
1:D:345:LEU:HD23	1:D:345:LEU:N	2.36	0.41
1:D:345:LEU:HD21	1:D:422:ILE:HD13	2.03	0.41
1:E:366:VAL:HG13	1:E:377:VAL:H	1.85	0.41
1:H:326:ASN:O	1:H:330:GLY:N	2.54	0.41
1:B:62:ARG:NH2	1:B:162:VAL:O	2.49	0.41
1:F:210:GLN:NE2	1:F:399:GLU:OE2	2.53	0.41
1:G:337:LYS:HA	1:G:360:GLU:HG3	2.03	0.41
1:A:132:LEU:HD12	1:A:132:LEU:N	2.35	0.40
1:B:568:THR:HG23	1:B:586:VAL:CG1	2.52	0.40
1:A:511:ILE:HG23	1:A:553:ALA:HB1	2.03	0.40
1:D:177:ASP:CG	1:D:178:GLU:H	2.29	0.40
1:D:177:ASP:CG	1:D:178:GLU:N	2.78	0.40
1:F:481:THR:HG21	1:F:496:TYR:CZ	2.57	0.40
1:H:80:VAL:HG12	1:H:130:ALA:HB3	2.03	0.40
1:A:41:LEU:HD12	1:A:41:LEU:N	2.37	0.40
1:A:114:GLY:O	1:A:115:HIS:CB	2.70	0.40
1:E:134:THR:HG23	1:E:137:ALA:H	1.87	0.40
1:E:330:GLY:N	1:E:331:PRO:CD	2.85	0.40
1:H:39:ARG:HH11	1:H:51:PRO:HB3	1.87	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	592/630 (94%)	568 (96%)	19 (3%)	5 (1%)	16	49
1	B	584/630 (93%)	559 (96%)	21 (4%)	4 (1%)	18	51
1	C	597/630 (95%)	581 (97%)	14 (2%)	2 (0%)	36	67
1	D	595/630 (94%)	572 (96%)	20 (3%)	3 (0%)	24	57
1	E	582/630 (92%)	557 (96%)	21 (4%)	4 (1%)	18	51
1	F	600/630 (95%)	572 (95%)	27 (4%)	1 (0%)	43	74
1	G	585/630 (93%)	565 (97%)	17 (3%)	3 (0%)	24	57
1	H	579/630 (92%)	550 (95%)	25 (4%)	4 (1%)	18	51
All	All	4714/5040 (94%)	4524 (96%)	164 (4%)	26 (1%)	21	54

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	475	ASP
1	E	475	ASP
1	G	13	ILE
1	H	244	ILE
1	A	44	SER
1	A	475	ASP
1	B	564	ILE
1	A	453	SER
1	E	453	SER
1	E	512	ARG
1	F	115	HIS
1	B	86	GLN
1	B	475	ASP
1	H	22	VAL
1	A	113	PRO
1	C	10	ASP
1	D	526	LEU
1	E	536	SER
1	G	112	GLU
1	B	193	ILE
1	H	349	THR
1	A	13	ILE
1	C	193	ILE
1	G	193	ILE
1	D	21	ILE
1	H	564	ILE

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	395/501 (79%)	381 (96%)	14 (4%)	32	57
1	B	352/501 (70%)	347 (99%)	5 (1%)	59	71
1	C	343/501 (68%)	333 (97%)	10 (3%)	37	60
1	D	355/501 (71%)	347 (98%)	8 (2%)	44	64
1	E	345/501 (69%)	334 (97%)	11 (3%)	34	59
1	F	380/501 (76%)	367 (97%)	13 (3%)	32	57
1	G	326/501 (65%)	310 (95%)	16 (5%)	22	48
1	H	277/501 (55%)	269 (97%)	8 (3%)	37	60
All	All	2773/4008 (69%)	2688 (97%)	85 (3%)	35	59

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	79	ARG
1	A	86	GLN
1	A	111	SER
1	A	118	ARG
1	A	119	LEU
1	A	174	ASP
1	A	364	ILE
1	A	371	LEU
1	A	450	THR
1	A	460	ASP
1	A	467	THR
1	A	501	GLU
1	A	528	ASP
1	B	12	GLN
1	B	215	LEU
1	B	240	LEU
1	B	359	GLU
1	B	535	HIS

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Mol	Chain	Res	Type
1	C	10	ASP
1	C	86	GLN
1	C	105	VAL
1	C	169	THR
1	C	174	ASP
1	C	200	THR
1	C	224	LEU
1	C	366	VAL
1	C	426	ASN
1	C	450	THR
1	D	79	ARG
1	D	193	ILE
1	D	287	ASP
1	D	364	ILE
1	D	387	VAL
1	D	450	THR
1	D	597	THR
1	D	599	SER
1	E	55	THR
1	E	75	GLN
1	E	79	ARG
1	E	171	VAL
1	E	345	LEU
1	E	377	VAL
1	E	450	THR
1	E	460	ASP
1	E	487	LEU
1	E	490	ILE
1	E	541	ASP
1	F	13	ILE
1	F	53	ASP
1	F	79	ARG
1	F	135	THR
1	F	157	ILE
1	F	162	VAL
1	F	200	THR
1	F	224	LEU
1	F	349	THR
1	F	450	THR
1	F	451	ASN
1	F	456	GLU
1	F	459	THR

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Mol	Chain	Res	Type
1	G	17	ASP
1	G	58	GLN
1	G	79	ARG
1	G	86	GLN
1	G	87	ASN
1	G	187	THR
1	G	224	LEU
1	G	355	THR
1	G	450	THR
1	G	459	THR
1	G	460	ASP
1	G	490	ILE
1	G	501	GLU
1	G	583	VAL
1	G	586	VAL
1	G	588	LEU
1	H	105	VAL
1	H	184	LEU
1	H	201	HIS
1	H	216	GLU
1	H	315	GLU
1	H	450	THR
1	H	467	THR
1	H	498	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	201	HIS
1	A	579	HIS
1	B	185	GLN
1	B	198	GLN
1	B	370	GLN
1	C	127	HIS
1	D	185	GLN
1	D	207	ASN
1	E	372	ASN
1	E	389	GLN
1	F	198	GLN
1	F	246	HIS
1	F	579	HIS

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Mol	Chain	Res	Type
1	G	185	GLN
1	G	416	GLN
1	G	444	ASN
1	G	525	GLN
1	G	533	ASN
1	H	495	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	5SV	E	701	-	38,38,45	1.25	3 (7%)	50,51,58	0.97	2 (4%)
2	5SV	F	701	-	36,36,45	1.11	3 (8%)	48,49,58	0.96	1 (2%)
2	5SV	C	701	-	38,38,45	1.13	3 (7%)	50,51,58	1.05	3 (6%)
2	5SV	G	701	-	36,36,45	1.22	3 (8%)	48,49,58	1.03	2 (4%)
2	5SV	H	701	-	37,37,45	1.13	2 (5%)	49,50,58	0.99	3 (6%)
3	GOL	E	702	-	5,5,5	0.43	0	5,5,5	0.20	0
3	GOL	F	702	-	5,5,5	0.37	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5SV	B	701	-	37,37,45	1.09	2 (5%)	49,50,58	1.00	2 (4%)
2	5SV	D	701	-	41,41,45	1.23	4 (9%)	53,54,58	1.00	1 (1%)
2	5SV	A	701	-	38,38,45	1.20	4 (10%)	50,51,58	1.04	2 (4%)

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	5SV	E	701	-	-	4/25/41/48	0/3/3/3
2	5SV	F	701	-	-	8/23/39/48	0/3/3/3
2	5SV	C	701	-	-	1/25/41/48	0/3/3/3
2	5SV	G	701	-	-	5/23/39/48	0/3/3/3
2	5SV	H	701	-	-	6/24/40/48	0/3/3/3
3	GOL	E	702	-	-	2/4/4/4	-
3	GOL	F	702	-	-	2/4/4/4	-
2	5SV	B	701	-	-	8/24/40/48	0/3/3/3
2	5SV	D	701	-	-	5/28/44/48	0/3/3/3
2	5SV	A	701	-	-	4/25/41/48	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	5SV	C8-N9	3.19	1.43	1.37
2	A	701	5SV	C8-N9	3.08	1.42	1.37
2	H	701	5SV	C8-N9	2.85	1.42	1.37
2	D	701	5SV	C8-N9	2.74	1.42	1.37
2	C	701	5SV	C8-N9	2.68	1.42	1.37
2	G	701	5SV	P-O1P	2.64	1.60	1.50
2	G	701	5SV	C8-N9	2.61	1.42	1.37
2	D	701	5SV	P-O1P	2.56	1.59	1.50
2	E	701	5SV	P-O1P	2.49	1.59	1.50
2	B	701	5SV	P-O1P	2.43	1.59	1.50
2	H	701	5SV	P-O1P	2.41	1.59	1.50
2	F	701	5SV	P-O1P	2.37	1.59	1.50
2	D	701	5SV	C24-C23	-2.28	1.34	1.50
2	B	701	5SV	C8-N9	2.26	1.41	1.37
2	A	701	5SV	P-O1P	2.25	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	5SV	C5-C4	2.22	1.43	1.39
2	C	701	5SV	P-O1P	2.18	1.58	1.50
2	F	701	5SV	C8-N9	2.17	1.41	1.37
2	A	701	5SV	C5-C4	2.16	1.42	1.39
2	F	701	5SV	O4'-C4'	-2.14	1.40	1.45
2	D	701	5SV	C5-C4	2.13	1.42	1.39
2	C	701	5SV	C2-N1	2.13	1.37	1.33
2	A	701	5SV	P-O2P	-2.04	1.45	1.55
2	G	701	5SV	C4-N3	2.02	1.38	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	5SV	O3P-P-O1P	-2.59	98.66	108.94
2	B	701	5SV	O5'-P-O1P	-2.59	98.68	108.94
2	C	701	5SV	O3P-P-O1P	-2.45	99.22	108.94
2	F	701	5SV	O3P-P-O1P	-2.45	99.22	108.94
2	E	701	5SV	O3P-P-O1P	-2.37	99.54	108.94
2	B	701	5SV	O3P-P-O1P	-2.34	99.66	108.94
2	H	701	5SV	O3P-P-O1P	-2.32	99.74	108.94
2	E	701	5SV	O5'-P-O1P	-2.26	99.97	108.94
2	A	701	5SV	O3'-C3'-C4'	-2.25	104.61	111.08
2	H	701	5SV	O5'-P-O1P	-2.24	100.06	108.94
2	D	701	5SV	O5'-P-O1P	-2.18	100.28	108.94
2	C	701	5SV	O5'-P-O1P	-2.16	100.37	108.94
2	G	701	5SV	O5'-P-O1P	-2.15	100.42	108.94
2	C	701	5SV	O4'-C4'-C3'	2.11	109.35	105.15
2	H	701	5SV	O3'-C3'-C4'	-2.11	105.02	111.08
2	G	701	5SV	O3P-P-O1P	-2.08	100.69	108.94

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	5SV	C9-O3P-P-O5'
2	B	701	5SV	C9-O3P-P-O5'
2	D	701	5SV	C9-O3P-P-O2P
2	D	701	5SV	C9-O3P-P-O5'
2	E	701	5SV	C9-O3P-P-O5'
2	F	701	5SV	C5'-O5'-P-O3P
2	G	701	5SV	C9-O3P-P-O2P
2	G	701	5SV	C9-O3P-P-O5'

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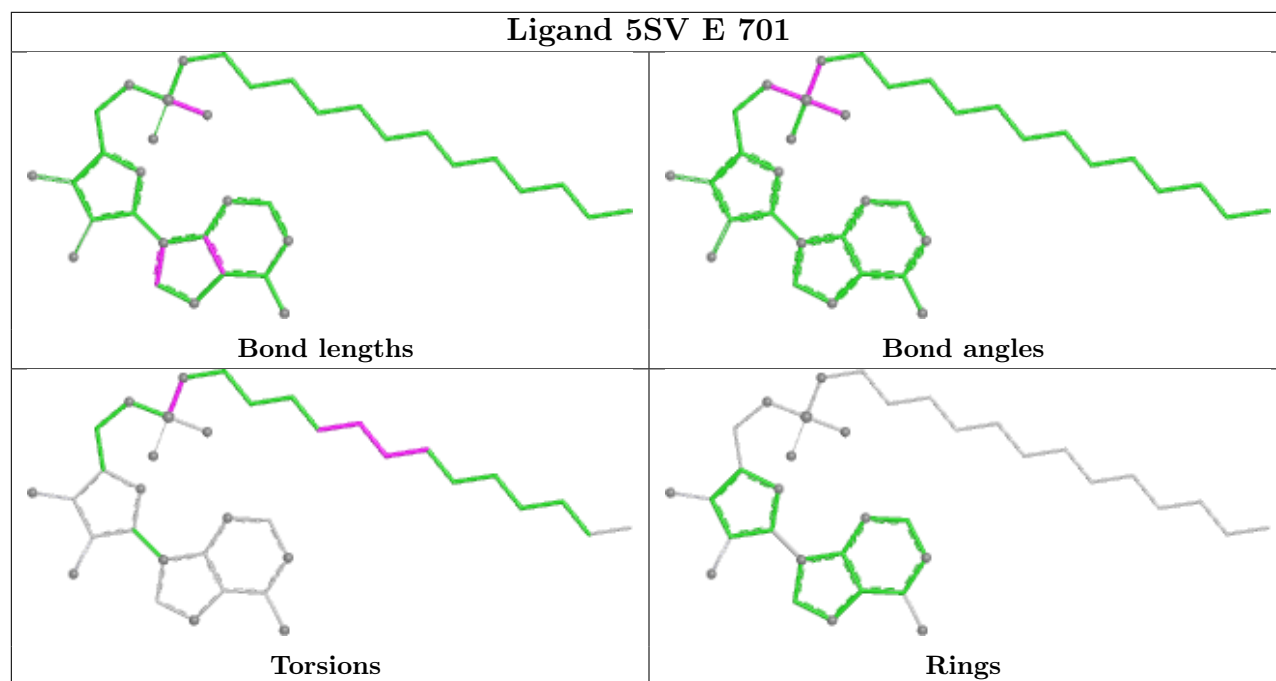
Mol	Chain	Res	Type	Atoms
3	E	702	GOL	O1-C1-C2-C3
3	F	702	GOL	O1-C1-C2-C3
2	B	701	5SV	C11-C12-C13-C14
2	F	701	5SV	C13-C14-C15-C16
3	E	702	GOL	O1-C1-C2-O2
3	F	702	GOL	O1-C1-C2-O2
2	G	701	5SV	C12-C13-C14-C15
2	E	701	5SV	C11-C12-C13-C14
2	A	701	5SV	C13-C14-C15-C16
2	H	701	5SV	C12-C13-C14-C15
2	A	701	5SV	C14-C15-C16-C17
2	F	701	5SV	C11-C12-C13-C14
2	B	701	5SV	C10-C11-C12-C13
2	G	701	5SV	C13-C14-C15-C16
2	C	701	5SV	C10-C11-C12-C13
2	G	701	5SV	C11-C12-C13-C14
2	D	701	5SV	C14-C15-C16-C17
2	D	701	5SV	C21-C22-C23-C24
2	B	701	5SV	C13-C14-C15-C16
2	D	701	5SV	C13-C14-C15-C16
2	A	701	5SV	C11-C10-C9-O3P
2	F	701	5SV	C12-C13-C14-C15
2	E	701	5SV	C12-C13-C14-C15
2	H	701	5SV	C11-C12-C13-C14
2	E	701	5SV	C13-C14-C15-C16
2	B	701	5SV	C12-C13-C14-C15
2	H	701	5SV	C10-C11-C12-C13
2	H	701	5SV	C13-C14-C15-C16
2	B	701	5SV	C9-O3P-P-O1P
2	F	701	5SV	C5'-O5'-P-O1P
2	F	701	5SV	C9-O3P-P-O5'
2	B	701	5SV	C15-C16-C17-C18
2	F	701	5SV	C10-C11-C12-C13
2	H	701	5SV	C3'-C4'-C5'-O5'
2	H	701	5SV	O4'-C4'-C5'-O5'
2	F	701	5SV	C15-C16-C17-C18
2	B	701	5SV	C11-C10-C9-O3P

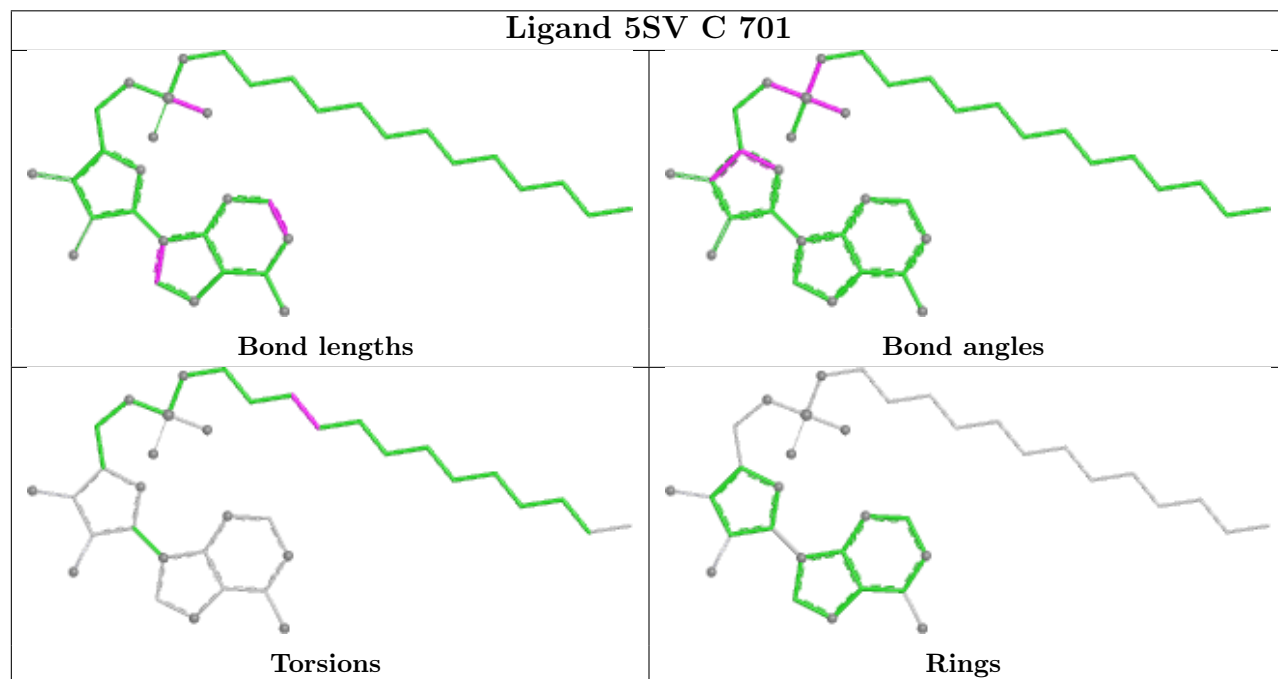
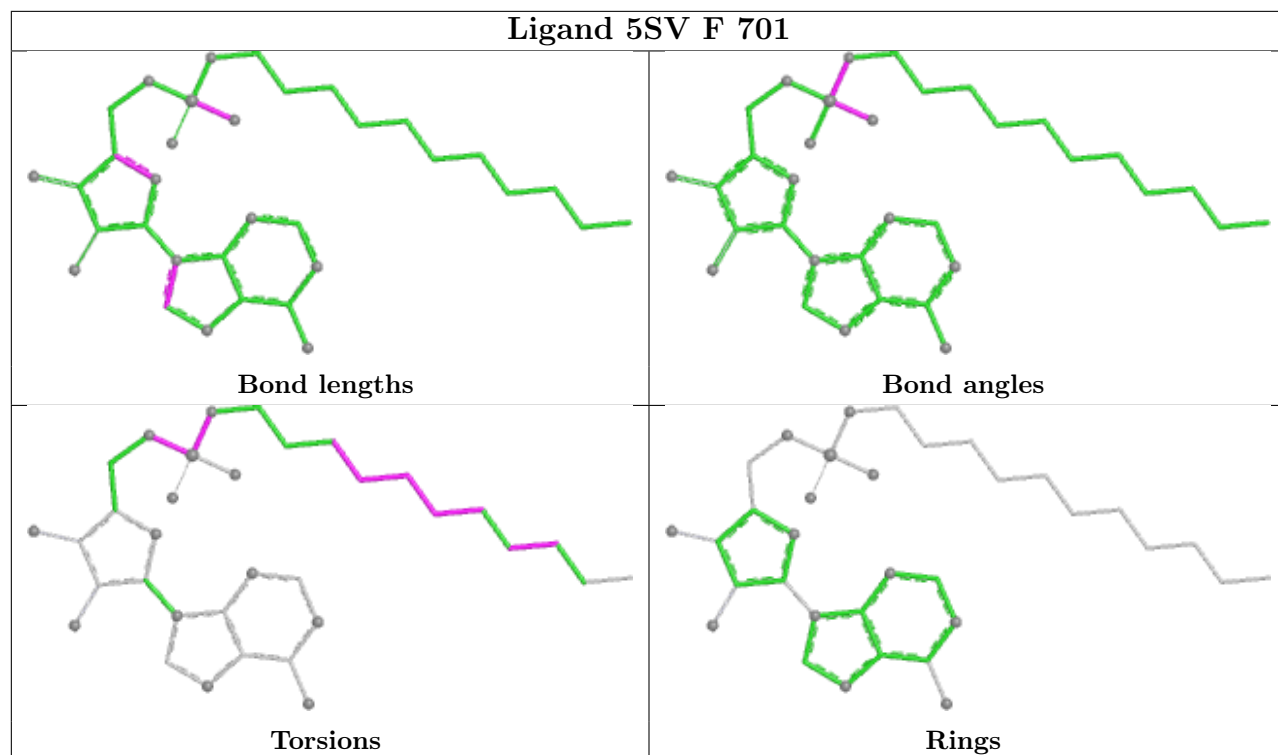
There are no ring outliers.

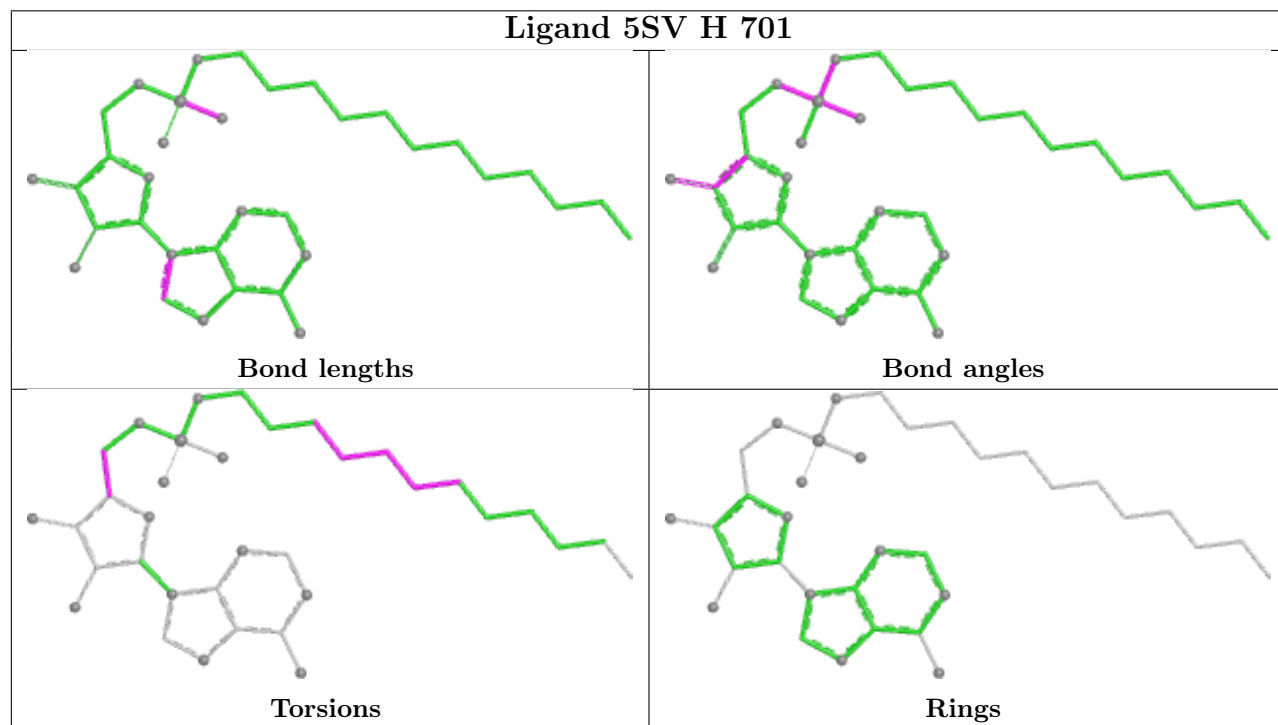
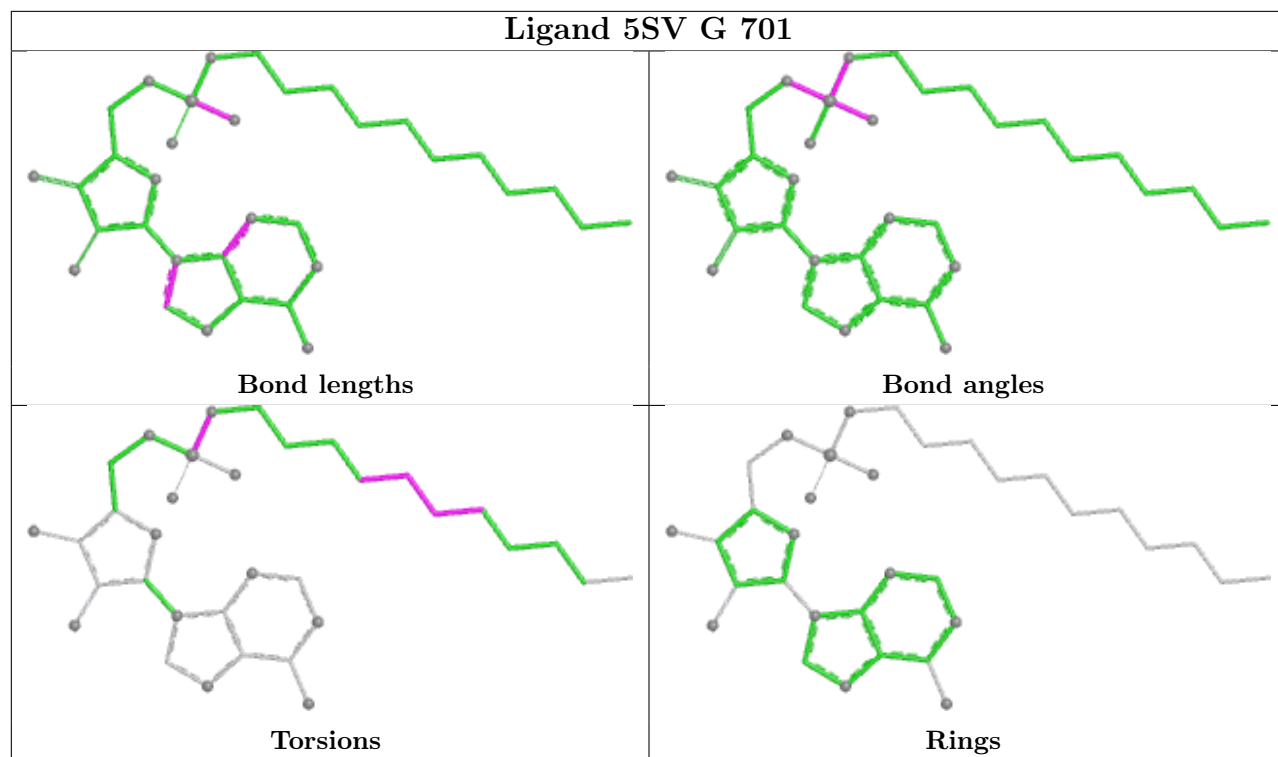
3 monomers are involved in 3 short contacts:

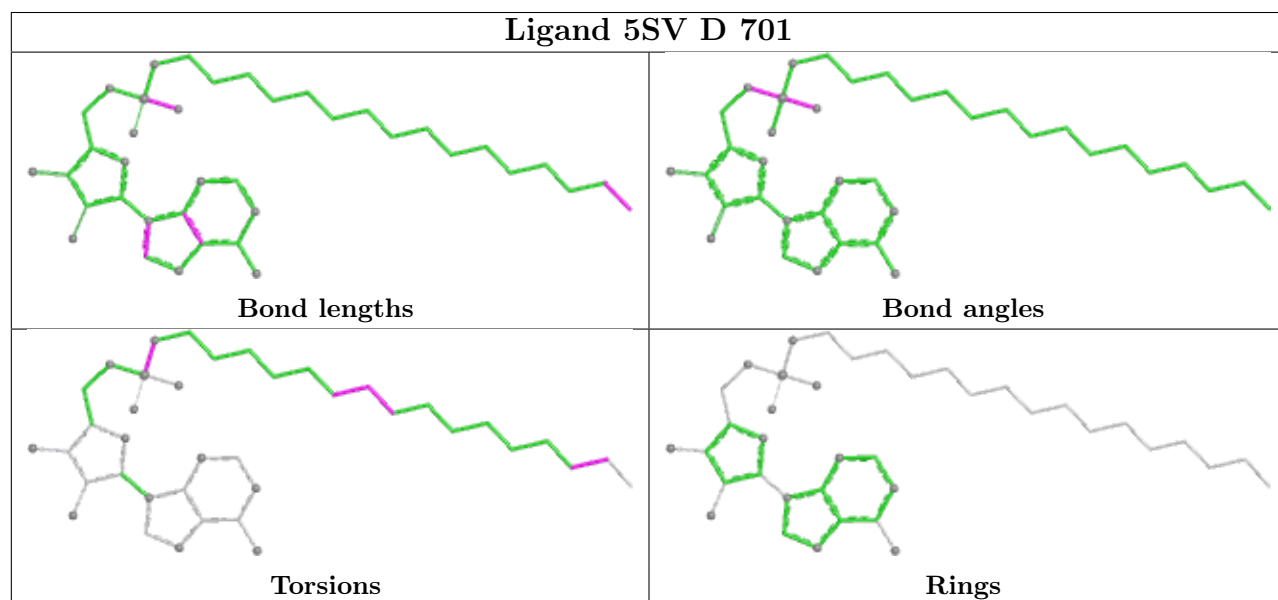
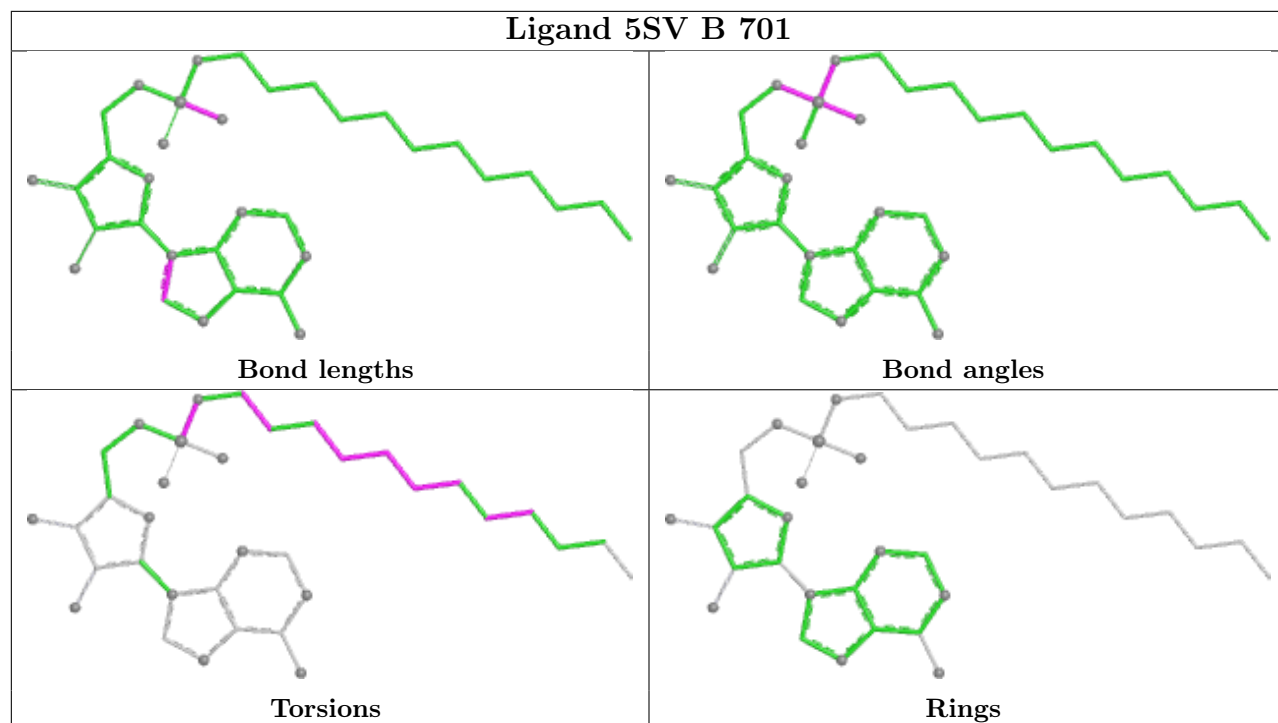
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	5SV	1	0
3	E	702	GOL	1	0
2	D	701	5SV	1	0

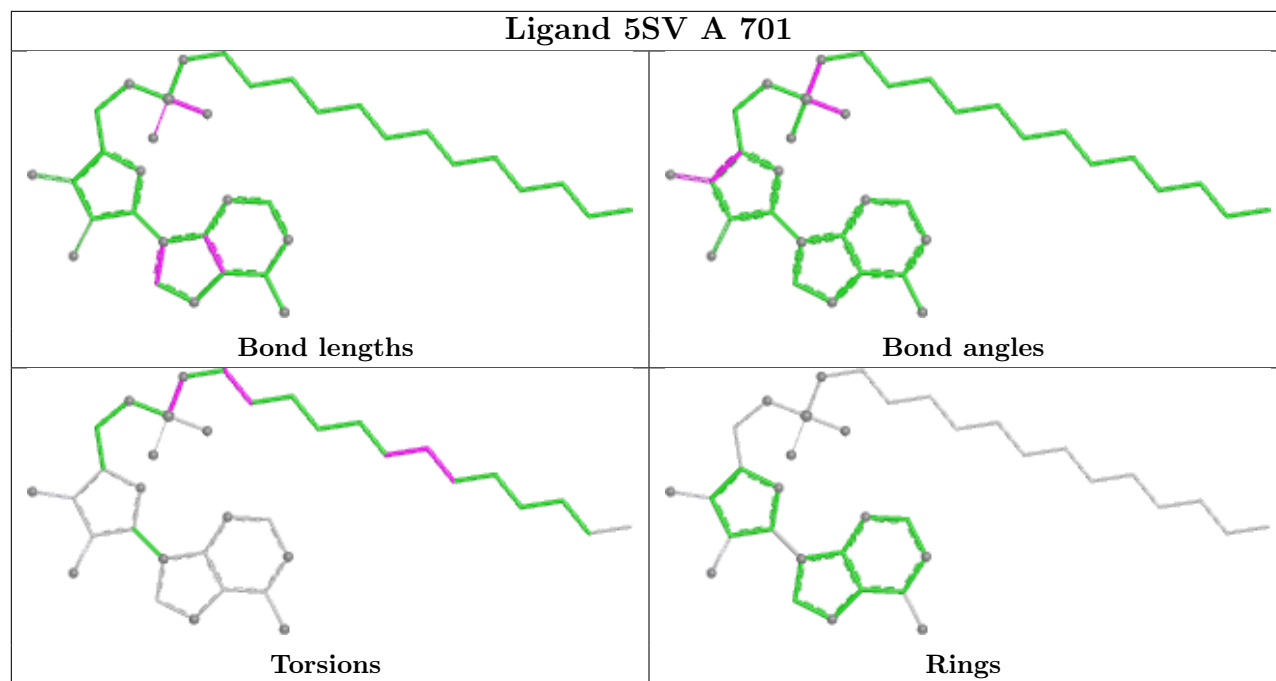
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	598/630 (94%)	-0.10	5 (0%) 82 60	32, 48, 94, 160	0
1	B	594/630 (94%)	-0.01	2 (0%) 90 76	38, 57, 105, 196	0
1	C	605/630 (96%)	-0.02	6 (0%) 79 56	38, 58, 99, 181	0
1	D	603/630 (95%)	-0.04	0 100 100	35, 54, 97, 171	0
1	E	592/630 (93%)	0.07	8 (1%) 73 48	37, 63, 115, 183	0
1	F	606/630 (96%)	-0.03	5 (0%) 82 60	33, 53, 101, 173	0
1	G	597/630 (94%)	0.04	5 (0%) 82 60	37, 64, 113, 187	0
1	H	595/630 (94%)	0.27	14 (2%) 59 35	38, 74, 123, 170	0
All	All	4790/5040 (95%)	0.02	45 (0%) 81 58	32, 58, 109, 196	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	205	ALA	3.8
1	H	283	ASN	3.6
1	G	407	GLU	3.0
1	C	528	ASP	2.9
1	C	115	HIS	2.8
1	A	452	PRO	2.8
1	G	19	SER	2.8
1	A	223	GLY	2.8
1	E	604	ARG	2.8
1	H	512	ARG	2.8
1	E	403	ILE	2.7
1	E	492	GLY	2.7
1	H	303	ASP	2.6
1	H	243	MET	2.6
1	H	115	HIS	2.6
1	F	598	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	48	ASP	2.5
1	H	87	ASN	2.4
1	E	543	ASP	2.3
1	H	248	PHE	2.3
1	E	491	ASP	2.3
1	A	12	GLN	2.3
1	E	215	LEU	2.3
1	F	10	ASP	2.3
1	B	78	ASP	2.2
1	E	115	HIS	2.2
1	H	472	ALA	2.2
1	A	13	ILE	2.2
1	H	237	THR	2.2
1	G	191	THR	2.2
1	F	297	PRO	2.1
1	C	17	ASP	2.1
1	C	558	GLY	2.1
1	E	189	GLY	2.1
1	F	557	PRO	2.1
1	G	556	ALA	2.1
1	F	49	GLY	2.1
1	C	512	ARG	2.1
1	H	607	CYS	2.1
1	G	309	ALA	2.1
1	H	485	LYS	2.0
1	A	46	GLU	2.0
1	H	20	SER	2.0
1	B	406	ALA	2.0
1	H	593	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

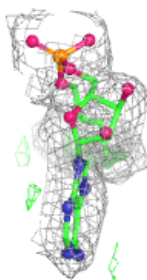
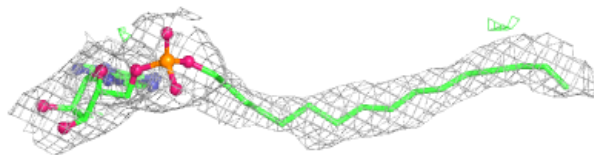
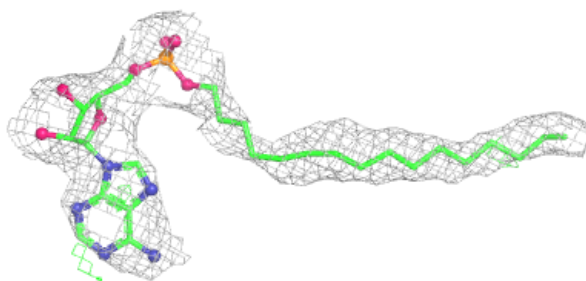
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	702	6/6	0.84	0.11	40,40,40,74	0
3	GOL	F	702	6/6	0.89	0.10	35,35,37,40	0
2	5SV	D	701	39/43	0.95	0.10	35,42,49,50	0
2	5SV	G	701	34/43	0.95	0.09	39,47,53,70	0
2	5SV	H	701	35/43	0.95	0.09	37,38,57,60	0
2	5SV	B	701	35/43	0.95	0.10	38,38,39,68	0
2	5SV	C	701	36/43	0.95	0.10	38,44,79,89	0
2	5SV	E	701	36/43	0.96	0.08	37,38,44,50	0
2	5SV	A	701	36/43	0.97	0.08	32,32,36,56	0
2	5SV	F	701	34/43	0.97	0.09	33,34,44,45	0

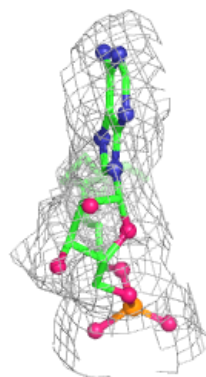
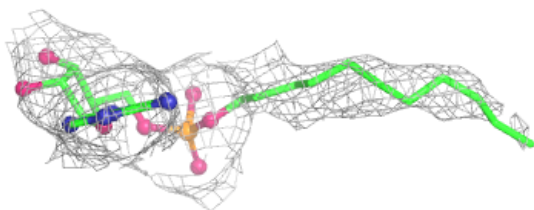
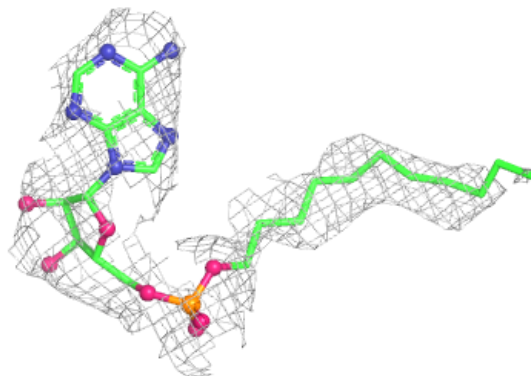
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5SV D 701:

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

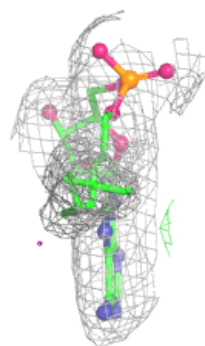
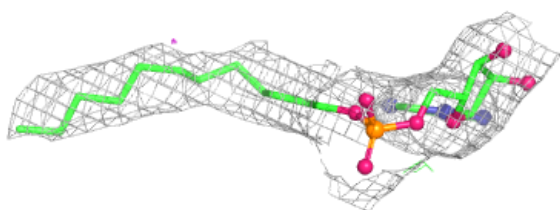
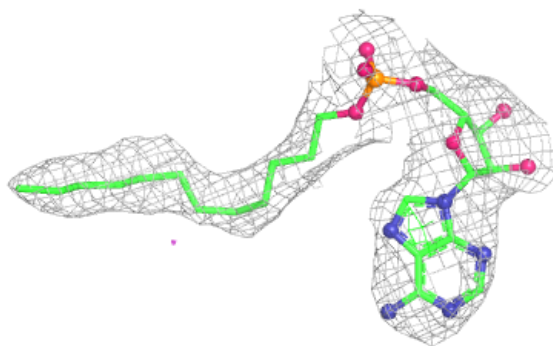
**Electron density around 5SV G 701:**

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

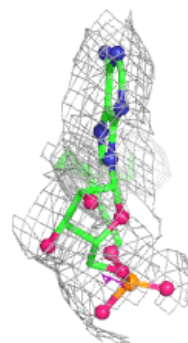
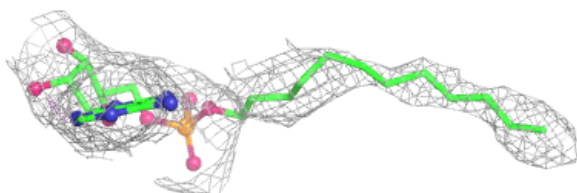
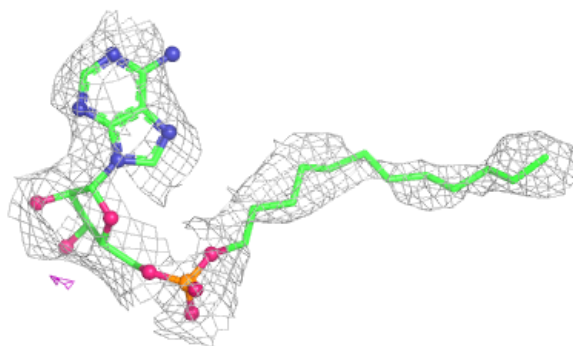


Electron density around 5SV H 701:

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

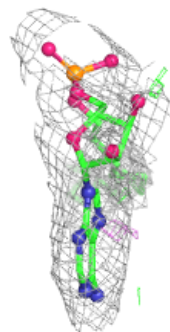
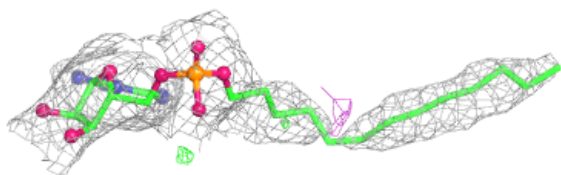
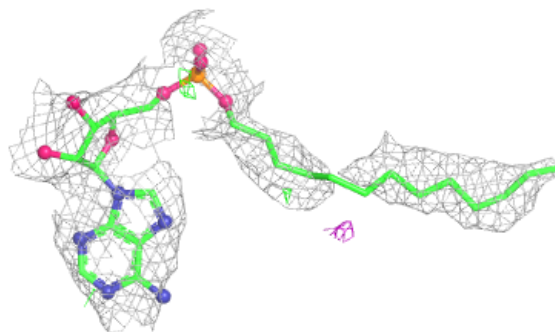
**Electron density around 5SV B 701:**

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

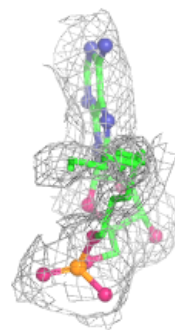
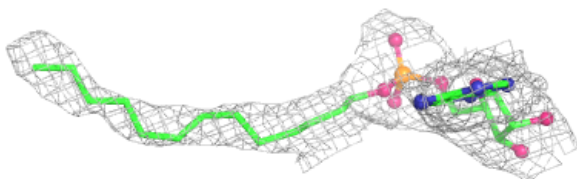
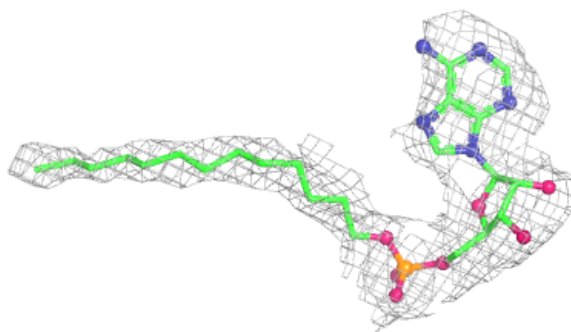


Electron density around 5SV C 701:

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

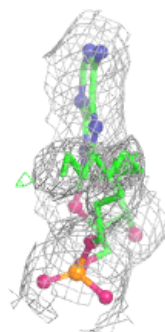
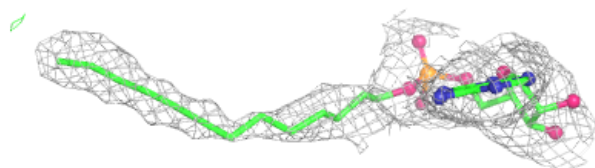
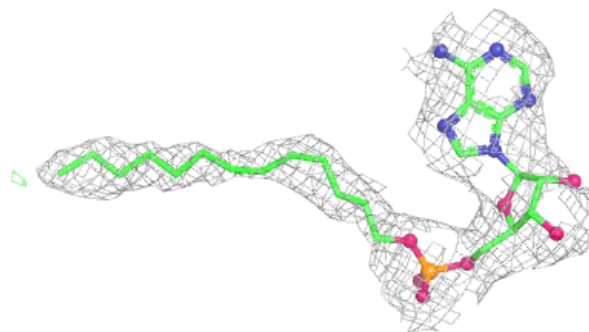
**Electron density around 5SV E 701:**

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

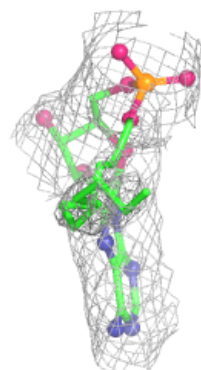
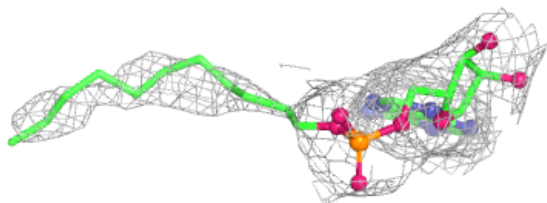
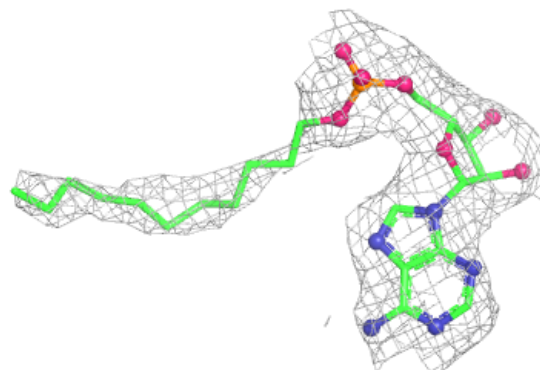


Electron density around 5SV A 701:

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

**Electron density around 5SV F 701:**

$2mF_o-DF_c$ (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.