Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 06:27 am BST

PDB ID	:	5HW8
Title	:	Candida albicans FKBP12 P104G protein bound with FK506 in C2 space group
Authors	:	Tonthat, N.K.; Schumacher, M.A.
Deposited on	:	2016-01-28
Resolution	:	2.86 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 (i) symbol.

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

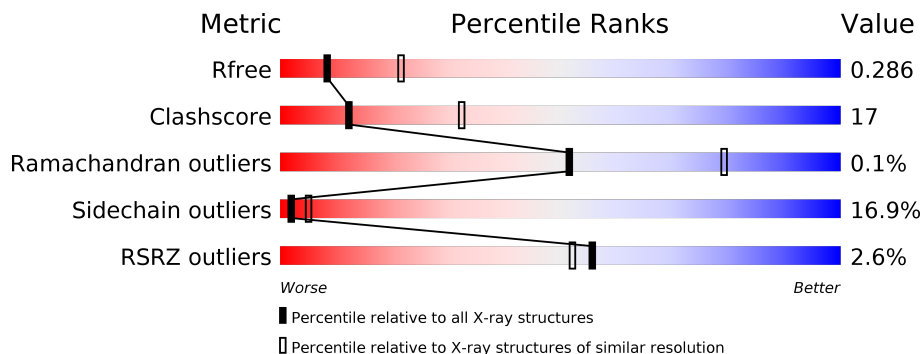|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.86 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		17
Ramachandran outliers		0.1%
Sidechain outliers		16.9%
RSRZ outliers		2.6%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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 <=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	122	65% 25% 9% ·
1	B	122	69% 30% ·
1	C	122	61% 33% 6% ·
1	D	122	% 69% 26% · ·
1	E	122	56% 34% 6% · ·
1	F	122	3% 51% 33% 7% 10%

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Mol	Chain	Length	Quality of chain
1	G	122	
1	H	122	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7289 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.
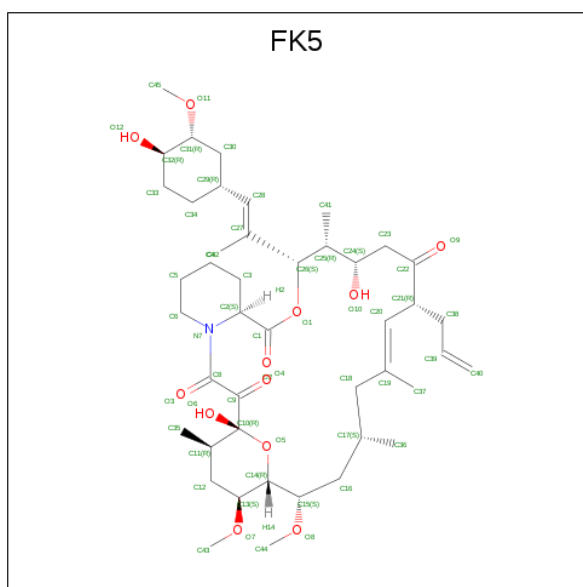
- Molecule 1 is a protein called FK506-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			875	558	149	167	1			
1	B	122	Total	C	N	O	S	0	0	0
			902	574	154	173	1			
1	C	121	Total	C	N	O	S	0	0	0
			874	555	148	170	1			
1	D	120	Total	C	N	O	S	0	0	0
			891	567	152	171	1			
1	E	118	Total	C	N	O	S	0	0	0
			860	550	146	163	1			
1	F	110	Total	C	N	O	S	0	0	0
			785	502	129	153	1			
1	G	121	Total	C	N	O	S	0	0	0
			866	552	144	169	1			
1	H	100	Total	C	N	O	S	0	0	0
			716	463	118	134	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLY	PRO	engineered mutation	UNP P28870
B	104	GLY	PRO	engineered mutation	UNP P28870
C	104	GLY	PRO	engineered mutation	UNP P28870
D	104	GLY	PRO	engineered mutation	UNP P28870
E	104	GLY	PRO	engineered mutation	UNP P28870
F	104	GLY	PRO	engineered mutation	UNP P28870
G	104	GLY	PRO	engineered mutation	UNP P28870
H	104	GLY	PRO	engineered mutation	UNP P28870

- Molecule 2 is 8-DEETHYL-8-[BUT-3-ENYL]-ASCOMYCIN (three-letter code: FK5) (formula: $C_{44}H_{69}NO_{12}$).

FK5

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 57	C 44	N 1	O 12	0	0
2	B	1	Total 57	C 44	N 1	O 12	0	0
2	C	1	Total 57	C 44	N 1	O 12	0	0
2	D	1	Total 57	C 44	N 1	O 12	0	0
2	E	1	Total 57	C 44	N 1	O 12	0	0
2	F	1	Total 57	C 44	N 1	O 12	0	0
2	G	1	Total 57	C 44	N 1	O 12	0	0
2	H	1	Total 57	C 44	N 1	O 12	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	7	Total 7	O 7	0	0
3	C	9	Total 9	O 9	0	0
3	D	10	Total 10	O 10	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	6	Total 6	O 6	0	0
3	F	8	Total 8	O 8	0	0
3	G	9	Total 9	O 9	0	0
3	H	7	Total 7	O 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
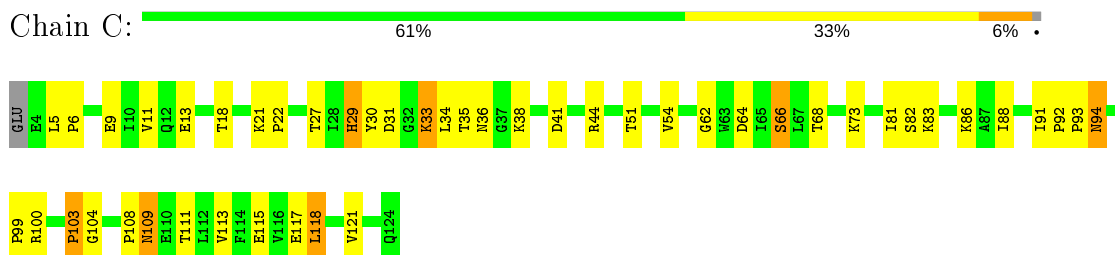
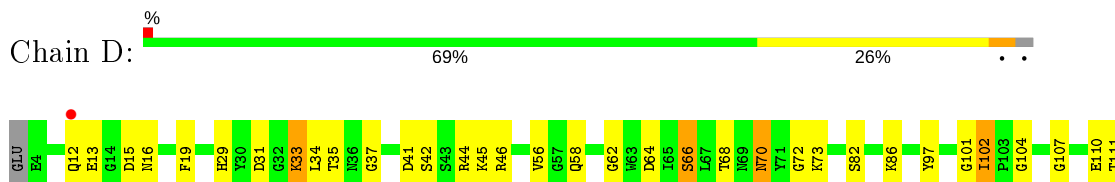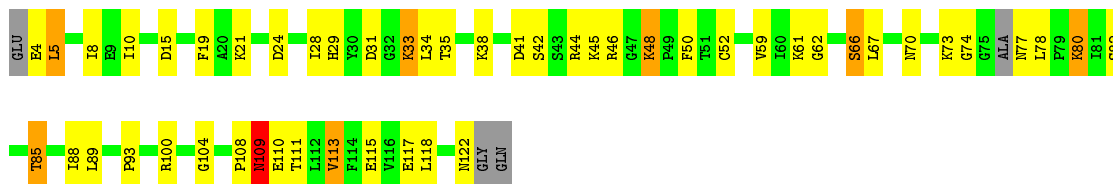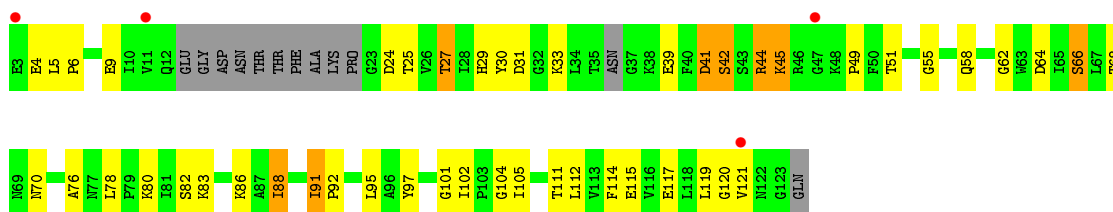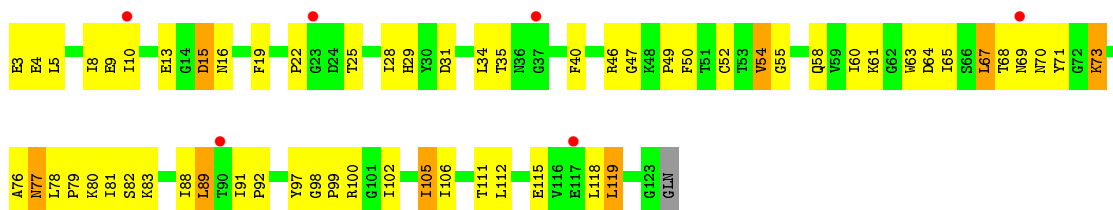- Molecule 1: FK506-binding protein 1
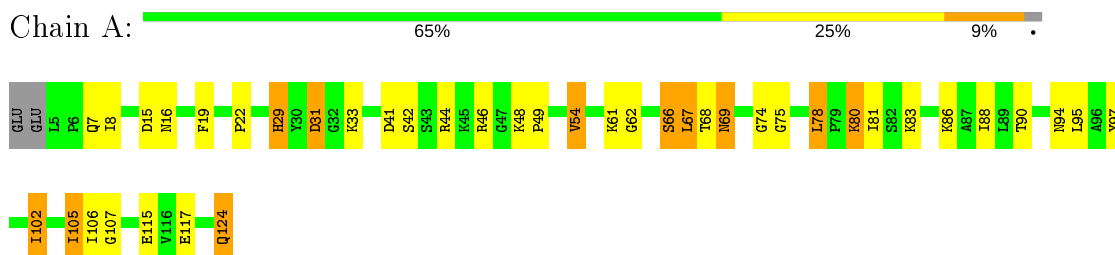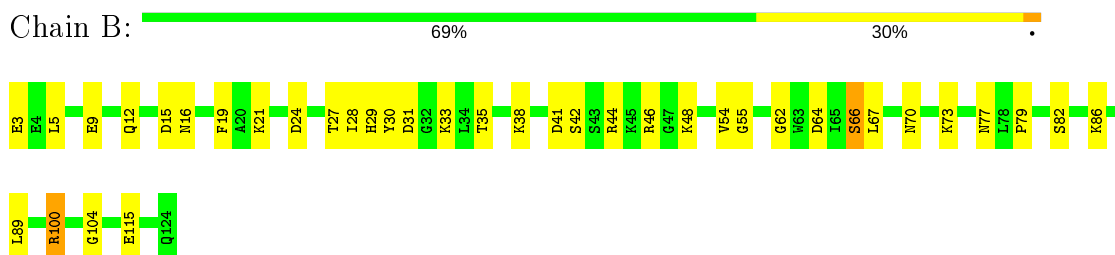
Chain A:

- Molecule 1: FK506-binding protein 1

Chain B:

- Molecule 1: FK506-binding protein 1

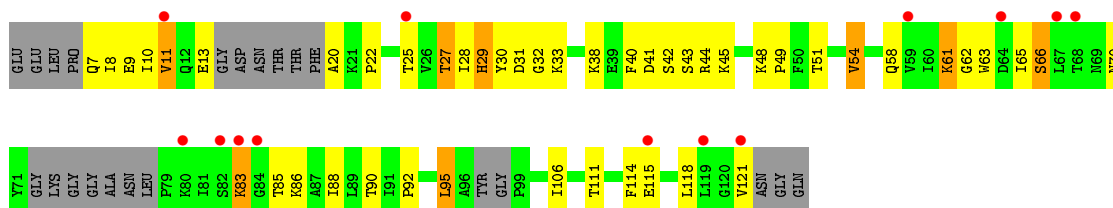Chain C:

- Molecule 1: FK506-binding protein 1

Chain D:

L112 V113 F114 E115 G123 GLN

• Molecule 1: FK506-binding protein 1

Chain E:

56% 34% 6% • •

GLU E4 L5 I8 E9 I10 D15 F19 A20 K21 D24 I28 H29 Y30 D31 G32 K33 L34 T35 K38 D41 S42 S43 R44 K45 R46 G47 K48 P49 F50 T51 C52 V59 I60 K61 G62 S66 L67 N70 K73 G74 G75 ALA N77 L78 P79 K80 I81 S82

T85 I88 L89 P93 R100 G104 P108 N109 E110 T111 L112 V113 F114 E115 V116 E117 L118 N122 GLY GLN

• Molecule 1: FK506-binding protein 1

Chain F:

3%
51% 33% 7% 10%

E3 E4 L5 P6 E9 I10 V11 Q12 GLU GLY ASP ASN THR PHE ALA LYS PRO G23 D24 T25 V26 T27 I28 H29 Y30 D31 G32 K33 L34 T35 ASN G37 K38 E39 F40 D41 S42 S43 R44 K45 R46 G47 K48 P49 F50 T51 G55 Q58 G62 W63 D64 I65 S66 L67 T68

N69 N70 A76 N77 L78 P79 K80 I81 S82 K83 K86 A87 I88 I91 P92 L95 A96 Y97 G101 I102 P103 G104 I105 T111 L112 V113 F114 E115 V116 E117 L118 L119 G120 V121 N122 G123 GLN

• Molecule 1: FK506-binding protein 1

Chain G:

5%
49% 43% 7% •

E3 E4 L5 I8 E9 I10 E13 G14 D15 N16 F19 P22 G23 D24 T25 I28 H29 Y30 D31 L34 T35 N36 G37 F40 R46 G47 K48 P49 F50 T51 C52 V54 G55 Q58 V59 I60 K61 G62 W63 D64 I65 S66 L67 T68 N69 N70 Y71 G72 K73

A76 N77 L78 P79 K80 I81 S82 K83 I88 L89 T90 I91 P92 Y97 G98 P99 R100 G101 I102 I105 I106 T111 L112 V116 E117 L118 L119 G123 GLN

• Molecule 1: FK506-binding protein 1

Chain H:

11%
43% 32% 7% 18%

GLU GLU LEU PRO Q7 I8 E9 I10 V11 Q12 E13 GLY ASP ASN THR THR PHE A20 K21 P22 T25 V26 T27 I28 H29 Y30 D31 G32 K33 K38 E39 F40 D41 S42 S43 R44 K45 K48 P49 F50 T51 V54 Q58 V59 I60 K61 G62 W63 D64 I65 S66 L67 T68 N69 N70

Y71 GLY LYS GLY GLY ALA ASN LEU P79 K80 I81 S82 K83 G84 T85 K86 A87 I88 L89 T90 I91 P92 L95 A96 TYR GLY P99 I106 T111 F114 E115 L118 L119 G120 V121 ASN GLY GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.42Å 84.18Å 116.72Å 90.00° 109.81° 90.00°	Depositor
Resolution (Å)	26.15 – 2.86 47.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (26.15-2.86) 84.1 (47.46-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.24 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.244 , 0.285 0.246 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (7.28%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.9	EDS
L-test for twinning[2]	$<|L|> = 0.45$, $<L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FK5

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	0.40	0/893	0.65	0/1215
1	B	0.36	0/920	0.58	0/1250
1	C	0.39	0/892	0.67	0/1214
1	D	0.39	0/909	0.68	0/1235
1	E	0.49	0/877	0.80	1/1192 (0.1%)
1	F	0.39	0/799	0.76	0/1090
1	G	0.37	0/884	0.73	1/1208 (0.1%)
1	H	0.38	0/727	0.70	0/985
All	All	0.40	0/6901	0.70	2/9389 (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	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	109	ASN	N-CA-C	6.61	128.84	111.00
1	G	89	LEU	CA-CB-CG	6.46	130.17	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	108	PRO	Peptide
1	F	42	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	875	0	872	31	0
1	B	902	0	904	23	0
1	C	874	0	852	26	0
1	D	891	0	898	24	0
1	E	860	0	848	28	0
1	F	785	0	755	33	0
1	G	866	0	832	40	0
1	H	716	0	721	31	0
2	A	57	0	69	3	0
2	B	57	0	69	1	0
2	C	57	0	69	5	0
2	D	57	0	69	3	0
2	E	57	0	69	3	0
2	F	57	0	69	4	0
2	G	57	0	69	3	0
2	H	57	0	69	5	0
3	A	8	0	0	2	0
3	B	7	0	0	2	0
3	C	9	0	0	3	0
3	D	10	0	0	4	0
3	E	6	0	0	4	0
3	F	8	0	0	2	0
3	G	9	0	0	6	0
3	H	7	0	0	0	0
All	All	7289	0	7234	246	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 17.

All (246) 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:G:76:ALA:O	1:G:77:ASN:ND2	1.85	1.10
1:D:107:GLY:O	3:D:301:HOH:O	1.85	0.94
1:F:45:LYS:NZ	3:F:301:HOH:O	2.02	0.92
1:B:3:GLU:OE1	3:B:301:HOH:O	1.93	0.85
1:E:45:LYS:NZ	3:E:301:HOH:O	2.11	0.82
1:A:46:ARG:NH2	3:A:302:HOH:O	2.13	0.81
1:F:92:PRO:HG2	1:F:95:LEU:HD12	1.60	0.81
1:H:7:GLN:N	1:H:90:THR:O	2.14	0.80
1:A:107:GLY:O	3:A:301:HOH:O	2.02	0.77
1:A:80:LYS:HD2	1:A:81:ILE:H	1.50	0.76
1:E:82:SER:O	1:E:85:THR:OG1	2.03	0.75
1:C:64:ASP:O	1:C:68:THR:OG1	2.03	0.74
1:F:64:ASP:O	1:F:68:THR:OG1	2.06	0.73
1:G:3:GLU:HG2	1:G:4:GLU:HA	1.70	0.73
1:D:115:GLU:OE1	3:D:302:HOH:O	2.08	0.70
1:H:48:LYS:HB3	1:H:49:PRO:HD2	1.74	0.70
1:F:41:ASP:HB3	1:F:42:SER:HB3	1.74	0.69
1:B:31:ASP:OD2	1:B:44:ARG:NH1	2.26	0.69
1:B:104:GLY:HA2	1:E:48:LYS:HB2	1.75	0.68
1:C:109:ASN:O	1:C:109:ASN:ND2	2.27	0.68
1:C:62:GLY:O	1:C:66:SER:OG	2.13	0.67
1:G:80:LYS:O	3:G:301:HOH:O	2.12	0.67
1:H:61:LYS:HB3	1:H:95:LEU:HD23	1.77	0.67
1:H:31:ASP:OD1	1:H:115:GLU:HB3	1.95	0.67
1:B:100:ARG:HD2	1:F:101:GLY:O	1.95	0.67
1:H:62:GLY:O	1:H:66:SER:OG	2.12	0.66
1:B:54:VAL:HG11	1:B:67:LEU:HD23	1.78	0.65
1:H:92:PRO:HA	1:H:111:THR:HG23	1.79	0.65
1:C:9:GLU:HB3	1:C:88:ILE:HB	1.78	0.65
1:F:5:LEU:HD11	1:F:76:ALA:HB1	1.77	0.65
1:F:104:GLY:O	1:G:47:GLY:HA2	1.96	0.65
1:A:19:PHE:CD1	1:A:80:LYS:HG3	2.31	0.64
1:D:86:LYS:NZ	3:D:303:HOH:O	2.25	0.64
1:E:41:ASP:OD2	3:E:302:HOH:O	2.14	0.63
1:E:70:ASN:HB3	1:E:74:GLY:HA3	1.80	0.63
1:C:73:LYS:NZ	3:C:304:HOH:O	2.30	0.62
1:A:19:PHE:HD1	1:A:80:LYS:HG3	1.63	0.62
1:B:62:GLY:O	1:B:66:SER:OG	2.18	0.62
1:D:62:GLY:O	1:D:66:SER:OG	2.15	0.62
1:D:70:ASN:O	1:D:70:ASN:ND2	2.31	0.61
1:G:76:ALA:C	1:G:77:ASN:HD22	1.95	0.61
1:B:41:ASP:OD1	1:B:46:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PRO:O	1:C:108:PRO:HB3	2.01	0.61
1:A:69:ASN:HD21	1:A:74:GLY:HA2	1.67	0.60
1:D:13:GLU:OE2	1:D:16:ASN:ND2	2.35	0.60
1:E:15:ASP:O	1:E:82:SER:OG	2.15	0.60
1:F:9:GLU:HB3	1:F:88:ILE:HG23	1.82	0.60
1:G:19:PHE:CE1	1:G:82:SER:HB3	2.36	0.60
1:H:10:ILE:CG2	1:H:13:GLU:HB2	2.32	0.60
1:A:105:ILE:HB	1:A:106:ILE:HD12	1.83	0.59
1:F:55:GLY:N	1:F:64:ASP:OD1	2.23	0.59
1:A:69:ASN:O	1:A:69:ASN:ND2	2.30	0.59
1:D:64:ASP:O	1:D:68:THR:OG1	2.18	0.58
1:B:12:GLN:OE1	1:B:86:LYS:NZ	2.36	0.58
2:C:201:FK5:H20	2:H:201:FK5:H431	1.86	0.58
1:C:109:ASN:OD1	3:C:301:HOH:O	2.17	0.58
1:G:31:ASP:OD1	1:G:31:ASP:N	2.37	0.58
1:B:48:LYS:HD2	1:E:104:GLY:HA2	1.85	0.58
1:E:80:LYS:NZ	1:E:80:LYS:HB2	2.19	0.58
1:A:97:TYR:CE1	1:A:102:ILE:HD11	2.39	0.57
1:G:55:GLY:N	1:G:64:ASP:OD1	2.23	0.57
1:H:27:THR:HG23	1:H:51:THR:HB	1.86	0.57
1:A:94:ASN:O	1:A:95:LEU:HB2	2.05	0.57
1:A:69:ASN:ND2	1:A:74:GLY:HA2	2.20	0.57
1:C:30:TYR:OH	1:C:41:ASP:OD2	2.12	0.56
1:D:33:LYS:HD2	1:D:37:GLY:HA2	1.86	0.56
2:H:201:FK5:H62	2:H:201:FK5:H411	1.86	0.56
1:G:61:LYS:HG3	3:G:306:HOH:O	2.04	0.56
1:D:70:ASN:O	1:D:72:GLY:N	2.38	0.56
1:F:62:GLY:HA3	1:F:91:ILE:HD13	1.88	0.56
1:H:29:HIS:CE1	1:H:44:ARG:HA	2.42	0.55
1:G:102:ILE:HD12	1:G:106:ILE:HG13	1.88	0.55
1:F:4:GLU:O	1:F:5:LEU:HD23	2.07	0.55
1:G:46:ARG:NH2	1:G:49:PRO:HG3	2.21	0.55
1:A:41:ASP:OD1	1:A:42:SER:N	2.39	0.55
1:F:30:TYR:HA	1:F:115:GLU:O	2.07	0.55
1:H:11:VAL:HG12	1:H:86:LYS:HB2	1.89	0.55
1:G:3:GLU:HB3	1:G:4:GLU:HG2	1.90	0.54
1:C:36:ASN:OD1	1:C:38:LYS:HG3	2.07	0.54
1:C:36:ASN:OD1	1:C:38:LYS:N	2.38	0.54
1:F:41:ASP:CB	1:F:42:SER:HB3	2.38	0.54
1:H:63:TRP:HZ2	1:H:114:PHE:CD1	2.25	0.54
1:H:32:GLY:N	1:H:41:ASP:O	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ARG:CZ	3:G:304:HOH:O	2.55	0.54
1:D:46:ARG:HH11	1:D:46:ARG:HG3	1.73	0.54
1:G:97:TYR:OH	2:G:201:FK5:O3	2.12	0.54
1:E:46:ARG:NH2	3:E:302:HOH:O	2.41	0.53
1:E:19:PHE:CE1	1:E:80:LYS:HD2	2.42	0.53
1:H:10:ILE:HG21	1:H:13:GLU:HB2	1.89	0.53
1:C:5:LEU:HG	1:C:6:PRO:HD2	1.90	0.53
1:H:20:ALA:HB2	1:H:121:VAL:HG21	1.90	0.53
1:F:58:GLN:NE2	3:F:303:HOH:O	2.42	0.52
1:E:62:GLY:O	1:E:66:SER:OG	2.25	0.52
1:A:80:LYS:HD2	1:A:81:ILE:N	2.23	0.52
1:F:6:PRO:HD3	1:F:95:LEU:HD13	1.92	0.52
1:C:31:ASP:OD1	1:C:33:LYS:HE3	2.10	0.52
1:G:54:VAL:HG11	1:G:67:LEU:HD23	1.92	0.52
1:E:4:GLU:O	1:E:5:LEU:HD13	2.10	0.51
1:D:44:ARG:NH1	3:D:303:HOH:O	2.39	0.51
1:G:68:THR:HG22	1:G:71:TYR:H	1.75	0.51
1:E:21:LYS:N	1:E:24:ASP:OD2	2.38	0.51
1:A:62:GLY:O	1:A:66:SER:OG	2.28	0.51
1:A:69:ASN:HB2	1:A:80:LYS:HD3	1.92	0.51
1:C:30:TYR:HA	1:C:115:GLU:O	2.10	0.51
1:H:31:ASP:HA	1:H:42:SER:HA	1.93	0.51
1:F:33:LYS:HA	1:F:39:GLU:HA	1.92	0.51
1:A:15:ASP:OD1	1:A:16:ASN:N	2.44	0.51
1:F:97:TYR:OH	2:F:201:FK5:O3	2.14	0.50
1:E:93:PRO:HB3	1:E:109:ASN:HB3	1.93	0.50
1:F:112:LEU:HD23	1:F:114:PHE:CZ	2.47	0.50
1:G:15:ASP:OD1	1:G:16:ASN:N	2.44	0.50
1:D:15:ASP:OD1	1:D:16:ASN:N	2.45	0.50
1:A:67:LEU:O	1:A:80:LYS:HE3	2.12	0.50
1:B:55:GLY:O	1:C:22:PRO:HG2	2.11	0.50
1:F:62:GLY:O	1:F:66:SER:OG	2.28	0.50
1:C:94:ASN:OD1	1:C:94:ASN:N	2.39	0.49
1:G:111:THR:O	3:G:302:HOH:O	2.19	0.49
1:G:28:ILE:HD12	1:G:63:TRP:CZ3	2.47	0.49
1:H:31:ASP:CB	1:H:42:SER:HB2	2.42	0.49
1:H:31:ASP:OD2	1:H:33:LYS:HE3	2.11	0.49
1:C:109:ASN:HB3	3:C:301:HOH:O	2.13	0.49
1:E:46:ARG:NH1	3:E:302:HOH:O	2.45	0.49
1:G:100:ARG:NH2	3:G:304:HOH:O	2.44	0.49
1:B:19:PHE:CE1	1:B:82:SER:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:GLN:O	2:H:201:FK5:O10	2.24	0.49
1:E:80:LYS:HZ3	1:E:80:LYS:HB2	1.76	0.49
1:F:5:LEU:CD1	1:F:76:ALA:HB1	2.40	0.49
1:C:27:THR:HG22	1:C:51:THR:HG23	1.95	0.48
1:D:70:ASN:HD22	1:D:70:ASN:C	2.16	0.48
1:G:50:PHE:CE2	1:G:52:CYS:HB3	2.48	0.48
1:D:73:LYS:O	1:D:73:LYS:HD3	2.13	0.48
1:G:31:ASP:OD1	1:G:115:GLU:HB3	2.13	0.48
1:H:30:TYR:CE2	1:H:43:SER:HB3	2.49	0.48
1:C:18:THR:HG23	1:D:35:THR:O	2.14	0.48
1:H:92:PRO:HG2	1:H:95:LEU:HD12	1.96	0.48
1:D:33:LYS:HE3	1:D:113:VAL:HG11	1.95	0.47
1:C:81:ILE:HG22	1:C:118:LEU:HD12	1.96	0.47
1:C:29:HIS:HB3	1:C:44:ARG:NH1	2.29	0.47
2:E:201:FK5:H421	2:E:201:FK5:H29	1.72	0.47
1:B:77:ASN:O	1:B:79:PRO:HD3	2.14	0.47
1:E:77:ASN:HB3	1:E:78:LEU:CA	2.45	0.47
1:E:33:LYS:HG3	1:E:113:VAL:HG23	1.96	0.47
1:B:64:ASP:OD2	3:B:302:HOH:O	2.20	0.47
1:A:75:GLY:HA3	1:A:78:LEU:HD12	1.95	0.47
1:E:44:ARG:C	1:E:46:ARG:H	2.18	0.47
1:F:83:LYS:HD2	1:F:120:GLY:HA3	1.95	0.47
1:C:93:PRO:HD3	1:C:111:THR:HG22	1.96	0.47
2:D:201:FK5:H442	2:D:201:FK5:H162	1.73	0.46
1:G:97:TYR:CE1	1:G:102:ILE:HD11	2.50	0.46
1:A:48:LYS:HD3	1:D:104:GLY:HA2	1.98	0.46
1:F:29:HIS:CE1	1:F:49:PRO:HA	2.51	0.46
1:F:29:HIS:HE1	1:F:49:PRO:HG3	1.81	0.46
1:G:65:ILE:O	1:G:68:THR:O	2.34	0.46
1:H:61:LYS:HB3	1:H:95:LEU:CD2	2.45	0.46
1:G:10:ILE:HD11	1:G:79:PRO:CB	2.46	0.46
2:E:201:FK5:H371	2:E:201:FK5:H21	1.72	0.46
1:F:97:TYR:CE1	1:F:102:ILE:HD11	2.52	0.45
1:G:91:ILE:HA	1:G:92:PRO:HD2	1.82	0.45
1:H:28:ILE:HD13	1:H:118:LEU:HA	1.97	0.45
1:H:22:PRO:O	1:H:54:VAL:O	2.34	0.45
1:G:70:ASN:O	1:G:73:LYS:HG3	2.16	0.45
1:C:86:LYS:HG3	1:C:117:GLU:HG3	1.99	0.45
1:H:13:GLU:HA	1:H:85:THR:HG23	1.99	0.45
1:D:15:ASP:O	1:D:16:ASN:HB2	2.16	0.45
1:E:34:LEU:HD12	1:E:38:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:HD3	1:F:102:ILE:HG12	1.98	0.45
1:B:31:ASP:OD1	1:B:42:SER:OG	2.23	0.45
1:H:30:TYR:HA	1:H:115:GLU:O	2.16	0.45
2:A:201:FK5:H371	2:A:201:FK5:H21	1.61	0.45
1:A:22:PRO:HD3	1:A:68:THR:HB	1.97	0.45
1:E:31:ASP:OD1	1:E:42:SER:OG	2.35	0.44
1:F:27:THR:HG22	1:F:49:PRO:HB2	2.00	0.44
1:G:22:PRO:HG3	1:G:68:THR:HG21	1.98	0.44
1:A:83:LYS:HD2	1:A:124:GLN:HG3	1.98	0.44
1:E:122:ASN:HB3	1:G:46:ARG:HH11	1.82	0.44
1:E:70:ASN:CB	1:E:74:GLY:HA3	2.46	0.44
2:F:201:FK5:H421	2:F:201:FK5:H29	1.71	0.44
1:A:29:HIS:NE2	1:A:49:PRO:HG3	2.32	0.44
1:A:31:ASP:OD1	1:A:31:ASP:N	2.51	0.44
1:D:41:ASP:OD1	1:D:42:SER:N	2.50	0.44
2:A:201:FK5:H15	2:A:201:FK5:H362	1.77	0.44
2:H:201:FK5:H161	2:H:201:FK5:H13	1.65	0.44
1:H:31:ASP:HB3	1:H:42:SER:HB2	2.00	0.44
2:C:201:FK5:H362	2:C:201:FK5:H15	1.82	0.44
1:C:108:PRO:HA	1:C:109:ASN:HA	1.58	0.44
1:D:101:GLY:O	1:E:100:ARG:HD2	2.18	0.44
2:A:201:FK5:H232	2:A:201:FK5:H413	1.70	0.43
1:B:30:TYR:OH	1:B:41:ASP:OD2	2.29	0.43
1:F:44:ARG:NH1	1:F:44:ARG:HB2	2.33	0.43
1:G:60:ILE:HA	3:G:306:HOH:O	2.17	0.43
1:A:7:GLN:HB2	1:A:90:THR:HB	2.00	0.43
1:A:97:TYR:CD1	1:A:102:ILE:HD11	2.52	0.43
2:C:201:FK5:H29	2:C:201:FK5:H421	1.74	0.43
2:F:201:FK5:H21	2:F:201:FK5:H371	1.81	0.43
1:D:97:TYR:CE1	1:D:102:ILE:HD11	2.54	0.43
1:H:61:LYS:O	1:H:65:ILE:HG13	2.18	0.43
1:F:105:ILE:HD11	2:G:201:FK5:H181	2.00	0.43
1:F:30:TYR:O	1:F:42:SER:OG	2.37	0.43
1:G:19:PHE:HD1	1:G:81:ILE:O	2.01	0.43
1:H:40:PHE:CD1	1:H:41:ASP:N	2.87	0.43
1:H:48:LYS:HB3	1:H:49:PRO:CD	2.44	0.43
2:C:201:FK5:H371	2:C:201:FK5:H21	1.73	0.42
1:B:21:LYS:N	1:B:24:ASP:OD2	2.46	0.42
2:E:201:FK5:H232	2:E:201:FK5:H413	1.81	0.42
1:F:83:LYS:HG3	1:F:120:GLY:CA	2.49	0.42
1:G:8:ILE:HG21	1:G:81:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:PHE:CE2	1:E:52:CYS:HB3	2.54	0.42
1:A:88:ILE:HG12	1:A:115:GLU:HG2	2.01	0.42
2:F:201:FK5:C18	1:G:105:ILE:HD11	2.49	0.42
1:A:49:PRO:HG2	1:B:27:THR:HG21	2.01	0.42
1:B:30:TYR:HA	1:B:115:GLU:O	2.20	0.42
1:G:78:LEU:HA	1:G:79:PRO:HD2	1.90	0.42
1:A:61:LYS:HB2	1:A:95:LEU:HA	2.02	0.42
1:C:103:PRO:HA	1:C:104:GLY:HA2	1.74	0.42
1:F:92:PRO:CG	1:F:95:LEU:HD12	2.42	0.42
2:G:201:FK5:H232	2:G:201:FK5:H413	1.82	0.42
1:E:77:ASN:HB3	1:E:78:LEU:CB	2.50	0.42
1:D:34:LEU:HD22	1:D:110:GLU:HG3	2.02	0.42
1:G:97:TYR:CZ	1:G:102:ILE:HD11	2.54	0.42
1:H:106:ILE:O	1:H:106:ILE:HG13	2.20	0.42
1:B:70:ASN:O	1:B:73:LYS:HB2	2.20	0.41
1:B:15:ASP:O	1:B:16:ASN:HB2	2.20	0.41
2:B:201:FK5:H14	2:B:201:FK5:H442	1.83	0.41
1:C:99:PRO:HD2	1:C:100:ARG:H	1.85	0.41
1:E:28:ILE:HG23	1:E:117:GLU:O	2.21	0.41
1:F:86:LYS:HA	1:F:117:GLU:HA	2.01	0.41
1:B:28:ILE:HD11	1:B:67:LEU:HD21	2.02	0.41
1:G:3:GLU:CG	1:G:4:GLU:HA	2.44	0.41
1:H:83:LYS:HE2	1:H:83:LYS:HB3	1.84	0.41
1:A:54:VAL:HG11	1:A:67:LEU:HD23	2.02	0.41
2:D:201:FK5:O7	2:D:201:FK5:H161	2.20	0.41
1:E:8:ILE:HD11	1:E:66:SER:HB3	2.02	0.41
1:A:86:LYS:HG2	1:A:117:GLU:HG3	2.03	0.41
1:G:119:LEU:HD12	1:G:119:LEU:HA	1.87	0.41
1:G:40:PHE:CE2	1:G:112:LEU:HD22	2.55	0.41
1:A:8:ILE:HD11	1:A:66:SER:HB3	2.03	0.41
1:B:15:ASP:OD1	1:B:16:ASN:N	2.54	0.41
1:D:56:VAL:HG23	1:D:58:GLN:HB2	2.02	0.41
1:G:28:ILE:HG12	1:G:118:LEU:HD12	2.03	0.41
2:H:201:FK5:H29	2:H:201:FK5:H421	1.87	0.41
1:D:19:PHE:CE1	1:D:82:SER:HB3	2.56	0.41
1:G:98:GLY:HA3	1:G:99:PRO:HD2	1.88	0.41
2:D:201:FK5:H443	2:D:201:FK5:H14	1.69	0.40
1:F:31:ASP:HA	1:F:42:SER:OG	2.21	0.40
2:C:201:FK5:H62	2:C:201:FK5:H411	2.03	0.40
1:C:91:ILE:HA	1:C:92:PRO:HD2	1.97	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	118/122 (97%)	113 (96%)	5 (4%)	0	100	100
1	B	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	C	119/122 (98%)	113 (95%)	5 (4%)	1 (1%)	19	46
1	D	118/122 (97%)	113 (96%)	5 (4%)	0	100	100
1	E	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
1	F	104/122 (85%)	100 (96%)	4 (4%)	0	100	100
1	G	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
1	H	92/122 (75%)	90 (98%)	2 (2%)	0	100	100
All	All	904/976 (93%)	873 (97%)	30 (3%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	103	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/100 (92%)	79 (86%)	13 (14%)	3	9
1	B	96/100 (96%)	87 (91%)	9 (9%)	8	23
1	C	90/100 (90%)	74 (82%)	16 (18%)	2	4
1	D	96/100 (96%)	87 (91%)	9 (9%)	8	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	E	89/100 (89%)	68 (76%)	21 (24%)		1	1
1	F	80/100 (80%)	63 (79%)	17 (21%)		1	2
1	G	88/100 (88%)	69 (78%)	19 (22%)		1	2
1	H	75/100 (75%)	60 (80%)	15 (20%)		1	3
All	All	706/800 (88%)	587 (83%)	119 (17%)		2	5

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	31	ASP
1	A	33	LYS
1	A	44	ARG
1	A	54	VAL
1	A	66	SER
1	A	67	LEU
1	A	69	ASN
1	A	78	LEU
1	A	80	LYS
1	A	102	ILE
1	A	105	ILE
1	A	124	GLN
1	B	5	LEU
1	B	9	GLU
1	B	29	HIS
1	B	33	LYS
1	B	35	THR
1	B	38	LYS
1	B	66	SER
1	B	89	LEU
1	B	100	ARG
1	C	11	VAL
1	C	13	GLU
1	C	21	LYS
1	C	29	HIS
1	C	33	LYS
1	C	34	LEU
1	C	35	THR
1	C	54	VAL
1	C	66	SER
1	C	82	SER

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Mol	Chain	Res	Type
1	C	83	LYS
1	C	94	ASN
1	C	109	ASN
1	C	113	VAL
1	C	118	LEU
1	C	121	VAL
1	D	12	GLN
1	D	29	HIS
1	D	31	ASP
1	D	33	LYS
1	D	45	LYS
1	D	66	SER
1	D	70	ASN
1	D	102	ILE
1	D	111	THR
1	E	5	LEU
1	E	10	ILE
1	E	29	HIS
1	E	33	LYS
1	E	35	THR
1	E	48	LYS
1	E	59	VAL
1	E	61	LYS
1	E	66	SER
1	E	67	LEU
1	E	73	LYS
1	E	80	LYS
1	E	85	THR
1	E	88	ILE
1	E	89	LEU
1	E	109	ASN
1	E	110	GLU
1	E	111	THR
1	E	113	VAL
1	E	115	GLU
1	E	118	LEU
1	F	24	ASP
1	F	25	THR
1	F	27	THR
1	F	41	ASP
1	F	44	ARG
1	F	45	LYS

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Mol	Chain	Res	Type
1	F	51	THR
1	F	66	SER
1	F	70	ASN
1	F	78	LEU
1	F	80	LYS
1	F	82	SER
1	F	88	ILE
1	F	91	ILE
1	F	111	THR
1	F	119	LEU
1	F	121	VAL
1	G	5	LEU
1	G	9	GLU
1	G	13	GLU
1	G	15	ASP
1	G	25	THR
1	G	29	HIS
1	G	34	LEU
1	G	35	THR
1	G	54	VAL
1	G	58	GLN
1	G	67	LEU
1	G	69	ASN
1	G	73	LYS
1	G	77	ASN
1	G	83	LYS
1	G	88	ILE
1	G	89	LEU
1	G	105	ILE
1	G	119	LEU
1	H	8	ILE
1	H	9	GLU
1	H	11	VAL
1	H	25	THR
1	H	27	THR
1	H	29	HIS
1	H	38	LYS
1	H	45	LYS
1	H	54	VAL
1	H	61	LYS
1	H	66	SER
1	H	70	ASN

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Mol	Chain	Res	Type
1	H	83	LYS
1	H	88	ILE
1	H	95	LEU

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

Mol	Chain	Res	Type
1	C	109	ASN
1	D	16	ASN
1	E	109	ASN
1	F	29	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	FK5	E	201	-	54,60,60	3.49	10 (18%)	64,86,86	1.89	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|>2$	Counts	RMSZ	#$|Z|>2$
2	FK5	H	201	-	54,60,60	3.66	11 (20%)	64,86,86	1.34	7 (10%)
2	FK5	A	201	-	54,60,60	3.54	11 (20%)	64,86,86	2.09	13 (20%)
2	FK5	G	201	-	54,60,60	3.58	11 (20%)	64,86,86	1.54	11 (17%)
2	FK5	C	201	-	54,60,60	3.57	11 (20%)	64,86,86	1.98	14 (21%)
2	FK5	F	201	-	54,60,60	3.55	10 (18%)	64,86,86	1.88	16 (25%)
2	FK5	D	201	-	54,60,60	3.60	11 (20%)	64,86,86	1.96	16 (25%)
2	FK5	B	201	-	54,60,60	3.59	11 (20%)	64,86,86	1.67	9 (14%)

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	FK5	E	201	-	-	6/68/114/114	0/3/4/4
2	FK5	H	201	-	-	12/68/114/114	0/3/4/4
2	FK5	A	201	-	-	6/68/114/114	0/3/4/4
2	FK5	G	201	-	-	2/68/114/114	0/3/4/4
2	FK5	C	201	-	-	9/68/114/114	0/3/4/4
2	FK5	F	201	-	-	7/68/114/114	0/3/4/4
2	FK5	D	201	-	-	20/68/114/114	0/3/4/4
2	FK5	B	201	-	-	11/68/114/114	0/3/4/4

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	FK5	O9-C22	11.91	1.42	1.21
2	G	201	FK5	O9-C22	11.79	1.42	1.21
2	D	201	FK5	C8-C9	-11.68	1.38	1.53
2	B	201	FK5	O9-C22	11.57	1.41	1.21
2	D	201	FK5	O9-C22	11.57	1.41	1.21
2	F	201	FK5	O9-C22	11.48	1.41	1.21
2	C	201	FK5	O9-C22	11.32	1.41	1.21
2	H	201	FK5	C8-C9	-11.25	1.39	1.53
2	A	201	FK5	O9-C22	11.21	1.41	1.21
2	C	201	FK5	O4-C9	11.18	1.42	1.22
2	E	201	FK5	O9-C22	11.12	1.40	1.21
2	B	201	FK5	C8-C9	-11.01	1.39	1.53
2	A	201	FK5	O4-C9	10.88	1.41	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	FK5	O4-C9	10.87	1.41	1.22
2	E	201	FK5	O4-C9	10.85	1.41	1.22
2	G	201	FK5	C8-C9	-10.81	1.39	1.53
2	A	201	FK5	C8-C9	-10.74	1.39	1.53
2	B	201	FK5	O4-C9	10.70	1.41	1.22
2	F	201	FK5	O4-C9	10.69	1.41	1.22
2	G	201	FK5	O4-C9	10.68	1.41	1.22
2	D	201	FK5	O4-C9	10.66	1.41	1.22
2	E	201	FK5	C8-C9	-10.63	1.40	1.53
2	F	201	FK5	C8-C9	-10.55	1.40	1.53
2	C	201	FK5	C8-C9	-10.45	1.40	1.53
2	H	201	FK5	C20-C19	9.74	1.48	1.33
2	F	201	FK5	C20-C19	9.61	1.48	1.33
2	B	201	FK5	C20-C19	9.41	1.47	1.33
2	C	201	FK5	C20-C19	9.37	1.47	1.33
2	G	201	FK5	C20-C19	9.34	1.47	1.33
2	A	201	FK5	C20-C19	9.26	1.47	1.33
2	D	201	FK5	C20-C19	9.24	1.47	1.33
2	G	201	FK5	O3-C8	8.82	1.41	1.23
2	C	201	FK5	O3-C8	8.81	1.41	1.23
2	E	201	FK5	O3-C8	8.72	1.41	1.23
2	H	201	FK5	O3-C8	8.68	1.41	1.23
2	D	201	FK5	O3-C8	8.64	1.41	1.23
2	F	201	FK5	O3-C8	8.56	1.41	1.23
2	E	201	FK5	C20-C19	8.55	1.46	1.33
2	B	201	FK5	O3-C8	8.53	1.41	1.23
2	A	201	FK5	O3-C8	8.49	1.41	1.23
2	A	201	FK5	O2-C1	8.38	1.42	1.21
2	F	201	FK5	O2-C1	8.25	1.41	1.21
2	B	201	FK5	O2-C1	8.24	1.41	1.21
2	E	201	FK5	O2-C1	8.12	1.41	1.21
2	G	201	FK5	O2-C1	8.08	1.41	1.21
2	D	201	FK5	O2-C1	8.02	1.41	1.21
2	H	201	FK5	O2-C1	8.01	1.41	1.21
2	C	201	FK5	O2-C1	7.87	1.41	1.21
2	H	201	FK5	C28-C27	7.10	1.48	1.33
2	C	201	FK5	C28-C27	6.99	1.48	1.33
2	B	201	FK5	C28-C27	6.69	1.47	1.33
2	G	201	FK5	C28-C27	6.66	1.47	1.33
2	E	201	FK5	C28-C27	6.64	1.47	1.33
2	D	201	FK5	C28-C27	6.56	1.47	1.33
2	F	201	FK5	C28-C27	6.49	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	FK5	C28-C27	6.43	1.47	1.33
2	B	201	FK5	O6-C10	4.00	1.46	1.39
2	H	201	FK5	O1-C1	-3.64	1.25	1.34
2	G	201	FK5	O6-C10	3.63	1.45	1.39
2	C	201	FK5	O1-C1	-3.63	1.25	1.34
2	F	201	FK5	O6-C10	3.62	1.45	1.39
2	D	201	FK5	O6-C10	3.56	1.45	1.39
2	D	201	FK5	O1-C1	-3.50	1.26	1.34
2	C	201	FK5	O6-C10	3.49	1.45	1.39
2	F	201	FK5	O1-C1	-3.47	1.26	1.34
2	E	201	FK5	O1-C1	-3.45	1.26	1.34
2	B	201	FK5	O1-C1	-3.42	1.26	1.34
2	G	201	FK5	O1-C1	-3.37	1.26	1.34
2	A	201	FK5	O1-C1	-3.31	1.26	1.34
2	H	201	FK5	O6-C10	3.27	1.44	1.39
2	A	201	FK5	O6-C10	3.24	1.44	1.39
2	E	201	FK5	C40-C39	2.87	1.48	1.28
2	B	201	FK5	C40-C39	2.87	1.48	1.28
2	G	201	FK5	C40-C39	2.86	1.47	1.28
2	F	201	FK5	C40-C39	2.85	1.47	1.28
2	D	201	FK5	C40-C39	2.81	1.47	1.28
2	H	201	FK5	C40-C39	2.78	1.47	1.28
2	C	201	FK5	C40-C39	2.74	1.47	1.28
2	A	201	FK5	C40-C39	2.73	1.47	1.28
2	E	201	FK5	O6-C10	2.56	1.43	1.39
2	G	201	FK5	O5-C14	-2.24	1.40	1.44
2	H	201	FK5	O5-C14	-2.20	1.40	1.44
2	C	201	FK5	O5-C14	-2.18	1.40	1.44
2	A	201	FK5	O5-C14	-2.10	1.40	1.44
2	B	201	FK5	O5-C14	-2.08	1.40	1.44
2	D	201	FK5	O5-C14	-2.02	1.40	1.44

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	FK5	C21-C20-C19	-10.57	116.81	127.64
2	E	201	FK5	C21-C20-C19	-9.27	118.14	127.64
2	C	201	FK5	C21-C20-C19	-8.10	119.34	127.64
2	F	201	FK5	C21-C20-C19	-7.67	119.78	127.64
2	D	201	FK5	C21-C20-C19	-7.66	119.79	127.64
2	B	201	FK5	C21-C20-C19	-7.35	120.10	127.64
2	C	201	FK5	O1-C1-C2	5.84	123.64	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201	FK5	C12-C11-C10	5.38	115.80	110.47
2	D	201	FK5	O1-C1-C2	5.09	122.00	110.78
2	E	201	FK5	O1-C1-C2	5.05	121.91	110.78
2	G	201	FK5	C21-C20-C19	-4.99	122.53	127.64
2	F	201	FK5	O1-C1-C2	4.94	121.66	110.78
2	B	201	FK5	O1-C26-C25	4.94	111.57	105.91
2	G	201	FK5	O1-C1-C2	4.88	121.53	110.78
2	H	201	FK5	O1-C1-C2	4.51	120.72	110.78
2	F	201	FK5	C12-C11-C10	4.41	114.84	110.47
2	B	201	FK5	O1-C1-C2	4.27	120.18	110.78
2	H	201	FK5	C21-C20-C19	-4.21	123.32	127.64
2	D	201	FK5	O1-C26-C25	4.21	110.73	105.91
2	A	201	FK5	C12-C11-C10	3.90	114.33	110.47
2	A	201	FK5	O1-C1-C2	3.88	119.33	110.78
2	F	201	FK5	O1-C26-C25	3.79	110.25	105.91
2	C	201	FK5	O1-C26-C25	3.74	110.20	105.91
2	A	201	FK5	O9-C22-C21	-3.62	117.39	121.13
2	E	201	FK5	O1-C26-C25	3.50	109.92	105.91
2	D	201	FK5	C15-C14-C13	3.48	118.90	113.57
2	G	201	FK5	O1-C26-C25	3.44	109.86	105.91
2	C	201	FK5	O1-C1-O2	-3.40	117.58	123.94
2	D	201	FK5	C17-C16-C15	-3.31	109.75	115.45
2	D	201	FK5	O4-C9-C8	-3.24	115.43	119.08
2	D	201	FK5	O9-C22-C21	-3.21	117.82	121.13
2	A	201	FK5	C42-C27-C26	3.09	121.02	115.68
2	E	201	FK5	O1-C1-O2	-2.79	118.73	123.94
2	F	201	FK5	O3-C8-C9	2.76	120.82	116.28
2	A	201	FK5	C23-C22-C21	2.76	121.29	117.75
2	D	201	FK5	C16-C17-C18	-2.72	107.34	111.57
2	E	201	FK5	C37-C19-C18	2.71	121.92	115.27
2	D	201	FK5	O2-C1-C2	-2.69	118.43	124.49
2	H	201	FK5	O1-C1-O2	-2.60	119.07	123.94
2	C	201	FK5	C3-C2-N7	-2.60	106.91	110.53
2	E	201	FK5	C37-C19-C20	-2.60	118.65	123.78
2	F	201	FK5	C9-C8-N7	2.58	122.20	119.25
2	C	201	FK5	O9-C22-C21	-2.58	118.47	121.13
2	F	201	FK5	O1-C1-O2	-2.57	119.14	123.94
2	G	201	FK5	O9-C22-C23	-2.56	117.96	121.41
2	G	201	FK5	O5-C14-C13	-2.56	105.66	109.42
2	C	201	FK5	C42-C27-C26	2.56	120.10	115.68
2	C	201	FK5	C37-C19-C20	-2.55	118.74	123.78
2	C	201	FK5	O2-C1-C2	-2.54	118.78	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	FK5	C16-C15-C14	2.53	118.19	113.34
2	F	201	FK5	C6-N7-C2	2.52	121.11	115.80
2	A	201	FK5	C34-C29-C28	-2.52	107.74	111.14
2	E	201	FK5	C5-C6-N7	-2.48	106.79	110.67
2	H	201	FK5	C6-N7-C2	2.47	121.00	115.80
2	F	201	FK5	O3-C8-N7	-2.45	116.98	122.15
2	C	201	FK5	C30-C29-C34	2.43	111.44	108.66
2	G	201	FK5	O2-C1-C2	-2.42	119.05	124.49
2	G	201	FK5	O1-C1-O2	-2.42	119.42	123.94
2	G	201	FK5	C24-C23-C22	-2.42	108.70	114.19
2	A	201	FK5	C37-C19-C20	-2.41	119.02	123.78
2	B	201	FK5	O1-C1-O2	-2.40	119.45	123.94
2	D	201	FK5	C42-C27-C26	2.37	119.78	115.68
2	D	201	FK5	C9-C8-N7	2.36	121.95	119.25
2	F	201	FK5	O2-C1-C2	-2.35	119.20	124.49
2	D	201	FK5	O1-C1-O2	-2.34	119.57	123.94
2	A	201	FK5	C3-C2-N7	-2.32	107.30	110.53
2	D	201	FK5	C34-C29-C28	-2.30	108.05	111.14
2	A	201	FK5	C5-C6-N7	-2.30	107.07	110.67
2	F	201	FK5	C42-C27-C26	2.29	119.65	115.68
2	D	201	FK5	C23-C22-C21	2.29	120.69	117.75
2	H	201	FK5	O3-C8-C9	2.29	120.04	116.28
2	B	201	FK5	O3-C8-C9	2.28	120.04	116.28
2	E	201	FK5	O2-C1-C2	-2.28	119.36	124.49
2	E	201	FK5	C9-C8-N7	2.27	121.84	119.25
2	A	201	FK5	O1-C26-C25	2.26	108.50	105.91
2	A	201	FK5	C6-N7-C2	2.23	120.50	115.80
2	E	201	FK5	C12-C11-C10	2.20	112.65	110.47
2	C	201	FK5	O3-C8-C9	2.20	119.89	116.28
2	B	201	FK5	C34-C29-C28	-2.18	108.20	111.14
2	H	201	FK5	C12-C11-C10	2.18	112.63	110.47
2	F	201	FK5	C34-C29-C28	-2.17	108.21	111.14
2	E	201	FK5	C17-C16-C15	-2.17	111.71	115.45
2	C	201	FK5	C17-C16-C15	-2.13	111.78	115.45
2	G	201	FK5	O3-C8-C9	2.13	119.78	116.28
2	H	201	FK5	O1-C26-C25	2.12	108.33	105.91
2	F	201	FK5	C16-C17-C18	-2.11	108.29	111.57
2	E	201	FK5	C26-O1-C1	-2.10	111.96	117.36
2	F	201	FK5	C16-C15-C14	-2.10	109.32	113.34
2	C	201	FK5	C37-C19-C18	2.09	120.41	115.27
2	A	201	FK5	C16-C17-C18	-2.08	108.34	111.57
2	B	201	FK5	C37-C19-C20	-2.08	119.67	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	201	FK5	C42-C27-C26	2.07	119.26	115.68
2	B	201	FK5	C6-N7-C2	2.06	120.14	115.80
2	F	201	FK5	C17-C16-C15	-2.06	111.90	115.45
2	D	201	FK5	C12-C11-C10	2.05	112.50	110.47
2	E	201	FK5	O3-C8-C9	2.03	119.61	116.28
2	G	201	FK5	C23-C22-C21	2.01	120.33	117.75
2	B	201	FK5	C37-C19-C18	2.01	120.21	115.27
2	F	201	FK5	C15-C14-C13	-2.01	110.50	113.57

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	201	FK5	C15-C16-C17-C36
2	H	201	FK5	C13-C14-C15-C16
2	H	201	FK5	C15-C16-C17-C18
2	H	201	FK5	C15-C16-C17-C36
2	H	201	FK5	C36-C17-C18-C19
2	A	201	FK5	C20-C21-C38-C39
2	A	201	FK5	C22-C21-C38-C39
2	A	201	FK5	C22-C23-C24-C25
2	G	201	FK5	C15-C16-C17-C36
2	G	201	FK5	C36-C17-C18-C19
2	C	201	FK5	C15-C16-C17-C36
2	C	201	FK5	C36-C17-C18-C19
2	C	201	FK5	C20-C21-C38-C39
2	F	201	FK5	C15-C16-C17-C36
2	F	201	FK5	C20-C21-C38-C39
2	F	201	FK5	C22-C21-C38-C39
2	D	201	FK5	C13-C14-C15-C16
2	D	201	FK5	C16-C17-C18-C19
2	D	201	FK5	C36-C17-C18-C19
2	D	201	FK5	C20-C21-C38-C39
2	D	201	FK5	C22-C21-C38-C39
2	D	201	FK5	C23-C24-C25-C26
2	D	201	FK5	C23-C24-C25-C41
2	D	201	FK5	O10-C24-C25-C26
2	D	201	FK5	O10-C24-C25-C41
2	D	201	FK5	C41-C25-C26-C27
2	B	201	FK5	C13-C14-C15-C16
2	B	201	FK5	C15-C16-C17-C18
2	B	201	FK5	C15-C16-C17-C36

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Mol	Chain	Res	Type	Atoms
2	B	201	FK5	C36-C17-C18-C19
2	F	201	FK5	C21-C38-C39-C40
2	B	201	FK5	C21-C38-C39-C40
2	H	201	FK5	C14-C15-C16-C17
2	A	201	FK5	C21-C38-C39-C40
2	D	201	FK5	C41-C25-C26-O1
2	H	201	FK5	C21-C38-C39-C40
2	D	201	FK5	O9-C22-C23-C24
2	H	201	FK5	C13-C14-C15-O8
2	D	201	FK5	C13-C14-C15-O8
2	B	201	FK5	C13-C14-C15-O8
2	B	201	FK5	C37-C19-C20-C21
2	D	201	FK5	C22-C23-C24-C25
2	E	201	FK5	C15-C16-C17-C18
2	C	201	FK5	C15-C16-C17-C18
2	C	201	FK5	C20-C21-C22-C23
2	D	201	FK5	C22-C23-C24-O10
2	H	201	FK5	C41-C25-C26-C27
2	E	201	FK5	C36-C17-C18-C19
2	H	201	FK5	O5-C14-C15-C16
2	A	201	FK5	C36-C17-C18-C19
2	F	201	FK5	C36-C17-C18-C19
2	E	201	FK5	C19-C20-C21-C22
2	H	201	FK5	C19-C20-C21-C22
2	A	201	FK5	C19-C20-C21-C22
2	F	201	FK5	C19-C20-C21-C22
2	B	201	FK5	C19-C20-C21-C22
2	H	201	FK5	O5-C14-C15-O8
2	D	201	FK5	C21-C38-C39-C40
2	E	201	FK5	C13-C14-C15-O8
2	E	201	FK5	C13-C14-C15-C16
2	C	201	FK5	C13-C14-C15-C16
2	B	201	FK5	O5-C14-C15-O8
2	D	201	FK5	C14-C15-O8-C44
2	B	201	FK5	C20-C21-C22-C23
2	D	201	FK5	C21-C22-C23-C24
2	H	201	FK5	C30-C31-O11-C45
2	F	201	FK5	C38-C21-C22-O9
2	B	201	FK5	C38-C21-C22-O9
2	C	201	FK5	C38-C21-C22-C23
2	D	201	FK5	O5-C14-C15-C16
2	C	201	FK5	C37-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	D	201	FK5	C37-C19-C20-C21
2	C	201	FK5	O2-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	FK5	3	0
2	H	201	FK5	5	0
2	A	201	FK5	3	0
2	G	201	FK5	3	0
2	C	201	FK5	5	0
2	F	201	FK5	4	0
2	D	201	FK5	3	0
2	B	201	FK5	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 then 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 FK5 E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 G 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 F 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FK5 B 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	120/122 (98%)	-0.26	0	100 100	26, 41, 57, 70	0
1	B	122/122 (100%)	-0.22	0	100 100	30, 41, 61, 79	0
1	C	121/122 (99%)	-0.28	0	100 100	29, 44, 76, 89	0
1	D	120/122 (98%)	-0.23	1 (0%)	86 85	26, 40, 57, 80	0
1	E	118/122 (96%)	-0.08	0	100 100	33, 50, 72, 82	0
1	F	110/122 (90%)	0.15	4 (3%)	42 37	48, 71, 101, 117	0
1	G	121/122 (99%)	0.29	6 (4%)	28 24	41, 62, 89, 102	0
1	H	100/122 (81%)	0.68	13 (13%)	3 2	46, 79, 107, 113	0
All	All	932/976 (95%)	-0.01	24 (2%)	56 52	26, 50, 89, 117	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	121	VAL	4.5
1	H	67	LEU	4.5
1	H	68	THR	3.5
1	H	11	VAL	3.2
1	H	59	VAL	3.1
1	G	10	ILE	2.8
1	H	84	GLY	2.7
1	G	69	ASN	2.7
1	H	64	ASP	2.7
1	F	3	GLU	2.7
1	H	82	SER	2.6
1	H	119	LEU	2.6
1	F	121	VAL	2.5
1	G	23	GLY	2.5
1	G	117	GLU	2.5
1	F	11	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	47	GLY	2.4
1	H	115	GLU	2.3
1	G	37	GLY	2.2
1	H	83	LYS	2.1
1	H	25	THR	2.1
1	H	80	LYS	2.1
1	G	90	THR	2.0
1	D	12	GLN	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 carbohydrates 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(Å^2)	Q<0.9
2	FK5	H	201	57/57	0.84	0.28	60,66,79,79	0
2	FK5	G	201	57/57	0.86	0.23	36,51,58,61	0
2	FK5	E	201	57/57	0.89	0.20	28,41,50,52	0
2	FK5	C	201	57/57	0.89	0.23	51,61,69,71	0
2	FK5	F	201	57/57	0.90	0.19	37,51,62,63	0
2	FK5	D	201	57/57	0.90	0.20	33,41,54,59	0
2	FK5	A	201	57/57	0.91	0.17	26,35,41,41	0
2	FK5	B	201	57/57	0.92	0.21	28,42,53,54	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.
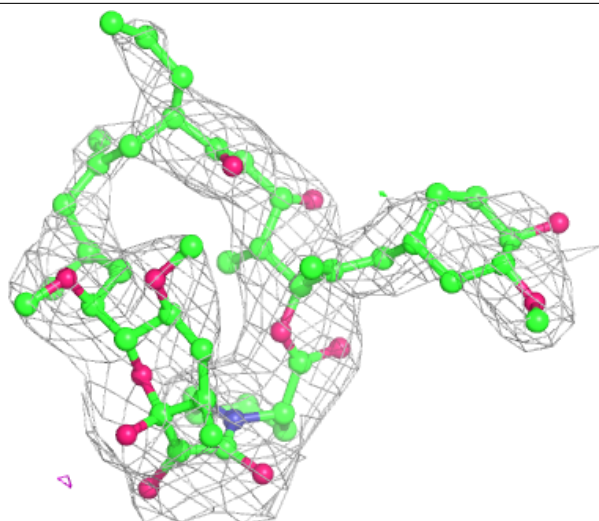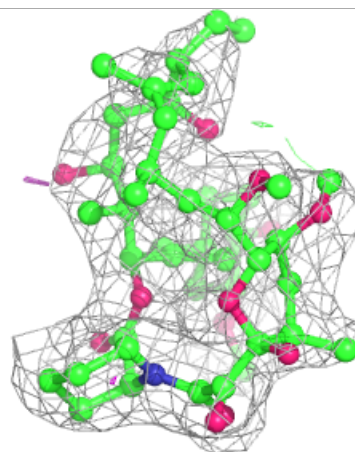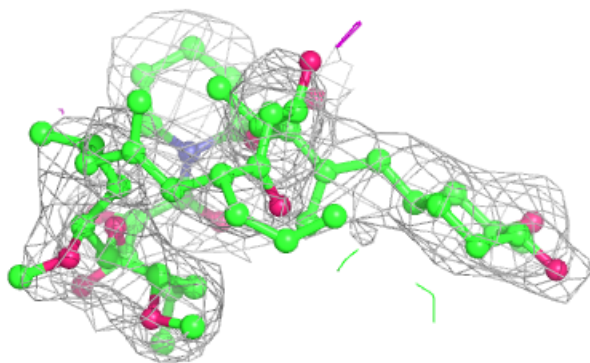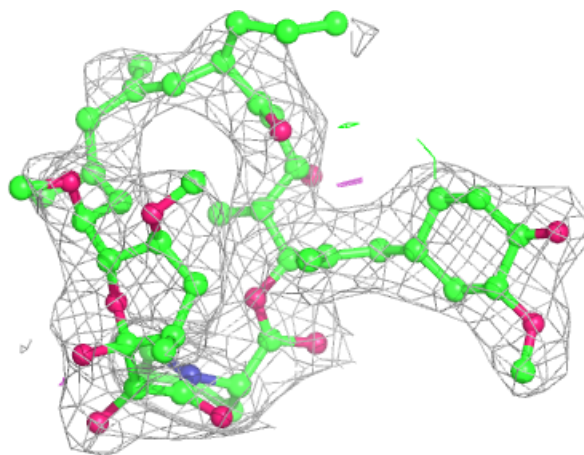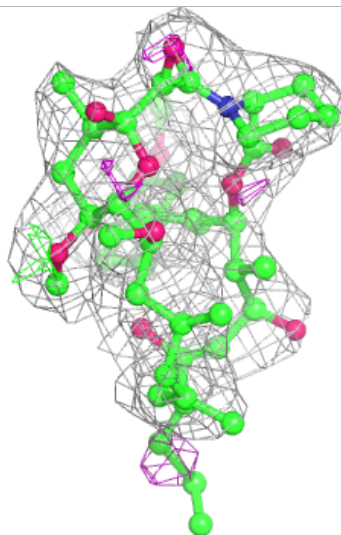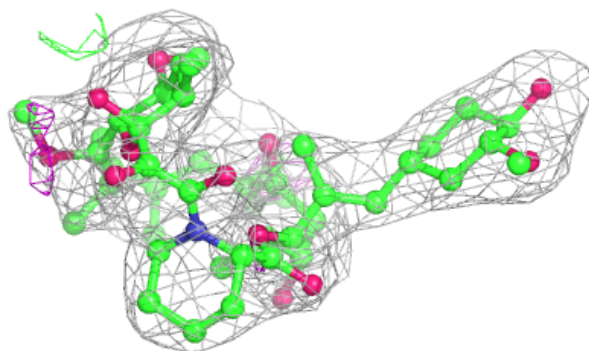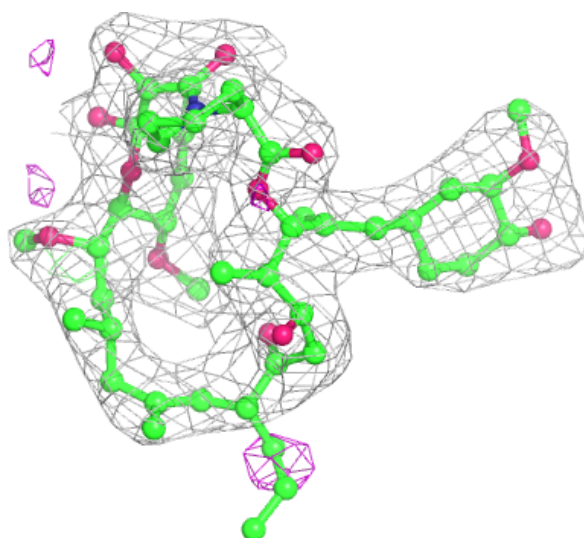
Electron density around FK5 H 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
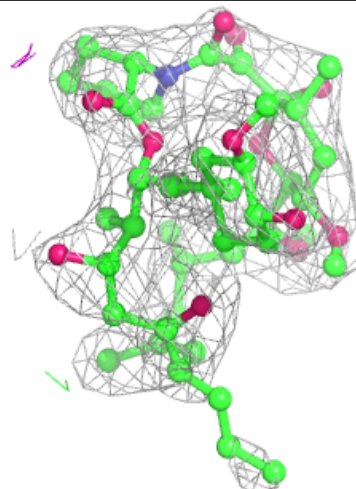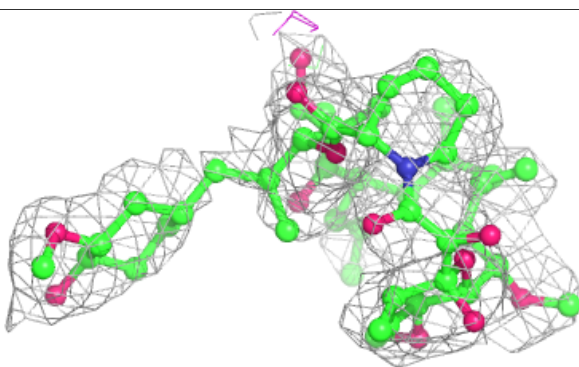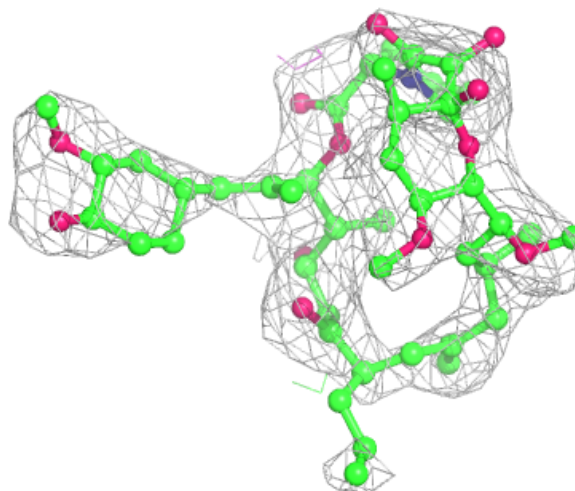
Electron density around FK5 G 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
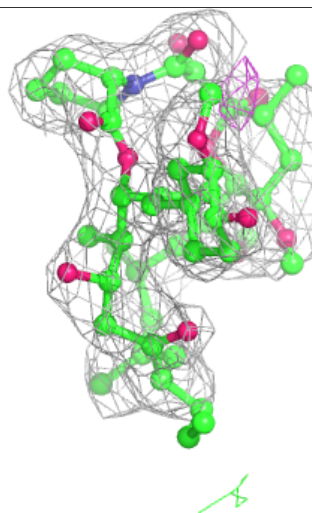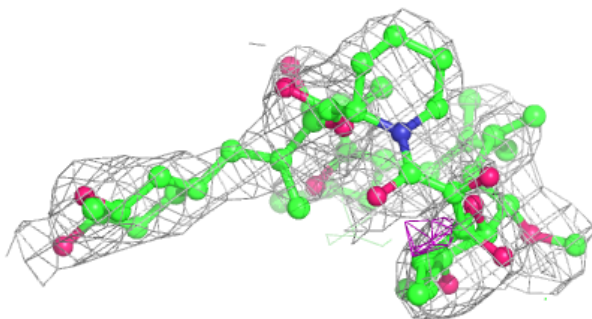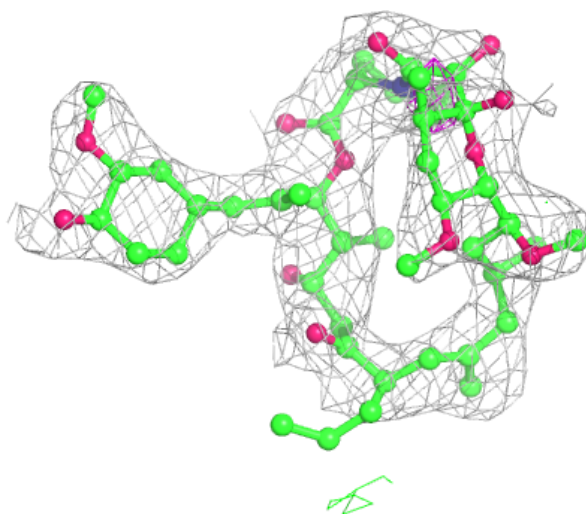
Electron density around FK5 E 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
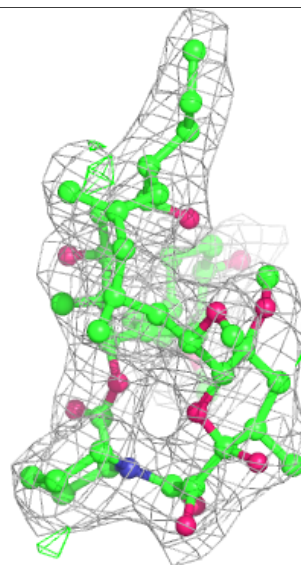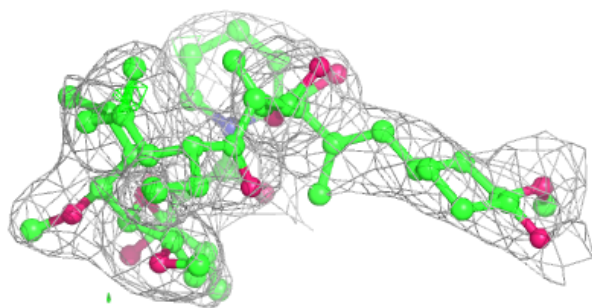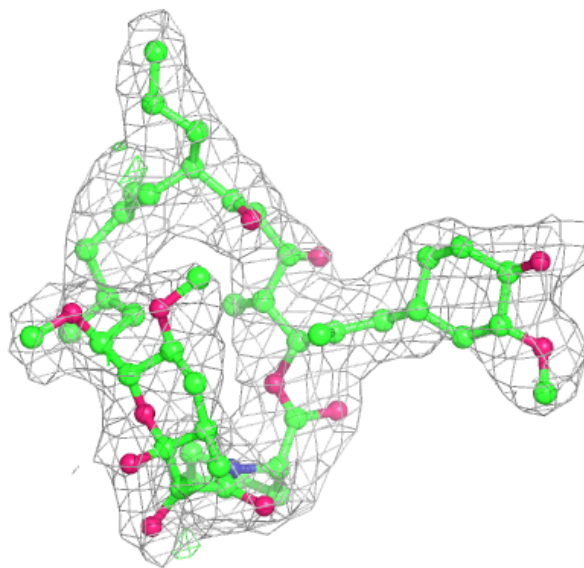
Electron density around FK5 C 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
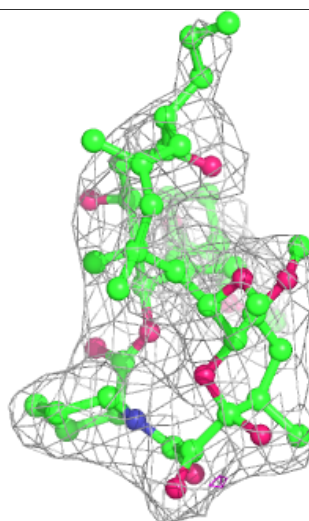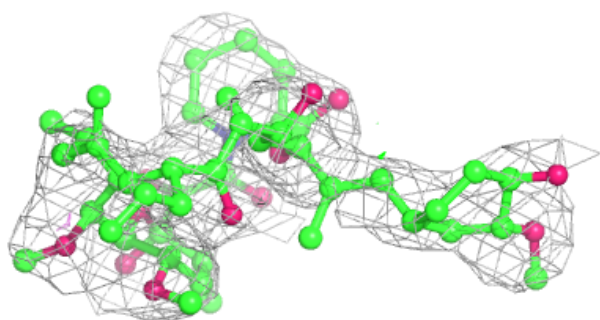
Electron density around FK5 F 201:

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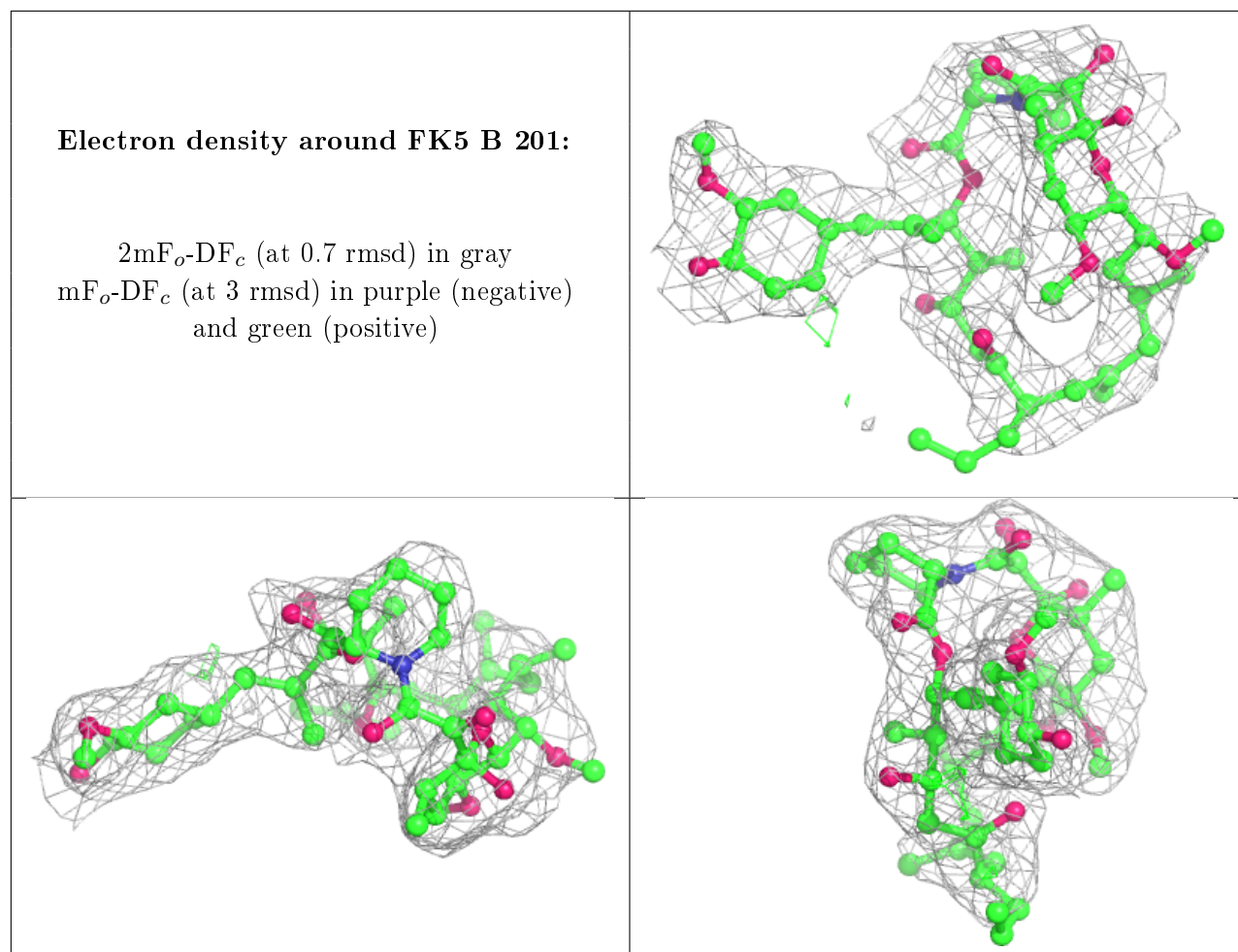and green (positive)

Electron density around FK5 D 201:

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

Electron density around FK5 A 201:

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

Electron density around FK5 B 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
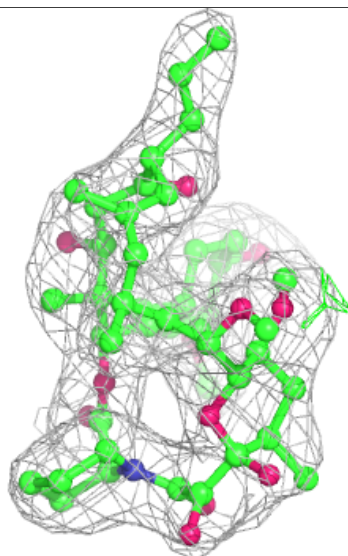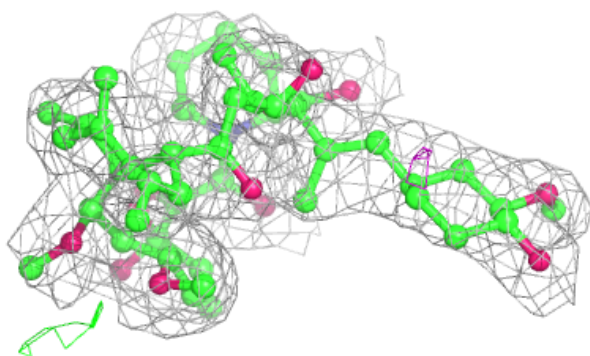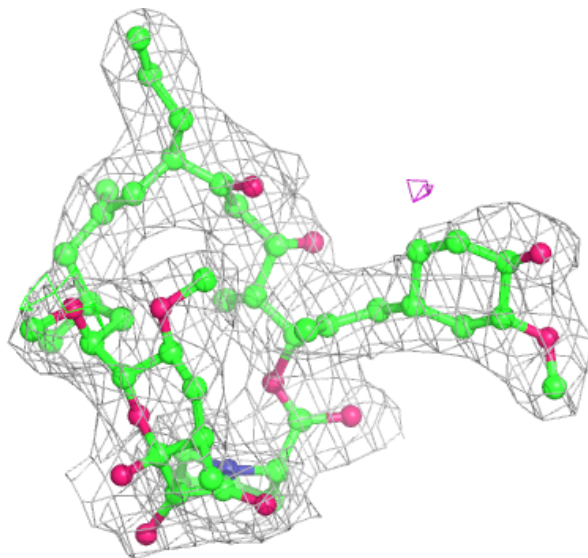
6.5 Other polymers (i)

There are no such residues in this entry.