



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:31 PM UTC

PDB ID : 8FAO / pdb_00008fao
Title : Bile Salt Hydrolase B from Lactobacillus gasseri with covalent inhibitor bound
Authors : Grundy, M.K.; Walker, M.E.; Redinbo, M.R.
Deposited on : 2022-11-28
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

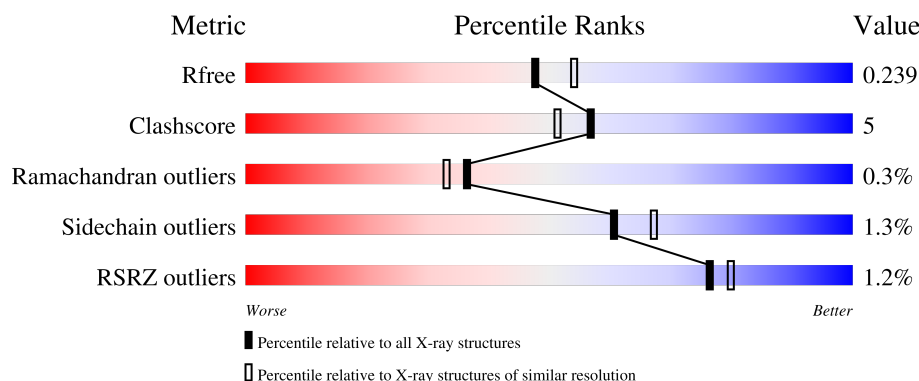
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	331	90% 9% .
1	B	331	89% 9% .
1	C	331	87% 10% ..
1	D	331	88% 11% .
1	E	331	3% 88% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	331	% 85% 14%
1	G	331	3% 84% 14%
1	H	331	88% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21015 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 Choloylglycine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	324	Total	C	N	O	S	0	1	0
			2505	1610	398	484	13			
1	A	329	Total	C	N	O	S	0	1	0
			2536	1626	412	485	13			
1	B	324	Total	C	N	O	S	0	1	0
			2472	1589	394	476	13			
1	C	324	Total	C	N	O	S	0	1	0
			2456	1572	391	480	13			
1	D	329	Total	C	N	O	S	0	1	0
			2554	1635	411	495	13			
1	E	327	Total	C	N	O	S	0	0	0
			2495	1593	408	482	12			
1	F	330	Total	C	N	O	S	0	1	0
			2546	1628	414	491	13			
1	G	324	Total	C	N	O	S	0	1	0
			2470	1584	396	477	13			

There are 48 discrepancies between the modelled and reference sequences:

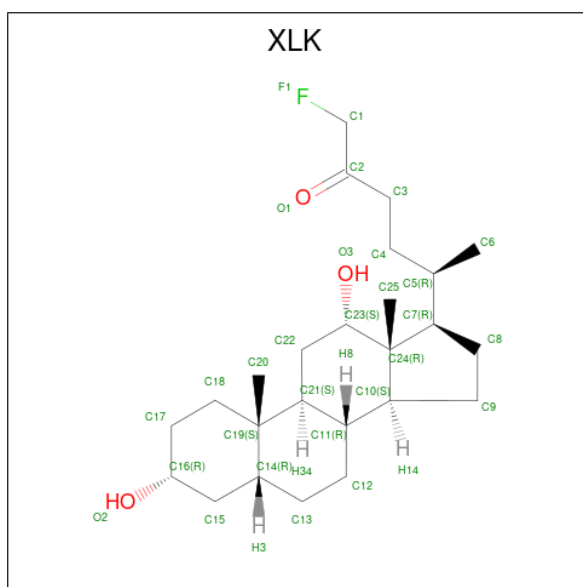
Chain	Residue	Modelled	Actual	Comment	Reference
H	326	HIS	-	expression tag	UNP A0A833FHE1
H	327	HIS	-	expression tag	UNP A0A833FHE1
H	328	HIS	-	expression tag	UNP A0A833FHE1
H	329	HIS	-	expression tag	UNP A0A833FHE1
H	330	HIS	-	expression tag	UNP A0A833FHE1
H	331	HIS	-	expression tag	UNP A0A833FHE1
A	326	HIS	-	expression tag	UNP A0A833FHE1
A	327	HIS	-	expression tag	UNP A0A833FHE1
A	328	HIS	-	expression tag	UNP A0A833FHE1
A	329	HIS	-	expression tag	UNP A0A833FHE1
A	330	HIS	-	expression tag	UNP A0A833FHE1
A	331	HIS	-	expression tag	UNP A0A833FHE1
B	326	HIS	-	expression tag	UNP A0A833FHE1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	327	HIS	-	expression tag	UNP A0A833FHE1
B	328	HIS	-	expression tag	UNP A0A833FHE1
B	329	HIS	-	expression tag	UNP A0A833FHE1
B	330	HIS	-	expression tag	UNP A0A833FHE1
B	331	HIS	-	expression tag	UNP A0A833FHE1
C	326	HIS	-	expression tag	UNP A0A833FHE1
C	327	HIS	-	expression tag	UNP A0A833FHE1
C	328	HIS	-	expression tag	UNP A0A833FHE1
C	329	HIS	-	expression tag	UNP A0A833FHE1
C	330	HIS	-	expression tag	UNP A0A833FHE1
C	331	HIS	-	expression tag	UNP A0A833FHE1
D	326	HIS	-	expression tag	UNP A0A833FHE1
D	327	HIS	-	expression tag	UNP A0A833FHE1
D	328	HIS	-	expression tag	UNP A0A833FHE1
D	329	HIS	-	expression tag	UNP A0A833FHE1
D	330	HIS	-	expression tag	UNP A0A833FHE1
D	331	HIS	-	expression tag	UNP A0A833FHE1
E	326	HIS	-	expression tag	UNP A0A833FHE1
E	327	HIS	-	expression tag	UNP A0A833FHE1
E	328	HIS	-	expression tag	UNP A0A833FHE1
E	329	HIS	-	expression tag	UNP A0A833FHE1
E	330	HIS	-	expression tag	UNP A0A833FHE1
E	331	HIS	-	expression tag	UNP A0A833FHE1
F	326	HIS	-	expression tag	UNP A0A833FHE1
F	327	HIS	-	expression tag	UNP A0A833FHE1
F	328	HIS	-	expression tag	UNP A0A833FHE1
F	329	HIS	-	expression tag	UNP A0A833FHE1
F	330	HIS	-	expression tag	UNP A0A833FHE1
F	331	HIS	-	expression tag	UNP A0A833FHE1
G	326	HIS	-	expression tag	UNP A0A833FHE1
G	327	HIS	-	expression tag	UNP A0A833FHE1
G	328	HIS	-	expression tag	UNP A0A833FHE1
G	329	HIS	-	expression tag	UNP A0A833FHE1
G	330	HIS	-	expression tag	UNP A0A833FHE1
G	331	HIS	-	expression tag	UNP A0A833FHE1

- Molecule 2 is (5R)-5-[(1R,3aS,3bR,5aR,7R,9aS,9bS,11S,11aR)-7,11-dihydroxy-9a,11a-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-1-yl]-1-fluorohexan-2-one (non-preferred name) (CCD ID: XLK) (formula: C₂₅H₄₁FO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			28	25	3		
2	A	1	Total	C	O	0	0
			28	25	3		
2	B	1	Total	C	O	0	0
			28	25	3		
2	C	1	Total	C	O	0	0
			28	25	3		
2	D	1	Total	C	O	0	0
			28	25	3		
2	E	1	Total	C	O	0	0
			28	25	3		
2	F	1	Total	C	O	0	0
			28	25	3		
2	G	1	Total	C	O	0	0
			28	25	3		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		

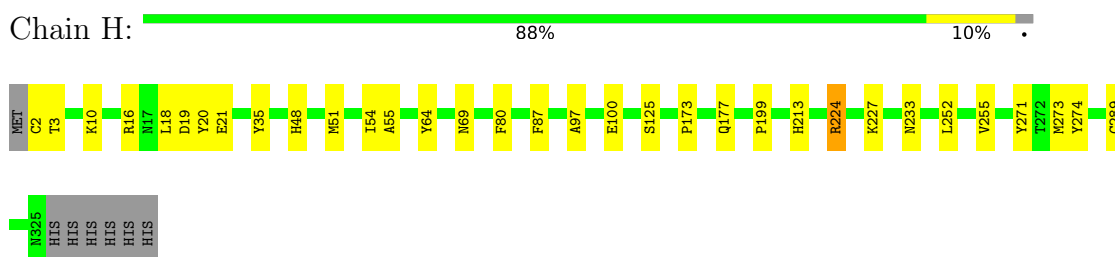
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	123	Total 123	O 123	0	0
4	A	127	Total 127	O 127	0	0
4	B	110	Total 110	O 110	0	0
4	C	82	Total 82	O 82	0	0
4	D	121	Total 121	O 121	0	0
4	E	70	Total 70	O 70	0	0
4	F	62	Total 62	O 62	0	0
4	G	60	Total 60	O 60	0	0

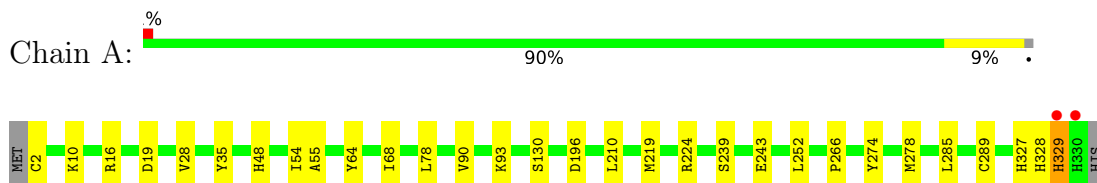
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

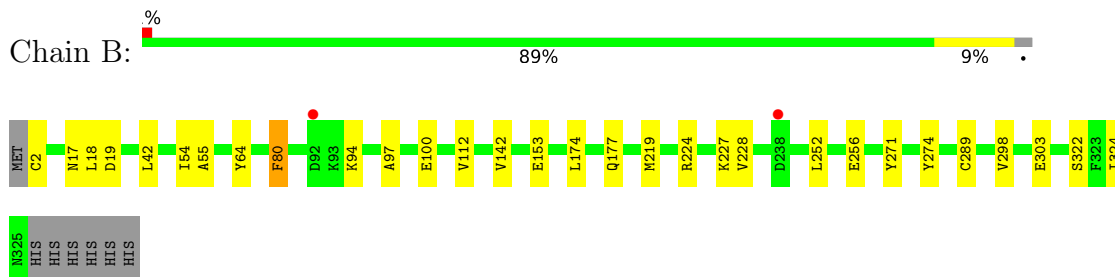
- Molecule 1: Choloylglycine hydrolase



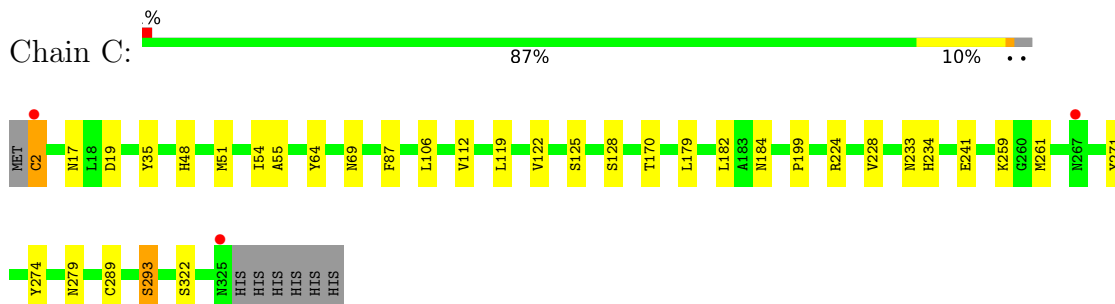
- Molecule 1: Choloylglycine hydrolase



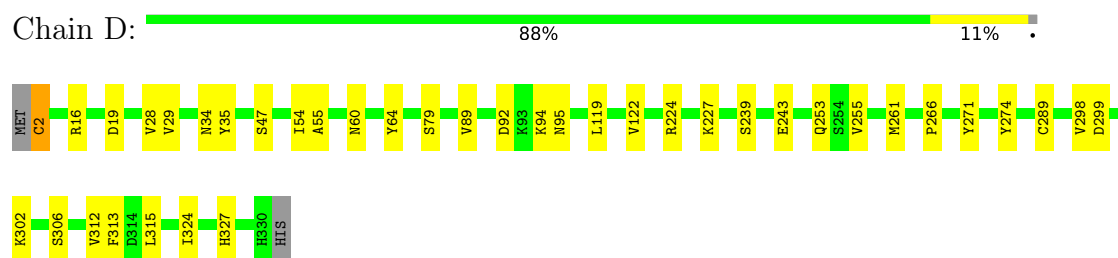
- Molecule 1: Choloylglycine hydrolase



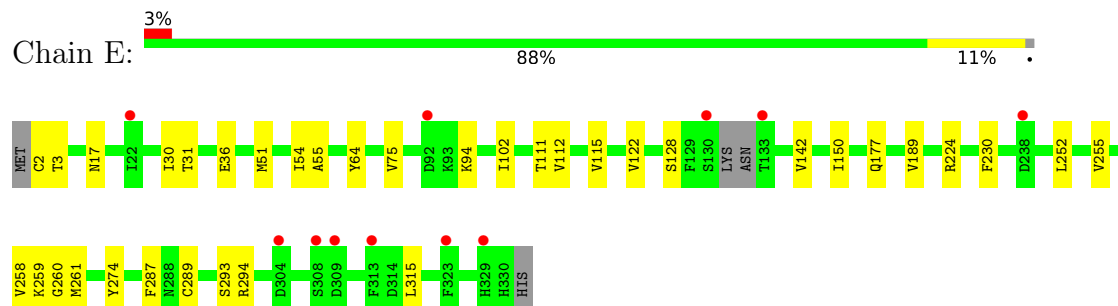
- Molecule 1: Choloylglycine hydrolase



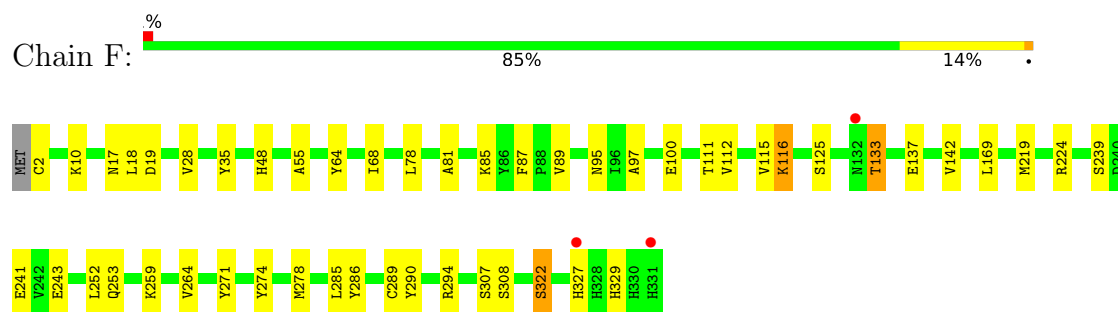
- Molecule 1: Choloylglycine hydrolase



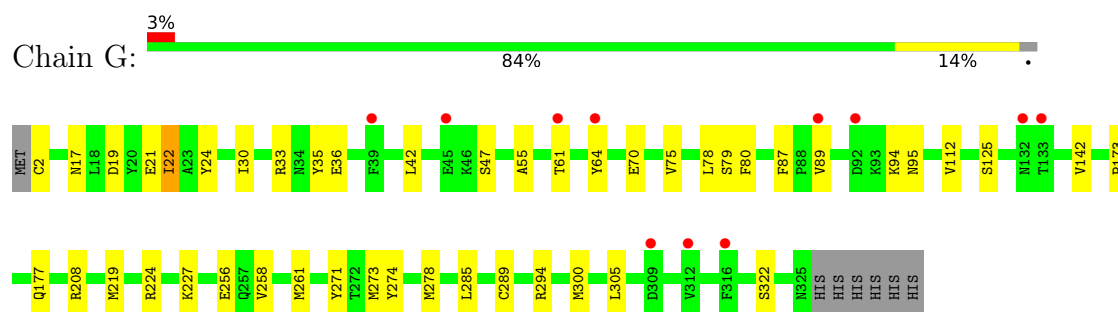
- Molecule 1: Choloylglycine hydrolase



- Molecule 1: Choloylglycine hydrolase



- Molecule 1: Choloylglycine hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.33Å 145.74Å 103.79Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	47.75 – 2.14 47.75 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.75-2.14) 99.9 (47.75-2.14)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.187 , 0.239 0.187 , 0.239	Depositor DCC
R_{free} test set	1995 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for l,k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21015	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: XLK, NI

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	0.39	0/2601	0.56	0/3544
1	B	0.35	0/2532	0.53	0/3452
1	C	0.33	0/2516	0.53	0/3431
1	D	0.36	0/2618	0.54	0/3565
1	E	0.32	0/2559	0.52	0/3487
1	F	0.31	0/2611	0.51	0/3557
1	G	0.29	0/2530	0.50	0/3448
1	H	0.37	0/2565	0.55	0/3491
All	All	0.34	0/20532	0.53	0/27975

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	224	ARG	Sidechain

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	2536	0	2356	20	0
1	B	2472	0	2302	22	0
1	C	2456	0	2250	22	0
1	D	2554	0	2378	28	0
1	E	2495	0	2275	21	0
1	F	2546	0	2366	32	0
1	G	2470	0	2293	26	0
1	H	2505	0	2357	26	0
2	A	28	0	0	0	0
2	B	28	0	0	1	0
2	C	28	0	0	0	0
2	D	28	0	0	2	0
2	E	28	0	0	0	0
2	F	28	0	0	1	0
2	G	28	0	0	0	0
2	H	28	0	0	1	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	127	0	0	0	0
4	B	110	0	0	1	0
4	C	82	0	0	1	0
4	D	121	0	0	1	0
4	E	70	0	0	1	0
4	F	62	0	0	0	0
4	G	60	0	0	1	0
4	H	123	0	0	1	0
All	All	21015	0	18577	178	0

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

All (178) 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:B:256:GLU:OE1	1:D:253:GLN:NE2	2.20	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:HIS:HD1	1:A:329:HIS:CE1	2.08	0.71
1:F:239:SER:HB2	1:F:243:GLU:HG2	1.72	0.71
1:C:2[B]:CYS:N	1:C:17:ASN:O	2.25	0.70
1:A:2[A]:CYS:O	1:A:224:ARG:NH2	2.25	0.70
1:F:2[B]:CYS:O	1:F:224:ARG:NH2	2.25	0.69
1:G:2[A]:CYS:N	1:G:17:ASN:O	2.26	0.69
1:D:239:SER:HB2	1:D:243:GLU:HG2	1.75	0.68
1:E:258:VAL:HB	1:E:261:MET:HE2	1.79	0.64
1:G:21:GLU:HG2	1:G:22:ILE:HG22	1.81	0.63
1:B:2[B]:CYS:O	1:B:224:ARG:NH2	2.32	0.63
1:E:2:CYS:O	1:E:224:ARG:NH2	2.32	0.62
1:C:35:TYR:O	1:C:48:HIS:NE2	2.29	0.62
1:B:42:LEU:HD21	1:B:94:LYS:HG3	1.82	0.62
1:C:2[A]:CYS:O	1:C:224:ARG:NH1	2.34	0.61
1:G:258:VAL:HB	1:G:261:MET:HE2	1.83	0.60
1:A:239:SER:HB2	1:A:243:GLU:HB3	1.85	0.58
1:B:2[A]:CYS:N	1:B:17:ASN:O	2.37	0.58
1:A:196:ASP:HB2	1:E:189:VAL:HG12	1.88	0.56
1:B:274:TYR:HA	1:B:289:CYS:HA	1.88	0.55
1:F:241:GLU:OE2	1:F:286:TYR:OH	2.18	0.55
1:F:112:VAL:HG22	1:F:142:VAL:HG12	1.89	0.55
1:A:274:TYR:HA	1:A:289:CYS:HA	1.89	0.55
1:G:227:LYS:NZ	4:G:504:HOH:O	2.39	0.55
1:G:42:LEU:HD21	1:G:94:LYS:HG3	1.88	0.54
1:H:2[B]:CYS:SG	1:H:16:ARG:NH2	2.78	0.54
1:A:28:VAL:HG13	1:A:285:LEU:HD23	1.89	0.54
1:C:55:ALA:HB2	1:C:64:TYR:CD1	2.43	0.53
1:C:241:GLU:OE2	1:C:279:ASN:ND2	2.40	0.53
1:G:274:TYR:HA	1:G:289:CYS:HA	1.90	0.53
1:B:219:MET:O	1:B:224:ARG:HD3	2.09	0.53
1:A:35:TYR:O	1:A:48:HIS:NE2	2.32	0.52
1:A:219:MET:O	1:A:224:ARG:HD3	2.09	0.52
1:A:2[B]:CYS:O	1:A:224:ARG:NH2	2.41	0.52
1:A:2[B]:CYS:SG	1:A:19:ASP:HB2	2.49	0.52
1:D:55:ALA:HB2	1:D:64:TYR:CD1	2.44	0.52
1:F:78:LEU:HD13	1:F:169:LEU:HD23	1.92	0.52
1:D:2[B]:CYS:O	1:D:224:ARG:NH2	2.43	0.52
1:F:259:LYS:HG3	1:F:290:TYR:CZ	2.44	0.52
1:F:327:HIS:ND1	1:F:329:HIS:NE2	2.55	0.52
1:G:75:VAL:HG22	1:G:142:VAL:HG22	1.92	0.52
1:D:92:ASP:OD1	1:D:92:ASP:N	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TYR:OH	1:D:60:ASN:O	2.20	0.51
1:E:31:THR:HB	1:E:51:MET:HG2	1.91	0.51
1:H:233:ASN:OD1	1:C:199:PRO:HD2	2.10	0.51
1:F:2[A]:CYS:N	1:F:17:ASN:O	2.43	0.51
1:D:299:ASP:HB3	1:D:302:LYS:HG3	1.92	0.51
1:E:55:ALA:HB2	1:E:64:TYR:CD1	2.46	0.51
1:F:111:THR:O	1:F:115:VAL:HG23	2.11	0.51
1:D:54:ILE:HD12	1:D:315:LEU:HD13	1.92	0.51
1:A:68:ILE:HD13	1:A:278:MET:HB3	1.93	0.50
1:C:179:LEU:O	1:C:182:LEU:HB2	2.10	0.50
1:E:75:VAL:HG22	1:E:142:VAL:HG22	1.93	0.50
1:H:2[A]:CYS:O	1:H:224:ARG:NH2	2.45	0.50
1:D:2[A]:CYS:SG	1:D:19:ASP:HB2	2.51	0.50
1:F:35:TYR:O	1:F:48:HIS:NE2	2.43	0.50
1:F:112:VAL:O	1:F:116:LYS:HG3	2.12	0.50
1:G:219:MET:O	1:G:224:ARG:NH1	2.43	0.49
1:F:133:THR:O	1:F:133:THR:OG1	2.27	0.49
1:G:22:ILE:C	1:G:273:MET:HE1	2.38	0.49
1:G:112:VAL:HG22	1:G:142:VAL:HG12	1.95	0.49
1:G:278:MET:HG2	1:G:285:LEU:HD13	1.93	0.49
1:E:75:VAL:HG12	1:E:102:ILE:HG12	1.94	0.49
1:C:261:MET:HE3	1:E:230:PHE:HD2	1.79	0.48
1:C:274:TYR:HA	1:C:289:CYS:HA	1.95	0.48
1:B:54:ILE:HG21	1:B:274:TYR:CZ	2.48	0.48
1:B:112:VAL:HG22	1:B:142:VAL:HG12	1.95	0.48
1:C:54:ILE:HG21	1:C:274:TYR:CZ	2.48	0.48
1:D:34:ASN:ND2	1:D:306:SER:O	2.44	0.48
1:F:85:LYS:HG2	1:F:87:PHE:CZ	2.49	0.48
1:F:322:SER:HB2	1:G:294:ARG:CZ	2.43	0.48
1:F:274:TYR:HA	1:F:289:CYS:HA	1.96	0.48
1:E:111:THR:O	1:E:115:VAL:HG23	2.14	0.47
1:H:20:TYR:O	1:H:273:MET:HE3	2.13	0.47
1:E:274:TYR:HA	1:E:289:CYS:HA	1.97	0.47
1:H:199:PRO:HD2	1:C:233:ASN:OD1	2.15	0.47
1:A:55:ALA:HB2	1:A:64:TYR:CD1	2.50	0.47
1:C:119:LEU:HD23	1:C:122:VAL:HG21	1.96	0.47
1:H:2[B]:CYS:CB	1:H:16:ARG:HH21	2.28	0.47
1:D:54:ILE:HG21	1:D:274:TYR:CZ	2.49	0.47
1:E:94:LYS:HB3	1:E:122:VAL:HG22	1.97	0.47
1:G:2[B]:CYS:HB3	1:G:78:LEU:HD23	1.97	0.47
1:G:70:GLU:HA	1:G:300:MET:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:ALA:HB2	1:F:64:TYR:CD1	2.50	0.46
1:F:219:MET:O	1:F:224:ARG:HD3	2.16	0.46
1:B:227:LYS:NZ	4:B:503:HOH:O	2.49	0.46
1:B:303:GLU:OE2	1:D:327:HIS:NE2	2.49	0.46
1:F:239:SER:HB2	1:F:243:GLU:CG	2.43	0.46
1:H:2[A]:CYS:SG	1:H:19:ASP:HB2	2.54	0.46
1:D:227:LYS:NZ	4:D:503:HOH:O	2.47	0.46
1:D:274:TYR:HA	1:D:289:CYS:HA	1.98	0.46
1:F:2[B]:CYS:HB3	1:F:78:LEU:HD23	1.98	0.46
1:G:89:VAL:HA	1:G:95:ASN:OD1	2.15	0.46
1:G:55:ALA:HB2	1:G:64:TYR:CD1	2.52	0.45
1:H:224:ARG:HG2	1:H:255:VAL:HB	1.97	0.45
1:B:2[B]:CYS:SG	1:B:18:LEU:HA	2.57	0.45
1:G:22:ILE:HD11	1:G:24:TYR:CZ	2.51	0.45
1:H:55:ALA:HB2	1:H:64:TYR:CD1	2.51	0.45
1:D:2[A]:CYS:N	1:D:16:ARG:HH21	2.15	0.45
1:D:2[B]:CYS:HB2	2:D:401:XLK:O1	2.15	0.45
1:H:2[B]:CYS:HB3	1:H:16:ARG:HH21	1.82	0.45
1:G:33:ARG:NH1	1:G:305:LEU:HB2	2.32	0.45
1:D:28:VAL:HB	1:D:313:PHE:HB2	1.99	0.45
1:C:293:SER:OG	1:E:293:SER:O	2.35	0.45
1:E:259:LYS:NZ	4:E:507:HOH:O	2.49	0.45
1:H:21:GLU:OE1	1:H:21:GLU:N	2.49	0.44
1:B:80:PHE:CE2	1:B:153:GLU:HG2	2.52	0.44
1:B:55:ALA:HB2	1:B:64:TYR:CD1	2.52	0.44
1:D:79:SER:HB3	2:D:401:XLK:O1	2.16	0.44
1:F:2[B]:CYS:SG	1:F:18:LEU:HA	2.57	0.44
1:A:54:ILE:HG21	1:A:274:TYR:CZ	2.52	0.44
1:B:174:LEU:HB2	1:B:177:GLN:HG3	2.00	0.44
1:H:87:PHE:O	1:H:125:SER:HA	2.18	0.44
1:H:173:PRO:HG2	1:H:177:GLN:HB2	1.99	0.44
1:G:173:PRO:HG2	1:G:177:GLN:HB2	1.99	0.44
1:H:51:MET:HA	1:H:69:ASN:HA	2.00	0.44
1:H:35:TYR:O	1:H:48:HIS:NE2	2.42	0.44
1:H:274:TYR:HA	1:H:289:CYS:HA	2.00	0.44
1:D:89:VAL:HG13	1:D:95:ASN:CG	2.42	0.44
1:A:2[A]:CYS:HB3	1:A:78:LEU:HD23	2.01	0.43
1:H:19:ASP:HA	1:H:271:TYR:O	2.19	0.43
1:H:54:ILE:HG21	1:H:274:TYR:CZ	2.53	0.43
1:H:213:HIS:CD2	1:C:184:ASN:HB3	2.54	0.43
1:A:328:HIS:O	1:A:329:HIS:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2[B]:CYS:HB2	2:F:401:XLK:O1	2.18	0.43
1:C:87:PHE:O	1:C:125:SER:HA	2.18	0.43
1:A:90:VAL:HG13	1:A:93:LYS:HB2	2.00	0.43
1:E:54:ILE:HD12	1:E:315:LEU:HD13	2.01	0.43
1:E:287:PHE:CD2	1:E:315:LEU:HD12	2.53	0.43
1:H:2[B]:CYS:HB2	2:H:401:XLK:O1	2.19	0.43
1:B:19:ASP:HA	1:B:271:TYR:O	2.19	0.43
1:C:2[B]:CYS:O	1:C:170:THR:HA	2.18	0.43
1:B:303:GLU:CD	1:D:327:HIS:HE2	2.27	0.43
1:A:2[B]:CYS:N	1:A:16:ARG:HH21	2.17	0.42
1:H:227:LYS:NZ	4:H:505:HOH:O	2.52	0.42
1:B:298:VAL:HG22	1:D:324:ILE:HB	2.00	0.42
1:F:68:ILE:HD13	1:F:278:MET:HB3	2.02	0.42
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.92	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.93	0.42
1:F:97:ALA:HB3	1:F:100:GLU:HG2	2.02	0.42
1:B:324:ILE:HB	1:D:298:VAL:HG22	2.02	0.42
1:F:87:PHE:O	1:F:125:SER:HA	2.20	0.42
1:F:253:GLN:NE2	1:G:256:GLU:OE1	2.51	0.42
1:C:69:ASN:HB3	1:C:106:LEU:HB3	2.01	0.41
1:C:259:LYS:NZ	4:C:506:HOH:O	2.52	0.41
1:D:19:ASP:HA	1:D:271:TYR:O	2.20	0.41
1:H:2[B]:CYS:SG	1:H:18:LEU:HG	2.59	0.41
1:C:322:SER:HB2	1:E:294:ARG:CZ	2.51	0.41
1:G:19:ASP:HA	1:G:271:TYR:O	2.20	0.41
1:C:234:HIS:O	1:E:260:GLY:HA3	2.21	0.41
1:F:89:VAL:HG13	1:F:95:ASN:CG	2.45	0.41
1:G:30:ILE:HD13	1:G:300:MET:HA	2.01	0.41
1:H:2[A]:CYS:HB3	1:H:224:ARG:NH2	2.35	0.41
1:D:224:ARG:HG2	1:D:255:VAL:HB	2.03	0.41
1:E:3:THR:HG21	1:E:255:VAL:HG21	2.02	0.41
1:E:142:VAL:HB	1:E:150:ILE:HG13	2.02	0.41
1:D:29:VAL:HG22	1:D:312:VAL:HG22	2.02	0.41
1:F:81:ALA:HA	1:F:137:GLU:OE1	2.21	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.91	0.41
1:B:97:ALA:HB3	1:B:100:GLU:HG2	2.03	0.41
1:F:264:VAL:HG11	1:G:208:ARG:NH1	2.36	0.41
1:G:35:TYR:OH	1:G:61:THR:HA	2.21	0.41
1:H:97:ALA:O	1:H:100:GLU:HG2	2.21	0.41
1:A:327:HIS:C	1:A:329:HIS:H	2.29	0.41
1:D:239:SER:HB2	1:D:243:GLU:CG	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:VAL:HG13	1:F:285:LEU:HD23	2.03	0.41
1:G:87:PHE:O	1:G:125:SER:HA	2.20	0.41
1:B:2[B]:CYS:HB2	2:B:401:XLK:O1	2.20	0.40
1:B:227:LYS:HE3	1:D:261:MET:HE1	2.03	0.40
1:F:252:LEU:HD23	1:F:252:LEU:HA	1.87	0.40
1:H:177:GLN:CD	1:E:177:GLN:HG2	2.46	0.40
1:D:119:LEU:HD23	1:D:122:VAL:HG21	2.03	0.40
1:E:17:ASN:OD1	1:E:252:LEU:HB3	2.21	0.40
1:F:294:ARG:CZ	1:G:322:SER:HB2	2.51	0.40
1:H:252:LEU:HD23	1:H:252:LEU:HA	1.91	0.40
1:C:19:ASP:HA	1:C:271:TYR:O	2.21	0.40
1:C:51:MET:HE2	1:C:51:MET:HB3	1.84	0.40
1:F:19:ASP:HA	1:F:271:TYR:O	2.21	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	327/331 (99%)	315 (96%)	9 (3%)	3 (1%)	14	8
1	B	322/331 (97%)	314 (98%)	8 (2%)	0	100	100
1	C	322/331 (97%)	309 (96%)	13 (4%)	0	100	100
1	D	327/331 (99%)	315 (96%)	11 (3%)	1 (0%)	36	33
1	E	323/331 (98%)	309 (96%)	14 (4%)	0	100	100
1	F	328/331 (99%)	315 (96%)	12 (4%)	1 (0%)	36	33
1	G	322/331 (97%)	301 (94%)	21 (6%)	0	100	100
1	H	322/331 (97%)	313 (97%)	7 (2%)	2 (1%)	21	15
All	All	2593/2648 (98%)	2491 (96%)	95 (4%)	7 (0%)	36	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	10	LYS
1	A	10	LYS
1	H	3	THR
1	H	10	LYS
1	A	329	HIS
1	D	266	PRO
1	A	266	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	265/291 (91%)	264 (100%)	1 (0%)	84	88
1	B	257/291 (88%)	254 (99%)	3 (1%)	63	69
1	C	254/291 (87%)	248 (98%)	6 (2%)	43	45
1	D	270/291 (93%)	266 (98%)	4 (2%)	57	63
1	E	258/291 (89%)	254 (98%)	4 (2%)	55	61
1	F	269/291 (92%)	264 (98%)	5 (2%)	50	55
1	G	259/291 (89%)	254 (98%)	5 (2%)	50	55
1	H	265/291 (91%)	264 (100%)	1 (0%)	84	88
All	All	2097/2328 (90%)	2068 (99%)	29 (1%)	61	65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	80	PHE
1	A	130	SER
1	B	80	PHE
1	B	228	VAL
1	B	322	SER
1	C	2[A]	CYS
1	C	2[B]	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	112	VAL
1	C	128	SER
1	C	228	VAL
1	C	293	SER
1	D	2[A]	CYS
1	D	2[B]	CYS
1	D	47	SER
1	D	94	LYS
1	E	30	ILE
1	E	36	GLU
1	E	112	VAL
1	E	128	SER
1	F	116	LYS
1	F	133	THR
1	F	307	SER
1	F	308	SER
1	F	322	SER
1	G	22	ILE
1	G	36	GLU
1	G	47	SER
1	G	79	SER
1	G	80	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	181	ASN
1	H	184	ASN
1	H	253	GLN
1	H	257	GLN
1	A	83	GLN
1	C	177	GLN
1	D	83	GLN
1	D	171	ASN
1	E	41	ASN
1	E	83	GLN
1	E	267	ASN
1	F	118	ASN
1	F	177	GLN
1	F	234	HIS
1	G	83	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XLK	B	401	1	31,31,32	0.36	0	49,49,50	1.00	2 (4%)
2	XLK	D	401	1	31,31,32	0.33	0	49,49,50	0.80	2 (4%)
2	XLK	E	401	1	31,31,32	0.37	0	49,49,50	0.73	1 (2%)
2	XLK	G	401	1	31,31,32	0.33	0	49,49,50	1.09	1 (2%)
2	XLK	F	401	1	31,31,32	0.34	0	49,49,50	0.87	1 (2%)
2	XLK	A	401	1	31,31,32	0.39	0	49,49,50	0.86	1 (2%)
2	XLK	H	401	1	31,31,32	0.34	0	49,49,50	0.79	1 (2%)
2	XLK	C	401	1	31,31,32	0.32	0	49,49,50	1.68	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	XLK	B	401	1	-	3/9/71/73	0/4/4/4
2	XLK	D	401	1	-	3/9/71/73	0/4/4/4
2	XLK	E	401	1	-	2/9/71/73	0/4/4/4
2	XLK	G	401	1	-	2/9/71/73	0/4/4/4
2	XLK	F	401	1	-	3/9/71/73	0/4/4/4
2	XLK	A	401	1	-	3/9/71/73	0/4/4/4
2	XLK	H	401	1	-	2/9/71/73	0/4/4/4
2	XLK	C	401	1	-	3/9/71/73	0/4/4/4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	XLK	C4-C3-C2	-10.50	98.38	114.77
2	G	401	XLK	C4-C3-C2	-6.02	105.38	114.77
2	F	401	XLK	C4-C3-C2	-4.57	107.63	114.77
2	B	401	XLK	C4-C3-C2	-4.44	107.85	114.77
2	A	401	XLK	C4-C3-C2	-3.64	109.09	114.77
2	E	401	XLK	C4-C3-C2	-3.15	109.85	114.77
2	D	401	XLK	C4-C3-C2	-2.57	110.75	114.77
2	C	401	XLK	C4-C5-C7	-2.51	105.13	110.33
2	H	401	XLK	C4-C3-C2	-2.49	110.88	114.77
2	D	401	XLK	C9-C10-C24	2.26	105.74	103.54
2	B	401	XLK	O3-C23-C24	-2.22	107.28	111.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	XLK	C1-C2-C3-C4
2	A	401	XLK	C1-C2-C3-C4
2	B	401	XLK	C1-C2-C3-C4
2	C	401	XLK	O1-C2-C3-C4
2	F	401	XLK	C1-C2-C3-C4
2	G	401	XLK	C1-C2-C3-C4
2	F	401	XLK	C3-C4-C5-C6
2	D	401	XLK	O1-C2-C3-C4
2	H	401	XLK	C1-C2-C3-C4
2	C	401	XLK	C1-C2-C3-C4
2	E	401	XLK	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

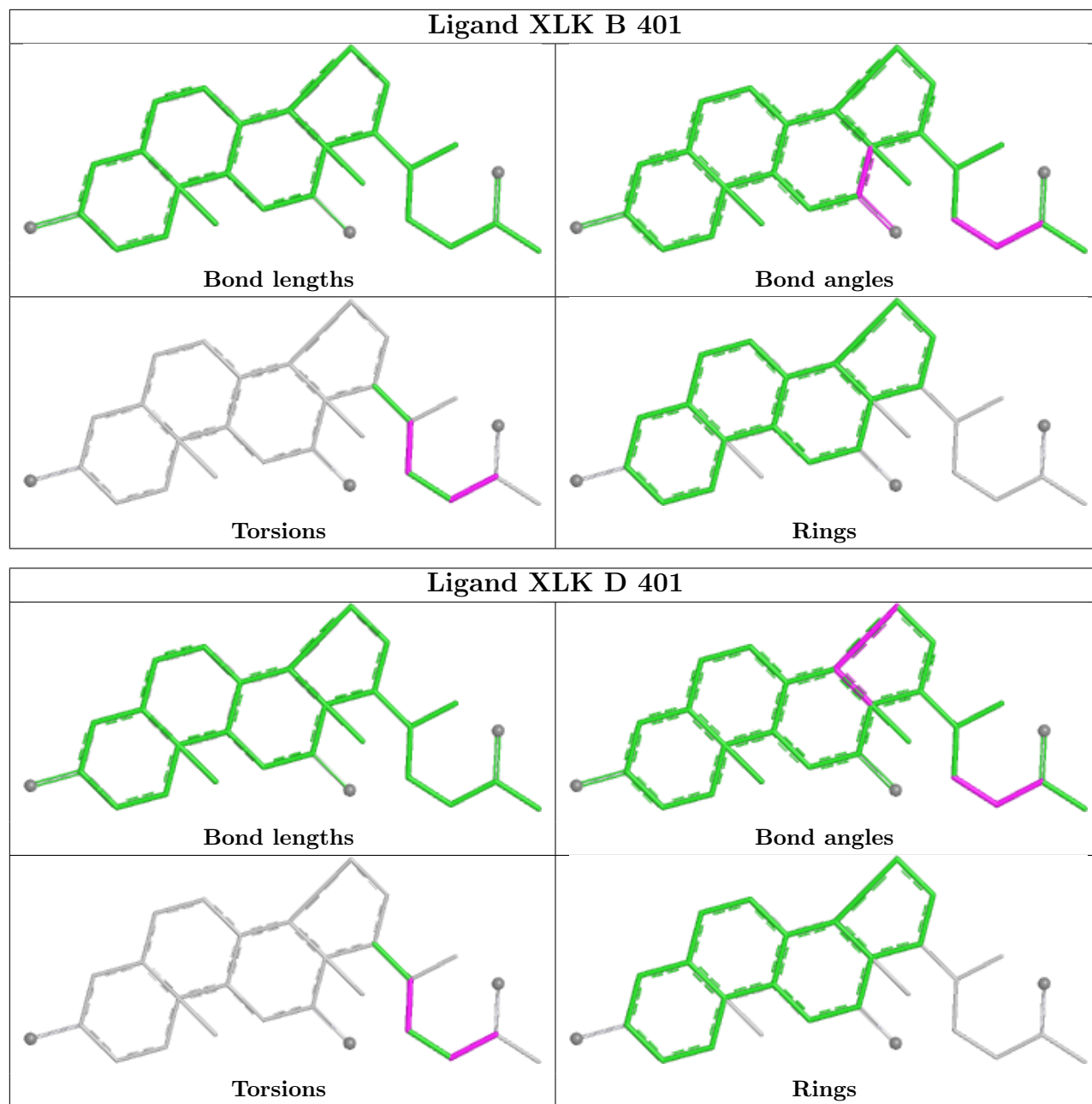
Mol	Chain	Res	Type	Atoms
2	F	401	XLK	O1-C2-C3-C4
2	B	401	XLK	C3-C4-C5-C6
2	D	401	XLK	C3-C4-C5-C6
2	A	401	XLK	O1-C2-C3-C4
2	B	401	XLK	O1-C2-C3-C4
2	E	401	XLK	O1-C2-C3-C4
2	G	401	XLK	O1-C2-C3-C4
2	C	401	XLK	C2-C3-C4-C5
2	H	401	XLK	O1-C2-C3-C4
2	A	401	XLK	C3-C4-C5-C6

There are no ring outliers.

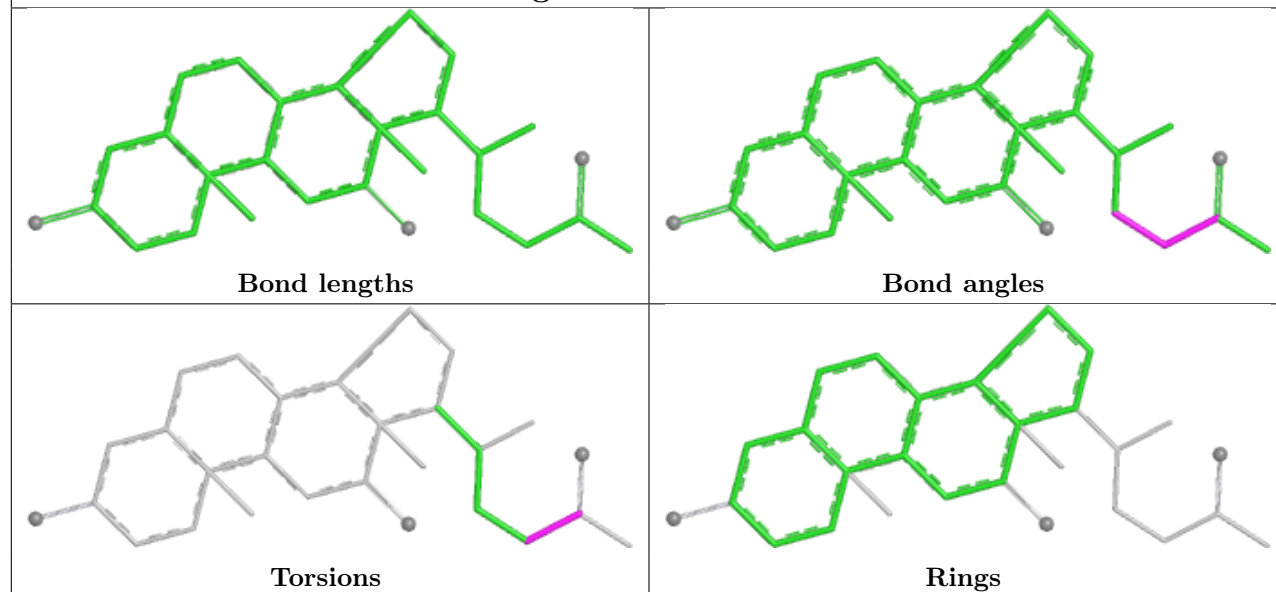
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	XLK	1	0
2	D	401	XLK	2	0
2	F	401	XLK	1	0
2	H	401	XLK	1	0

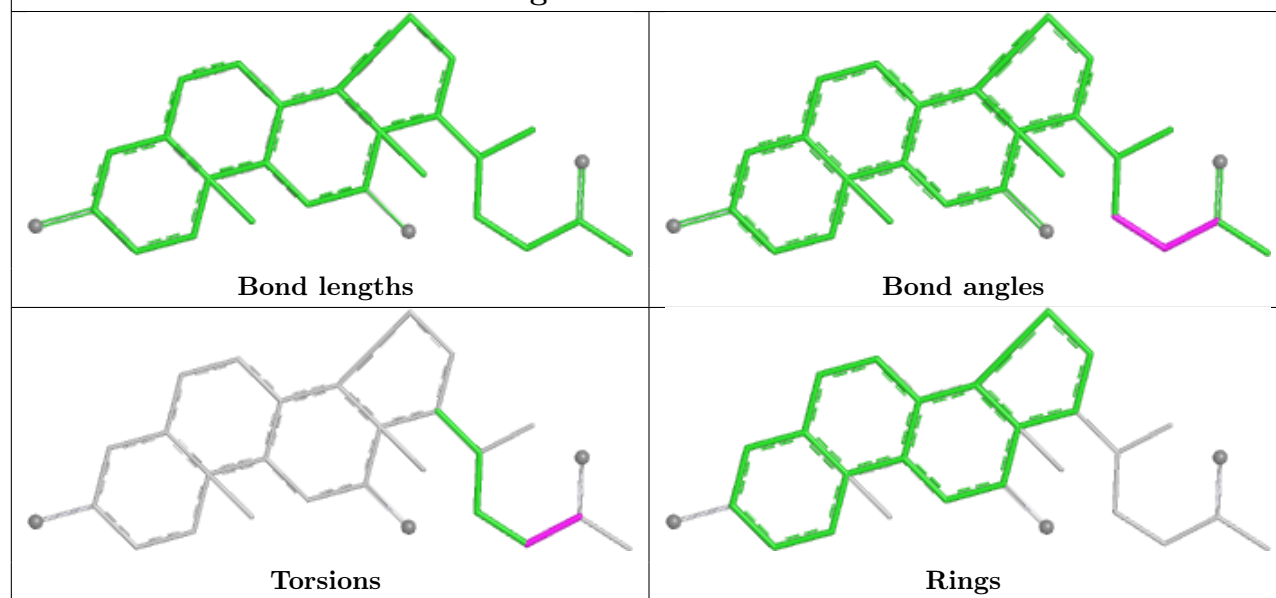
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



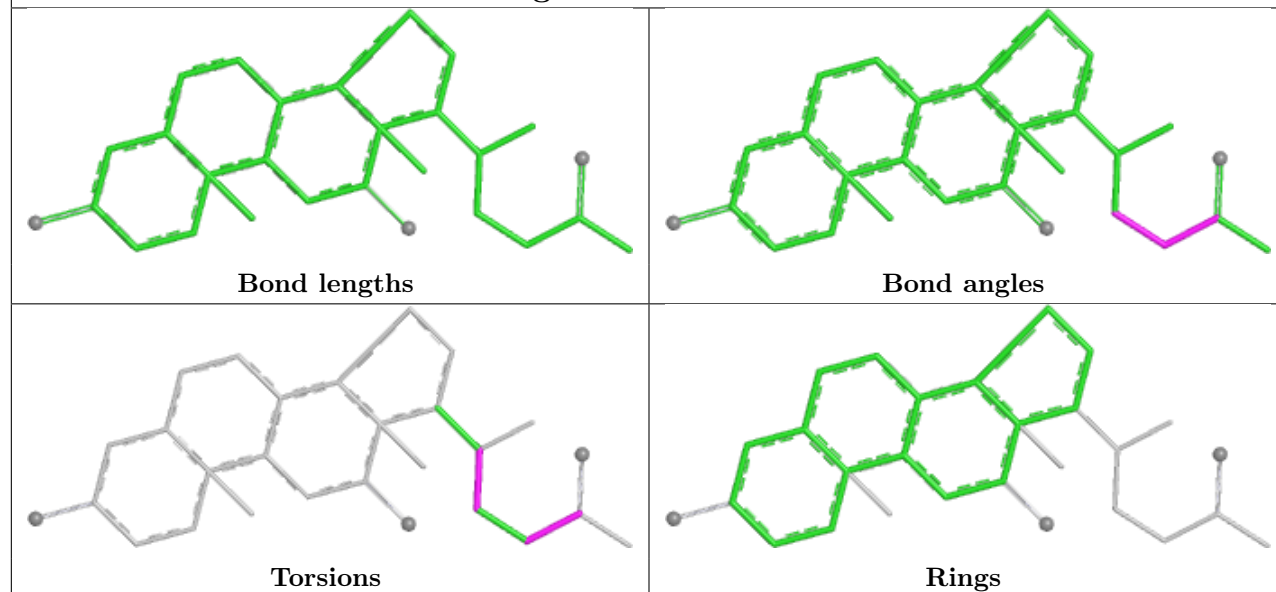
Ligand XLK E 401



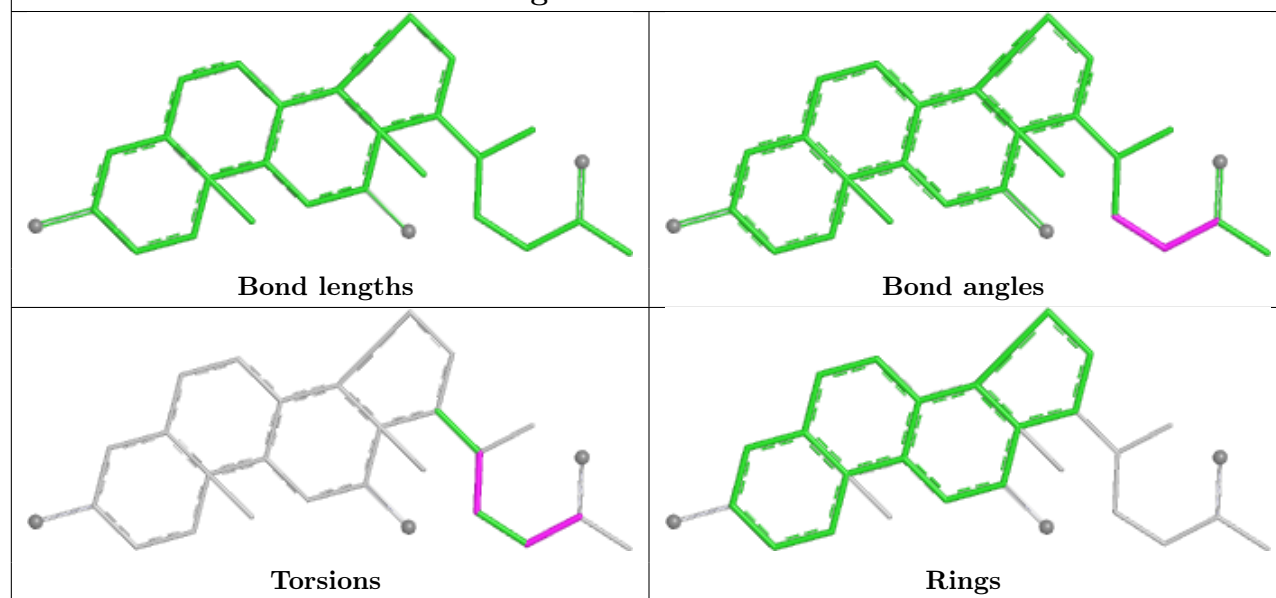
Ligand XLK G 401

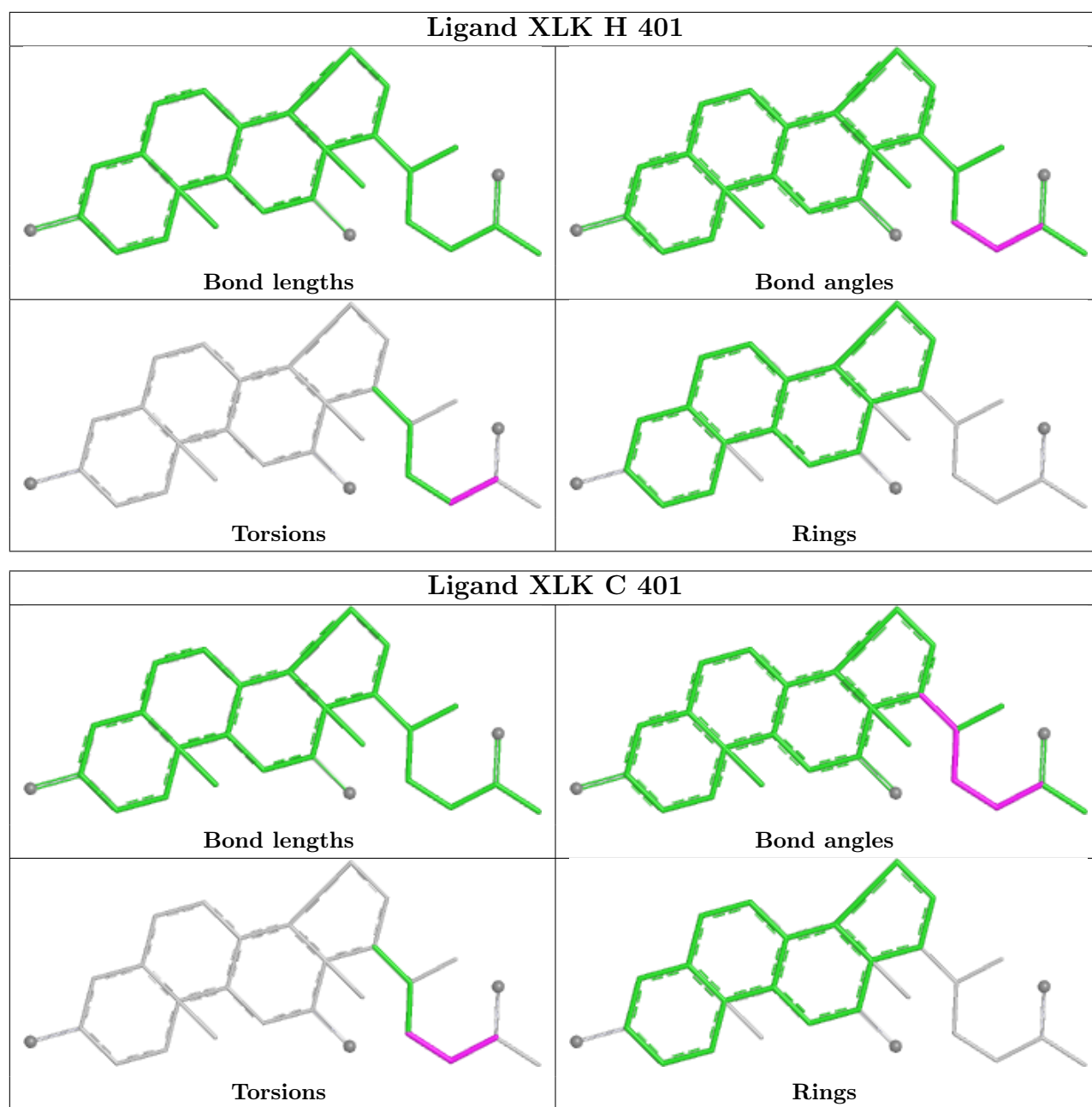


Ligand XLK F 401



Ligand XLK A 401





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	329/331 (99%)	-0.24	2 (0%) 85 88	18, 38, 53, 59	1 (0%)
1	B	324/331 (97%)	-0.15	2 (0%) 85 88	19, 40, 56, 67	1 (0%)
1	C	324/331 (97%)	0.13	3 (0%) 81 84	21, 46, 61, 67	1 (0%)
1	D	329/331 (99%)	-0.14	0 100 100	18, 40, 55, 73	1 (0%)
1	E	327/331 (98%)	0.34	11 (3%) 48 52	33, 49, 65, 70	0
1	F	330/331 (99%)	0.25	3 (0%) 81 84	22, 49, 62, 70	1 (0%)
1	G	324/331 (97%)	0.47	11 (3%) 48 52	24, 53, 71, 78	1 (0%)
1	H	324/331 (97%)	-0.29	0 100 100	18, 38, 49, 60	1 (0%)
All	All	2611/2648 (98%)	0.05	32 (1%) 76 80	18, 44, 62, 78	7 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	130	SER	4.5
1	F	327	HIS	3.9
1	C	2[A]	CYS	3.4
1	E	329	HIS	3.2
1	B	92	ASP	3.1
1	G	92	ASP	3.1
1	A	329	HIS	3.0
1	G	133	THR	3.0
1	E	304	ASP	3.0
1	G	132	ASN	3.0
1	G	89	VAL	2.9
1	F	331	HIS	2.9
1	G	61	THR	2.9
1	E	133	THR	2.8
1	B	238	ASP	2.6
1	E	238	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	312	VAL	2.5
1	F	132	ASN	2.5
1	E	308	SER	2.4
1	G	309	ASP	2.4
1	E	309	ASP	2.3
1	C	267	ASN	2.3
1	E	323	PHE	2.2
1	E	22	ILE	2.2
1	E	92	ASP	2.2
1	G	45	GLU	2.1
1	G	64	TYR	2.1
1	E	313	PHE	2.1
1	G	39	PHE	2.1
1	G	316	PHE	2.0
1	C	325	ASN	2.0
1	A	330	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

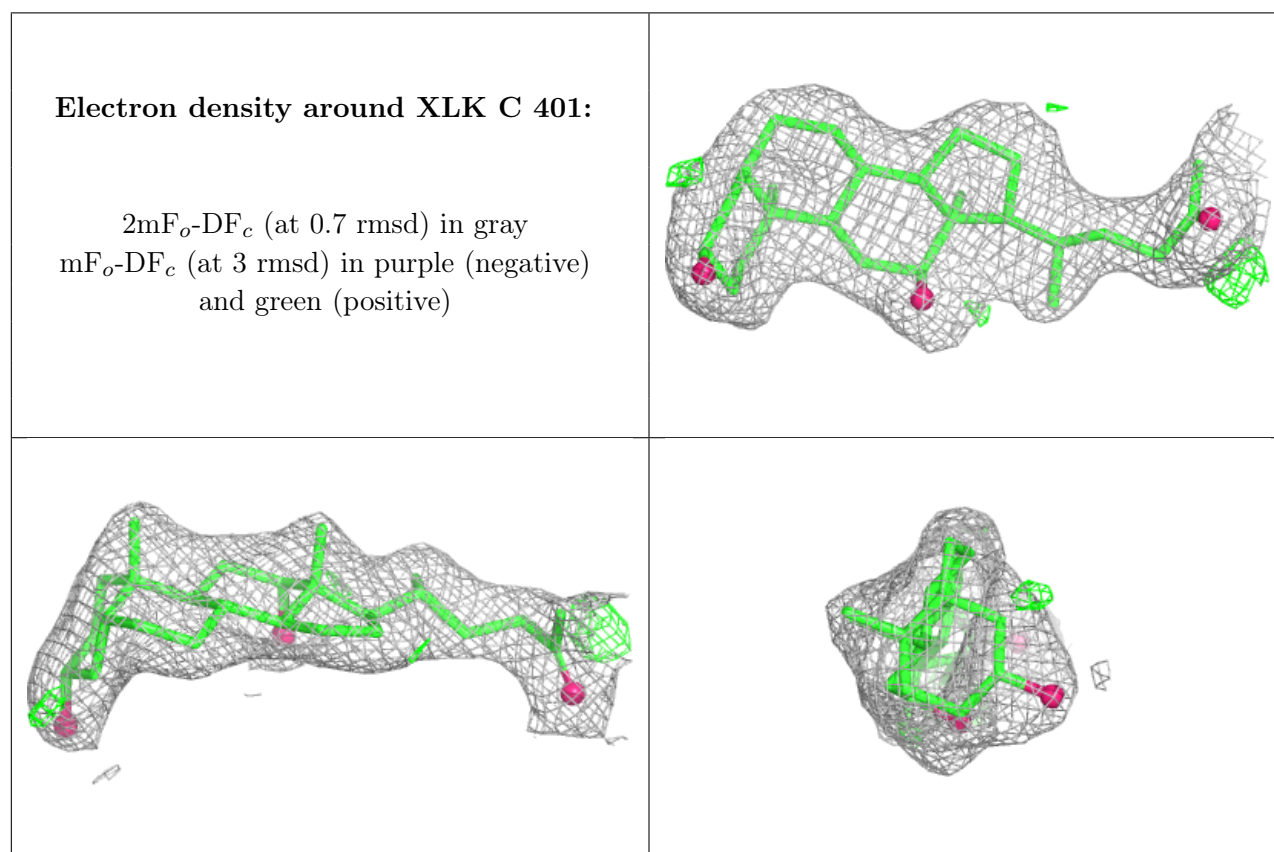
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XLK	C	401	28/29	0.92	0.10	40,45,49,51	0
2	XLK	E	401	28/29	0.92	0.10	42,49,53,58	0
2	XLK	G	401	28/29	0.93	0.10	49,53,57,64	0
2	XLK	D	401	28/29	0.94	0.09	32,37,47,49	0
2	XLK	A	401	28/29	0.94	0.08	31,36,41,47	0
2	XLK	F	401	28/29	0.94	0.09	37,42,46,54	0
2	XLK	H	401	28/29	0.94	0.08	29,34,42,49	0

Continued on next page...

Continued from previous page...

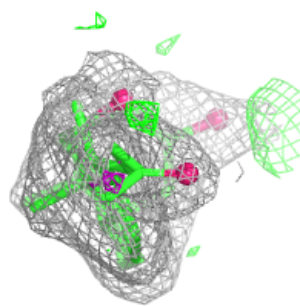
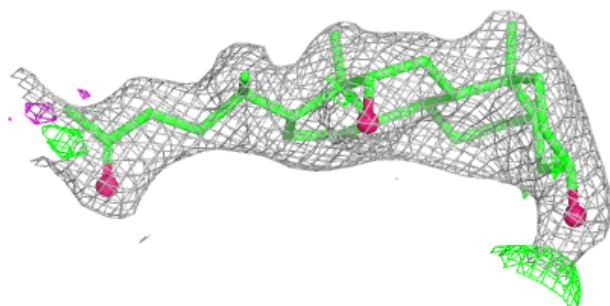
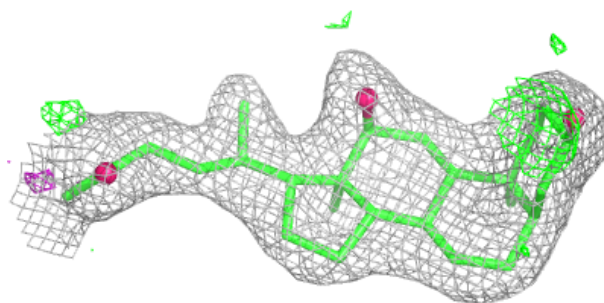
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XLK	B	401	28/29	0.95	0.08	33,38,44,45	0
3	NI	A	402	1/1	0.99	0.04	45,45,45,45	0
3	NI	D	402	1/1	1.00	0.01	50,50,50,50	0

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.

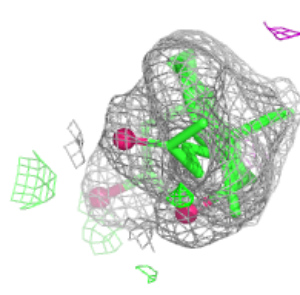
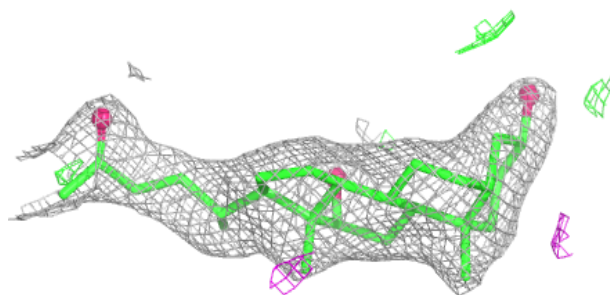
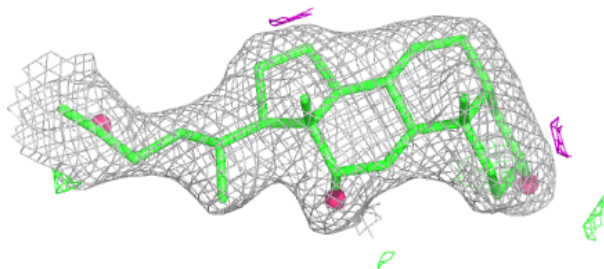


Electron density around XLK E 401:

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

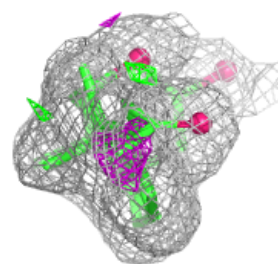
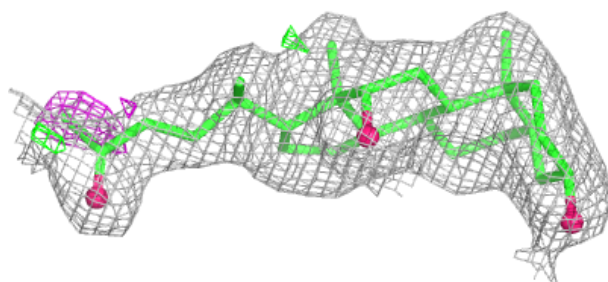
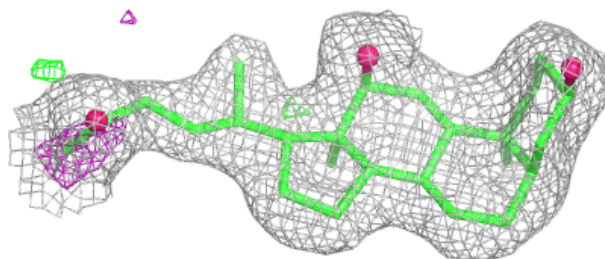
**Electron density around XLK G 401:**

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

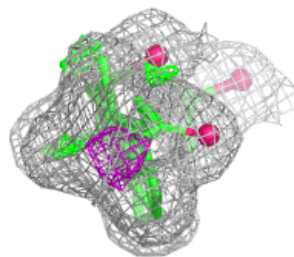
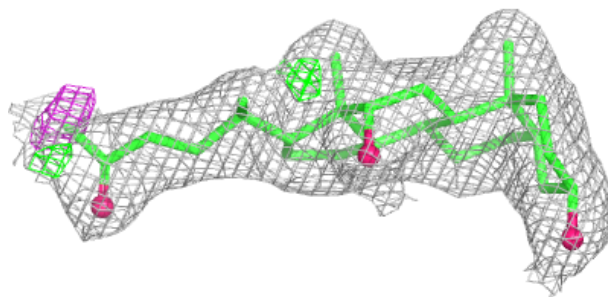
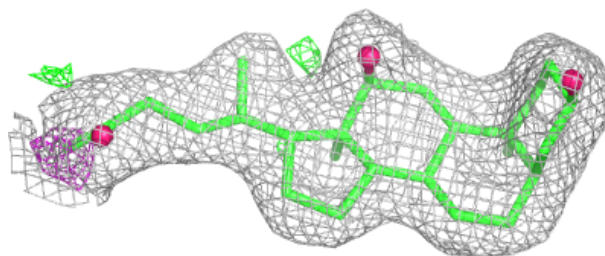


Electron density around XLK D 401:

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

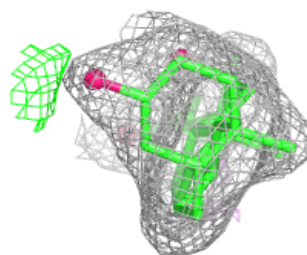
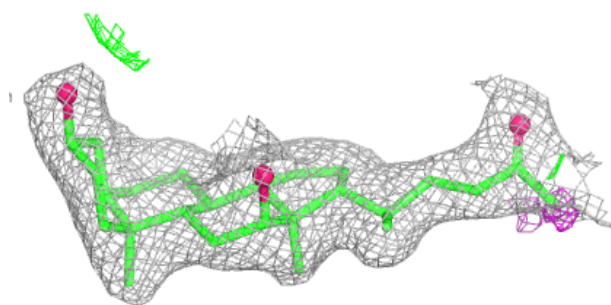
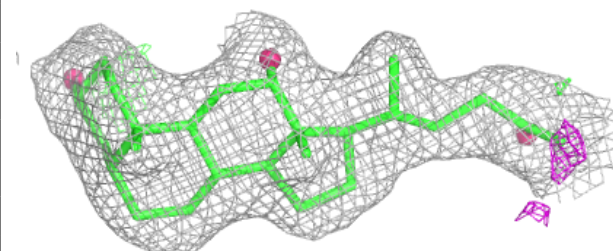
**Electron density around XLK A 401:**

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

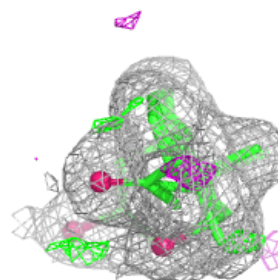
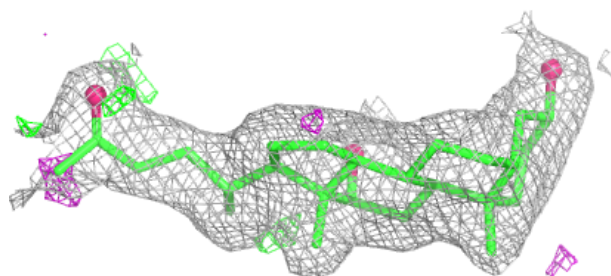
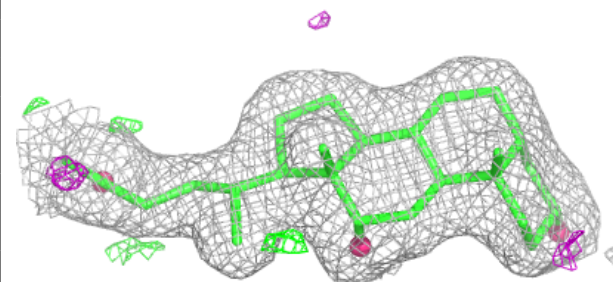


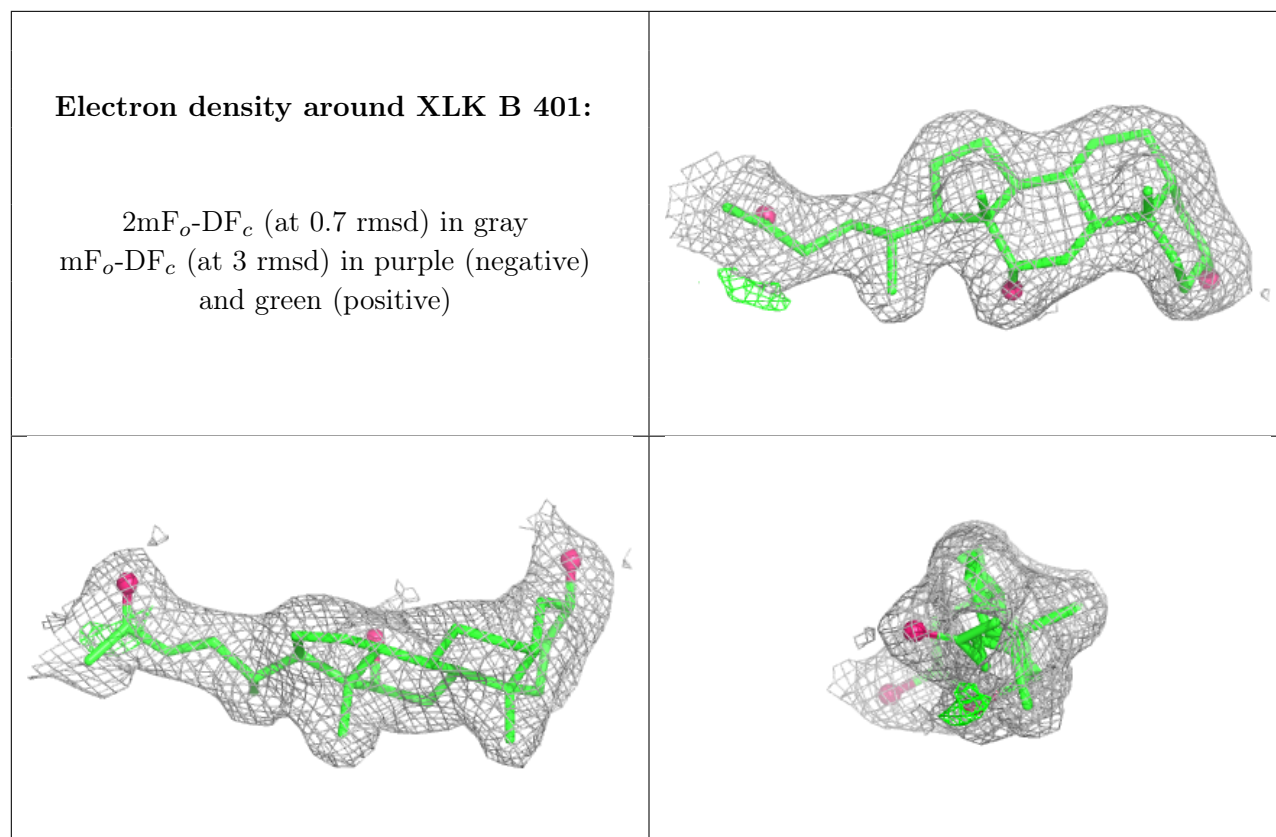
Electron density around XLK F 401:

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

**Electron density around XLK H 401:**

$2mF_o-DF_c$ (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.