



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:52 AM UTC

PDB ID : 2PNJ / pdb_00002pnj
Title : Crystal structure of human ferrochelatase mutant with Phe 337 replaced by Ala
Authors : Dailey, H.A.; Wu, C.-K.; Horanyi, P.; Medlock, A.E.; Najahi-Missaoui, W.; Burden, A.E.; Dailey, T.A.; Rose, J.P.
Deposited on : 2007-04-24
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

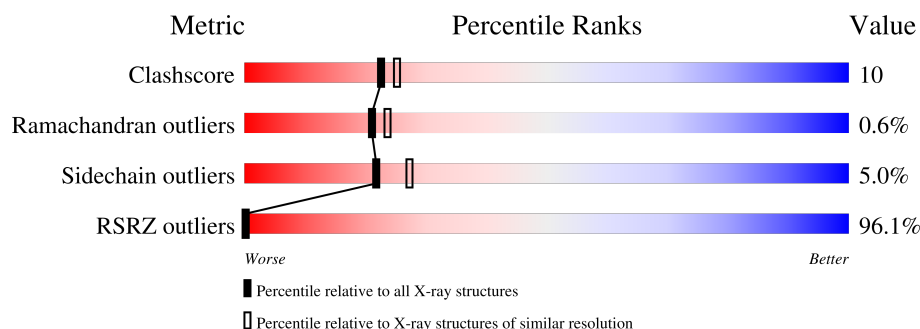
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	359	91% 78% 18% ..
1	B	359	99% 76% 18% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CHD	B	503	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6166 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.

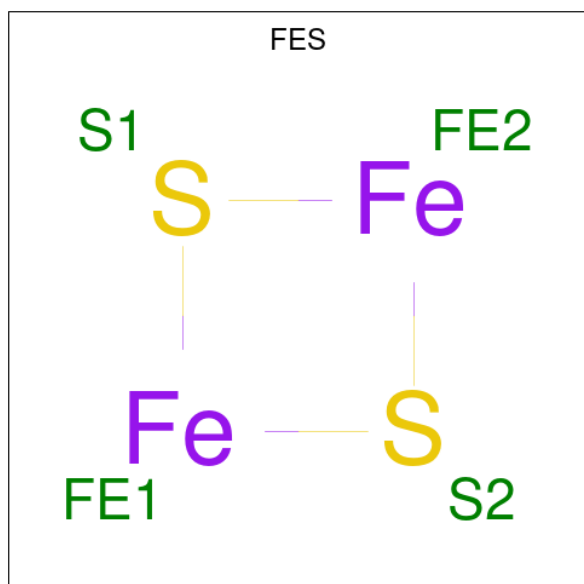
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2815	1794	481	522	18			
1	B	356	Total	C	N	O	S	0	0	0
			2827	1803	484	522	18			

There are 4 discrepancies between the modelled and reference sequences:

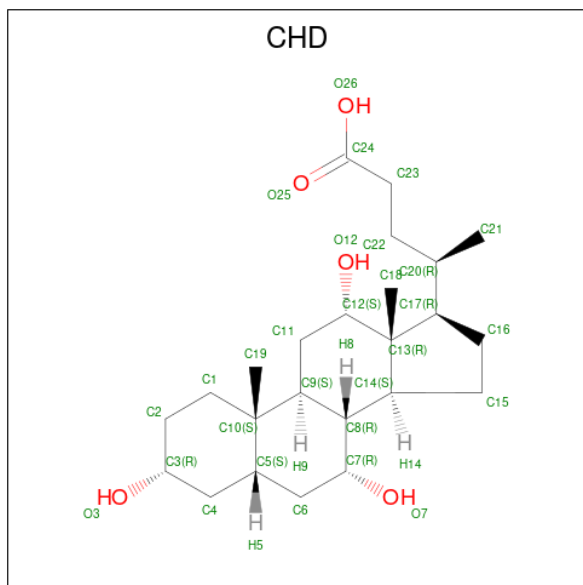
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	engineered mutation	UNP P22830
A	337	ALA	PHE	engineered mutation	UNP P22830
B	115	LEU	ARG	engineered mutation	UNP P22830
B	337	ALA	PHE	engineered mutation	UNP P22830

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			29	24	5		
3	A	1	Total	C	O	0	0
			29	24	5		
3	A	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		

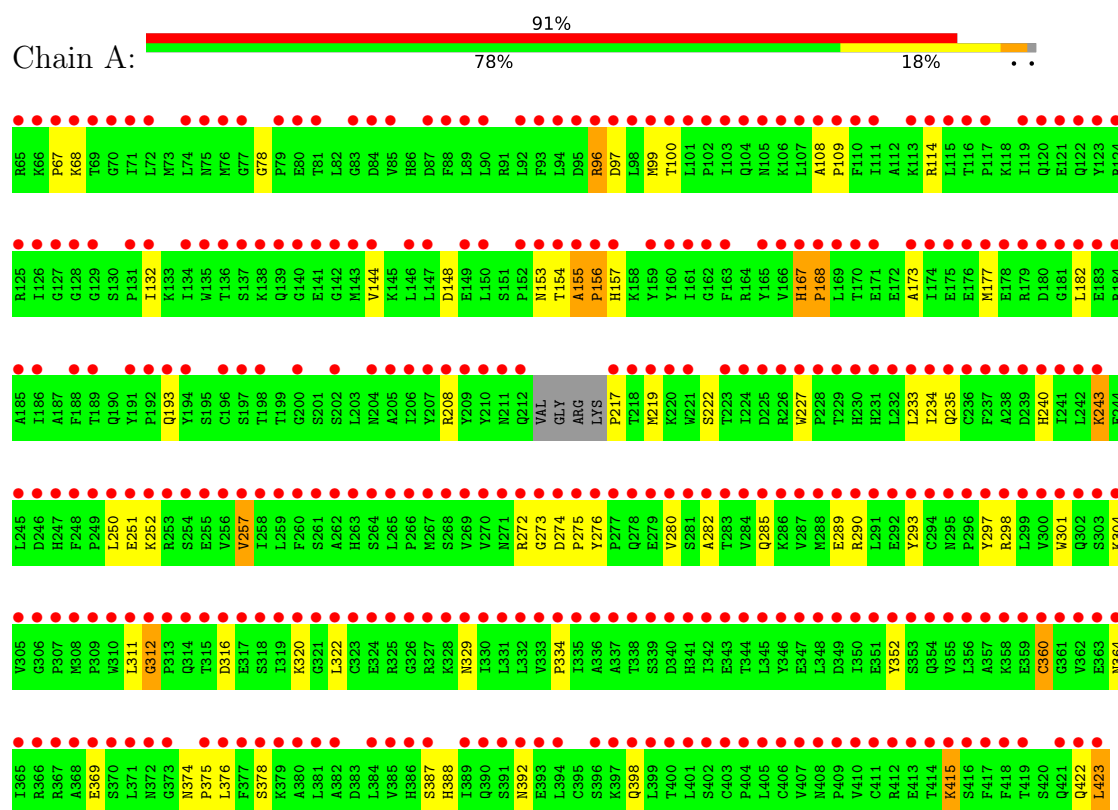
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172	172		
4	B	170	Total	O	0	0
			170	170		

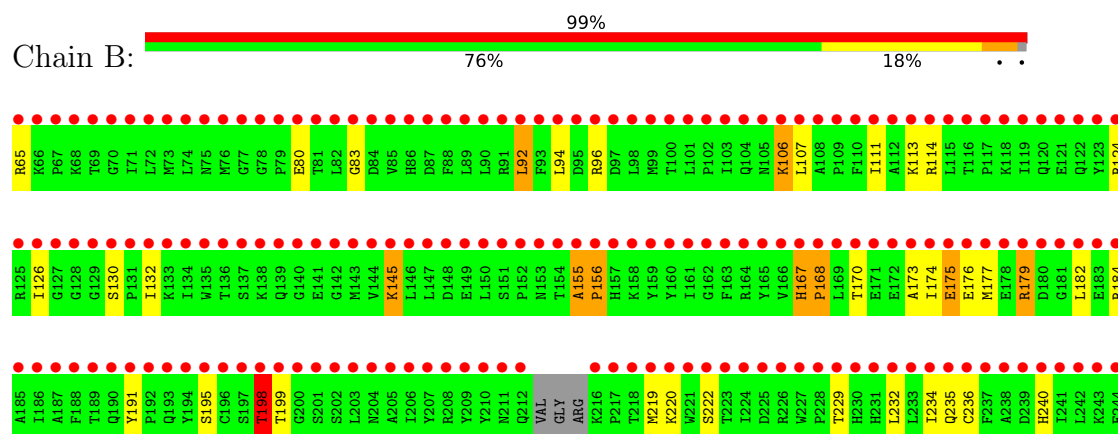
3 Residue-property plots

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: Ferrochelatase, mitochondrial



• Molecule 1: Ferrochelatase, mitochondrial



L365	V305	L245	G306	D246	L245	L371	L311	G312	K252	R253	S254	E255	V256	V257	I258	L259	F260	S261	A262	H263	S264	L265	P266	M267	S268	V269	V270	M271	R272	G273	D274	P275	Y276	F277	Q278	E279	V280	S281	A282	T283	V284	Q285	K286	V287	M288	E289	R290	L291	Y292	T293	C294	M295	P296	Y297	R298	L299	V300	M301	Q302	S303	K304
R366	G306	D246	P307	H247	L245	S370	L311	G312	K252	R253	S254	E255	V256	V257	I258	L259	F260	S261	A262	H263	S264	L265	P266	M267	S268	V269	V270	M271	R272	G273	D274	P275	Y276	F277	Q278	E279	V280	S281	A282	T283	V284	Q285	K286	V287	M288	E289	R290	L291	Y292	T293	C294	M295	P296	Y297	R298	L299	V300	M301	Q302	S303	K304
R367	G306	D246	P307	H247	L245	S370	L311	G312	K252	R253	S254	E255	V256	V257	I258	L259	F260	S261	A262	H263	S264	L265	P266	M267	S268	V269	V270	M271	R272	G273	D274	P275	Y276	F277	Q278	E279	V280	S281	A282	T283	V284	Q285	K286	V287	M288	E289	R290	L291	Y292	T293	C294	M295	P296	Y297	R298	L299	V300	M301	Q302	S303	K304
A368	M308	F248	P309	F248	L245	S370	L311	G312	K252	R253	S254	E255	V256	V257	I258	L259	F260	S261	A262	H263	S264	L265	P266	M267	S268	V269	V270	M271	R272	G273	D274	P275	Y276	F277	Q278	E279	V280	S281	A282	T283	V284	Q285	K286	V287	M288	E289	R290	L291	Y292	T293	C294	M295	P296	Y297	R298	L299	V300	M301	Q302	S303	K304
E369	P309	F248	P309	F248	L245	S370	L311	G312	K252	R253	S254	E255	V256	V257	I258	L259	F260	S261	A262	H263	S264	L265	P266	M267	S268	V269	V270	M271	R272	G273	D274	P275	Y276	F277	Q278	E279	V280	S281	A282	T283	V284	Q285	K286	V287	M288	E289	R290	L291	Y292	T293	C294	M295	P296	Y297	R298	L299	V300	M301	Q302	S303	K304
L371	L311	G312	P313	Q314	T315	D316	F317	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364							
N372	G312	P313	Q314	T315	D316	F317	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364								
G373	P313	Q314	T315	D316	F317	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364									
N374	Q314	T315	D316	F317	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364										
P375	T315	D316	F317	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364											
F377	F317	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364													
S378	S318	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364														
K379	I319	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364															
A380	K320	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																
L381	G321	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																	
A382	L322	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																		
D383	C323	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																			
L384	E324	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																				
V385	R325	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																					
H386	G326	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																						
S387	R327	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																							
H388	K328	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																								
T389	M329	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																									
Q390	T330	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																										
S391	L331	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																											
N392	L332	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																												
E393	V333	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																													
L394	P334	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																														
C395	T335	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																															
S396	A336	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																																
K397	A337	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																																	
Q398	T338	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																																		
L399	S339	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																																			
T400	D340	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																																				
L401	H341	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364																																					
S402	T342	E343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354																																																

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 94.05Å 113.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 2.35 43.44 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.44-2.35) 93.2 (43.44-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.192 , 0.253 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5269e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.95	4/2883 (0.1%)	1.13	8/3916 (0.2%)
1	B	0.96	2/2895 (0.1%)	1.16	10/3931 (0.3%)
All	All	0.96	6/5778 (0.1%)	1.15	18/7847 (0.2%)

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	A	0	4
1	B	0	5
All	All	0	9

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ILE	CA-CB	6.43	1.61	1.54
1	A	312	GLY	N-CA	5.97	1.52	1.44
1	A	312	GLY	CA-C	-5.64	1.43	1.51
1	B	342	ILE	CA-CB	5.27	1.60	1.54
1	A	234	ILE	CA-CB	5.18	1.60	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	HIS	CA-C-N	18.63	143.13	119.84
1	B	167	HIS	C-N-CA	18.63	143.13	119.84
1	A	155	ALA	CA-C-N	12.82	135.87	119.84
1	A	155	ALA	C-N-CA	12.82	135.87	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	HIS	CA-C-N	10.90	133.47	119.84

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ALA	Peptide
1	A	167	HIS	Mainchain,Peptide
1	A	311	LEU	Peptide
1	B	155	ALA	Mainchain,Peptide
1	B	167	HIS	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	2815	0	2769	56	8
1	B	2827	0	2790	68	5
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	87	0	117	2	0
3	B	87	0	117	4	0
4	A	172	0	0	13	2
4	B	170	0	0	20	7
All	All	6166	0	5793	122	11

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 10.

The worst 5 of 122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HD2	4:A:616:HOH:O	1.28	1.31
1:B:410:VAL:HB	4:B:633:HOH:O	1.43	1.18
1:B:323:CYS:HB3	4:B:602:HOH:O	1.47	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLN:HE22	1:B:297:TYR:H	1.15	0.94
1:B:272:ARG:NH1	4:B:673:HOH:O	2.01	0.93

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:645:HOH:O	4:B:628:HOH:O[3_655]	0.89	1.31
1:B:80:GLU:OE1	4:A:620:HOH:O[3_645]	1.08	1.12
1:A:252:LYS:CE	4:B:599:HOH:O[3_655]	1.09	1.11
1:A:252:LYS:CD	4:B:599:HOH:O[3_655]	1.66	0.54
1:A:251:GLU:CB	1:B:83:GLY:O[3_655]	1.75	0.45

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/359 (98%)	338 (96%)	11 (3%)	2 (1%)	21	24
1	B	352/359 (98%)	340 (97%)	10 (3%)	2 (1%)	21	24
All	All	703/718 (98%)	678 (96%)	21 (3%)	4 (1%)	21	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	B	168	PRO
1	A	168	PRO
1	B	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/323 (96%)	296 (96%)	14 (4%)	24	32
1	B	311/323 (96%)	294 (94%)	17 (6%)	19	24
All	All	621/646 (96%)	590 (95%)	31 (5%)	22	27

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	LEU
1	B	341	HIS
1	B	145	LYS
1	B	374	ASN
1	B	257	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	240	HIS
1	B	341	HIS
1	B	329	ASN
1	B	364	ASN
1	A	364	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	FES	B	499	1	0,4,4	-	-	-		
3	CHD	B	502	-	32,32,32	0.58	0	51,51,51	1.84	12 (23%)
3	CHD	A	502	-	32,32,32	0.61	0	51,51,51	1.86	14 (27%)
3	CHD	B	503	-	32,32,32	0.63	0	51,51,51	1.52	11 (21%)
2	FES	A	499	1	0,4,4	-	-	-		
3	CHD	A	503	-	32,32,32	0.65	0	51,51,51	1.46	11 (21%)
3	CHD	B	501	-	32,32,32	0.76	0	51,51,51	1.90	12 (23%)
3	CHD	A	501	-	32,32,32	0.66	0	51,51,51	1.83	14 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHD	B	502	-	-	5/9/74/74	0/4/4/4
2	FES	B	499	1	-	-	0/1/1/1
3	CHD	A	502	-	-	6/9/74/74	0/4/4/4
3	CHD	B	503	-	-	7/9/74/74	0/4/4/4
2	FES	A	499	1	-	-	0/1/1/1
3	CHD	A	503	-	-	3/9/74/74	0/4/4/4
3	CHD	B	501	-	-	9/9/74/74	0/4/4/4
3	CHD	A	501	-	-	7/9/74/74	0/4/4/4

There are no bond length outliers.

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	CHD	C6-C5-C4	-4.65	105.91	111.23
3	B	501	CHD	C13-C17-C20	-4.62	113.89	119.48
3	A	501	CHD	C16-C17-C20	4.61	119.16	112.18
3	A	502	CHD	C6-C5-C4	-4.53	106.05	111.23
3	B	501	CHD	C6-C5-C4	-4.50	106.08	111.23

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

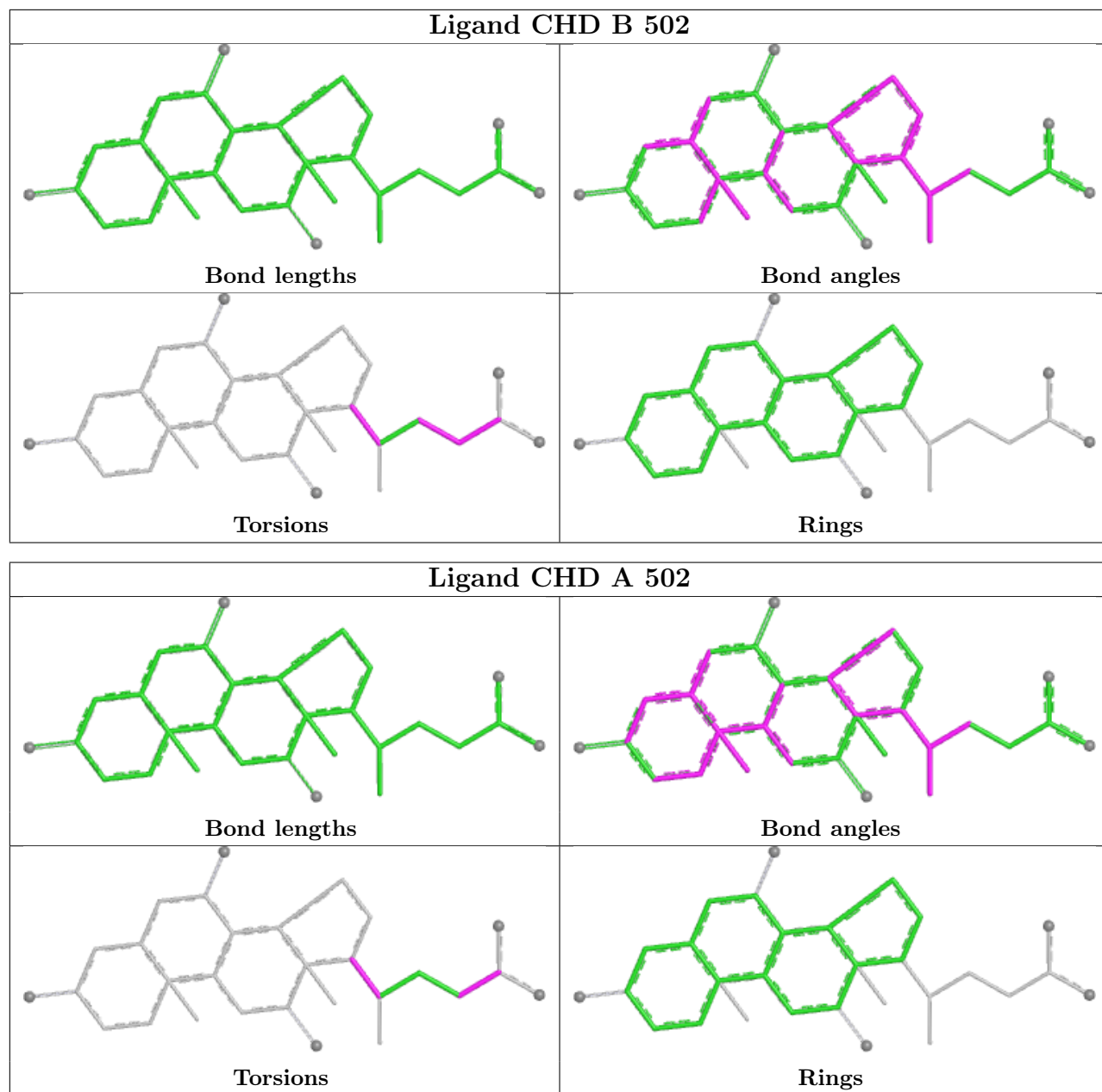
Mol	Chain	Res	Type	Atoms
3	A	502	CHD	C13-C17-C20-C21
3	B	501	CHD	C21-C20-C22-C23
3	B	501	CHD	C17-C20-C22-C23
3	A	501	CHD	C13-C17-C20-C22
3	B	503	CHD	C16-C17-C20-C21

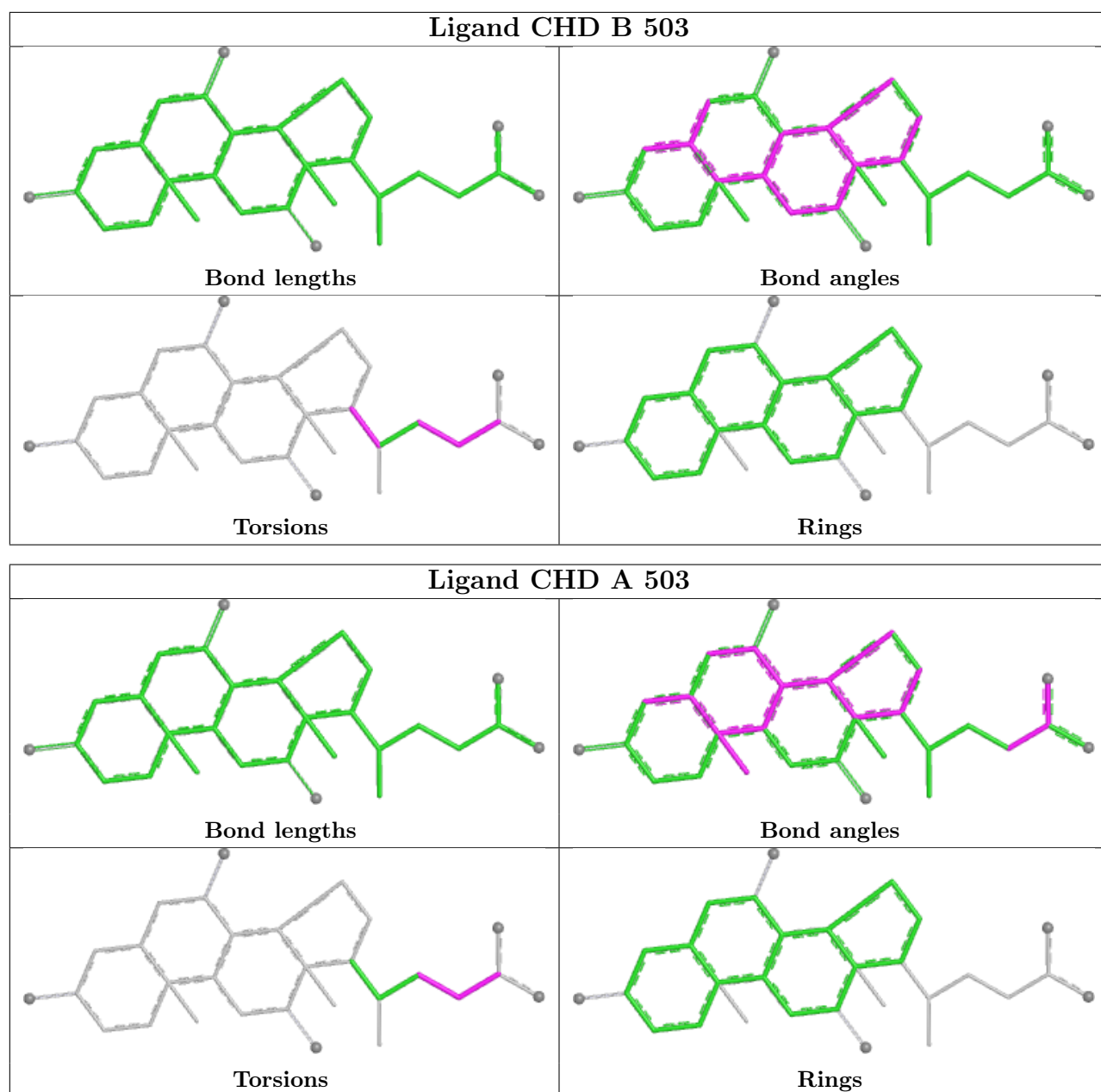
There are no ring outliers.

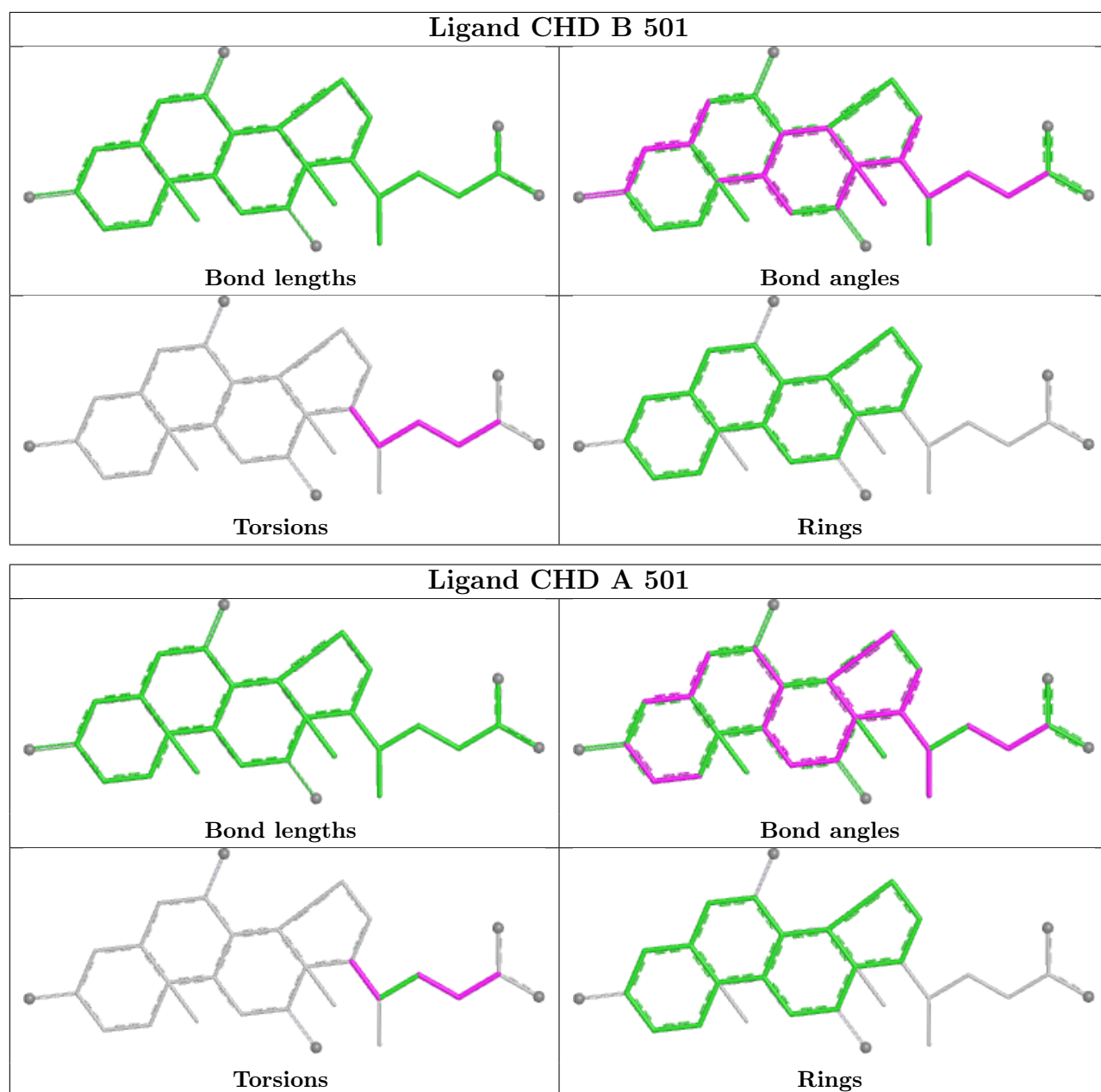
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	CHD	1	0
3	B	503	CHD	1	0
3	B	501	CHD	3	0
3	A	501	CHD	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 [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	355/359 (98%)	3.98	327 (92%) 0 0	14, 23, 40, 50	0
1	B	356/359 (99%)	6.05	356 (100%) 0 0	13, 23, 41, 48	0
All	All	711/718 (99%)	5.02	683 (96%) 0 0	13, 23, 41, 50	0

The worst 5 of 683 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	GLY	14.7
1	B	206	ILE	11.9
1	B	382	ALA	11.5
1	B	168	PRO	11.4
1	B	342	ILE	11.4

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

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

6.3 Carbohydrates [i](#)

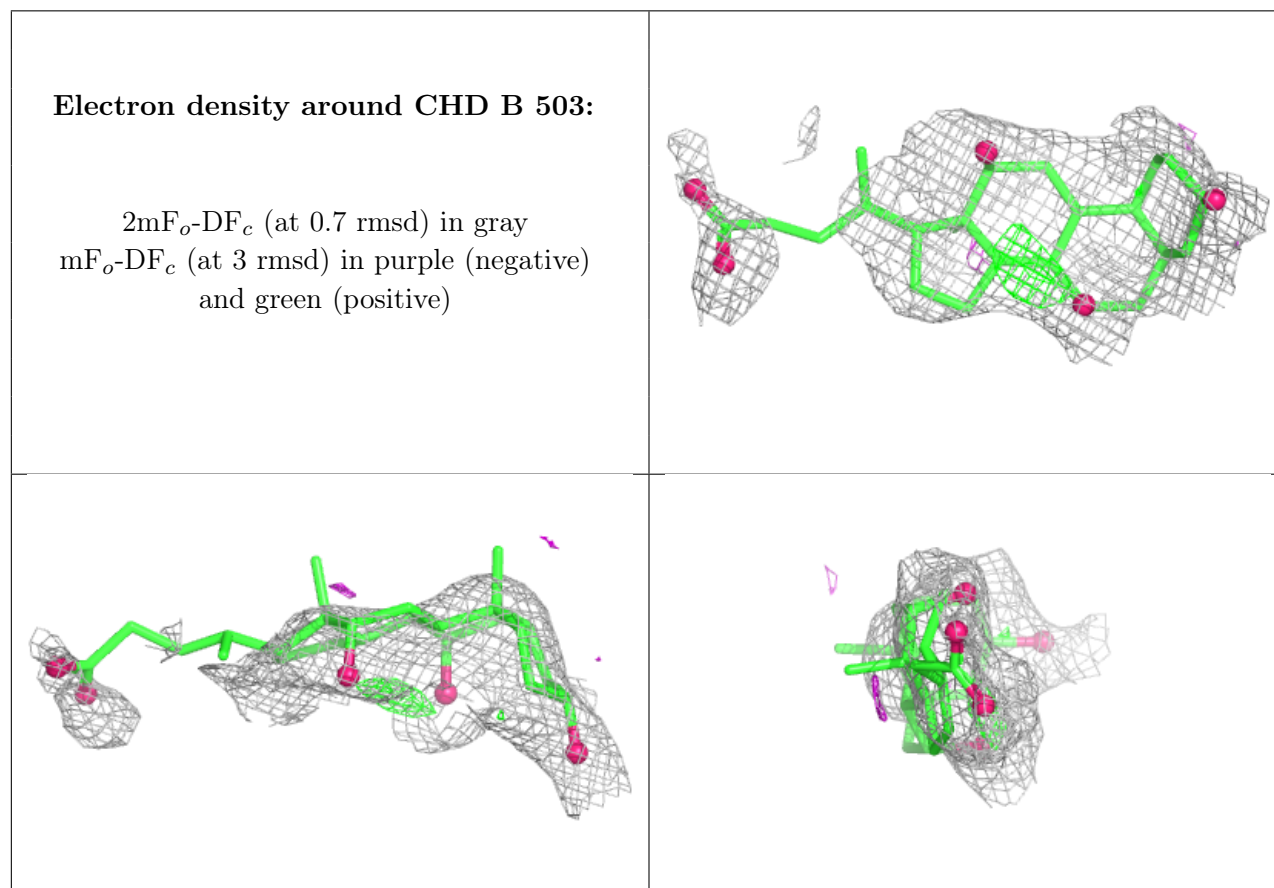
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

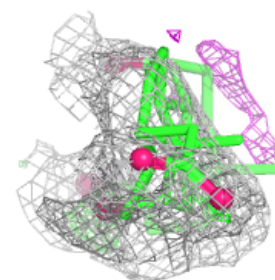
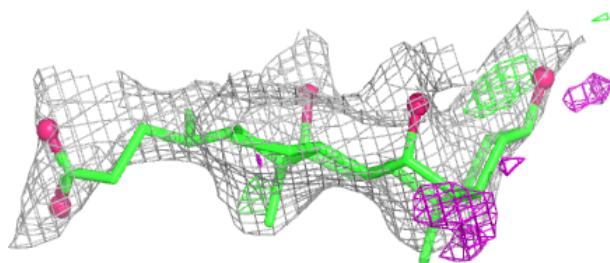
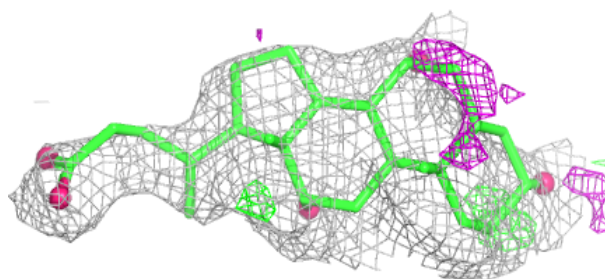
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CHD	B	503	29/29	0.34	0.42	45,48,63,64	0
3	CHD	B	501	29/29	0.48	0.40	28,29,41,45	0
3	CHD	B	502	29/29	0.57	0.38	34,38,51,53	0
3	CHD	A	502	29/29	0.59	0.29	37,41,49,51	0
2	FES	B	499	4/4	0.61	0.22	20,20,22,23	0
3	CHD	A	503	29/29	0.62	0.26	43,47,50,51	0
3	CHD	A	501	29/29	0.72	0.26	26,31,47,48	0
2	FES	A	499	4/4	0.84	0.12	16,17,18,18	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.

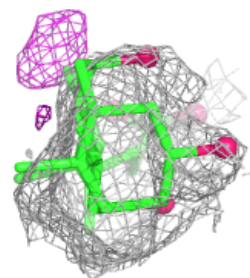
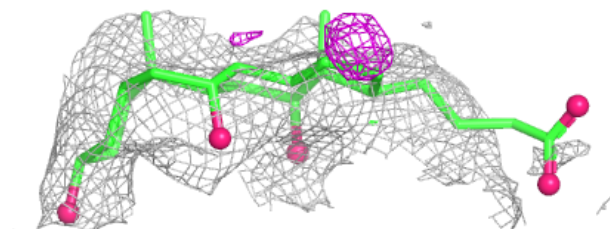
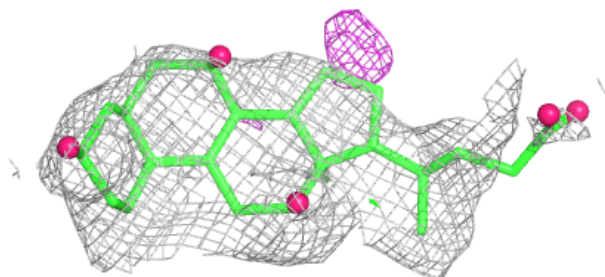


Electron density around CHD B 501:

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

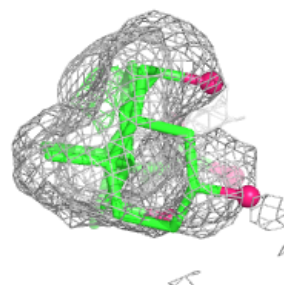
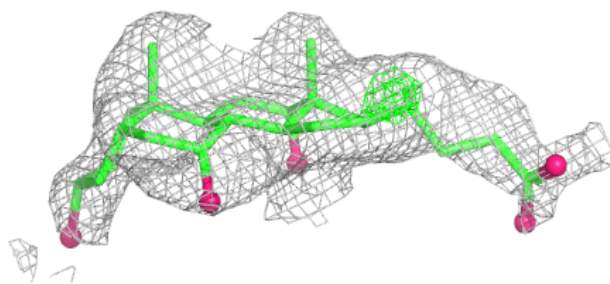
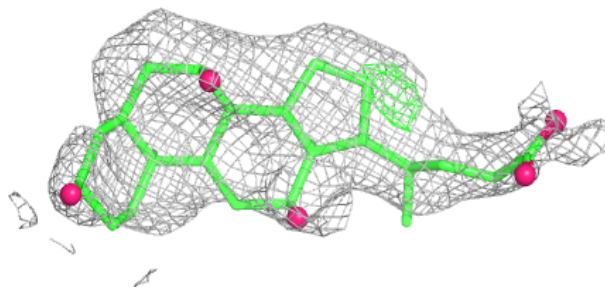
**Electron density around CHD B 502:**

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

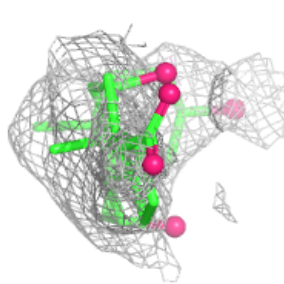
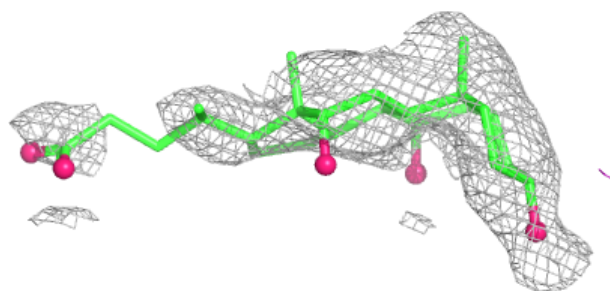
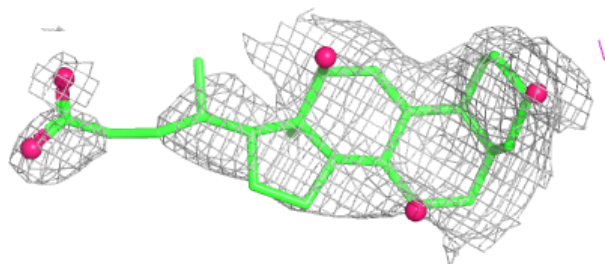


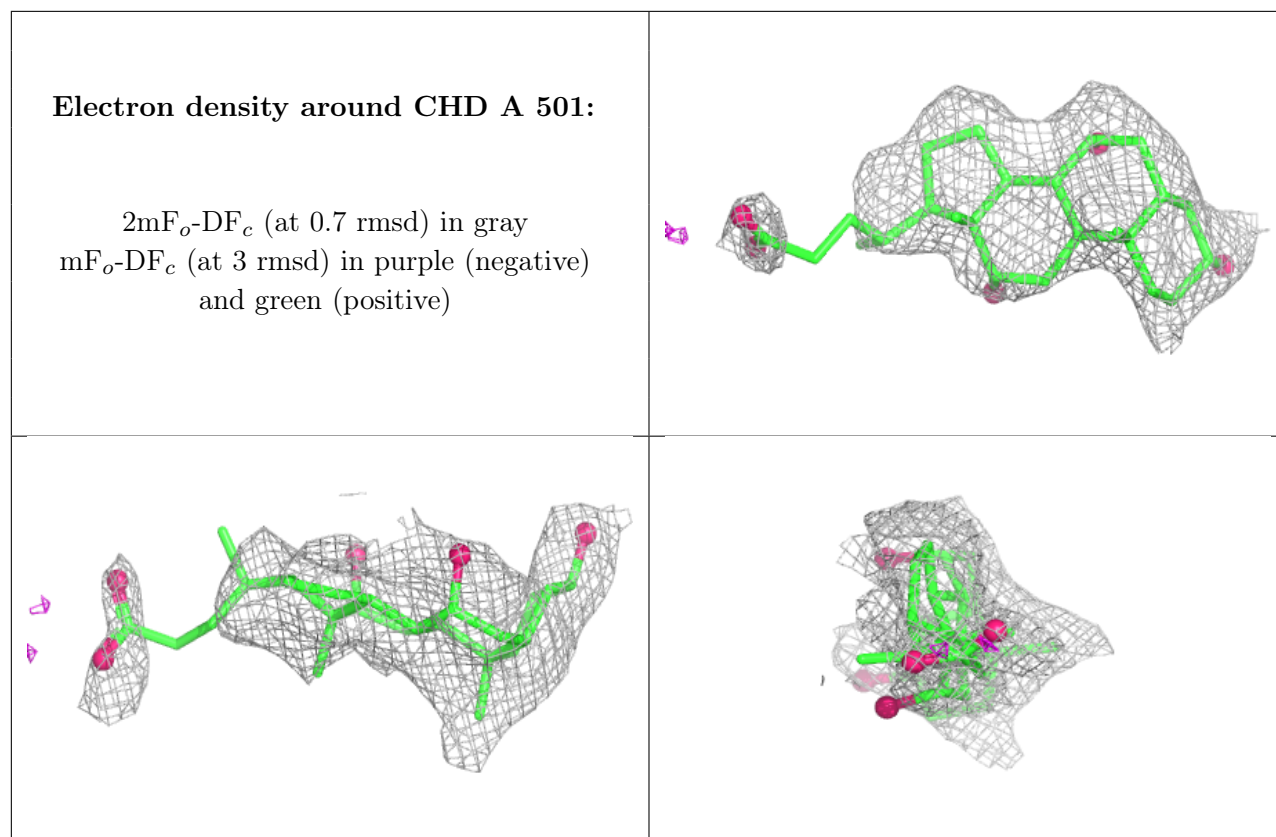
Electron density around CHD A 502:

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

**Electron density around CHD A 503:**

$2mF_o-DF_c$ (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.