



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 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 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

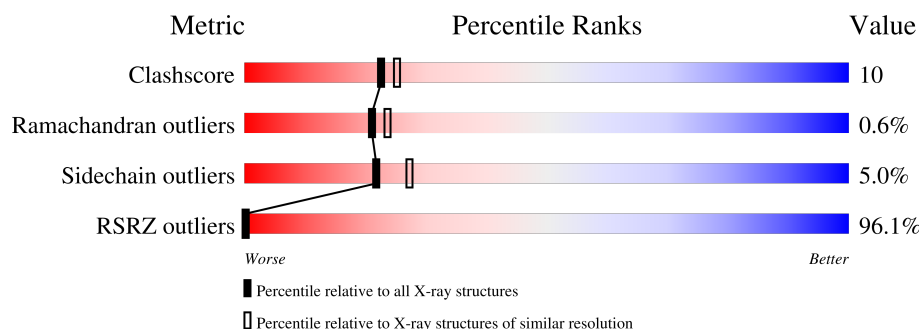
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.

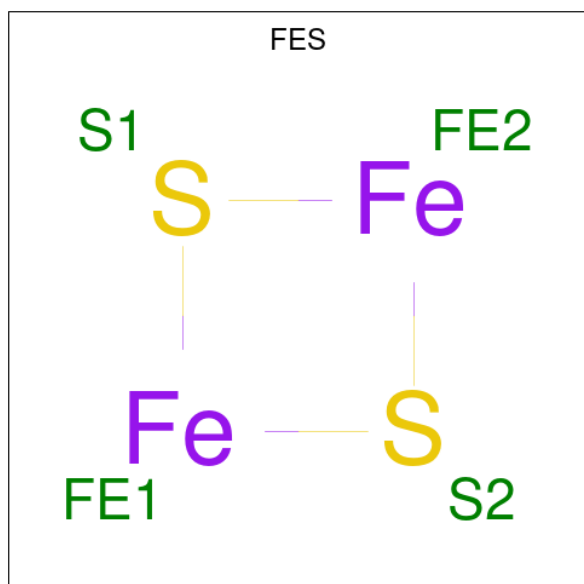
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

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:

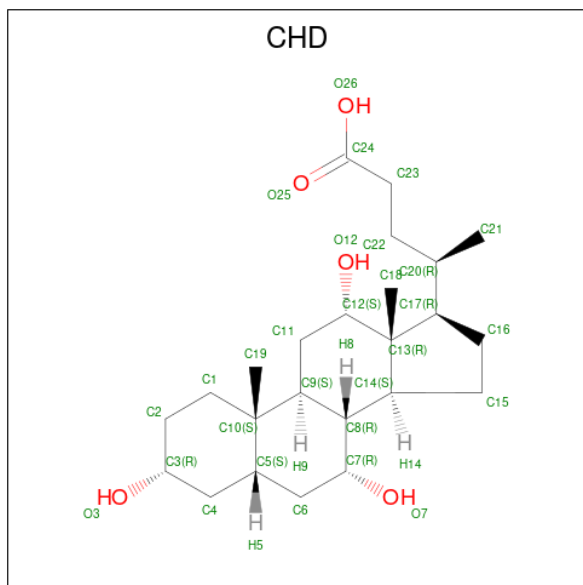
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	engineered mutation	UNP P22830
A	337	ALA	PHE	engineered mutation	UNP P22830
B	115	LEU	ARG	engineered mutation	UNP P22830
B	337	ALA	PHE	engineered mutation	UNP P22830

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



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

- 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 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0

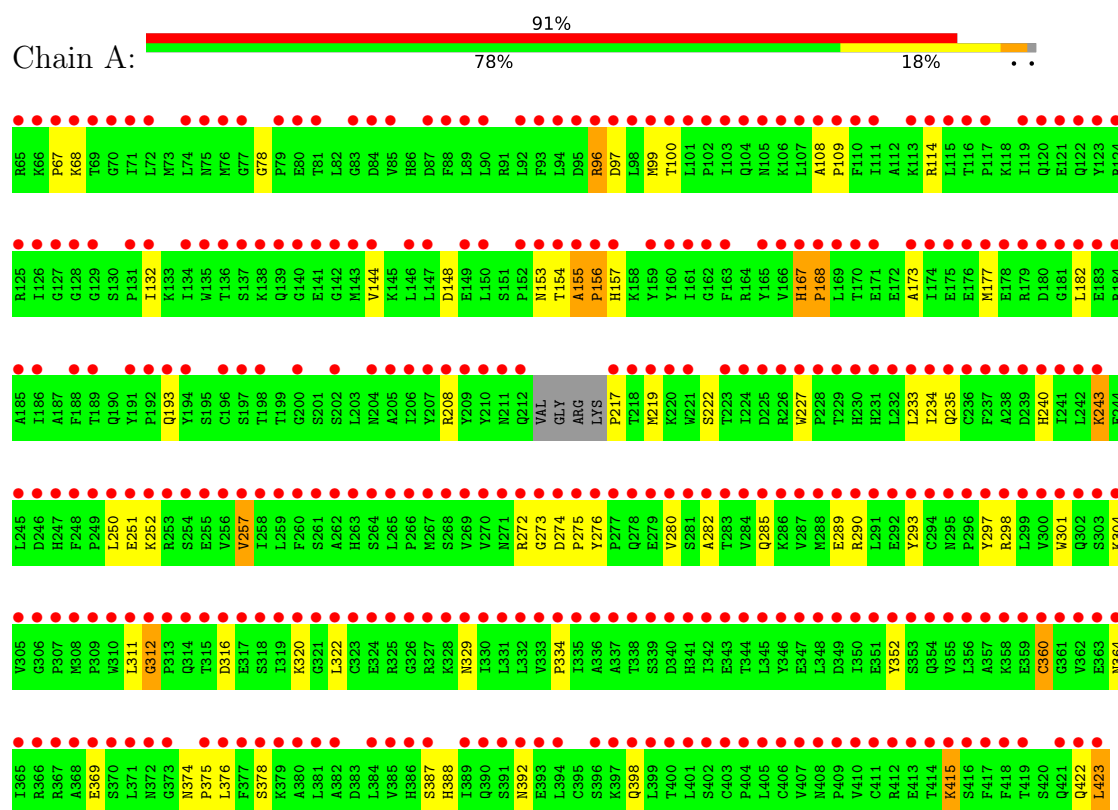
- Molecule 4 is water.

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

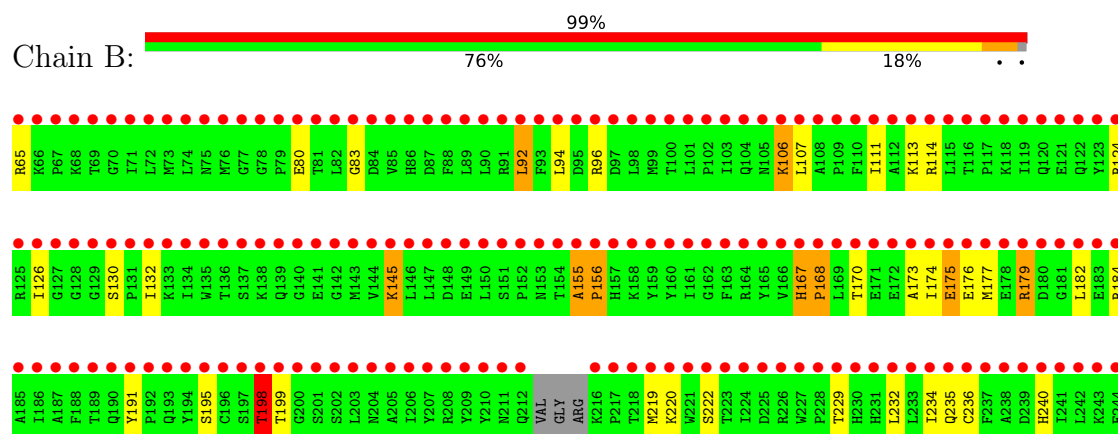
3 Residue-property plots

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	R366	R367	A368	E369	S370	L371	N372	G373	N374	P375	L376	F377	S378	K379	A380	L381	A382	D383	L384	V385	H386	S387	H388	T389	Q390	S391	N392	E393	L394	C395	S396	K397	Q398	L399	T400	L401	S402	C403	P404	L405	C406	V407	M408	P409	V410	C411	R412	F413	T414	K415	S416	F417	F418	T419	S420	Q421	Q422	L423	
V305	G306	P307	M308	P309	W310	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
L245	L246	D247	H248	F249	L250	E251	K252	R253	S254	E255	V256	V257	I258	L259	F260	A261	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	E292	Y293	C294	M295	P296	Y297	R298	L299	V300	M301	Q302	S303	K304

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

All (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
1	B	126	ILE	CA-CB	5.12	1.60	1.54

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ALA	C-N-CA	12.82	135.87	119.84
1	A	167	HIS	CA-C-N	10.90	133.47	119.84
1	A	167	HIS	C-N-CA	10.90	133.47	119.84
1	A	312	GLY	N-CA-C	-7.87	96.29	112.34
1	B	155	ALA	CA-C-N	7.31	128.98	119.84
1	B	155	ALA	C-N-CA	7.31	128.98	119.84
1	B	274	ASP	CA-C-N	6.70	126.39	119.82
1	B	274	ASP	C-N-CA	6.70	126.39	119.82
1	B	167	HIS	C-N-CD	-6.29	99.19	125.00
1	B	156	PRO	N-CA-C	-6.15	99.81	112.47
1	B	155	ALA	N-CA-C	5.78	116.94	109.72
1	A	78	GLY	CA-C-N	5.74	126.03	119.83
1	A	78	GLY	C-N-CA	5.74	126.03	119.83
1	A	78	GLY	N-CA-C	-5.47	101.18	112.34
1	B	198	THR	CB-CA-C	5.25	120.86	110.42

There are no chirality outliers.

All (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
1	B	312	GLY	Mainchain,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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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
1:B:323:CYS:CB	4:B:602:HOH:O	2.09	0.86
1:A:240:HIS:O	1:A:243:LYS:HE3	1.75	0.85
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.42	0.84
1:B:323:CYS:SG	4:B:602:HOH:O	2.35	0.83
1:B:198:THR:HG22	1:B:199:THR:H	1.42	0.83
1:A:67:PRO:HA	1:A:156:PRO:HB2	1.60	0.82
1:A:388:HIS:HD2	4:A:561:HOH:O	1.69	0.76
1:B:300:VAL:HG12	1:B:313:PRO:HG2	1.70	0.74
1:B:198:THR:HG21	4:B:517:HOH:O	1.87	0.74
1:B:176:GLU:HG3	4:B:609:HOH:O	1.87	0.73
1:A:297:TYR:H	1:B:398:GLN:HE22	1.33	0.73
1:B:334:PRO:CG	4:B:564:HOH:O	2.37	0.72
1:A:222:SER:OG	1:A:388:HIS:HE1	1.73	0.71
1:A:217:PRO:N	4:A:504:HOH:O	2.23	0.70
1:B:222:SER:OG	1:B:388:HIS:HE1	1.75	0.70
1:B:334:PRO:HG3	4:B:564:HOH:O	1.90	0.70
1:B:402:SER:CB	4:B:551:HOH:O	2.40	0.70
1:A:392:ASN:ND2	4:A:605:HOH:O	2.26	0.68
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.59	0.67
1:B:298:ARG:HG2	4:B:565:HOH:O	1.95	0.65
1:A:240:HIS:HD2	1:A:369:GLU:O	1.79	0.64
1:B:422:GLN:O	1:B:423:LEU:HB2	1.98	0.64
1:B:402:SER:HB3	4:B:551:HOH:O	1.98	0.63
1:A:329:ASN:ND2	1:A:364:ASN:HB2	2.12	0.63
1:B:175:GLU:O	1:B:179:ARG:HG2	1.99	0.62
1:A:114:ARG:HG3	4:A:585:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:HIS:HD2	1:B:369:GLU:O	1.83	0.61
1:A:422:GLN:O	1:A:423:LEU:HB2	2.01	0.61
1:A:398:GLN:HE22	1:B:297:TYR:N	1.93	0.60
1:B:168:PRO:HD3	4:B:639:HOH:O	2.00	0.60
1:B:198:THR:CG2	1:B:199:THR:H	2.16	0.58
1:A:97:ASP:CG	1:A:208:ARG:HH22	2.11	0.58
1:B:388:HIS:HD2	1:B:393:GLU:OE1	1.86	0.58
1:B:386:HIS:O	1:B:390:GLN:HG3	2.04	0.57
1:A:273:GLY:O	1:B:298:ARG:HD3	2.04	0.57
1:B:191:TYR:CD1	1:B:198:THR:HG23	2.40	0.57
1:B:402:SER:HB2	4:B:551:HOH:O	2.04	0.56
1:A:240:HIS:HA	1:A:243:LYS:HE3	1.87	0.56
1:B:195:SER:HB3	1:B:198:THR:HB	1.87	0.56
1:B:229:THR:HB	1:B:286:LYS:HE2	1.87	0.55
1:A:334:PRO:HG2	4:A:578:HOH:O	2.05	0.54
1:B:173:ALA:O	1:B:177:MET:HG3	2.08	0.54
1:A:97:ASP:OD1	1:A:208:ARG:NH2	2.41	0.53
1:A:243:LYS:CD	4:A:616:HOH:O	2.08	0.53
1:A:374:ASN:C	1:A:374:ASN:HD22	2.16	0.53
1:A:68:LYS:NZ	1:A:153:ASN:O	2.41	0.52
1:A:168:PRO:HD3	4:A:626:HOH:O	2.08	0.52
1:B:222:SER:OG	1:B:388:HIS:CE1	2.60	0.52
1:A:240:HIS:C	1:A:243:LYS:HE3	2.34	0.52
1:B:177:MET:HB2	1:B:219:MET:HE1	1.90	0.52
1:A:240:HIS:HA	1:A:243:LYS:CE	2.40	0.52
1:B:232:LEU:HD22	1:B:376:LEU:HD11	1.92	0.52
1:B:392:ASN:HB2	4:B:660:HOH:O	2.09	0.52
1:B:229:THR:HB	1:B:286:LYS:CE	2.40	0.51
1:A:154:THR:OG1	1:A:157:HIS:HE1	1.94	0.51
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.26	0.51
1:A:374:ASN:HD22	1:A:375:PRO:N	2.09	0.50
1:B:416:SER:O	1:B:420:SER:HB2	2.10	0.50
1:B:235:GLN:HG3	1:B:290:ARG:CZ	2.42	0.49
1:A:243:LYS:CE	4:A:616:HOH:O	2.50	0.49
1:B:198:THR:HG22	1:B:199:THR:N	2.19	0.49
1:B:92:LEU:HD11	3:B:501:CHD:H62	1.95	0.49
1:A:240:HIS:CA	1:A:243:LYS:HE3	2.42	0.49
1:B:320:LYS:O	1:B:324:GLU:HG3	2.13	0.49
1:A:148:ASP:OD1	1:A:157:HIS:HD2	1.94	0.49
1:B:94:LEU:O	1:B:96:ARG:NH1	2.44	0.48
1:A:374:ASN:ND2	1:A:376:LEU:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:SER:OG	1:A:388:HIS:CE1	2.61	0.48
1:B:252:LYS:NZ	4:B:631:HOH:O	2.47	0.48
1:A:320:LYS:HG3	1:A:360:CYS:SG	2.53	0.47
1:B:198:THR:CG2	1:B:199:THR:N	2.74	0.47
1:A:154:THR:OG1	1:A:157:HIS:CE1	2.68	0.47
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.95	0.47
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.48	0.47
1:A:301:TRP:CD1	1:A:312:GLY:HA3	2.50	0.47
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.77	0.46
1:B:130:SER:OG	1:B:132:ILE:HG13	2.16	0.46
1:A:97:ASP:HB2	4:A:665:HOH:O	2.15	0.46
1:B:65:ARG:N	4:B:601:HOH:O	2.49	0.46
1:B:113:LYS:HG2	4:B:661:HOH:O	2.15	0.46
1:B:235:GLN:HG3	1:B:290:ARG:NH1	2.30	0.46
1:A:285:GLN:HG2	1:B:282:ALA:HB1	1.98	0.46
1:B:334:PRO:HG2	4:B:564:HOH:O	2.07	0.46
1:A:415:LYS:CE	4:A:563:HOH:O	2.64	0.45
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.17	0.45
1:A:257:VAL:HG21	1:A:322:LEU:HD13	1.99	0.45
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.99	0.43
1:A:173:ALA:O	1:A:177:MET:HG3	2.17	0.43
1:B:234:ILE:HG13	1:B:286:LYS:HE3	2.00	0.43
1:B:398:GLN:NE2	1:B:398:GLN:HA	2.33	0.43
1:B:177:MET:CB	1:B:219:MET:HE1	2.49	0.43
1:A:282:ALA:HB1	1:B:285:GLN:HG2	1.99	0.42
3:A:501:CHD:H222	3:A:501:CHD:C18	2.50	0.42
1:B:374:ASN:HD22	1:B:374:ASN:C	2.27	0.42
1:B:374:ASN:HD22	1:B:376:LEU:H	1.67	0.42
1:B:329:ASN:ND2	1:B:364:ASN:HB2	2.30	0.42
3:B:501:CHD:H212	3:B:501:CHD:H12	2.01	0.42
1:A:177:MET:HB3	1:A:182:LEU:HD12	2.01	0.42
1:A:285:GLN:O	1:A:289:GLU:HG3	2.20	0.42
1:B:170:THR:O	1:B:174:ILE:HG13	2.20	0.42
1:A:374:ASN:HD22	1:A:376:LEU:H	1.67	0.42
1:A:304:LYS:HE2	4:A:635:HOH:O	2.19	0.42
1:A:227:TRP:CZ3	1:A:233:LEU:HD13	2.55	0.41
1:A:96:ARG:HA	1:A:99:MET:O	2.19	0.41
1:B:412:ARG:HH11	1:B:412:ARG:HG2	1.85	0.41
1:A:276:TYR:O	1:A:280:VAL:HG23	2.20	0.41
3:B:501:CHD:H183	3:B:501:CHD:H20	1.92	0.41
1:A:235:GLN:HG3	1:A:290:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:503:CHD:H162	3:B:503:CHD:H222	1.79	0.41
1:B:107:LEU:O	1:B:111:ILE:HG13	2.20	0.41
1:B:145:LYS:NZ	1:B:145:LYS:HB3	2.36	0.41
1:B:357:ALA:HB1	1:B:362:VAL:HG11	2.03	0.40
1:B:236:CYS:HB3	1:B:371:LEU:HD22	2.03	0.40
3:A:502:CHD:H112	3:A:502:CHD:H12A	1.90	0.40
4:A:624:HOH:O	1:B:286:LYS:HD3	2.20	0.40
1:B:341:HIS:HE1	4:B:563:HOH:O	2.03	0.40
1:A:273:GLY:HA2	1:B:313:PRO:HG3	2.04	0.40

All (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
1:B:124:ARG:O	4:B:521:HOH:O[3_645]	1.79	0.41
1:A:251:GLU:CA	1:B:83:GLY:O[3_655]	1.91	0.29
1:A:251:GLU:OE1	4:B:567:HOH:O[3_655]	2.00	0.20
1:A:251:GLU:CG	4:B:567:HOH:O[3_655]	2.01	0.19
1:A:251:GLU:O	1:B:83:GLY:CA[3_655]	2.03	0.17
1:A:251:GLU:CD	4:B:567:HOH:O[3_655]	2.05	0.15

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	351/359 (98%)	338 (96%)	11 (3%)	2 (1%)	21 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	100	THR
1	A	144	VAL
1	A	219	MET
1	A	243	LYS
1	A	250	LEU
1	A	257	VAL
1	A	272	ARG
1	A	298	ARG
1	A	360	CYS
1	A	378	SER
1	A	387	SER

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Mol	Chain	Res	Type
1	A	415	LYS
1	A	423	LEU
1	B	92	LEU
1	B	106	LYS
1	B	114	ARG
1	B	145	LYS
1	B	175	GLU
1	B	179	ARG
1	B	182	LEU
1	B	184	ARG
1	B	198	THR
1	B	220	LYS
1	B	257	VAL
1	B	272	ARG
1	B	298	ARG
1	B	341	HIS
1	B	362	VAL
1	B	374	ASN
1	B	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	211	ASN
1	A	240	HIS
1	A	314	GLN
1	A	329	ASN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	386	HIS
1	A	388	HIS
1	A	398	GLN
1	A	421	GLN
1	B	167	HIS
1	B	235	GLN
1	B	240	HIS
1	B	314	GLN
1	B	329	ASN
1	B	341	HIS
1	B	364	ASN

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Mol	Chain	Res	Type
1	B	374	ASN
1	B	388	HIS
1	B	390	GLN
1	B	398	GLN
1	B	421	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

All (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
3	B	502	CHD	C15-C14-C13	4.46	107.87	103.54
3	B	502	CHD	C17-C13-C14	-4.45	95.65	100.11
3	B	501	CHD	C23-C22-C20	-4.37	106.29	114.46
3	A	503	CHD	C15-C14-C13	4.10	107.52	103.54
3	B	501	CHD	C16-C17-C20	3.93	118.12	112.18
3	A	502	CHD	C21-C20-C17	3.72	118.46	112.88
3	B	502	CHD	C1-C10-C5	3.68	113.03	107.75
3	B	501	CHD	C14-C13-C12	3.58	110.69	107.42
3	A	501	CHD	C14-C13-C12	3.58	110.69	107.42
3	B	502	CHD	C6-C5-C4	-3.57	107.15	111.23
3	B	503	CHD	C15-C14-C13	3.55	106.99	103.54
3	A	501	CHD	C22-C23-C24	-3.40	103.42	112.49
3	A	502	CHD	C13-C17-C20	3.39	123.59	119.48
3	B	502	CHD	C19-C10-C5	-3.37	104.80	110.44
3	B	503	CHD	C16-C17-C13	3.34	106.78	103.54
3	A	502	CHD	C9-C10-C5	3.33	113.14	108.51
3	B	503	CHD	C9-C10-C5	3.33	113.14	108.51
3	B	502	CHD	C13-C17-C20	3.32	123.50	119.48
3	B	501	CHD	C11-C9-C10	-3.31	110.34	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CHD	C17-C13-C14	-3.26	96.84	100.11
3	B	502	CHD	C22-C20-C17	-3.13	103.84	110.33
3	A	501	CHD	C13-C17-C20	-3.09	115.75	119.48
3	A	501	CHD	C15-C14-C13	3.00	106.45	103.54
3	A	501	CHD	C21-C20-C17	-2.97	108.42	112.88
3	B	503	CHD	C4-C5-C10	2.96	115.81	112.66
3	A	501	CHD	C9-C11-C12	2.95	118.16	114.29
3	A	502	CHD	C1-C10-C5	2.89	111.89	107.75
3	A	503	CHD	C10-C9-C8	2.88	115.05	111.84
3	A	503	CHD	C6-C7-C8	2.85	114.61	111.50
3	A	502	CHD	C2-C1-C10	2.78	117.43	112.74
3	A	502	CHD	C22-C20-C17	-2.77	104.59	110.33
3	A	501	CHD	C11-C9-C8	2.74	114.96	110.89
3	B	502	CHD	C21-C20-C17	2.73	116.99	112.88
3	A	503	CHD	C9-C10-C5	2.72	112.29	108.51
3	A	501	CHD	C9-C8-C7	-2.71	108.45	111.86
3	B	501	CHD	C22-C23-C24	-2.67	105.38	112.49
3	A	502	CHD	C6-C5-C10	2.65	115.48	112.66
3	B	501	CHD	C17-C13-C12	-2.64	115.29	117.67
3	B	503	CHD	C11-C12-C13	2.63	113.94	111.26
3	B	501	CHD	C11-C9-C8	2.61	114.76	110.89
3	A	502	CHD	C19-C10-C1	-2.58	104.21	108.31
3	A	502	CHD	C15-C14-C13	2.55	106.01	103.54
3	A	501	CHD	C16-C17-C13	2.54	106.00	103.54
3	A	503	CHD	C14-C8-C9	-2.53	106.21	109.75
3	B	503	CHD	C17-C13-C14	-2.53	97.58	100.11
3	B	501	CHD	O3-C3-C4	-2.45	104.96	109.84
3	B	501	CHD	C18-C13-C12	2.44	111.50	109.06
3	A	503	CHD	C4-C5-C10	2.38	115.19	112.66
3	B	502	CHD	C11-C9-C8	2.37	114.41	110.89
3	A	502	CHD	C21-C20-C22	-2.36	106.69	110.34
3	A	503	CHD	C14-C8-C7	2.32	114.93	111.85
3	B	503	CHD	C14-C8-C9	-2.29	106.55	109.75
3	A	501	CHD	C17-C13-C14	-2.29	97.82	100.11
3	B	502	CHD	C16-C17-C20	-2.25	108.78	112.18
3	B	503	CHD	C14-C13-C12	2.20	109.42	107.42
3	A	502	CHD	C5-C4-C3	2.19	116.01	112.71
3	A	503	CHD	C19-C10-C5	-2.15	106.85	110.44
3	B	502	CHD	C16-C15-C14	-2.12	101.00	105.14
3	B	502	CHD	C16-C17-C13	2.11	105.58	103.54
3	B	501	CHD	C13-C14-C8	-2.09	112.06	114.72
3	A	501	CHD	C11-C12-C13	2.07	113.37	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	CHD	C10-C9-C8	2.07	114.14	111.84
3	A	503	CHD	C9-C8-C7	2.06	114.45	111.86
3	B	503	CHD	C6-C5-C4	-2.05	108.88	111.23
3	B	503	CHD	C11-C9-C8	2.03	113.89	110.89
3	A	502	CHD	C11-C9-C8	2.03	113.89	110.89
3	A	503	CHD	O26-C24-C23	2.02	120.39	114.00
3	A	503	CHD	C16-C17-C13	2.02	105.50	103.54
3	A	501	CHD	C1-C2-C3	-2.01	107.82	110.48

There are no chirality outliers.

All (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
3	A	501	CHD	C20-C22-C23-C24
3	A	501	CHD	C16-C17-C20-C21
3	A	501	CHD	C13-C17-C20-C21
3	B	503	CHD	C16-C17-C20-C22
3	B	501	CHD	C20-C22-C23-C24
3	B	503	CHD	C20-C22-C23-C24
3	A	502	CHD	C16-C17-C20-C22
3	B	503	CHD	C13-C17-C20-C22
3	B	502	CHD	C13-C17-C20-C21
3	A	502	CHD	C13-C17-C20-C22
3	B	503	CHD	C13-C17-C20-C21
3	B	501	CHD	C13-C17-C20-C22
3	B	502	CHD	C20-C22-C23-C24
3	B	501	CHD	C13-C17-C20-C21
3	A	503	CHD	C20-C22-C23-C24
3	B	501	CHD	C16-C17-C20-C22
3	B	501	CHD	C16-C17-C20-C21
3	B	502	CHD	C22-C23-C24-O26
3	B	502	CHD	C22-C23-C24-O25
3	B	501	CHD	C22-C23-C24-O25
3	A	501	CHD	C22-C23-C24-O26
3	A	503	CHD	C22-C23-C24-O25
3	A	502	CHD	C22-C23-C24-O26
3	A	501	CHD	C22-C23-C24-O25

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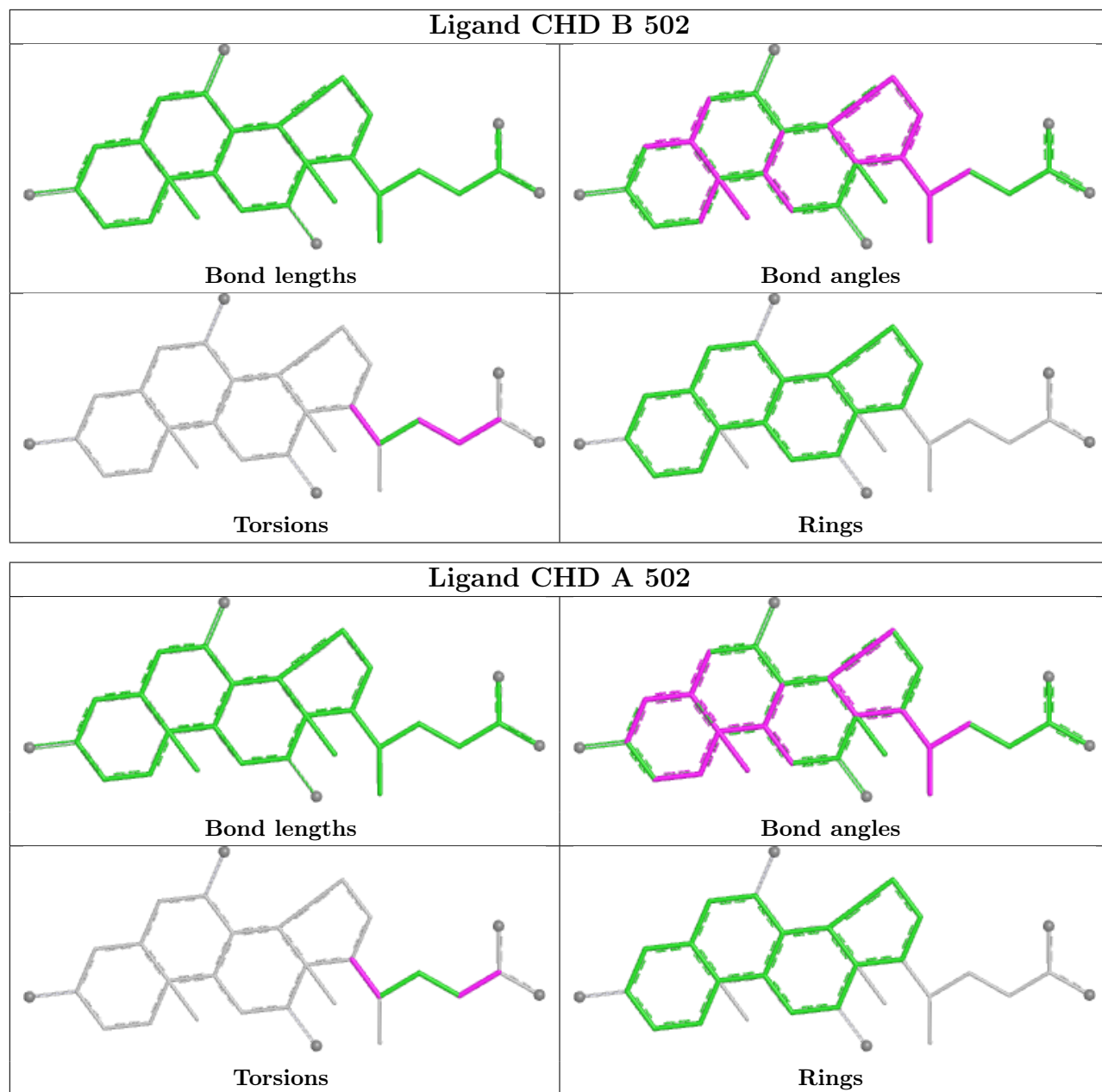
Mol	Chain	Res	Type	Atoms
3	A	502	CHD	C22-C23-C24-O25
3	A	503	CHD	C22-C23-C24-O26
3	B	501	CHD	C22-C23-C24-O26
3	A	501	CHD	C16-C17-C20-C22
3	B	502	CHD	C16-C17-C20-C22
3	A	502	CHD	C16-C17-C20-C21
3	B	503	CHD	C22-C23-C24-O26
3	B	503	CHD	C22-C23-C24-O25

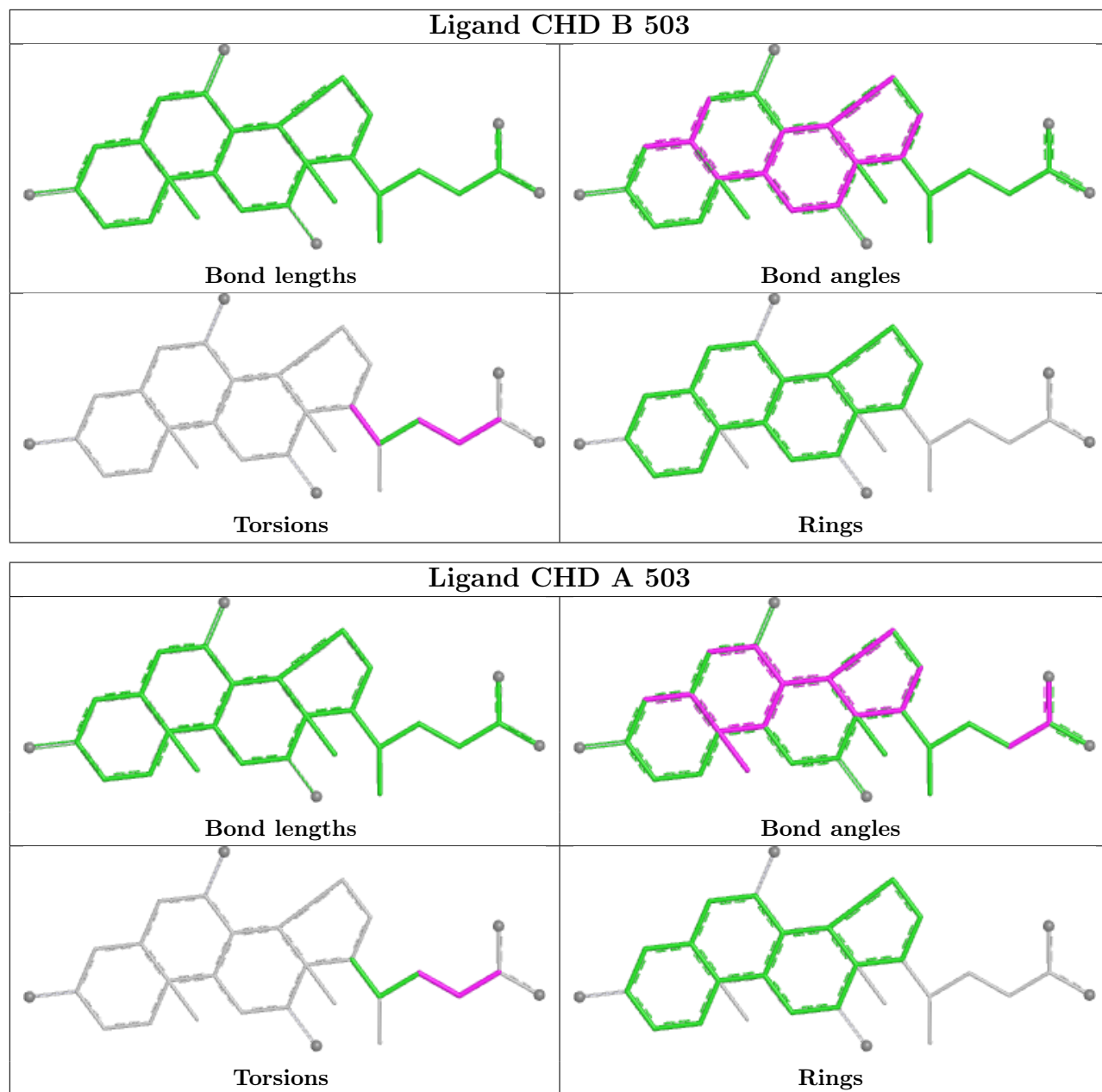
There are no ring outliers.

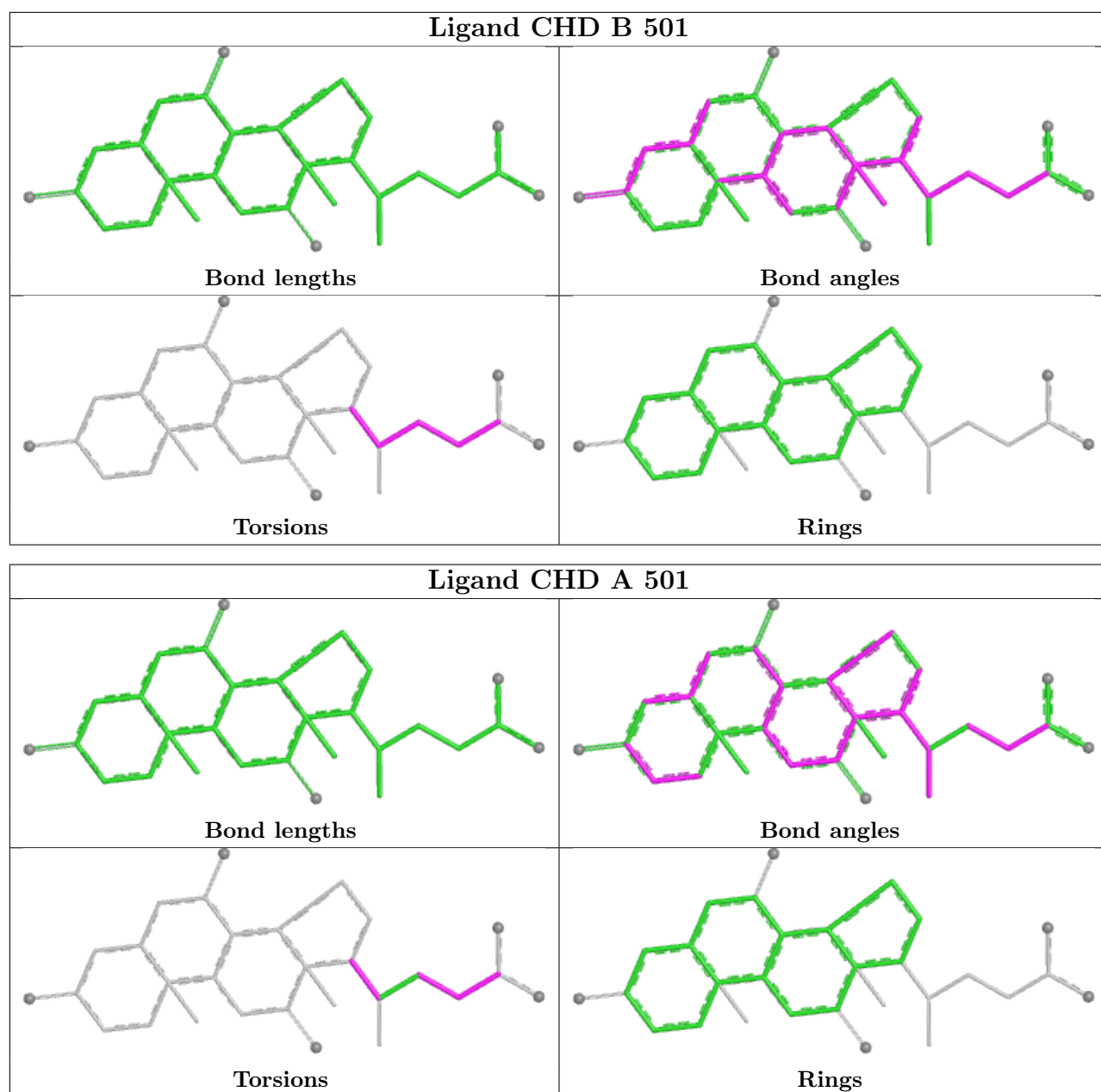
4 monomers are involved in 6 short contacts:

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

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	355/359 (98%)	3.98	327 (92%)  	14, 23, 40, 50	0
1	B	356/359 (99%)	6.05	356 (100%)  	13, 23, 41, 48	0
All	All	711/718 (99%)	5.02	683 (96%)  	13, 23, 41, 50	0

All (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
1	B	210	TYR	11.2
1	B	418	PHE	11.2
1	B	134	ILE	10.9
1	B	77	GLY	10.8
1	B	205	ALA	10.6
1	B	161	ILE	10.6
1	B	73	MET	10.5
1	B	385	VAL	10.4
1	B	181	GLY	10.4
1	B	169	LEU	10.4
1	B	218	THR	10.3
1	B	378	SER	10.2
1	B	163	PHE	10.2
1	A	238	ALA	10.2
1	B	71	ILE	10.1
1	A	273	GLY	10.0
1	B	159	TYR	10.0
1	A	322	LEU	9.8
1	B	207	TYR	9.8

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Mol	Chain	Res	Type	RSRZ
1	B	101	LEU	9.7
1	B	65	ARG	9.7
1	B	123	TYR	9.7
1	A	326	GLY	9.6
1	B	132	ILE	9.6
1	B	135	TRP	9.6
1	B	276	TYR	9.6
1	A	293	TYR	9.5
1	B	219	MET	9.4
1	A	297	TYR	9.3
1	B	227	TRP	9.3
1	B	414	THR	9.2
1	B	346	TYR	9.2
1	B	420	SER	9.2
1	B	76	MET	9.2
1	B	108	ALA	9.2
1	A	254	SER	9.1
1	B	98	LEU	9.0
1	B	81	THR	9.0
1	A	321	GLY	9.0
1	B	410	VAL	9.0
1	B	381	LEU	8.8
1	B	375	PRO	8.7
1	B	176	GLU	8.7
1	B	130	SER	8.7
1	A	357	ALA	8.6
1	B	372	ASN	8.6
1	B	187	ALA	8.6
1	B	211	ASN	8.5
1	A	314	GLN	8.5
1	B	128	GLY	8.5
1	B	136	THR	8.5
1	B	92	LEU	8.5
1	B	386	HIS	8.5
1	B	70	GLY	8.4
1	B	129	GLY	8.4
1	B	110	PHE	8.4
1	B	221	TRP	8.4
1	A	352	TYR	8.4
1	B	72	LEU	8.4
1	B	352	TYR	8.4
1	A	318	SER	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	258	ILE	8.2
1	B	209	TYR	8.2
1	B	185	ALA	8.1
1	B	340	ASP	8.1
1	B	99	MET	8.1
1	A	325	ARG	8.1
1	B	196	CYS	7.9
1	A	353	SER	7.9
1	B	394	LEU	7.9
1	B	106	LYS	7.8
1	B	411	CYS	7.8
1	B	109	PRO	7.8
1	A	356	LEU	7.8
1	A	270	VAL	7.8
1	B	201	SER	7.7
1	A	361	GLY	7.7
1	B	345	LEU	7.7
1	B	78	GLY	7.7
1	B	202	SER	7.7
1	B	273	GLY	7.6
1	B	392	ASN	7.6
1	B	165	TYR	7.6
1	B	370	SER	7.5
1	B	120	GLN	7.5
1	B	156	PRO	7.5
1	B	188	PHE	7.5
1	B	293	TYR	7.5
1	B	224	ILE	7.5
1	B	112	ALA	7.5
1	B	164	ARG	7.4
1	B	93	PHE	7.4
1	B	406	CYS	7.4
1	A	315	THR	7.4
1	B	311	LEU	7.3
1	B	117	PRO	7.3
1	B	334	PRO	7.3
1	B	180	ASP	7.3
1	B	90	LEU	7.3
1	B	192	PRO	7.3
1	B	144	VAL	7.2
1	B	126	ILE	7.2
1	A	251	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	305	VAL	7.1
1	B	333	VAL	7.1
1	B	167	HIS	7.0
1	B	389	ILE	7.0
1	B	269	VAL	7.0
1	B	86	HIS	7.0
1	B	199	THR	7.0
1	B	339	SER	7.0
1	B	173	ALA	7.0
1	A	323	CYS	6.9
1	B	119	ILE	6.9
1	B	265	LEU	6.9
1	A	335	ILE	6.9
1	B	393	GLU	6.9
1	B	140	GLY	6.9
1	A	234	ILE	6.9
1	B	84	ASP	6.8
1	B	82	LEU	6.8
1	B	270	VAL	6.8
1	B	186	ILE	6.8
1	B	395	CYS	6.8
1	A	360	CYS	6.8
1	B	191	TYR	6.8
1	B	124	ARG	6.7
1	B	353	SER	6.7
1	A	294	CYS	6.7
1	A	245	LEU	6.7
1	B	137	SER	6.7
1	B	95	ASP	6.7
1	A	380	ALA	6.7
1	B	85	VAL	6.7
1	A	237	PHE	6.6
1	B	408	ASN	6.6
1	A	255	GLU	6.6
1	B	423	LEU	6.6
1	B	360	CYS	6.6
1	A	252	LYS	6.6
1	B	287	VAL	6.6
1	B	74	LEU	6.6
1	B	384	LEU	6.6
1	B	358	LYS	6.6
1	B	391	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	6.5
1	A	296	PRO	6.5
1	B	409	PRO	6.4
1	A	329	ASN	6.4
1	A	235	GLN	6.4
1	B	145	LYS	6.4
1	A	366	ARG	6.4
1	B	100	THR	6.4
1	B	275	PRO	6.4
1	B	197	SER	6.4
1	A	253	ARG	6.4
1	B	198	THR	6.3
1	A	362	VAL	6.3
1	B	308	MET	6.3
1	B	69	THR	6.3
1	B	116	THR	6.3
1	B	338	THR	6.3
1	B	235	GLN	6.3
1	B	380	ALA	6.3
1	A	319	ILE	6.3
1	B	103	ILE	6.3
1	B	272	ARG	6.3
1	A	299	LEU	6.3
1	B	162	GLY	6.2
1	B	190	GLN	6.2
1	B	237	PHE	6.2
1	B	111	ILE	6.2
1	B	257	VAL	6.2
1	B	153	ASN	6.2
1	B	94	LEU	6.2
1	A	288	MET	6.2
1	B	189	THR	6.2
1	B	160	TYR	6.2
1	B	297	TYR	6.2
1	A	332	LEU	6.2
1	B	195	SER	6.2
1	A	292	GLU	6.1
1	B	306	GLY	6.1
1	B	407	VAL	6.1
1	B	131	PRO	6.1
1	B	170	THR	6.1
1	B	138	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	233	LEU	6.0
1	B	286	LYS	6.0
1	B	421	GLN	6.0
1	B	422	GLN	6.0
1	B	377	PHE	6.0
1	B	172	GLU	6.0
1	B	142	GLY	6.0
1	B	182	LEU	6.0
1	B	75	ASN	5.9
1	A	241	ILE	5.9
1	A	358	LYS	5.9
1	B	315	THR	5.9
1	B	80	GLU	5.9
1	B	148	ASP	5.9
1	A	108	ALA	5.9
1	B	194	TYR	5.9
1	B	295	ASN	5.9
1	B	107	LEU	5.9
1	A	281	SER	5.9
1	A	287	VAL	5.9
1	B	318	SER	5.9
1	A	286	LYS	5.9
1	A	331	LEU	5.8
1	B	354	GLN	5.8
1	A	328	LYS	5.8
1	B	413	GLU	5.8
1	B	223	THR	5.8
1	B	400	THR	5.8
1	A	250	LEU	5.8
1	A	311	LEU	5.8
1	B	166	VAL	5.8
1	B	323	CYS	5.8
1	B	143	MET	5.8
1	B	174	ILE	5.8
1	B	415	LYS	5.8
1	B	155	ALA	5.8
1	B	280	VAL	5.8
1	B	361	GLY	5.8
1	B	193	GLN	5.7
1	B	150	LEU	5.7
1	A	339	SER	5.7
1	B	204	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	77	GLY	5.7
1	A	423	LEU	5.7
1	B	89	LEU	5.7
1	B	337	ALA	5.7
1	B	113	LYS	5.7
1	B	171	GLU	5.7
1	B	203	LEU	5.7
1	B	309	PRO	5.7
1	B	416	SER	5.7
1	A	257	VAL	5.7
1	B	417	PHE	5.7
1	B	403	CYS	5.7
1	B	91	ARG	5.6
1	B	177	MET	5.6
1	B	147	LEU	5.6
1	B	228	PRO	5.6
1	B	184	ARG	5.6
1	B	262	ALA	5.6
1	B	388	HIS	5.5
1	A	295	ASN	5.5
1	A	344	THR	5.5
1	B	405	LEU	5.5
1	B	149	GLU	5.5
1	A	348	LEU	5.4
1	B	307	PRO	5.4
1	B	379	LYS	5.4
1	B	412	ARG	5.4
1	A	107	LEU	5.4
1	B	178	GLU	5.4
1	B	104	GLN	5.4
1	A	387	SER	5.4
1	A	336	ALA	5.3
1	A	405	LEU	5.3
1	B	355	VAL	5.3
1	B	68	LYS	5.3
1	B	253	ARG	5.3
1	B	264	SER	5.3
1	A	355	VAL	5.3
1	B	234	ILE	5.3
1	B	122	GLN	5.3
1	B	348	LEU	5.3
1	B	258	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	365	ILE	5.2
1	B	313	PRO	5.2
1	B	175	GLU	5.2
1	B	367	ARG	5.2
1	A	310	TRP	5.2
1	B	115	LEU	5.2
1	B	263	HIS	5.2
1	B	303	SER	5.2
1	A	205	ALA	5.2
1	B	238	ALA	5.2
1	B	383	ASP	5.2
1	A	264	SER	5.2
1	B	152	PRO	5.2
1	B	341	HIS	5.1
1	B	401	LEU	5.1
1	B	419	THR	5.1
1	B	268	SER	5.1
1	A	312	GLY	5.1
1	B	373	GLY	5.1
1	B	277	PRO	5.1
1	B	259	LEU	5.1
1	B	183	GLU	5.1
1	B	279	GLU	5.1
1	B	404	PRO	5.1
1	A	364	ASN	5.1
1	B	230	HIS	5.1
1	B	200	GLY	5.1
1	B	397	LYS	5.1
1	B	154	THR	5.0
1	A	390	GLN	5.0
1	A	407	VAL	5.0
1	B	79	PRO	5.0
1	B	267	MET	5.0
1	A	354	GLN	5.0
1	B	245	LEU	5.0
1	A	284	VAL	5.0
1	A	100	THR	5.0
1	B	283	THR	5.0
1	A	246	ASP	5.0
1	A	275	PRO	4.9
1	B	67	PRO	4.9
1	B	300	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	220	LYS	4.9
1	B	225	ASP	4.9
1	B	236	CYS	4.9
1	A	123	TYR	4.9
1	A	350	ILE	4.9
1	B	350	ILE	4.9
1	B	146	LEU	4.9
1	B	349	ASP	4.9
1	B	374	ASN	4.9
1	B	282	ALA	4.9
1	B	336	ALA	4.9
1	B	158	LYS	4.9
1	B	362	VAL	4.9
1	B	88	PHE	4.9
1	B	319	ILE	4.9
1	A	265	LEU	4.9
1	B	387	SER	4.9
1	A	194	TYR	4.9
1	A	346	TYR	4.9
1	A	98	LEU	4.8
1	B	246	ASP	4.9
1	B	371	LEU	4.8
1	B	301	TRP	4.8
1	B	330	ILE	4.8
1	A	324	GLU	4.8
1	B	289	GLU	4.8
1	B	271	ASN	4.8
1	A	285	GLN	4.8
1	A	337	ALA	4.8
1	B	266	PRO	4.8
1	B	179	ARG	4.8
1	B	376	LEU	4.8
1	B	278	GLN	4.8
1	A	289	GLU	4.8
1	B	335	ILE	4.7
1	A	96	ARG	4.7
1	A	263	HIS	4.7
1	B	331	LEU	4.7
1	A	248	PHE	4.7
1	A	406	CYS	4.7
1	B	105	ASN	4.7
1	B	232	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	157	HIS	4.7
1	A	277	PRO	4.7
1	B	251	GLU	4.7
1	B	212	GLN	4.7
1	A	342	ILE	4.7
1	B	302	GLN	4.6
1	B	390	GLN	4.6
1	A	150	LEU	4.6
1	A	371	LEU	4.6
1	A	365	ILE	4.6
1	B	121	GLU	4.6
1	B	359	GLU	4.6
1	B	329	ASN	4.6
1	B	248	PHE	4.6
1	B	87	ASP	4.6
1	A	351	GLU	4.6
1	A	269	VAL	4.6
1	A	280	VAL	4.6
1	A	200	GLY	4.5
1	A	313	PRO	4.5
1	B	368	ALA	4.5
1	B	320	LYS	4.5
1	B	241	ILE	4.5
1	B	312	GLY	4.5
1	A	247	HIS	4.5
1	A	363	GLU	4.5
1	A	368	ALA	4.5
1	B	310	TRP	4.5
1	B	66	LYS	4.5
1	A	92	LEU	4.5
1	B	366	ARG	4.5
1	B	274	ASP	4.5
1	B	252	LYS	4.5
1	B	242	LEU	4.4
1	B	139	GLN	4.4
1	A	301	TRP	4.4
1	A	85	VAL	4.4
1	A	320	LYS	4.4
1	A	276	TYR	4.4
1	A	128	GLY	4.4
1	A	397	LYS	4.4
1	A	307	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	302	GLN	4.4
1	B	343	GLU	4.3
1	A	89	LEU	4.3
1	A	249	PRO	4.3
1	A	378	SER	4.3
1	A	239	ASP	4.3
1	A	274	ASP	4.3
1	B	97	ASP	4.3
1	B	208	ARG	4.3
1	A	218	THR	4.3
1	A	272	ARG	4.3
1	A	347	GLU	4.3
1	B	260	PHE	4.3
1	A	376	LEU	4.3
1	A	398	GLN	4.3
1	B	363	GLU	4.2
1	A	97	ASP	4.2
1	A	116	THR	4.2
1	A	229	THR	4.2
1	A	370	SER	4.2
1	B	299	LEU	4.2
1	B	399	LEU	4.2
1	A	95	ASP	4.2
1	B	226	ARG	4.2
1	A	186	ILE	4.2
1	A	330	ILE	4.2
1	A	392	ASN	4.2
1	A	382	ALA	4.2
1	A	377	PHE	4.2
1	A	408	ASN	4.1
1	B	216	LYS	4.1
1	B	304	LYS	4.1
1	A	334	PRO	4.1
1	A	343	GLU	4.1
1	A	282	ALA	4.1
1	B	357	ALA	4.1
1	A	170	THR	4.1
1	A	298	ARG	4.1
1	A	228	PRO	4.1
1	B	351	GLU	4.1
1	A	129	GLY	4.1
1	A	135	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	317	GLU	4.0
1	B	102	PRO	4.0
1	A	212	GLN	4.0
1	A	219	MET	4.0
1	B	288	MET	4.0
1	A	305	VAL	4.0
1	B	141	GLU	4.0
1	A	114	ARG	4.0
1	B	364	ASN	4.0
1	B	290	ARG	3.9
1	A	422	GLN	3.9
1	B	151	SER	3.9
1	A	404	PRO	3.9
1	B	296	PRO	3.9
1	B	291	LEU	3.9
1	B	96	ARG	3.9
1	B	369	GLU	3.9
1	A	399	LEU	3.9
1	A	262	ALA	3.9
1	B	133	LYS	3.9
1	A	196	CYS	3.9
1	B	261	SER	3.9
1	A	131	PRO	3.9
1	A	389	ILE	3.9
1	A	393	GLU	3.9
1	A	300	VAL	3.9
1	A	179	ARG	3.9
1	B	239	ASP	3.8
1	A	110	PHE	3.8
1	A	402	SER	3.8
1	B	314	GLN	3.8
1	A	76	MET	3.8
1	B	284	VAL	3.8
1	A	142	GLY	3.8
1	A	181	GLY	3.8
1	A	231	HIS	3.8
1	A	316	ASP	3.8
1	A	132	ILE	3.8
1	A	134	ILE	3.8
1	A	291	LEU	3.8
1	A	171	GLU	3.8
1	B	254	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	156	PRO	3.8
1	A	260	PHE	3.8
1	A	283	THR	3.7
1	A	87	ASP	3.7
1	A	271	ASN	3.7
1	A	102	PRO	3.7
1	B	332	LEU	3.7
1	A	66	LYS	3.7
1	A	211	ASN	3.7
1	A	372	ASN	3.7
1	A	409	PRO	3.7
1	A	208	ARG	3.7
1	A	242	LEU	3.7
1	A	256	VAL	3.7
1	B	324	GLU	3.7
1	A	159	TYR	3.7
1	A	119	ILE	3.7
1	B	243	LYS	3.7
1	B	344	THR	3.7
1	B	114	ARG	3.7
1	B	255	GLU	3.6
1	A	232	LEU	3.6
1	A	349	ASP	3.6
1	A	160	TYR	3.6
1	B	217	PRO	3.6
1	B	231	HIS	3.6
1	B	240	HIS	3.6
1	A	220	LYS	3.6
1	A	317	GLU	3.6
1	A	327	ARG	3.6
1	B	125	ARG	3.6
1	B	250	LEU	3.6
1	B	402	SER	3.6
1	B	285	GLN	3.6
1	A	105	ASN	3.6
1	A	173	ALA	3.6
1	A	359	GLU	3.6
1	B	281	SER	3.5
1	A	224	ILE	3.5
1	A	101	LEU	3.5
1	A	93	PHE	3.5
1	A	309	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLN	3.5
1	A	278	GLN	3.5
1	A	412	ARG	3.5
1	B	398	GLN	3.5
1	B	222	SER	3.5
1	A	127	GLY	3.5
1	A	175	GLU	3.5
1	B	118	LYS	3.5
1	B	328	LYS	3.4
1	A	207	TYR	3.4
1	B	356	LEU	3.4
1	A	417	PHE	3.4
1	A	396	SER	3.4
1	A	138	LYS	3.4
1	A	345	LEU	3.4
1	A	65	ARG	3.4
1	A	185	ALA	3.4
1	A	259	LEU	3.3
1	A	143	MET	3.3
1	A	209	TYR	3.3
1	B	316	ASP	3.3
1	A	381	LEU	3.3
1	A	401	LEU	3.3
1	A	197	SER	3.3
1	B	326	GLY	3.3
1	A	243	LYS	3.3
1	A	136	THR	3.3
1	A	141	GLU	3.2
1	A	403	CYS	3.2
1	A	227	TRP	3.2
1	A	83	GLY	3.2
1	A	163	PHE	3.2
1	A	385	VAL	3.2
1	A	149	GLU	3.2
1	A	180	ASP	3.2
1	A	340	ASP	3.2
1	B	229	THR	3.2
1	A	99	MET	3.2
1	A	375	PRO	3.2
1	A	166	VAL	3.1
1	A	182	LEU	3.1
1	A	81	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	303	SER	3.1
1	A	386	HIS	3.1
1	A	192	PRO	3.1
1	B	322	LEU	3.1
1	A	267	MET	3.1
1	A	223	THR	3.1
1	B	127	GLY	3.1
1	A	139	GLN	3.1
1	A	155	ALA	3.1
1	B	325	ARG	3.1
1	A	308	MET	3.1
1	A	391	SER	3.0
1	A	225	ASP	3.0
1	A	394	LEU	3.0
1	A	111	ILE	3.0
1	A	379	LYS	3.0
1	A	88	PHE	3.0
1	A	373	GLY	3.0
1	A	304	LYS	3.0
1	A	189	THR	3.0
1	A	367	ARG	3.0
1	A	109	PRO	3.0
1	A	144	VAL	2.9
1	A	191	TYR	2.9
1	A	147	LEU	2.9
1	A	341	HIS	2.9
1	B	327	ARG	2.9
1	A	421	GLN	2.9
1	A	154	THR	2.9
1	A	221	TRP	2.9
1	A	290	ARG	2.9
1	A	146	LEU	2.9
1	A	411	CYS	2.9
1	A	414	THR	2.9
1	A	193	GLN	2.8
1	A	94	LEU	2.8
1	A	233	LEU	2.8
1	A	198	THR	2.8
1	A	266	PRO	2.8
1	B	249	PRO	2.8
1	A	121	GLU	2.8
1	A	306	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	120	GLN	2.8
1	A	369	GLU	2.8
1	A	113	LYS	2.8
1	A	126	ILE	2.8
1	A	75	ASN	2.8
1	A	115	LEU	2.8
1	A	168	PRO	2.7
1	A	236	CYS	2.7
1	B	347	GLU	2.7
1	A	106	LYS	2.7
1	A	210	TYR	2.7
1	B	298	ARG	2.7
1	A	157	HIS	2.7
1	A	230	HIS	2.7
1	A	69	THR	2.7
1	A	70	GLY	2.7
1	A	206	ILE	2.7
1	A	79	PRO	2.7
1	B	244	GLU	2.7
1	B	396	SER	2.7
1	A	74	LEU	2.7
1	A	240	HIS	2.7
1	B	256	VAL	2.7
1	A	178	GLU	2.7
1	A	140	GLY	2.7
1	A	162	GLY	2.6
1	A	226	ARG	2.6
1	A	268	SER	2.6
1	A	400	THR	2.6
1	A	80	GLU	2.6
1	A	174	ILE	2.6
1	A	167	HIS	2.6
1	A	415	LYS	2.6
1	A	122	GLN	2.5
1	A	153	ASN	2.5
1	A	418	PHE	2.5
1	A	137	SER	2.5
1	A	333	VAL	2.5
1	B	292	GLU	2.5
1	A	90	LEU	2.5
1	A	125	ARG	2.5
1	B	247	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	188	PHE	2.5
1	A	217	PRO	2.5
1	A	72	LEU	2.4
1	A	165	TYR	2.4
1	A	68	LYS	2.4
1	A	338	THR	2.4
1	A	419	THR	2.4
1	A	413	GLU	2.4
1	A	117	PRO	2.4
1	A	384	LEU	2.3
1	A	416	SER	2.3
1	A	84	ASP	2.3
1	A	279	GLU	2.3
1	A	161	ILE	2.3
1	A	177	MET	2.2
1	A	184	ARG	2.2
1	A	152	PRO	2.2
1	A	410	VAL	2.2
1	A	67	PRO	2.2
1	A	71	ILE	2.2
1	A	124	ARG	2.2
1	B	321	GLY	2.1
1	A	202	SER	2.1
1	B	294	CYS	2.1
1	A	204	ASN	2.1
1	A	261	SER	2.0
1	A	176	GLU	2.0
1	A	169	LEU	2.0
1	A	183	GLU	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](#)

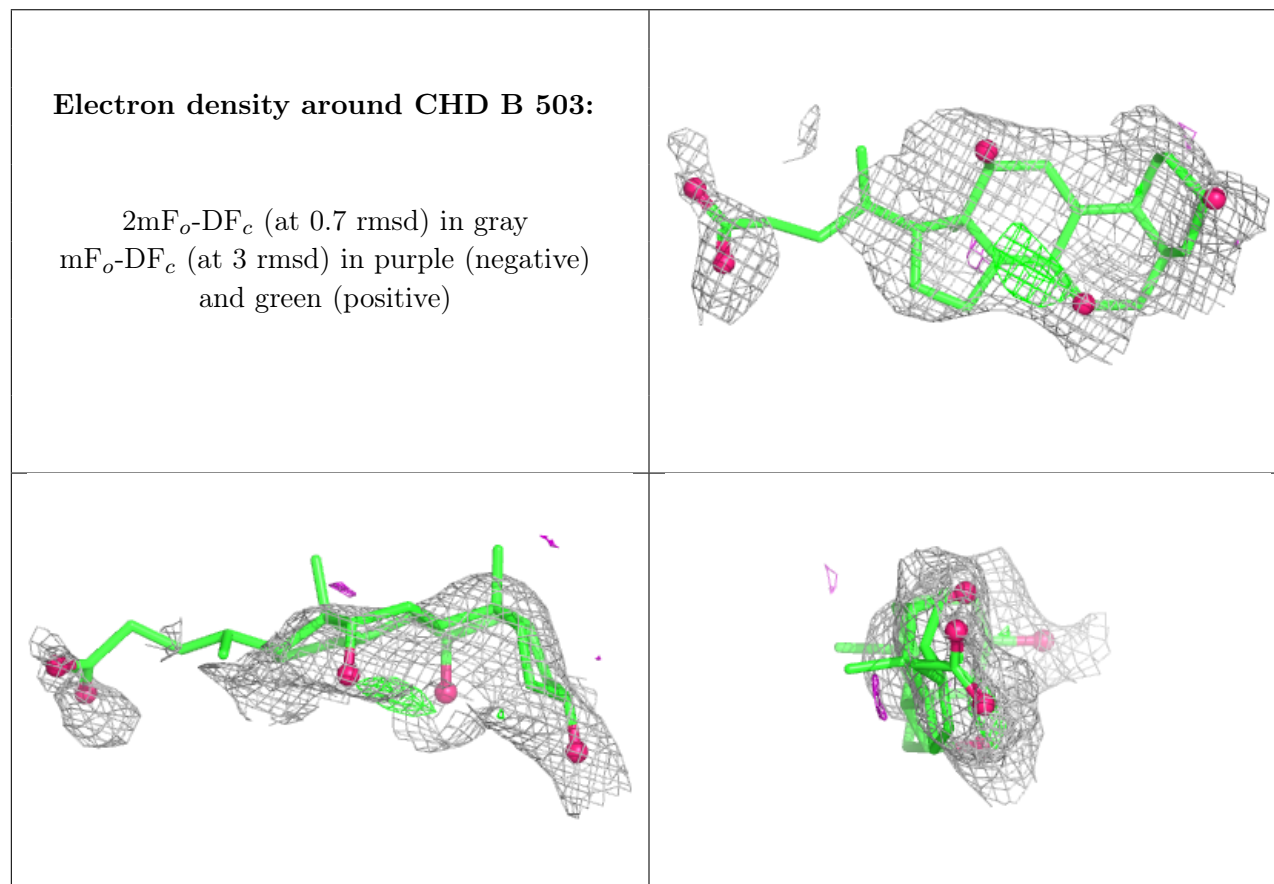
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

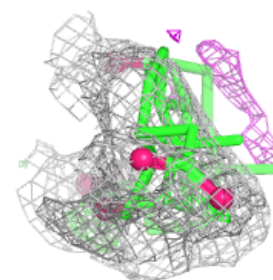
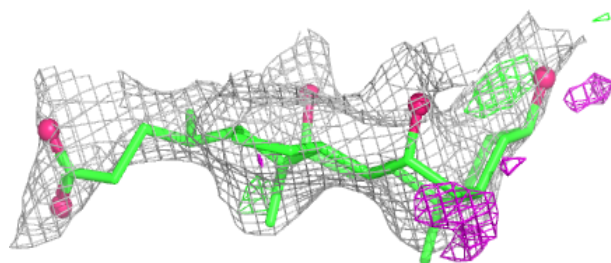
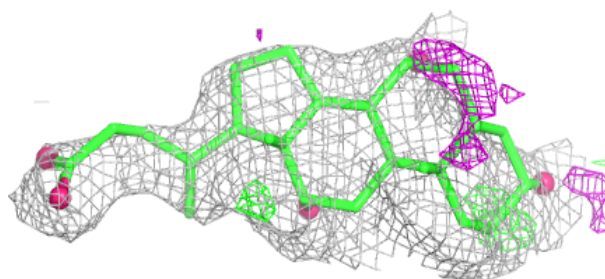
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CHD	B	503	29/29	0.34	0.42	45,48,63,64	0
3	CHD	B	501	29/29	0.48	0.40	28,29,41,45	0
3	CHD	B	502	29/29	0.57	0.38	34,38,51,53	0
3	CHD	A	502	29/29	0.59	0.29	37,41,49,51	0
2	FES	B	499	4/4	0.61	0.22	20,20,22,23	0
3	CHD	A	503	29/29	0.62	0.26	43,47,50,51	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.

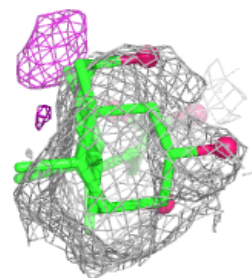
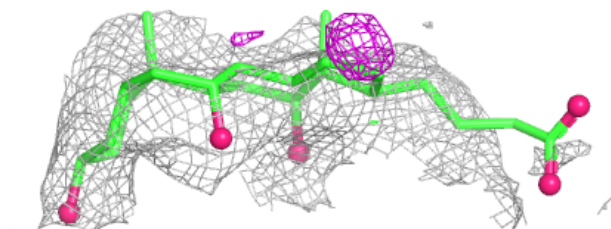
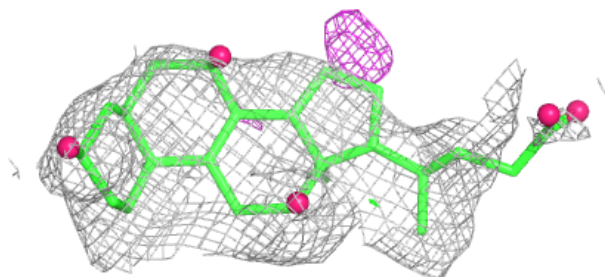


Electron density around CHD B 501:

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

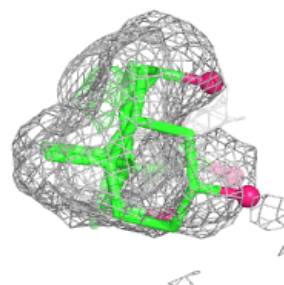
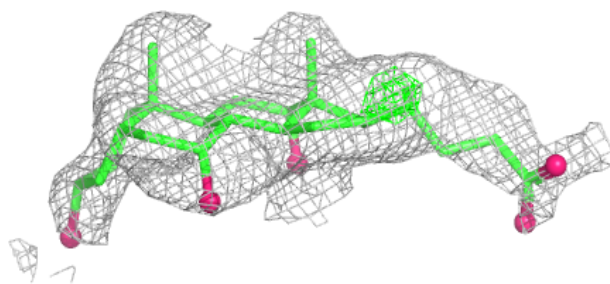
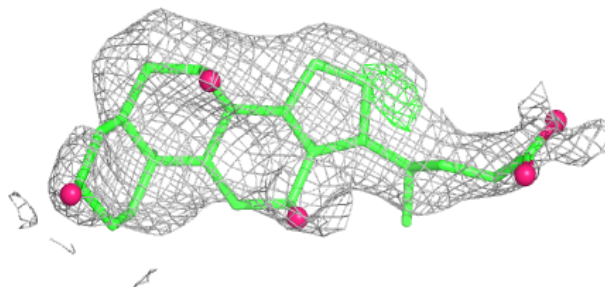
**Electron density around CHD B 502:**

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

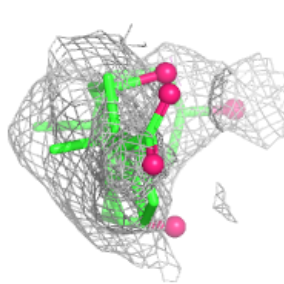
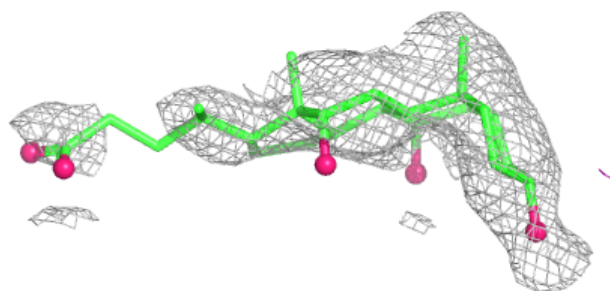
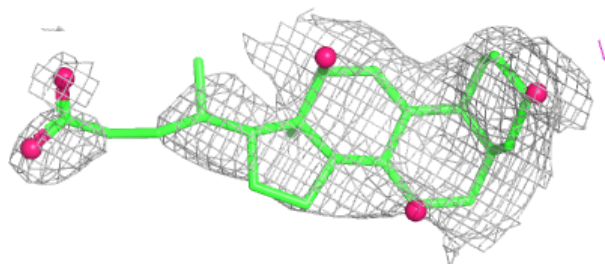


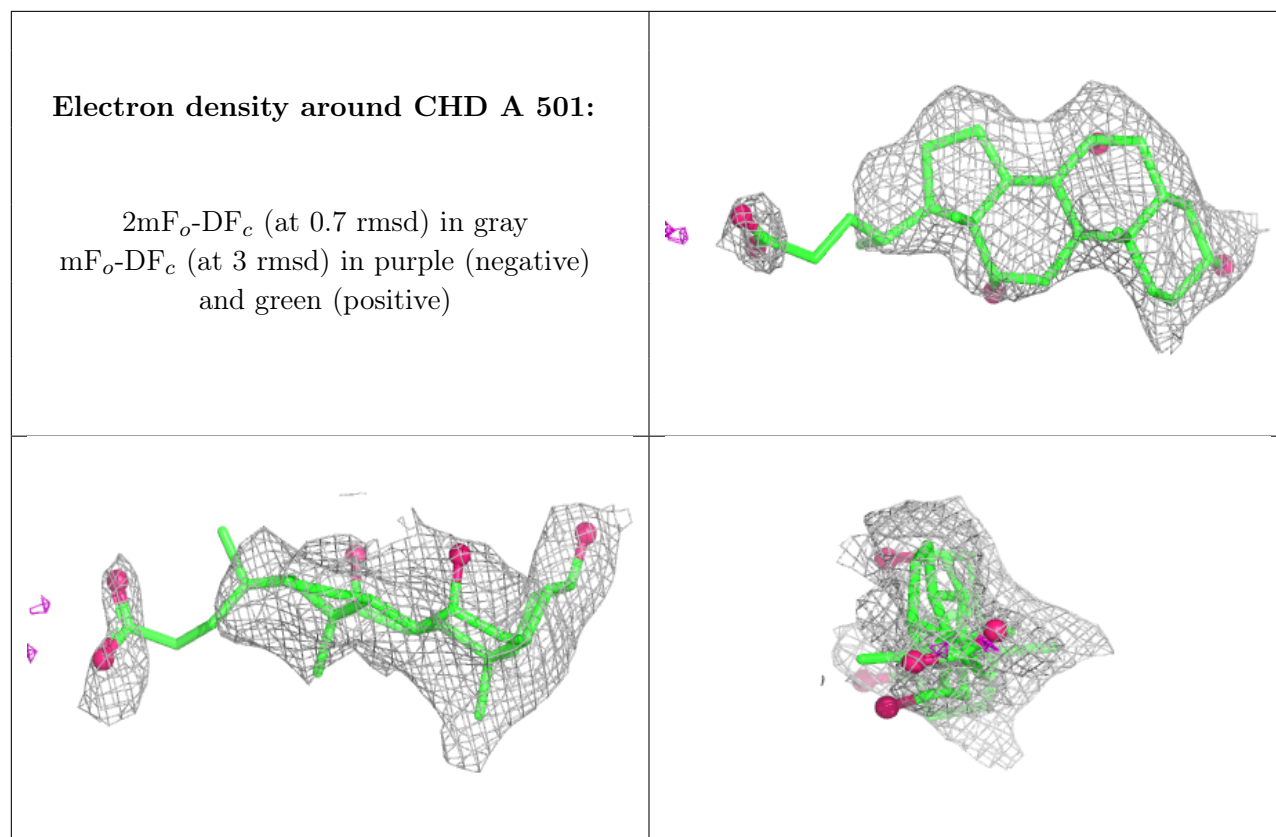
Electron density around CHD A 502:

$2mF_o-DF_c$ (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.