



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:04 AM UTC

PDB ID : 1HRK / pdb_00001hrk
Title : CRYSTAL STRUCTURE OF HUMAN FERROCHELATASE
Authors : Wu, C.K.; Dailey, H.A.; Rose, J.P.; Burden, A.; Sellers, V.M.; Wang, B.-C.
Deposited on : 2000-12-21
Resolution : 2.00 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

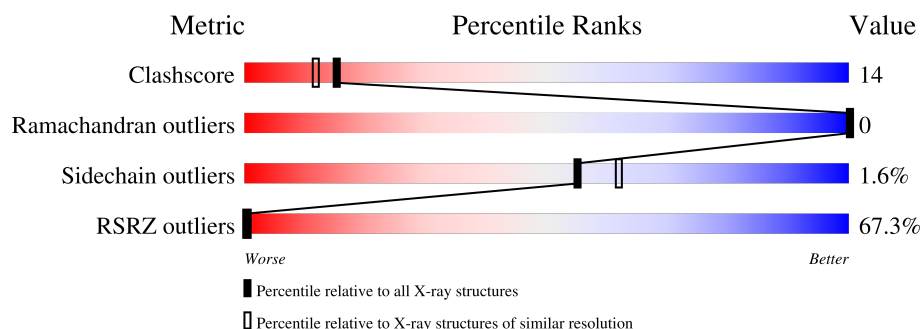
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	65% 74% 25% .
1	B	359	70% 75% 23% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6486 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.

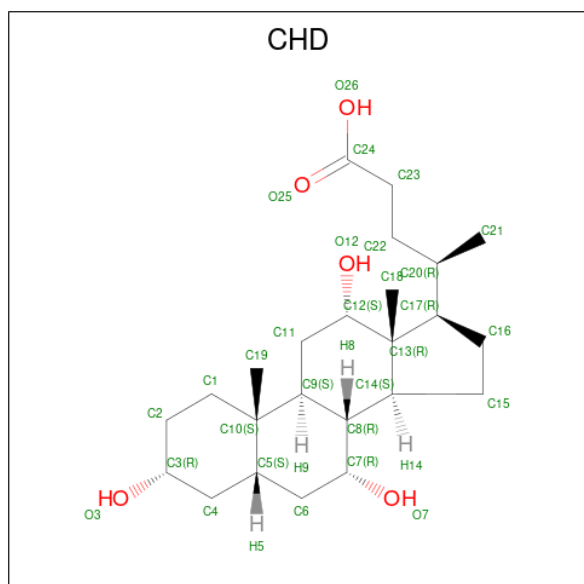
- Molecule 1 is a protein called FERROCHELATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2854	1819	491	526	18			
1	B	359	Total	C	N	O	S	0	0	0
			2854	1819	491	526	18			

There are 4 discrepancies between the modelled and reference sequences:

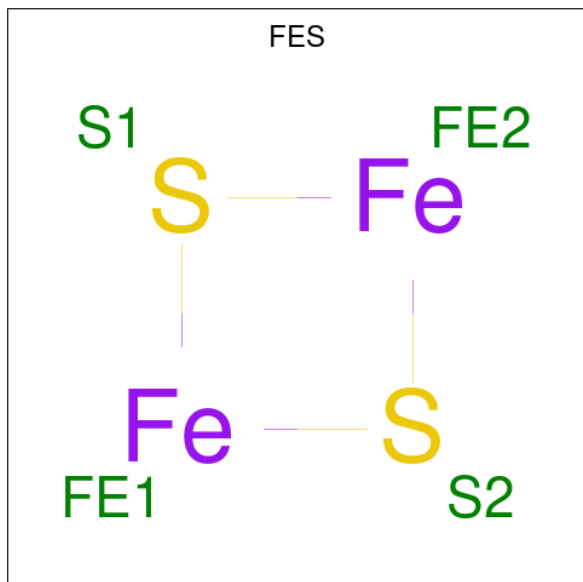
Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ARG	GLN	engineered mutation	UNP P22830
A	115	LEU	ARG	engineered mutation	UNP P22830
B	96	ARG	GLN	engineered mutation	UNP P22830
B	115	LEU	ARG	engineered mutation	UNP P22830

- Molecule 2 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

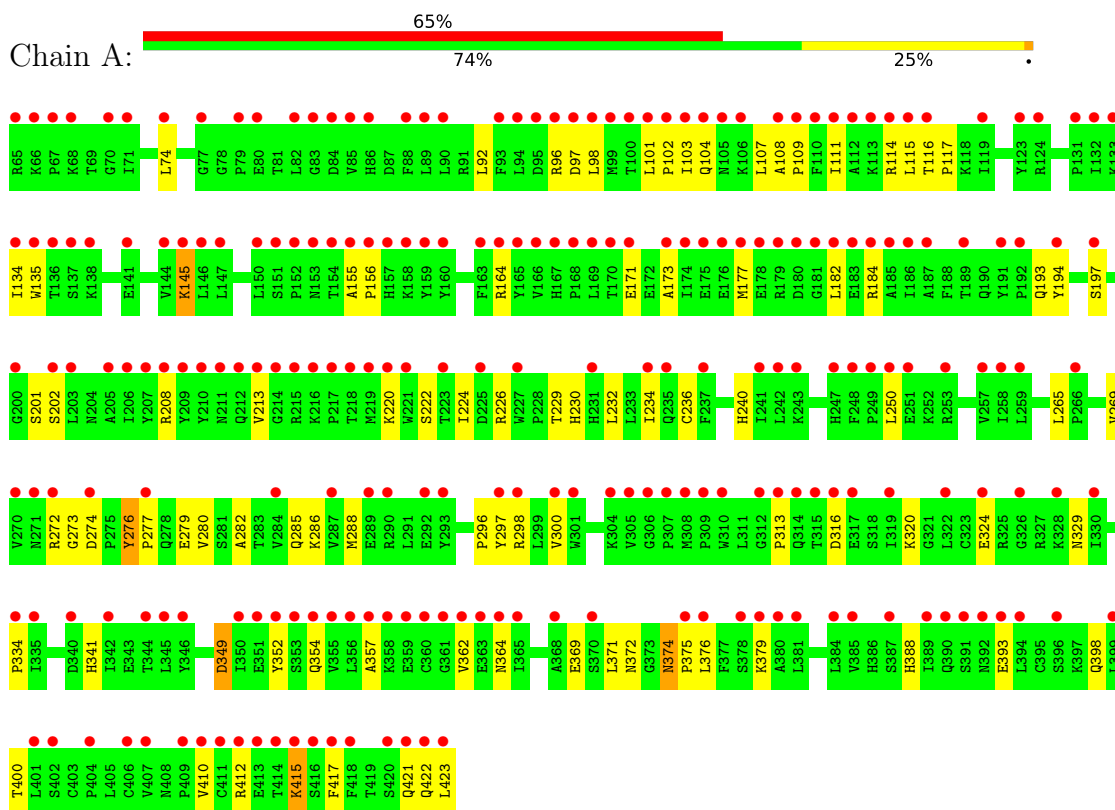
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	291	Total O 291 291	0	0
4	B	305	Total O 305 305	0	0

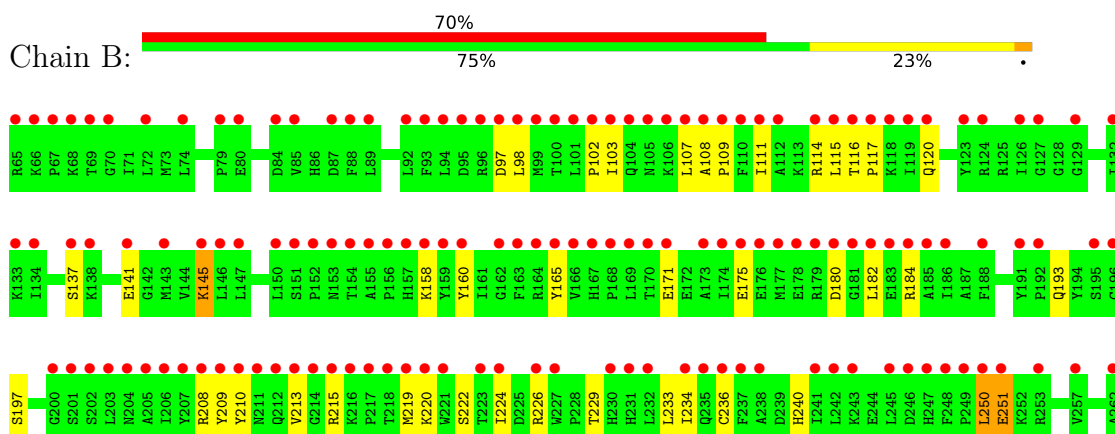
3 Residue-property plots

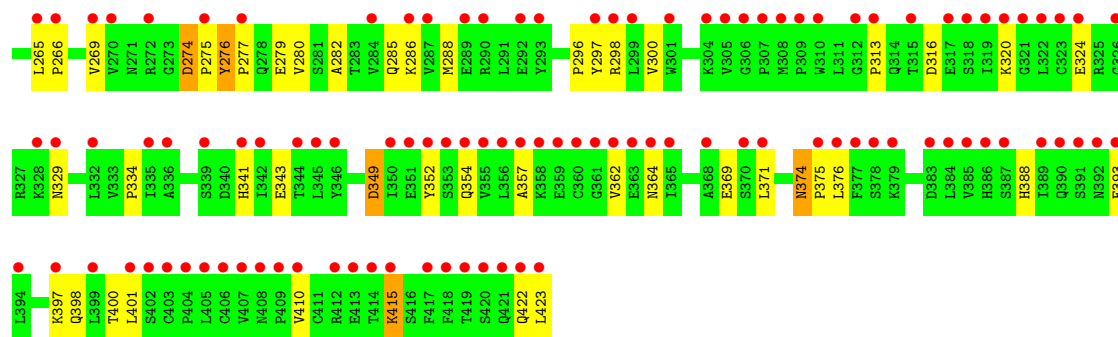
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: FERROCHELATASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.43Å 87.57Å 109.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.00 19.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.87-2.00) 98.3 (19.87-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 1.84Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.202 , 0.226 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	6486	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 43.66 % 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 1.7074e-04. 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: CHD, FES

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	0.36	0/2924	0.87	7/3971 (0.2%)
1	B	0.35	0/2924	0.86	9/3971 (0.2%)
All	All	0.35	0/5848	0.87	16/7942 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ILE	N-CA-C	-6.64	95.52	109.34
1	A	224	ILE	N-CA-C	-6.38	96.07	109.34
1	A	274	ASP	CA-C-N	5.95	125.57	119.56
1	A	274	ASP	C-N-CA	5.95	125.57	119.56
1	B	349	ASP	N-CA-C	5.87	117.75	111.36
1	B	233	LEU	N-CA-C	-5.42	105.28	111.14
1	A	194	TYR	N-CA-C	5.34	117.97	109.96
1	A	349	ASP	N-CA-C	5.33	116.89	111.14
1	B	274	ASP	CA-C-N	5.18	124.79	119.56
1	B	274	ASP	C-N-CA	5.18	124.79	119.56
1	A	276	TYR	N-CA-C	5.18	121.25	109.81
1	B	165	TYR	N-CA-C	5.16	120.22	112.94
1	B	276	TYR	N-CA-C	5.14	121.17	109.81
1	A	334	PRO	N-CA-C	-5.13	102.64	110.95
1	B	334	PRO	N-CA-C	-5.12	102.65	110.95
1	B	397	LYS	N-CA-C	-5.02	106.00	111.82

There are no chirality outliers.

There are no planarity outliers.

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	2854	0	2821	80	0
1	B	2854	0	2821	79	0
2	A	87	0	117	12	0
2	B	87	0	117	12	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	291	0	0	9	0
4	B	305	0	0	6	0
All	All	6486	0	5876	160	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 14.

All (160) 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:297:TYR:H	1:B:398:GLN:HE22	1.13	0.96
1:A:208:ARG:NH2	1:A:410:VAL:HG21	1.81	0.96
1:A:398:GLN:HE22	1:B:297:TYR:H	1.15	0.93
1:B:250:LEU:HD12	1:B:250:LEU:H	1.34	0.91
1:B:208:ARG:NH2	1:B:410:VAL:HG21	1.88	0.87
1:A:250:LEU:HD12	1:A:250:LEU:H	1.40	0.85
1:A:422:GLN:O	1:A:423:LEU:HB2	1.79	0.82
1:B:422:GLN:O	1:B:423:LEU:HB2	1.79	0.81
1:A:229:THR:HB	1:A:286:LYS:HE2	1.62	0.80
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.65	0.78
1:B:415:LYS:HB3	1:B:415:LYS:HZ3	1.46	0.77
1:B:300:VAL:HG12	1:B:313:PRO:HG2	1.67	0.74
1:A:269:VAL:O	1:A:272:ARG:HG2	1.87	0.74
2:B:2501:CHD:H12	2:B:2501:CHD:H212	1.70	0.74
1:A:234:ILE:HG13	1:A:286:LYS:HE3	1.69	0.74
1:B:208:ARG:HH21	1:B:410:VAL:HG21	1.49	0.74
1:B:171:GLU:O	1:B:175:GLU:HG3	1.88	0.73
1:B:98:LEU:HD11	2:B:2501:CHD:H162	1.70	0.73
1:B:229:THR:HB	1:B:286:LYS:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HG13	1:B:286:LYS:HE3	1.70	0.72
1:B:265:LEU:HD22	2:B:2501:CHD:O26	1.91	0.71
1:B:250:LEU:H	1:B:250:LEU:CD1	2.05	0.70
1:A:222:SER:OG	1:A:388:HIS:HE1	1.75	0.70
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.73	0.69
1:A:197:SER:HB3	2:A:1501:CHD:O25	1.92	0.69
2:A:1501:CHD:H212	2:A:1501:CHD:H12	1.75	0.68
1:B:222:SER:OG	1:B:388:HIS:HE1	1.76	0.68
1:A:265:LEU:HD22	2:A:1501:CHD:O26	1.93	0.68
1:B:357:ALA:HB1	1:B:362:VAL:HG11	1.74	0.67
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.77	0.67
1:B:374:ASN:HD22	1:B:374:ASN:C	2.02	0.66
1:B:298:ARG:HD3	4:B:3003:HOH:O	1.94	0.66
1:B:250:LEU:HD12	1:B:250:LEU:N	2.09	0.65
1:A:115:LEU:HD21	2:A:1502:CHD:H231	1.78	0.65
1:A:374:ASN:C	1:A:374:ASN:HD22	2.05	0.65
1:B:220:LYS:HD3	1:B:423:LEU:HG	1.79	0.63
1:A:415:LYS:HZ3	1:A:415:LYS:HB3	1.64	0.63
1:B:210:TYR:HA	1:B:213:VAL:HG12	1.79	0.63
1:B:374:ASN:HD22	1:B:375:PRO:N	1.97	0.63
1:A:220:LYS:HD2	1:A:423:LEU:HG	1.80	0.62
1:A:297:TYR:N	1:B:398:GLN:HE22	1.90	0.62
1:B:240:HIS:HD2	1:B:369:GLU:O	1.82	0.62
1:A:398:GLN:HE22	1:B:297:TYR:N	1.91	0.61
1:A:250:LEU:H	1:A:250:LEU:CD1	2.13	0.61
1:A:114:ARG:HD3	2:A:1502:CHD:O26	2.00	0.60
1:A:357:ALA:HB1	1:A:362:VAL:HG11	1.83	0.60
1:A:208:ARG:HH21	1:A:410:VAL:HG21	1.61	0.60
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.83	0.60
1:A:282:ALA:HB1	1:B:285:GLN:HG2	1.83	0.60
1:B:197:SER:HB3	2:B:2501:CHD:O25	2.01	0.60
1:B:400:THR:HA	1:B:415:LYS:HD2	1.84	0.60
1:B:374:ASN:ND2	1:B:376:LEU:H	1.99	0.59
1:A:374:ASN:HD22	1:A:375:PRO:N	1.99	0.59
1:A:349:ASP:O	1:A:354:GLN:HG3	2.02	0.59
1:A:240:HIS:HD2	1:A:369:GLU:O	1.85	0.59
1:A:415:LYS:HB3	1:A:415:LYS:NZ	2.18	0.58
1:B:251:GLU:H	1:B:251:GLU:CD	2.10	0.58
1:A:320:LYS:O	1:A:324:GLU:HG3	2.03	0.58
1:A:285:GLN:HG2	1:B:282:ALA:HB1	1.85	0.58
1:A:400:THR:HA	1:A:415:LYS:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.70	0.57
2:B:2502:CHD:H213	4:B:3264:HOH:O	2.04	0.57
1:B:213:VAL:CG2	1:B:215:ARG:HH21	2.18	0.56
1:A:374:ASN:ND2	1:A:376:LEU:H	2.04	0.56
1:A:184:ARG:NH2	4:A:1553:HOH:O	2.35	0.55
1:B:115:LEU:HD21	2:B:2502:CHD:H231	1.87	0.55
1:B:111:ILE:HA	1:B:114:ARG:HG2	1.89	0.54
1:A:250:LEU:HD12	1:A:250:LEU:N	2.17	0.54
1:B:320:LYS:O	1:B:324:GLU:HG3	2.08	0.53
1:A:145:LYS:HB3	1:A:145:LYS:NZ	2.24	0.52
1:A:296:PRO:HB2	1:B:401:LEU:HB2	1.91	0.52
1:A:341:HIS:HE1	4:A:1651:HOH:O	1.92	0.52
1:B:349:ASP:O	1:B:354:GLN:HG3	2.09	0.52
2:A:1503:CHD:H212	2:A:1503:CHD:H12	1.90	0.52
1:A:135:TRP:CE3	1:A:372:ASN:HB3	2.45	0.52
1:B:341:HIS:HE1	4:B:3148:HOH:O	1.93	0.51
1:B:415:LYS:HB3	1:B:415:LYS:NZ	2.21	0.51
1:A:98:LEU:HD11	2:A:1501:CHD:H162	1.92	0.51
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.76	0.51
1:B:102:PRO:O	1:B:103:ILE:C	2.53	0.51
1:B:388:HIS:HD2	1:B:393:GLU:CD	2.19	0.50
2:B:2503:CHD:H212	2:B:2503:CHD:H12	1.93	0.50
1:A:135:TRP:CZ3	1:A:372:ASN:HB3	2.48	0.49
1:B:269:VAL:HG21	2:B:2501:CHD:C24	2.42	0.49
1:B:208:ARG:HH11	1:B:208:ARG:HG3	1.76	0.49
1:A:341:HIS:HD2	4:A:1650:HOH:O	1.95	0.49
1:A:379:LYS:HE3	4:A:1620:HOH:O	2.12	0.49
1:A:102:PRO:O	1:A:103:ILE:C	2.56	0.49
1:B:213:VAL:HG21	1:B:215:ARG:HH21	1.77	0.49
1:B:145:LYS:NZ	1:B:145:LYS:HB3	2.28	0.49
1:A:96:ARG:C	1:A:98:LEU:H	2.20	0.48
1:A:422:GLN:HG2	1:A:423:LEU:HD23	1.95	0.48
1:B:213:VAL:HG22	1:B:215:ARG:HE	1.78	0.48
1:A:388:HIS:HD2	1:A:393:GLU:CD	2.21	0.47
1:B:175:GLU:HG2	1:B:209:TYR:OH	2.15	0.47
1:A:177:MET:HB3	1:A:182:LEU:HD12	1.96	0.47
1:B:103:ILE:HG13	1:B:107:LEU:HG	1.97	0.47
1:A:173:ALA:O	1:A:177:MET:HG3	2.15	0.47
1:A:103:ILE:HG13	1:A:107:LEU:HG	1.95	0.47
1:A:273:GLY:O	1:B:298:ARG:HD2	2.15	0.47
1:B:357:ALA:HB1	1:B:362:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:H	1:A:171:GLU:CD	2.23	0.46
2:B:2502:CHD:H12	2:B:2502:CHD:H212	1.97	0.46
1:B:236:CYS:HB3	1:B:371:LEU:HD22	1.97	0.46
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.50	0.46
1:B:341:HIS:CE1	1:B:343:GLU:HB2	2.51	0.46
1:B:102:PRO:O	1:B:107:LEU:HD12	2.15	0.46
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.97	0.45
1:B:116:THR:HB	1:B:117:PRO:HD3	1.99	0.45
1:A:116:THR:HB	1:A:117:PRO:HD3	1.98	0.45
1:A:111:ILE:HA	1:A:114:ARG:HG2	1.99	0.45
1:A:145:LYS:HB3	1:A:145:LYS:HZ3	1.82	0.45
1:A:417:PHE:O	1:A:421:GLN:HG2	2.15	0.45
1:B:374:ASN:HD22	1:B:376:LEU:H	1.65	0.45
1:B:341:HIS:HD2	4:B:3150:HOH:O	2.00	0.45
1:A:155:ALA:HB1	1:A:156:PRO:HA	1.99	0.45
1:A:296:PRO:HA	1:B:398:GLN:NE2	2.32	0.45
1:A:298:ARG:HD3	4:A:1512:HOH:O	2.16	0.45
2:A:1501:CHD:H212	2:A:1502:CHD:H193	1.99	0.45
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.99	0.44
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.52	0.44
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.81	0.44
1:B:220:LYS:HD2	4:B:3267:HOH:O	2.16	0.44
2:B:2501:CHD:H212	2:B:2502:CHD:H193	1.99	0.44
1:A:269:VAL:HG21	2:A:1501:CHD:C24	2.47	0.43
1:B:288:MET:HG3	1:B:297:TYR:CD2	2.53	0.43
1:A:101:LEU:HB2	1:A:104:GLN:HG3	2.00	0.43
1:A:412:ARG:HG2	1:A:412:ARG:HH11	1.82	0.43
1:B:226:ARG:HD3	1:B:279:GLU:OE1	2.19	0.43
1:A:97:ASP:OD2	1:A:208:ARG:NH1	2.34	0.43
1:A:236:CYS:HB3	1:A:371:LEU:HD22	1.99	0.43
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.32	0.43
2:A:1501:CHD:H232	2:A:1501:CHD:H211	1.75	0.43
1:A:164:ARG:HD2	1:A:201:SER:OG	2.18	0.43
2:A:1502:CHD:H213	4:A:1713:HOH:O	2.18	0.43
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.53	0.43
1:B:266:PRO:HG2	2:B:2502:CHD:H11	1.99	0.43
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.84	0.43
1:A:92:LEU:C	1:A:92:LEU:HD23	2.44	0.43
4:A:1618:HOH:O	1:B:286:LYS:HD3	2.19	0.42
2:A:1502:CHD:H12	2:A:1502:CHD:H212	2.00	0.42
1:B:266:PRO:CG	2:B:2502:CHD:H11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASN:C	1:A:374:ASN:ND2	2.76	0.42
1:B:180:ASP:HB2	1:B:182:LEU:HD13	2.01	0.42
1:B:116:THR:O	1:B:120:GLN:HG3	2.20	0.42
1:A:230:HIS:CE1	1:A:232:LEU:HB2	2.55	0.42
1:A:226:ARG:HD3	1:A:279:GLU:OE1	2.19	0.41
1:B:171:GLU:H	1:B:171:GLU:CD	2.28	0.41
1:A:74:LEU:HD13	1:A:202:SER:HB3	2.01	0.41
1:A:134:ILE:HG13	4:A:1586:HOH:O	2.21	0.41
1:B:158:LYS:HD3	1:B:160:TYR:OH	2.20	0.41
1:A:96:ARG:NH2	4:A:1691:HOH:O	2.53	0.41
1:A:111:ILE:O	1:A:114:ARG:HG3	2.21	0.41
1:A:398:GLN:NE2	1:B:296:PRO:HA	2.36	0.41
1:B:422:GLN:O	1:B:423:LEU:CB	2.58	0.41
1:B:184:ARG:NH2	4:B:3056:HOH:O	2.50	0.40
1:B:208:ARG:HG3	1:B:208:ARG:NH1	2.35	0.40
1:A:108:ALA:HB3	1:A:109:PRO:CD	2.51	0.40
1:B:97:ASP:CG	1:B:208:ARG:HH12	2.28	0.40
1:B:137:SER:O	1:B:141:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

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	357/359 (99%)	346 (97%)	11 (3%)	0	100	100
1	B	357/359 (99%)	348 (98%)	9 (2%)	0	100	100
All	All	714/718 (99%)	694 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	316/324 (98%)	312 (99%)	4 (1%)	61	68
1	B	316/324 (98%)	310 (98%)	6 (2%)	50	56
All	All	632/648 (98%)	622 (98%)	10 (2%)	55	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	A	213	VAL
1	A	374	ASN
1	A	415	LYS
1	B	145	LYS
1	B	219	MET
1	B	250	LEU
1	B	251	GLU
1	B	374	ASN
1	B	415	LYS

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	120	GLN
1	A	211	ASN
1	A	235	GLN
1	A	240	HIS
1	A	314	GLN
1	A	329	ASN
1	A	341	HIS
1	A	354	GLN
1	A	374	ASN
1	A	388	HIS
1	A	392	ASN
1	A	398	GLN

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Mol	Chain	Res	Type
1	A	421	GLN
1	B	235	GLN
1	B	240	HIS
1	B	314	GLN
1	B	329	ASN
1	B	341	HIS
1	B	354	GLN
1	B	364	ASN
1	B	374	ASN
1	B	388	HIS
1	B	398	GLN
1	B	421	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](#)

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	CHD	B	2503	-	32,32,32	0.82	2 (6%)	51,51,51	1.16	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHD	A	1501	-	32,32,32	0.82	1 (3%)	51,51,51	1.60	8 (15%)
3	FES	B	2999	1	0,4,4	-	-	-	-	-
2	CHD	A	1502	-	32,32,32	0.83	2 (6%)	51,51,51	1.13	3 (5%)
2	CHD	B	2501	-	32,32,32	0.80	1 (3%)	51,51,51	1.67	8 (15%)
3	FES	A	1499	1	0,4,4	-	-	-	-	-
2	CHD	A	1503	-	32,32,32	0.81	1 (3%)	51,51,51	1.13	3 (5%)
2	CHD	B	2502	-	32,32,32	0.80	2 (6%)	51,51,51	1.11	3 (5%)

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	CHD	B	2503	-	-	0/9/74/74	0/4/4/4
2	CHD	A	1501	-	-	2/9/74/74	0/4/4/4
3	FES	B	2999	1	-	-	0/1/1/1
2	CHD	A	1502	-	-	0/9/74/74	0/4/4/4
2	CHD	B	2501	-	-	2/9/74/74	0/4/4/4
3	FES	A	1499	1	-	-	0/1/1/1
2	CHD	A	1503	-	-	2/9/74/74	0/4/4/4
2	CHD	B	2502	-	-	0/9/74/74	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1502	CHD	C11-C12	2.43	1.57	1.53
2	B	2502	CHD	O12-C12	-2.37	1.39	1.43
2	B	2503	CHD	C11-C12	2.35	1.57	1.53
2	B	2502	CHD	C11-C12	2.28	1.56	1.53
2	A	1501	CHD	C11-C12	2.26	1.56	1.53
2	A	1503	CHD	C11-C12	2.22	1.56	1.53
2	B	2503	CHD	O12-C12	-2.20	1.40	1.43
2	B	2501	CHD	C11-C12	2.16	1.56	1.53
2	A	1502	CHD	O12-C12	-2.05	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2501	CHD	C13-C17-C20	-6.21	111.96	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	CHD	C13-C17-C20	-5.45	112.88	119.48
2	B	2501	CHD	C23-C22-C20	-3.32	108.27	114.46
2	A	1501	CHD	C11-C12-C13	-3.25	107.96	111.26
2	B	2501	CHD	C21-C20-C22	-3.23	105.34	110.34
2	B	2501	CHD	C11-C12-C13	-3.21	108.00	111.26
2	A	1503	CHD	C4-C5-C10	-3.18	109.27	112.66
2	A	1501	CHD	C21-C20-C22	-2.96	105.76	110.34
2	A	1501	CHD	C1-C2-C3	-2.92	106.61	110.48
2	A	1501	CHD	C23-C22-C20	-2.91	109.03	114.46
2	B	2501	CHD	C4-C5-C10	-2.70	109.79	112.66
2	B	2503	CHD	C4-C5-C10	-2.66	109.83	112.66
2	B	2502	CHD	C4-C5-C10	-2.53	109.97	112.66
2	B	2503	CHD	C13-C17-C20	-2.52	116.43	119.48
2	B	2501	CHD	C1-C2-C3	-2.49	107.19	110.48
2	B	2503	CHD	C11-C12-C13	-2.47	108.76	111.26
2	A	1502	CHD	C4-C5-C10	-2.39	110.11	112.66
2	A	1501	CHD	C4-C5-C10	-2.34	110.17	112.66
2	A	1503	CHD	C13-C17-C20	-2.27	116.73	119.48
2	A	1502	CHD	C1-C2-C3	-2.27	107.47	110.48
2	B	2501	CHD	C13-C14-C8	-2.21	111.91	114.72
2	B	2501	CHD	C11-C9-C10	-2.19	111.48	113.70
2	A	1503	CHD	C11-C12-C13	-2.15	109.07	111.26
2	A	1502	CHD	C11-C12-C13	-2.14	109.08	111.26
2	B	2502	CHD	C1-C2-C3	-2.13	107.66	110.48
2	A	1501	CHD	C6-C5-C4	2.13	113.66	111.23
2	B	2502	CHD	C11-C12-C13	-2.10	109.12	111.26
2	A	1501	CHD	C19-C10-C1	-2.01	105.11	108.31
2	B	2503	CHD	C1-C2-C3	-2.00	107.83	110.48

There are no chirality outliers.

All (6) torsion outliers are listed below:

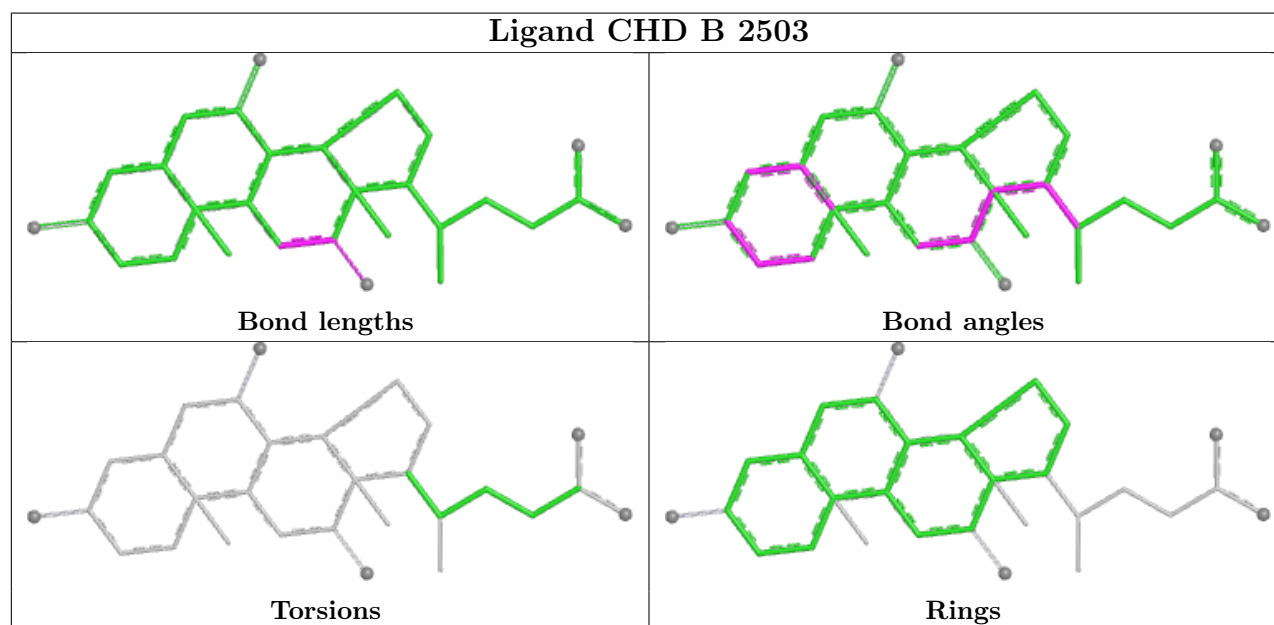
Mol	Chain	Res	Type	Atoms
2	B	2501	CHD	C22-C23-C24-O25
2	A	1501	CHD	C22-C23-C24-O26
2	B	2501	CHD	C22-C23-C24-O26
2	A	1501	CHD	C22-C23-C24-O25
2	A	1503	CHD	C22-C23-C24-O26
2	A	1503	CHD	C22-C23-C24-O25

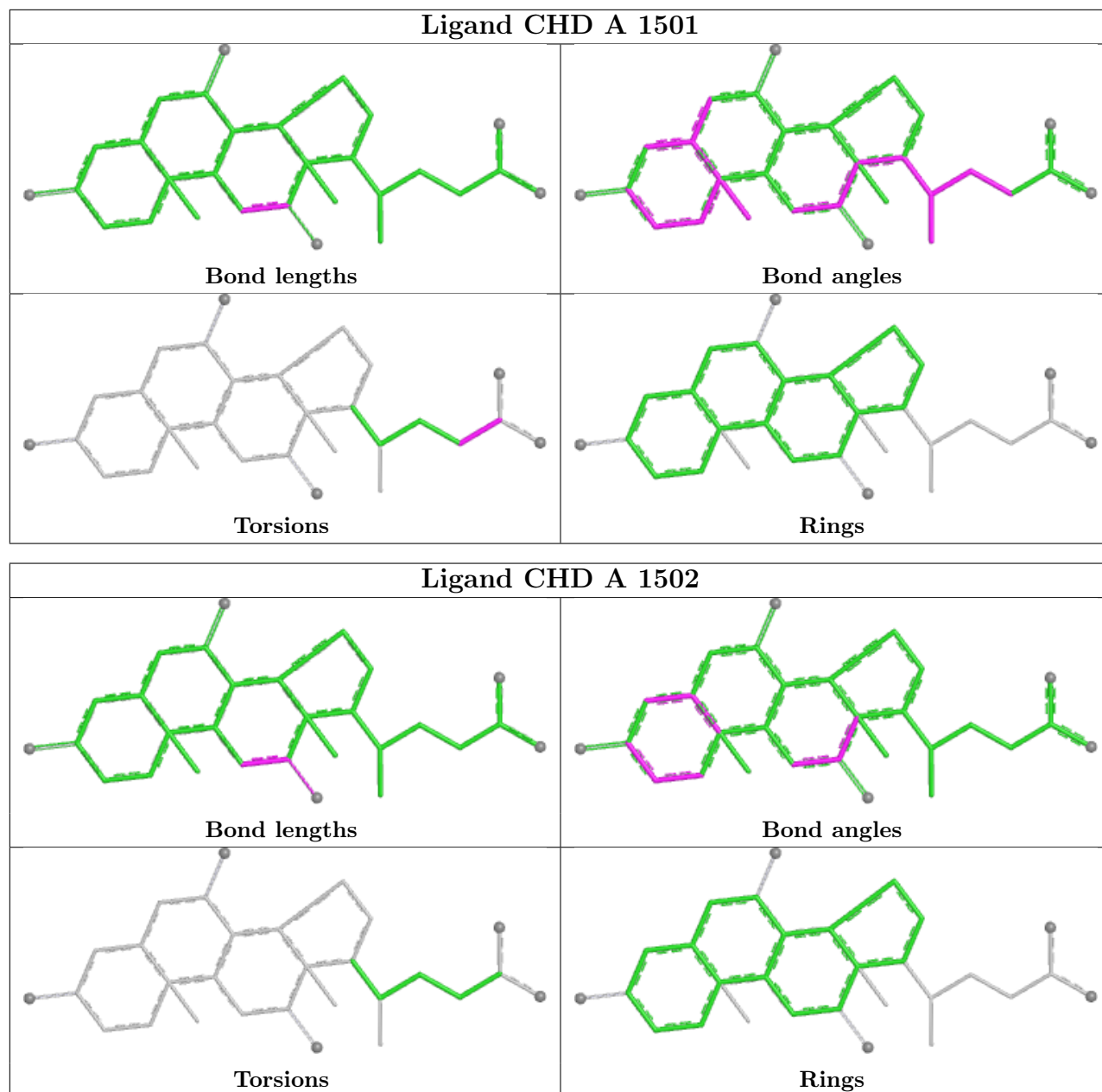
There are no ring outliers.

6 monomers are involved in 24 short contacts:

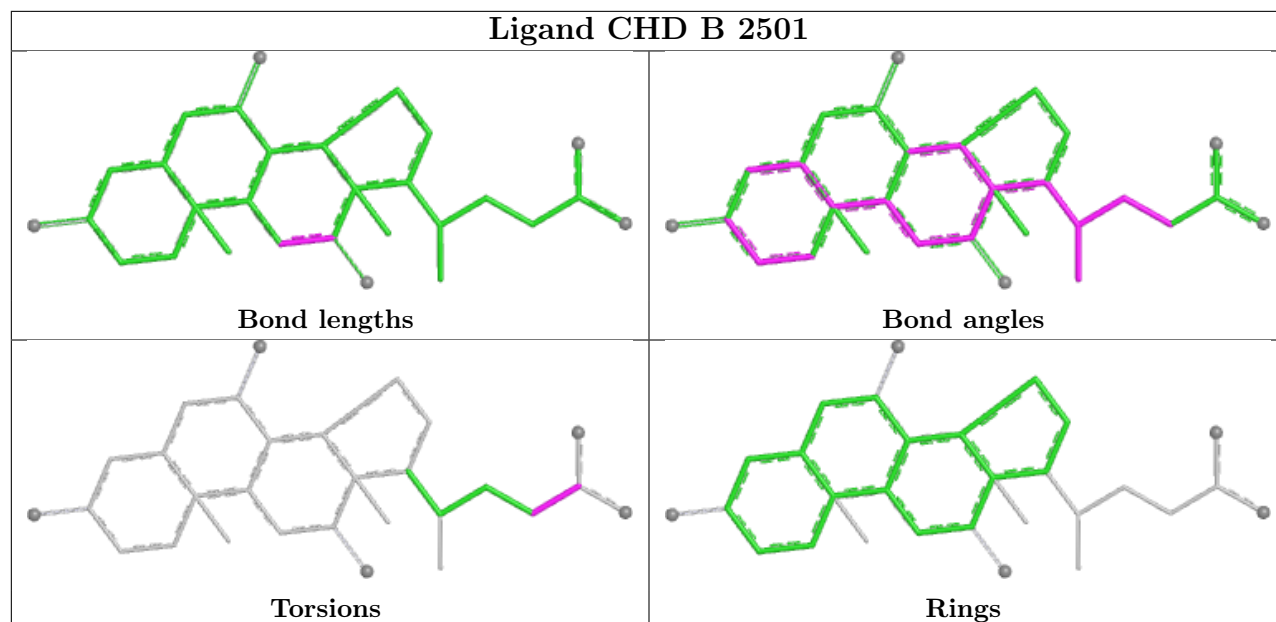
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2503	CHD	1	0
2	A	1501	CHD	7	0
2	A	1502	CHD	5	0
2	B	2501	CHD	6	0
2	A	1503	CHD	1	0
2	B	2502	CHD	6	0

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.

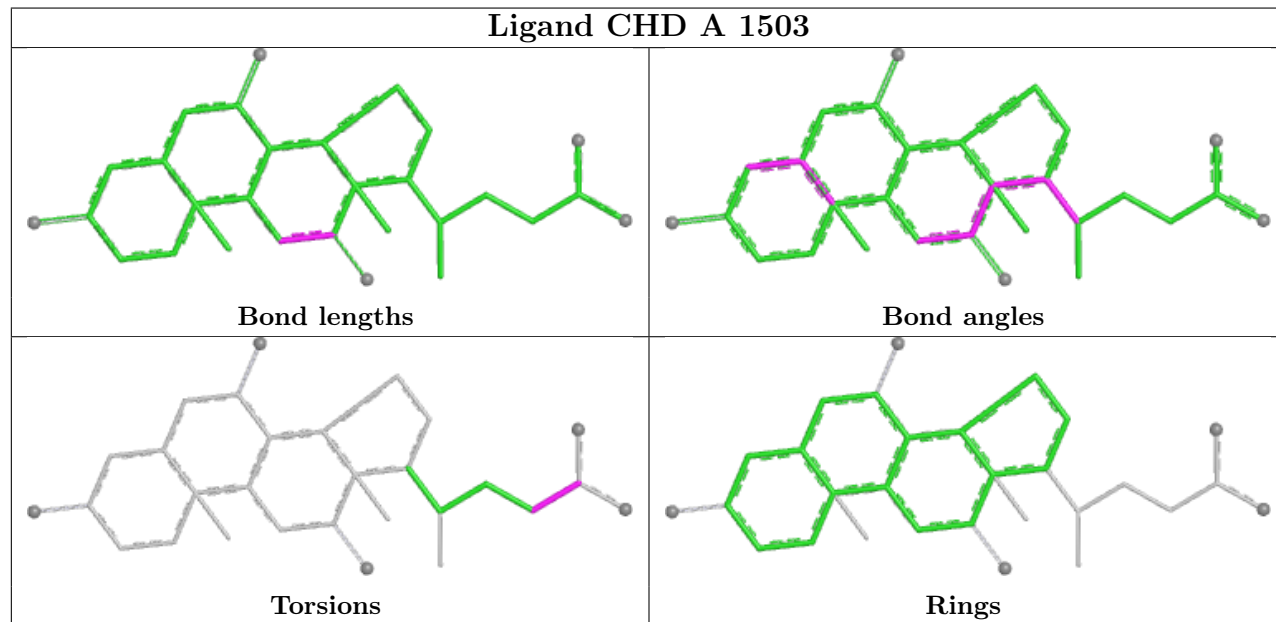


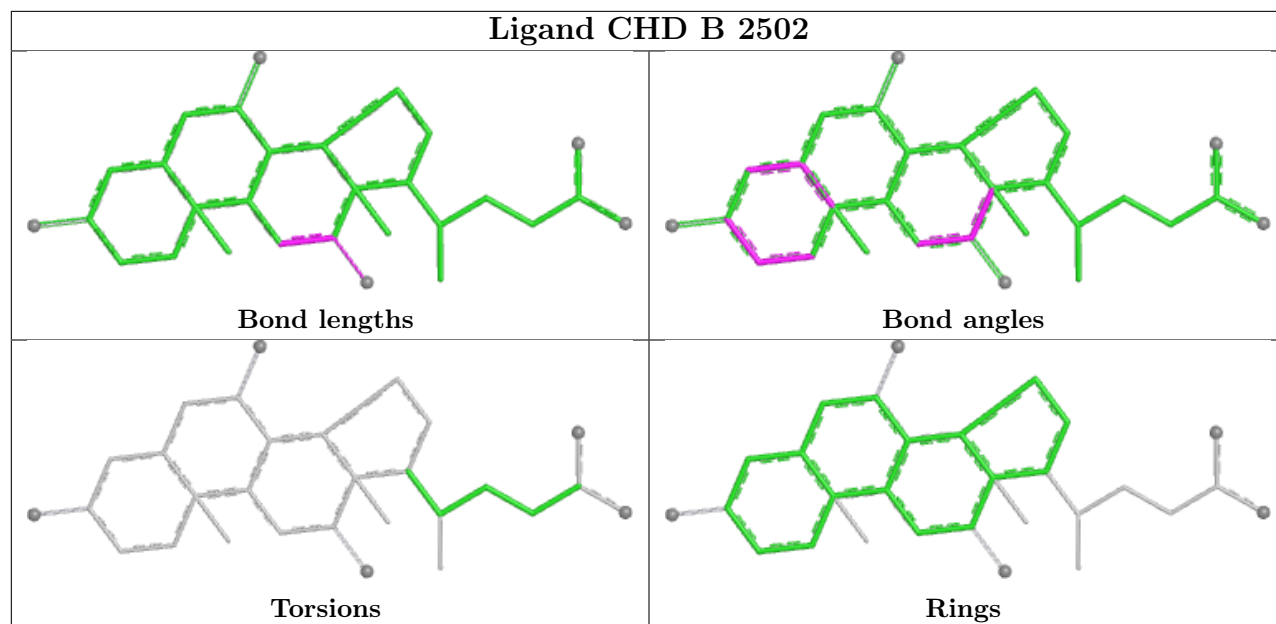


Ligand CHD B 2501



Ligand CHD A 1503





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	359/359 (100%)	2.66	232 (64%)  	7, 17, 28, 33	0
1	B	359/359 (100%)	2.72	251 (69%)  	8, 17, 28, 34	0
All	All	718/718 (100%)	2.69	483 (67%)  	7, 17, 28, 34	0

All (483) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	VAL	9.5
1	B	423	LEU	8.7
1	A	213	VAL	8.5
1	A	423	LEU	7.8
1	A	214	GLY	7.7
1	B	214	GLY	7.7
1	B	182	LEU	7.4
1	B	98	LEU	6.7
1	B	358	LYS	6.7
1	A	250	LEU	6.6
1	B	215	ARG	6.4
1	B	250	LEU	6.2
1	B	212	GLN	6.2
1	A	212	GLN	6.0
1	B	174	ILE	6.0
1	A	293	TYR	6.0
1	B	150	LEU	5.9
1	A	207	TYR	5.8
1	B	66	LYS	5.8
1	B	357	ALA	5.8
1	B	375	PRO	5.8
1	A	103	ILE	5.7
1	A	358	LYS	5.7
1	A	355	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	360	CYS	5.5
1	B	391	SER	5.5
1	B	351	GLU	5.5
1	A	65	ARG	5.4
1	A	418	PHE	5.4
1	A	185	ALA	5.4
1	A	211	ASN	5.3
1	B	209	TYR	5.2
1	B	175	GLU	5.2
1	B	218	THR	5.2
1	B	101	LEU	5.2
1	A	360	CYS	5.1
1	A	218	THR	5.1
1	A	384	LEU	5.0
1	B	154	THR	5.0
1	B	221	TRP	5.0
1	A	217	PRO	4.9
1	A	105	ASN	4.9
1	B	99	MET	4.9
1	A	215	ARG	4.9
1	B	153	ASN	4.8
1	B	393	GLU	4.8
1	A	381	LEU	4.8
1	B	217	PRO	4.7
1	B	361	GLY	4.7
1	A	96	ARG	4.7
1	B	100	THR	4.7
1	B	164	ARG	4.7
1	A	101	LEU	4.6
1	A	351	GLU	4.6
1	A	66	LYS	4.6
1	B	65	ARG	4.6
1	B	103	ILE	4.6
1	A	253	ARG	4.6
1	A	407	VAL	4.5
1	B	200	GLY	4.5
1	A	200	GLY	4.5
1	B	96	ARG	4.5
1	A	150	LEU	4.5
1	A	164	ARG	4.5
1	B	94	LEU	4.5
1	B	394	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	313	PRO	4.5
1	A	390	GLN	4.4
1	A	231	HIS	4.4
1	A	362	VAL	4.4
1	A	98	LEU	4.4
1	A	319	ILE	4.4
1	B	352	TYR	4.4
1	A	163	PHE	4.4
1	B	317	GLU	4.4
1	B	418	PHE	4.4
1	A	144	VAL	4.4
1	A	357	ALA	4.4
1	B	69	THR	4.4
1	A	153	ASN	4.4
1	A	202	SER	4.4
1	B	132	ILE	4.4
1	A	307	PRO	4.3
1	B	249	PRO	4.3
1	A	134	ILE	4.3
1	A	160	TYR	4.3
1	A	412	ARG	4.3
1	B	184	ARG	4.3
1	A	221	TRP	4.3
1	A	205	ALA	4.3
1	B	362	VAL	4.3
1	B	155	ALA	4.2
1	B	231	HIS	4.2
1	A	145	LYS	4.2
1	B	108	ALA	4.2
1	A	219	MET	4.2
1	B	219	MET	4.2
1	B	363	GLU	4.2
1	A	352	TYR	4.2
1	B	145	LYS	4.2
1	A	178	GLU	4.2
1	B	257	VAL	4.2
1	B	405	LEU	4.1
1	B	67	PRO	4.1
1	A	68	LYS	4.1
1	B	165	TYR	4.1
1	B	211	ASN	4.1
1	A	97	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	104	GLN	4.1
1	B	359	GLU	4.1
1	B	185	ALA	4.0
1	B	97	ASP	4.0
1	B	160	TYR	4.0
1	B	115	LEU	4.0
1	A	100	THR	4.0
1	B	112	ALA	4.0
1	A	346	TYR	4.0
1	A	313	PRO	4.0
1	A	132	ILE	4.0
1	A	180	ASP	4.0
1	B	95	ASP	4.0
1	A	356	LEU	3.9
1	A	154	THR	3.9
1	A	106	LYS	3.9
1	B	114	ARG	3.9
1	B	305	VAL	3.9
1	B	378	SER	3.9
1	A	181	GLY	3.8
1	B	234	ILE	3.8
1	A	137	SER	3.8
1	B	251	GLU	3.8
1	A	210	TYR	3.8
1	A	363	GLU	3.8
1	B	247	HIS	3.8
1	B	68	LYS	3.8
1	B	134	ILE	3.8
1	B	293	TYR	3.8
1	B	203	LEU	3.8
1	A	375	PRO	3.8
1	B	355	VAL	3.8
1	B	407	VAL	3.8
1	A	209	TYR	3.7
1	B	168	PRO	3.7
1	A	359	GLU	3.7
1	A	257	VAL	3.7
1	B	417	PHE	3.7
1	A	115	LEU	3.7
1	B	323	CYS	3.7
1	B	364	ASN	3.7
1	A	138	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	106	LYS	3.7
1	B	354	GLN	3.7
1	A	159	TYR	3.7
1	B	207	TYR	3.7
1	B	181	GLY	3.6
1	A	284	VAL	3.6
1	A	110	PHE	3.6
1	B	110	PHE	3.6
1	A	94	LEU	3.6
1	A	99	MET	3.6
1	A	394	LEU	3.6
1	B	392	ASN	3.6
1	B	286	LYS	3.6
1	A	206	ILE	3.6
1	B	389	ILE	3.6
1	A	192	PRO	3.6
1	A	77	GLY	3.6
1	A	151	SER	3.6
1	A	93	PHE	3.6
1	A	330	ILE	3.6
1	A	179	ARG	3.6
1	A	227	TRP	3.5
1	B	111	ILE	3.5
1	B	192	PRO	3.5
1	B	216	LYS	3.5
1	A	182	LEU	3.5
1	B	412	ARG	3.5
1	A	155	ALA	3.5
1	B	322	LEU	3.5
1	B	179	ARG	3.5
1	B	186	ILE	3.5
1	B	180	ASP	3.5
1	B	210	TYR	3.5
1	B	329	ASN	3.5
1	B	387	SER	3.4
1	A	216	LYS	3.4
1	B	178	GLU	3.4
1	B	272	ARG	3.4
1	B	105	ASN	3.4
1	A	174	ILE	3.4
1	A	391	SER	3.4
1	A	317	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	290	ARG	3.4
1	A	308	MET	3.4
1	B	176	GLU	3.4
1	A	168	PRO	3.4
1	A	379	LYS	3.4
1	B	205	ALA	3.4
1	A	247	HIS	3.3
1	A	183	GLU	3.3
1	B	80	GLU	3.3
1	B	339	SER	3.3
1	B	350	ILE	3.3
1	B	408	ASN	3.3
1	A	411	CYS	3.3
1	B	406	CYS	3.3
1	B	220	LYS	3.3
1	A	67	PRO	3.3
1	A	380	ALA	3.3
1	A	389	ILE	3.3
1	B	336	ALA	3.3
1	B	232	LEU	3.3
1	B	141	GLU	3.3
1	A	83	GLY	3.3
1	A	298	ARG	3.3
1	B	227	TRP	3.2
1	A	156	PRO	3.2
1	A	114	ARG	3.2
1	A	141	GLU	3.2
1	A	189	THR	3.2
1	A	152	PRO	3.2
1	A	306	GLY	3.2
1	B	183	GLU	3.2
1	A	270	VAL	3.2
1	B	410	VAL	3.2
1	A	71	ILE	3.2
1	B	248	PHE	3.2
1	A	167	HIS	3.2
1	A	70	GLY	3.2
1	B	277	PRO	3.2
1	A	410	VAL	3.1
1	A	184	ARG	3.1
1	A	220	LYS	3.1
1	A	334	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	3.1
1	A	187	ALA	3.1
1	A	305	VAL	3.1
1	B	119	ILE	3.1
1	A	416	SER	3.1
1	A	223	THR	3.1
1	A	248	PHE	3.1
1	B	309	PRO	3.1
1	B	157	HIS	3.1
1	B	320	LYS	3.1
1	A	421	GLN	3.1
1	A	123	TYR	3.0
1	A	165	TYR	3.0
1	B	253	ARG	3.0
1	A	157	HIS	3.0
1	B	243	LYS	3.0
1	B	202	SER	3.0
1	B	306	GLY	3.0
1	A	297	TYR	3.0
1	B	292	GLU	3.0
1	B	413	GLU	3.0
1	B	93	PHE	3.0
1	B	151	SER	3.0
1	A	186	ILE	3.0
1	A	131	PRO	3.0
1	B	328	LYS	3.0
1	B	88	PHE	3.0
1	A	259	LEU	3.0
1	B	204	ASN	3.0
1	B	324	GLU	3.0
1	A	116	THR	3.0
1	A	277	PRO	3.0
1	B	118	LYS	3.0
1	A	177	MET	3.0
1	A	173	ALA	2.9
1	A	392	ASN	2.9
1	B	365	ILE	2.9
1	B	304	LYS	2.9
1	B	109	PRO	2.9
1	A	378	SER	2.9
1	A	387	SER	2.9
1	A	102	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	353	SER	2.9
1	A	243	LYS	2.9
1	A	354	GLN	2.9
1	A	364	ASN	2.9
1	B	310	TRP	2.9
1	A	74	LEU	2.8
1	B	146	LEU	2.8
1	B	383	ASP	2.8
1	B	290	ARG	2.8
1	A	309	PRO	2.8
1	A	402	SER	2.8
1	B	147	LEU	2.8
1	A	119	ILE	2.8
1	B	298	ARG	2.8
1	B	163	PHE	2.8
1	B	156	PRO	2.8
1	A	241	ILE	2.8
1	A	420	SER	2.8
1	A	314	GLN	2.8
1	A	176	GLU	2.8
1	A	194	TYR	2.8
1	B	265	LEU	2.8
1	B	138	LYS	2.8
1	B	152	PRO	2.8
1	A	166	VAL	2.8
1	A	301	TRP	2.8
1	B	390	GLN	2.7
1	B	318	SER	2.7
1	B	208	ARG	2.7
1	B	307	PRO	2.7
1	A	171	GLU	2.7
1	B	312	GLY	2.7
1	A	170	THR	2.7
1	B	72	LEU	2.7
1	A	324	GLU	2.7
1	A	335	ILE	2.7
1	B	241	ILE	2.7
1	A	133	LYS	2.7
1	A	82	LEU	2.7
1	A	315	THR	2.7
1	A	376	LEU	2.7
1	B	376	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	270	VAL	2.7
1	A	235	GLN	2.6
1	B	171	GLU	2.6
1	A	203	LEU	2.6
1	A	322	LEU	2.6
1	A	401	LEU	2.6
1	B	414	THR	2.6
1	B	117	PRO	2.6
1	A	415	LYS	2.6
1	A	258	ILE	2.6
1	A	365	ILE	2.6
1	B	166	VAL	2.6
1	B	120	GLN	2.6
1	B	421	GLN	2.6
1	A	251	GLU	2.6
1	A	413	GLU	2.6
1	A	414	THR	2.6
1	B	169	LEU	2.6
1	A	225	ASP	2.6
1	B	297	TYR	2.6
1	A	422	GLN	2.6
1	B	235	GLN	2.6
1	B	284	VAL	2.6
1	B	92	LEU	2.6
1	B	370	SER	2.6
1	A	104	GLN	2.5
1	B	70	GLY	2.5
1	B	326	GLY	2.5
1	B	236	CYS	2.5
1	A	89	LEU	2.5
1	A	146	LEU	2.5
1	B	242	LEU	2.5
1	B	401	LEU	2.5
1	B	422	GLN	2.5
1	A	350	ILE	2.5
1	B	123	TYR	2.5
1	B	159	TYR	2.5
1	A	344	THR	2.5
1	A	289	GLU	2.5
1	A	396	SER	2.5
1	B	195	SER	2.5
1	B	262	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	353	SER	2.5
1	B	74	LEU	2.5
1	B	245	LEU	2.5
1	A	361	GLY	2.5
1	A	85	VAL	2.5
1	B	85	VAL	2.5
1	B	226	ARG	2.5
1	A	80	GLU	2.5
1	A	242	LEU	2.5
1	B	385	VAL	2.4
1	B	402	SER	2.4
1	A	79	PRO	2.4
1	A	404	PRO	2.4
1	B	102	PRO	2.4
1	A	158	LYS	2.4
1	B	133	LYS	2.4
1	B	384	LEU	2.4
1	A	292	GLU	2.4
1	A	300	VAL	2.4
1	A	316	ASP	2.4
1	A	342	ILE	2.4
1	A	385	VAL	2.4
1	B	116	THR	2.4
1	B	404	PRO	2.4
1	B	173	ALA	2.4
1	A	399	LEU	2.4
1	B	332	LEU	2.4
1	A	326	GLY	2.4
1	A	237	PHE	2.4
1	B	188	PHE	2.4
1	A	84	ASP	2.4
1	B	269	VAL	2.4
1	A	310	TRP	2.4
1	B	409	PRO	2.4
1	B	386	HIS	2.4
1	A	108	ALA	2.4
1	B	167	HIS	2.4
1	B	191	TYR	2.3
1	A	112	ALA	2.3
1	A	393	GLU	2.3
1	B	107	LEU	2.3
1	B	345	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	88	PHE	2.3
1	A	197	SER	2.3
1	A	191	TYR	2.3
1	A	368	ALA	2.3
1	B	127	GLY	2.3
1	B	246	ASP	2.3
1	B	124	ARG	2.3
1	B	420	SER	2.3
1	B	223	THR	2.3
1	B	419	THR	2.3
1	A	208	ARG	2.3
1	A	113	LYS	2.3
1	A	370	SER	2.3
1	B	137	SER	2.3
1	B	335	ILE	2.3
1	A	406	CYS	2.3
1	B	196	CYS	2.3
1	A	340	ASP	2.3
1	B	158	LYS	2.3
1	B	379	LYS	2.3
1	A	147	LEU	2.3
1	B	371	LEU	2.3
1	B	206	ILE	2.2
1	B	287	VAL	2.2
1	B	238	ALA	2.2
1	A	124	ARG	2.2
1	A	111	ILE	2.2
1	A	266	PRO	2.2
1	B	224	ILE	2.2
1	A	287	VAL	2.2
1	B	87	ASP	2.2
1	B	308	MET	2.2
1	B	346	TYR	2.2
1	A	272	ARG	2.2
1	A	109	PRO	2.2
1	A	136	THR	2.2
1	A	234	ILE	2.2
1	A	417	PHE	2.2
1	B	266	PRO	2.2
1	B	275	PRO	2.2
1	A	274	ASP	2.2
1	B	289	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	2.2
1	A	345	LEU	2.2
1	B	403	CYS	2.2
1	A	135	TRP	2.2
1	B	177	MET	2.2
1	B	79	PRO	2.1
1	B	170	THR	2.2
1	B	315	THR	2.2
1	B	342	ILE	2.1
1	A	312	GLY	2.1
1	B	129	GLY	2.1
1	B	299	LEU	2.1
1	B	201	SER	2.1
1	A	175	GLU	2.1
1	B	301	TRP	2.1
1	B	126	ILE	2.1
1	A	169	LEU	2.1
1	B	415	LYS	2.1
1	A	271	ASN	2.1
1	B	377	PHE	2.1
1	B	368	ALA	2.1
1	B	89	LEU	2.1
1	B	356	LEU	2.1
1	B	143	MET	2.1
1	A	95	ASP	2.1
1	A	86	HIS	2.1
1	A	409	PRO	2.1
1	B	162	GLY	2.1
1	B	321	GLY	2.1
1	B	237	PHE	2.1
1	B	399	LEU	2.0
1	B	84	ASP	2.0
1	B	341	HIS	2.0
1	A	304	LYS	2.0
1	B	319	ILE	2.0
1	B	230	HIS	2.0
1	A	328	LYS	2.0
1	B	397	LYS	2.0
1	B	344	THR	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](#)

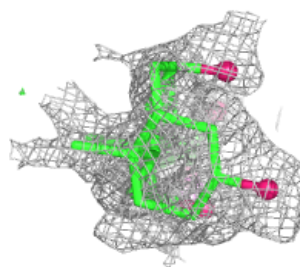
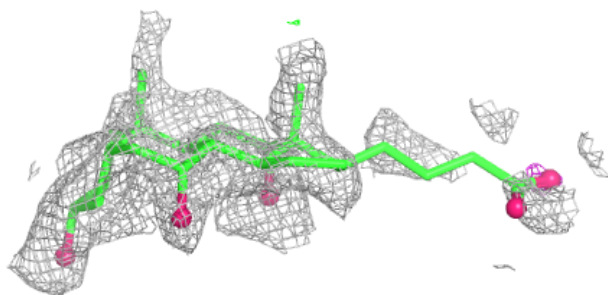
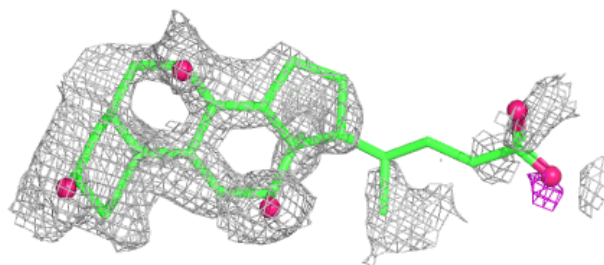
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CHD	B	2503	29/29	0.49	0.28	33,35,42,43	0
2	CHD	A	1503	29/29	0.50	0.29	32,33,39,40	0
2	CHD	A	1502	29/29	0.64	0.23	24,24,33,34	0
2	CHD	B	2502	29/29	0.68	0.21	24,25,33,35	0
2	CHD	B	2501	29/29	0.71	0.23	18,19,35,37	0
2	CHD	A	1501	29/29	0.77	0.20	16,18,36,39	0
3	FES	A	1499	4/4	0.98	0.06	13,14,14,14	0
3	FES	B	2999	4/4	0.98	0.04	14,15,15,15	0

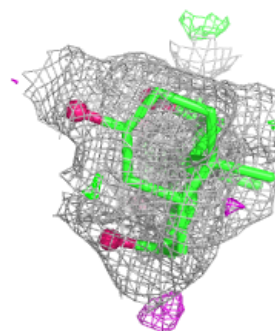
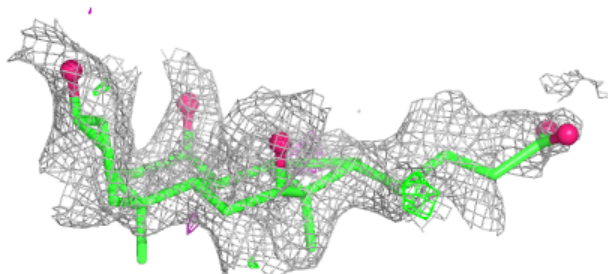
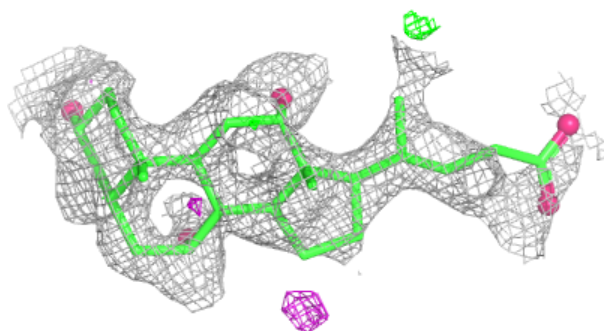
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD B 2503:

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

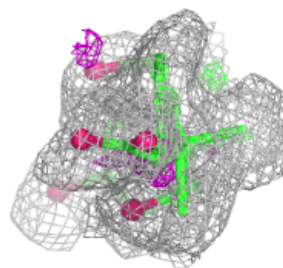
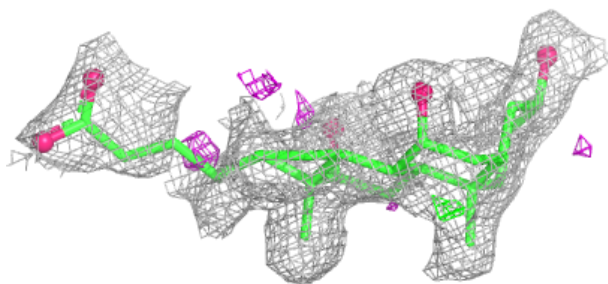
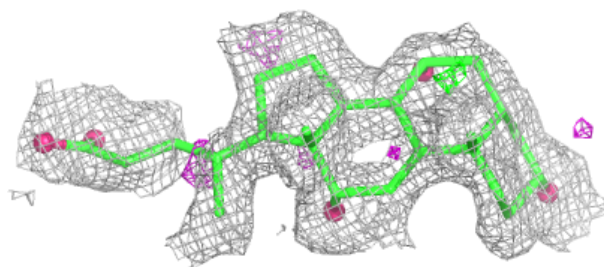
**Electron density around CHD A 1503:**

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

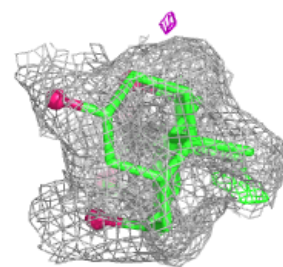
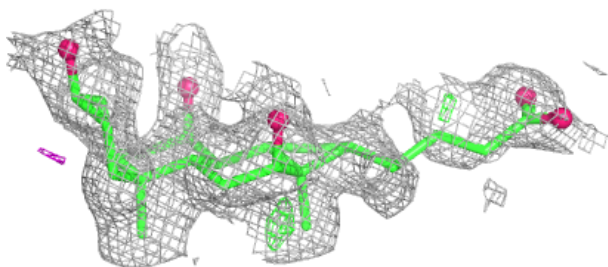
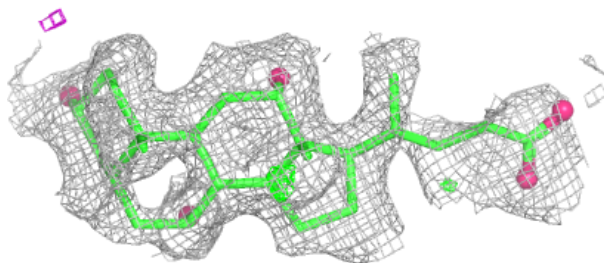


Electron density around CHD A 1502:

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

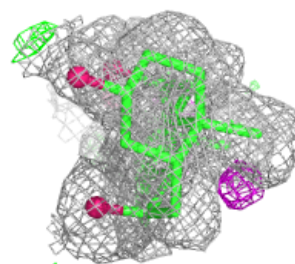
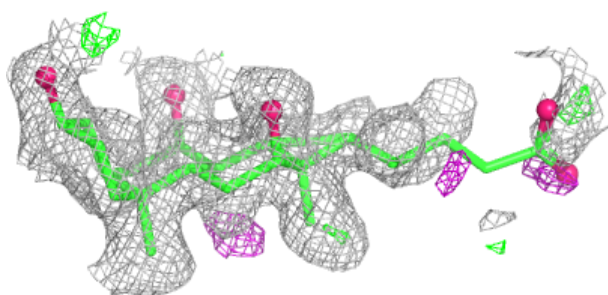
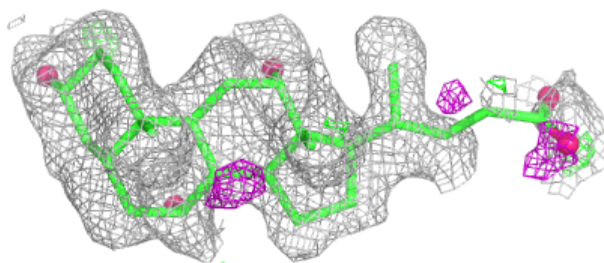
**Electron density around CHD B 2502:**

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

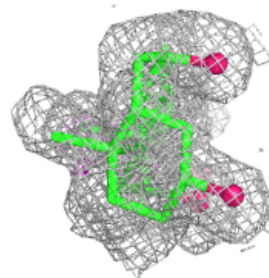
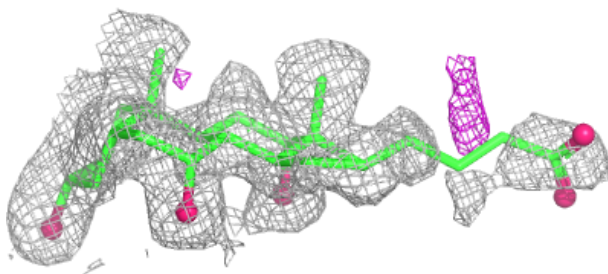
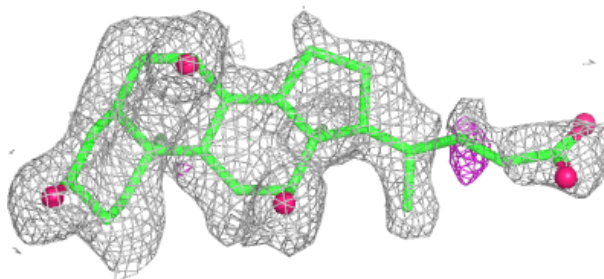


Electron density around CHD B 2501:

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

**Electron density around CHD A 1501:**

$2mF_o-DF_c$ (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.