



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 4KLA / pdb_00004kla
Title : E343D variant of human ferrochelatase
Authors : Lanzilotta, W.N.; Medlock, A.E.
Deposited on : 2013-05-07
Resolution : 2.60 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

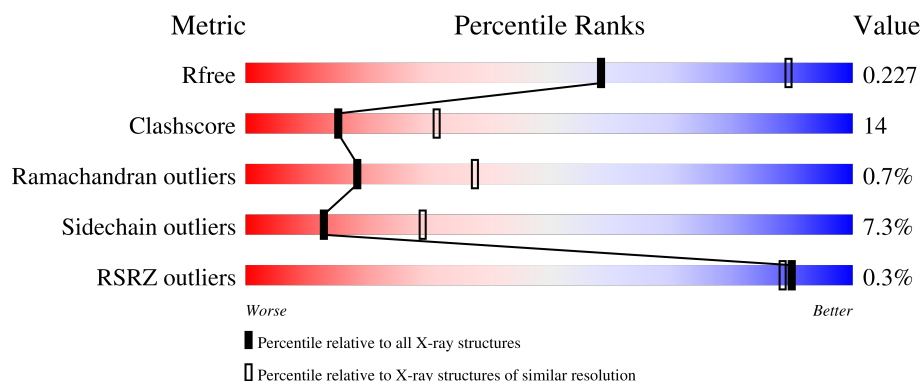
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 74% 23% . .
1	B	359	 68% 28% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6184 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.

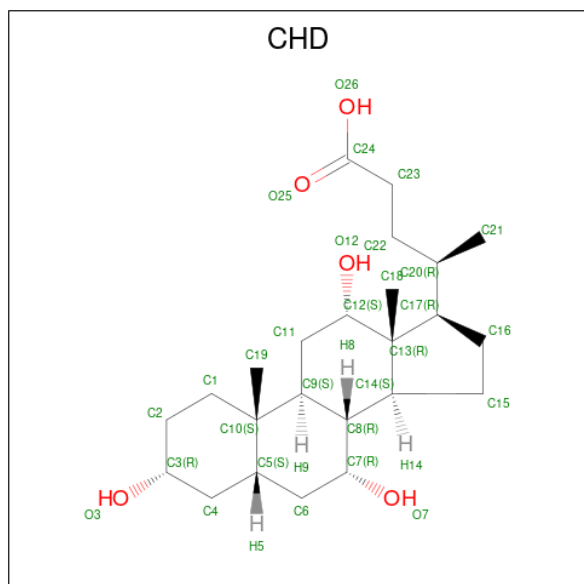
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2890	1840	503	529	18			
1	B	359	Total	C	N	O	S	0	1	0
			2896	1845	504	529	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	ASP	GLU	engineered mutation	UNP P22830
B	343	ASP	GLU	engineered mutation	UNP P22830

- Molecule 2 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



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

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



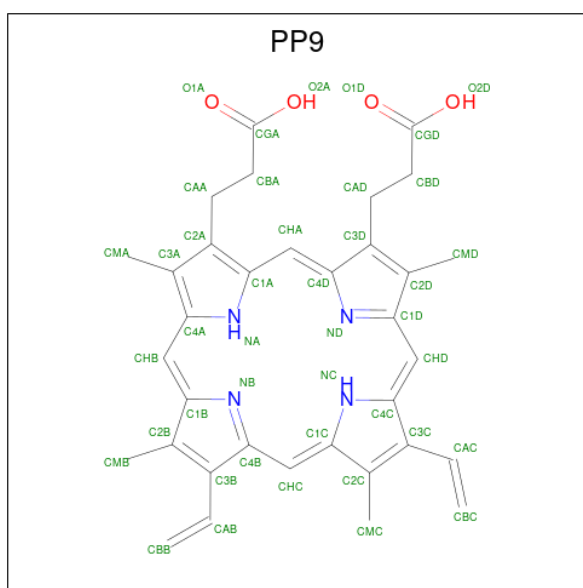
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 5 is PROTOPORPHYRIN IX (CCD ID: PP9) (formula: $C_{34}H_{34}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			42	34	4	4		

- Molecule 6 is water.

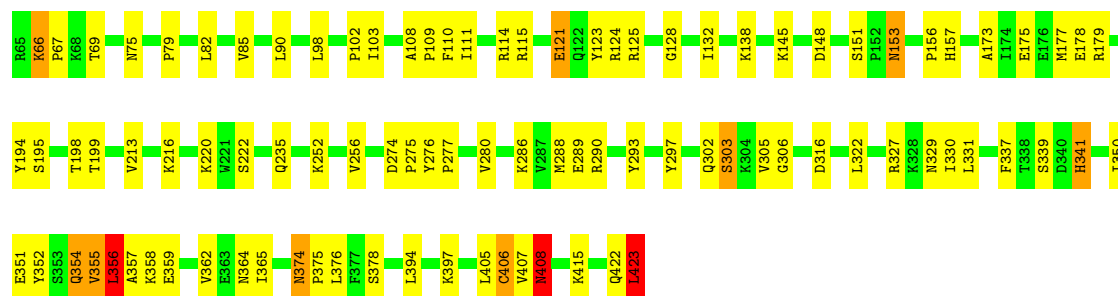
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total 142	O 142	0	0
6	B	113	Total 113	O 113	0	0

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.

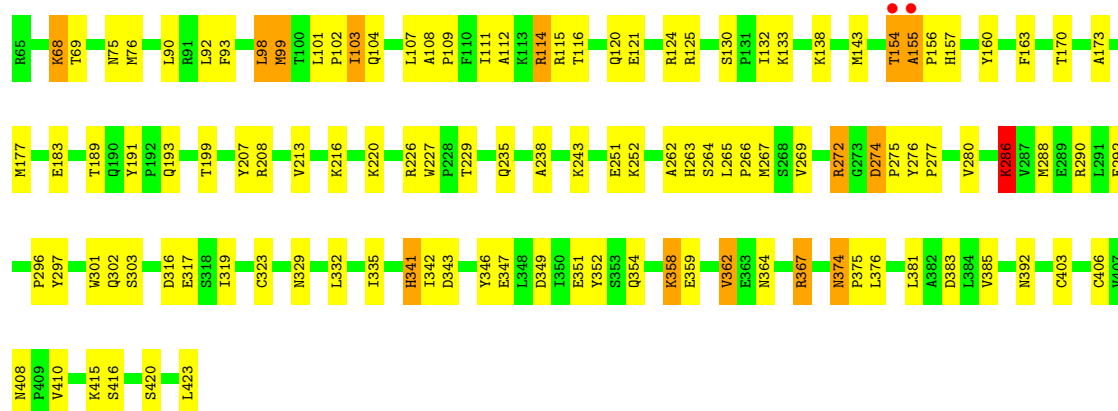
• Molecule 1: Ferrochelatase, mitochondrial

Chain A: 



• Molecule 1: Ferrochelatase, mitochondrial

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.99Å 93.43Å 111.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.68 – 2.60 71.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.68-2.60) 99.7 (71.67-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.212 , 0.285 (Not available) , 0.227	Depositor DCC
R_{free} test set	1473 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6184	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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 56.66 % 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 2.6504e-05. 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, GOL, PP9, 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	0.81	0/2960	1.06	8/4010 (0.2%)
1	B	0.91	7/2969 (0.2%)	1.02	3/4021 (0.1%)
All	All	0.86	7/5929 (0.1%)	1.04	11/8031 (0.1%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	LEU	C-O	-13.79	1.06	1.24
1	B	99	MET	C-O	-9.21	1.13	1.23
1	B	98	LEU	CG-CD2	-9.09	1.22	1.52
1	B	99	MET	CA-C	-7.30	1.44	1.52
1	B	99	MET	CG-SD	-5.44	1.67	1.80
1	B	286[A]	LYS	N-CA	5.32	1.52	1.46
1	B	286[B]	LYS	N-CA	5.32	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ASN	CA-C-N	8.33	128.06	119.56
1	A	408	ASN	C-N-CA	8.33	128.06	119.56
1	B	130	SER	N-CA-C	6.55	117.90	109.65
1	A	66	LYS	CA-C-N	6.54	126.90	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	LYS	C-N-CA	6.54	126.90	119.83
1	A	423	LEU	CA-CB-CG	5.79	136.58	116.30
1	B	98	LEU	CB-CG-CD2	-5.53	94.10	110.70
1	A	85	VAL	N-CA-C	5.43	115.63	110.42
1	A	280	VAL	N-CA-C	-5.32	105.35	110.72
1	A	151	SER	N-CA-C	5.19	116.23	108.76
1	B	274	ASP	N-CA-C	5.08	116.80	109.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	406	CYS	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	2890	0	2895	59	0
1	B	2896	0	2910	95	0
2	A	58	0	78	11	0
2	B	29	0	39	6	0
3	A	6	0	8	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	B	42	0	32	7	0
6	A	142	0	0	5	0
6	B	113	0	0	1	0
All	All	6184	0	5962	162	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 (162) 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:220:LYS:HE3	1:A:423:LEU:HD11	1.17	1.14
1:B:155:ALA:HB1	1:B:156:PRO:CD	1.85	1.05
1:B:155:ALA:HB1	1:B:156:PRO:HD2	1.39	1.01
3:A:503:GOL:H2	1:B:277:PRO:HB3	1.53	0.88
2:B:501:CHD:H192	5:B:502:PP9:HMB3	1.53	0.87
2:A:501:CHD:H212	2:A:501:CHD:H12	1.58	0.86
1:A:115:ARG:HD2	2:A:501:CHD:H231	1.58	0.85
1:B:115:ARG:HH21	2:B:501:CHD:H231	1.43	0.83
2:B:501:CHD:C19	5:B:502:PP9:HMB3	2.09	0.82
1:B:155:ALA:CB	1:B:156:PRO:CD	2.62	0.75
1:A:115:ARG:NH1	2:A:501:CHD:H222	2.02	0.74
2:B:501:CHD:H192	5:B:502:PP9:CMB	2.17	0.74
1:A:374:ASN:ND2	1:A:376:LEU:H	1.84	0.74
1:A:374:ASN:HD22	1:A:375:PRO:N	1.85	0.72
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.56	0.70
3:A:503:GOL:H2	1:B:277:PRO:CB	2.22	0.69
1:B:75:ASN:OD1	1:B:132:ILE:HD11	1.92	0.69
1:A:220:LYS:HD3	1:A:423:LEU:HD21	1.76	0.67
1:A:374:ASN:HD22	1:A:374:ASN:C	2.03	0.66
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.77	0.66
1:A:153:ASN:H	1:A:153:ASN:ND2	1.95	0.65
1:A:355:VAL:O	1:A:356:LEU:C	2.41	0.64
1:B:68:LYS:HB2	1:B:155:ALA:HB3	1.80	0.63
1:A:305:VAL:HG21	2:A:502:CHD:H161	1.81	0.63
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.82	0.62
1:A:355:VAL:O	1:A:358:LYS:N	2.32	0.61
1:B:68:LYS:CB	1:B:155:ALA:HB3	2.30	0.61
1:A:330:ILE:HB	1:A:365:ILE:HD12	1.83	0.61
1:A:306:GLY:HA2	6:A:675:HOH:O	2.00	0.60
1:A:110:PHE:CZ	1:A:114:ARG:HD2	2.37	0.59
1:B:115:ARG:NH2	2:B:501:CHD:H231	2.17	0.58
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.15	0.58
1:A:357:ALA:HB1	1:A:362:VAL:HG11	1.84	0.58
1:A:350:ILE:O	1:A:354:GLN:HB2	2.03	0.58
1:B:229:THR:HB	1:B:286[A]:LYS:HE3	1.84	0.58
1:B:269:VAL:HG21	5:B:502:PP9:HBB2	1.85	0.58
1:B:155:ALA:CB	1:B:156:PRO:HD2	2.24	0.57
1:A:375:PRO:O	1:A:378:SER:HB2	2.05	0.56
1:B:121:GLU:O	1:B:125:ARG:HG2	2.05	0.56
1:B:374:ASN:ND2	1:B:376:LEU:H	2.04	0.56
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.80	0.56
1:A:148:ASP:OD2	1:A:157:HIS:ND1	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MET:HG2	1:B:101:LEU:HG	1.87	0.56
1:B:173:ALA:O	1:B:177:MET:HG3	2.06	0.56
1:A:194:TYR:HA	6:A:615:HOH:O	2.06	0.56
1:B:133:LYS:HG3	1:B:163:PHE:HE1	1.71	0.55
1:B:229:THR:HB	1:B:286[A]:LYS:HD3	1.88	0.55
1:B:229:THR:O	1:B:286[A]:LYS:HE3	2.07	0.55
1:B:132:ILE:HG23	1:B:133:LYS:N	2.22	0.54
1:B:93:PHE:HB2	1:B:108:ALA:HB1	1.89	0.54
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.43	0.54
1:A:198:THR:OG1	1:A:199:THR:N	2.41	0.54
1:B:102:PRO:C	1:B:103:ILE:HG13	2.34	0.53
1:B:408:ASN:OD1	1:B:410:VAL:HG12	2.08	0.53
1:B:374:ASN:HD22	1:B:376:LEU:H	1.56	0.53
1:B:115:ARG:NH1	6:B:602:HOH:O	2.37	0.53
1:B:235:GLN:HG3	1:B:290:ARG:CZ	2.39	0.53
1:B:102:PRO:O	1:B:103:ILE:C	2.51	0.53
1:B:319:ILE:HD11	1:B:332:LEU:HD21	1.90	0.53
1:A:405:LEU:HD11	1:B:317:GLU:HB3	1.90	0.52
1:B:374:ASN:HD22	1:B:374:ASN:C	2.16	0.52
1:A:121:GLU:O	1:A:125:ARG:HG2	2.10	0.52
2:A:501:CHD:H12	2:A:501:CHD:C21	2.36	0.52
1:A:374:ASN:ND2	1:A:374:ASN:C	2.68	0.51
1:A:102:PRO:O	1:A:103:ILE:HG13	2.09	0.51
1:B:189:THR:HB	1:B:199:THR:HG23	1.93	0.51
1:B:235:GLN:HG3	1:B:290:ARG:NH2	2.26	0.51
1:A:82:LEU:HD21	1:A:128:GLY:HA2	1.93	0.51
1:B:154:THR:OG1	1:B:157:HIS:NE2	2.41	0.50
1:A:98:LEU:HD13	6:A:658:HOH:O	2.12	0.50
1:B:349:ASP:OD2	1:B:367:ARG:NH2	2.45	0.50
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.47	0.49
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.47	0.49
1:A:341:HIS:CD2	1:A:341:HIS:N	2.81	0.49
1:A:422:GLN:HG2	6:A:721:HOH:O	2.11	0.49
1:B:354:GLN:O	1:B:358:LYS:HB2	2.12	0.49
1:B:238:ALA:CB	1:B:290:ARG:HD3	2.43	0.49
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.95	0.48
1:B:343:ASP:O	1:B:347:GLU:HB3	2.13	0.48
1:B:116:THR:O	1:B:120:GLN:HG3	2.13	0.48
1:B:323:CYS:SG	1:B:362:VAL:HG23	2.53	0.48
1:A:407:VAL:O	1:A:408:ASN:CB	2.62	0.48
1:A:79:PRO:HD2	1:A:123:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:O	1:B:104:GLN:HG3	2.14	0.47
1:B:112:ALA:C	1:B:114:ARG:N	2.71	0.47
1:B:381:LEU:O	1:B:385:VAL:HG23	2.14	0.47
1:B:265:LEU:HD11	1:B:276:TYR:CD2	2.49	0.47
1:B:302:GLN:HG3	1:B:303:SER:OG	2.14	0.47
1:B:238:ALA:HB3	1:B:290:ARG:HD3	1.97	0.47
1:B:329:ASN:ND2	1:B:364:ASN:HB2	2.27	0.47
1:B:416:SER:O	1:B:420:SER:OG	2.24	0.47
1:B:347:GLU:HA	1:B:351:GLU:HG2	1.97	0.47
1:B:262:ALA:O	1:B:301:TRP:HA	2.15	0.47
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.14	0.47
1:A:406:CYS:SG	1:A:407:VAL:O	2.72	0.47
1:A:111:ILE:O	1:A:115:ARG:HG2	2.14	0.46
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.30	0.46
1:B:342:ILE:HG21	5:B:502:PP9:HAD2	1.97	0.46
1:B:341:HIS:N	1:B:341:HIS:CD2	2.82	0.46
1:A:69:THR:HB	1:A:157:HIS:CD2	2.50	0.46
1:B:90:LEU:HD13	1:B:109:PRO:HA	1.97	0.46
1:B:102:PRO:O	1:B:107:LEU:HD12	2.15	0.46
2:A:502:CHD:H41	2:A:502:CHD:O7	2.15	0.46
1:B:374:ASN:HD22	1:B:375:PRO:N	2.13	0.46
1:B:342:ILE:CG2	5:B:502:PP9:HAD2	2.46	0.46
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.81	0.45
1:B:226:ARG:C	1:B:227:TRP:CD1	2.94	0.45
1:B:374:ASN:HD22	1:B:376:LEU:N	2.14	0.45
2:A:501:CHD:H12A	2:A:501:CHD:H112	1.65	0.45
1:B:288:MET:HG3	1:B:297:TYR:CD2	2.52	0.45
1:B:115:ARG:HH21	2:B:501:CHD:C23	2.23	0.45
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.98	0.45
2:A:501:CHD:C21	2:A:501:CHD:C12	2.94	0.45
1:B:403:CYS:HB2	1:B:406:CYS:HB2	1.99	0.45
1:B:229:THR:HB	1:B:286[A]:LYS:CD	2.47	0.45
1:B:263:HIS:HB3	5:B:502:PP9:HBC1	1.99	0.44
1:A:173:ALA:O	1:A:177:MET:HG3	2.16	0.44
1:A:90:LEU:HD13	1:A:109:PRO:HA	1.99	0.44
1:B:154:THR:HG1	1:B:157:HIS:CE1	2.33	0.44
1:B:335:ILE:O	1:B:335:ILE:HG13	2.17	0.44
1:B:68:LYS:HD3	1:B:183:GLU:OE1	2.18	0.44
1:B:272:ARG:O	1:B:272:ARG:HG2	2.16	0.43
1:A:322:LEU:HB3	1:A:327:ARG:HB2	1.99	0.43
1:B:76:MET:HG2	1:B:191:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.87	0.43
1:B:101:LEU:HB2	1:B:104:GLN:HG3	2.00	0.43
1:B:251:GLU:HG2	1:B:252:LYS:HG2	2.01	0.43
1:A:195:SER:HB2	1:A:276:TYR:HB2	2.00	0.42
1:B:133:LYS:HG3	1:B:163:PHE:CE1	2.53	0.42
1:B:288:MET:HG3	1:B:297:TYR:CE2	2.54	0.42
1:A:75:ASN:OD1	1:A:337:PHE:CZ	2.72	0.42
1:A:115:ARG:HD2	2:A:501:CHD:C23	2.41	0.42
1:B:160:TYR:CD1	1:B:177:MET:HE3	2.55	0.42
1:B:69:THR:HB	1:B:157:HIS:CD2	2.54	0.42
1:B:69:THR:HB	1:B:157:HIS:HD2	1.85	0.42
1:A:222:SER:HB2	1:A:394:LEU:HA	2.01	0.42
1:A:175:GLU:HG2	1:A:179:ARG:HH22	1.85	0.41
1:B:112:ALA:C	1:B:114:ARG:H	2.28	0.41
1:B:160:TYR:CD2	1:B:177:MET:HG2	2.55	0.41
1:B:346:TYR:O	1:B:347:GLU:C	2.63	0.41
1:A:302:GLN:O	1:A:303:SER:HB2	2.20	0.41
1:B:68:LYS:HB3	1:B:154:THR:O	2.21	0.41
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.74	0.41
1:A:252:LYS:O	1:A:256:VAL:HG23	2.19	0.41
1:B:132:ILE:HG23	1:B:133:LYS:H	1.85	0.41
1:B:143:MET:HE2	1:B:143:MET:HB3	1.95	0.41
1:B:69:THR:OG1	1:B:154:THR:HB	2.21	0.41
1:B:207:TYR:O	1:B:208:ARG:C	2.64	0.41
1:A:67:PRO:HA	1:A:156:PRO:HG2	2.02	0.41
1:A:288:MET:HG3	1:A:297:TYR:CE2	2.56	0.41
1:A:330:ILE:O	1:A:365:ILE:HA	2.21	0.41
1:A:75:ASN:ND2	6:A:729:HOH:O	2.53	0.41
1:B:264:SER:HB2	1:B:301:TRP:HB3	2.03	0.41
1:B:154:THR:OG1	1:B:157:HIS:CE1	2.74	0.41
1:A:397:LYS:HD2	1:B:296:PRO:HD3	2.03	0.40
1:B:265:LEU:HD11	1:B:276:TYR:HB3	2.04	0.40
1:A:422:GLN:O	1:A:423:LEU:HD22	2.21	0.40
2:A:501:CHD:C18	2:A:502:CHD:H162	2.51	0.40
2:A:502:CHD:H212	2:A:502:CHD:H12	2.03	0.40
1:B:111:ILE:O	1:B:111:ILE:HG22	2.21	0.40
1:A:297:TYR:CD1	1:A:297:TYR:C	2.99	0.40
1:B:266:PRO:O	1:B:267:MET:C	2.64	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%)	332 (93%)	21 (6%)	4 (1%)	11	25
1	B	358/359 (100%)	328 (92%)	29 (8%)	1 (0%)	36	58
All	All	715/718 (100%)	660 (92%)	50 (7%)	5 (1%)	18	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	VAL
1	A	303	SER
1	B	155	ALA
1	A	356	LEU
1	A	408	ASN

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	324/324 (100%)	303 (94%)	21 (6%)	15	35
1	B	325/324 (100%)	298 (92%)	27 (8%)	10	23
All	All	649/648 (100%)	601 (93%)	48 (7%)	13	29

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	121	GLU
1	A	124	ARG
1	A	132	ILE
1	A	138	LYS
1	A	145	LYS
1	A	153	ASN
1	A	178	GLU
1	A	213	VAL
1	A	216	LYS
1	A	286	LYS
1	A	331	LEU
1	A	339	SER
1	A	341	HIS
1	A	351	GLU
1	A	354	GLN
1	A	356	LEU
1	A	359	GLU
1	A	374	ASN
1	A	415	LYS
1	A	423	LEU
1	B	68	LYS
1	B	92	LEU
1	B	98	LEU
1	B	103	ILE
1	B	114	ARG
1	B	124	ARG
1	B	138	LYS
1	B	154	THR
1	B	170	THR
1	B	213	VAL
1	B	216	LYS
1	B	220	LYS
1	B	243	LYS
1	B	272	ARG
1	B	286[A]	LYS
1	B	286[B]	LYS
1	B	292	GLU
1	B	341	HIS
1	B	358	LYS
1	B	359	GLU
1	B	362	VAL
1	B	367	ARG

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Mol	Chain	Res	Type
1	B	374	ASN
1	B	383	ASP
1	B	392	ASN
1	B	415	LYS
1	B	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	153	ASN
1	A	212	GLN
1	A	329	ASN
1	A	364	ASN
1	A	374	ASN
1	A	386	HIS
1	A	390	GLN
1	A	421	GLN
1	B	105	ASN
1	B	231	HIS
1	B	314	GLN
1	B	329	ASN
1	B	364	ASN
1	B	374	ASN
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

7 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	501	-	32,32,32	0.75	0	51,51,51	2.46	19 (37%)
2	CHD	A	501	-	32,32,32	0.87	1 (3%)	51,51,51	2.47	20 (39%)
3	GOL	A	503	-	5,5,5	0.57	0	5,5,5	0.82	0
2	CHD	A	502	-	32,32,32	0.76	0	51,51,51	1.56	10 (19%)
4	FES	B	503	1	0,4,4	-	-	-		
4	FES	A	504	1	0,4,4	-	-	-		
5	PP9	B	502	-	36,46,46	3.04	8 (22%)	28,68,68	4.62	18 (64%)

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	501	-	-	0/9/74/74	0/4/4/4
2	CHD	A	501	-	-	1/9/74/74	0/4/4/4
3	GOL	A	503	-	-	2/4/4/4	-
2	CHD	A	502	-	-	1/9/74/74	0/4/4/4
4	FES	B	503	1	-	-	0/1/1/1
4	FES	A	504	1	-	-	0/1/1/1
5	PP9	B	502	-	-	8/12/62/62	0/4/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PP9	C1C-C2C	9.24	1.49	1.39
5	B	502	PP9	C1A-C2A	8.09	1.48	1.39
5	B	502	PP9	C3C-C4C	7.67	1.49	1.41
5	B	502	PP9	C4A-C3A	6.66	1.46	1.39
5	B	502	PP9	C3C-C2C	5.40	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PP9	C3B-C2B	3.69	1.44	1.37
5	B	502	PP9	C2A-C3A	2.42	1.44	1.37
5	B	502	PP9	C4A-NA	-2.19	1.34	1.38
2	A	501	CHD	C13-C14	-2.16	1.51	1.55

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	PP9	C3A-C4A-NA	10.73	117.19	109.43
5	B	502	PP9	C2C-C1C-NC	10.07	116.71	109.43
5	B	502	PP9	C3C-C4C-NC	9.11	113.40	107.46
5	B	502	PP9	C2A-C1A-NA	7.91	115.15	109.43
5	B	502	PP9	CBA-CAA-C2A	-7.49	99.95	112.54
5	B	502	PP9	CBB-CAB-C3B	-6.78	112.48	125.93
2	A	501	CHD	C9-C8-C7	-5.79	104.57	111.86
2	B	501	CHD	C17-C13-C14	-5.69	94.41	100.11
2	A	501	CHD	C9-C10-C5	5.53	116.20	108.51
2	A	501	CHD	C4-C5-C10	5.34	118.34	112.66
2	B	501	CHD	C4-C5-C10	5.15	118.14	112.66
2	B	501	CHD	C18-C13-C14	5.06	119.13	111.20
2	B	501	CHD	C13-C17-C20	4.98	125.52	119.48
2	B	501	CHD	C17-C13-C12	4.93	122.10	117.67
5	B	502	PP9	CMB-C2B-C1B	4.93	133.60	124.73
2	B	501	CHD	C13-C14-C8	4.71	120.68	114.72
2	B	501	CHD	C9-C10-C5	4.58	114.88	108.51
2	B	501	CHD	C9-C8-C7	-4.58	106.09	111.86
2	A	501	CHD	C13-C17-C20	-4.52	114.01	119.48
5	B	502	PP9	C4A-NA-C1A	-4.52	102.23	108.82
2	A	501	CHD	C17-C13-C12	-4.12	113.96	117.67
2	A	501	CHD	C4-C3-C2	-3.81	105.97	110.62
2	A	501	CHD	C16-C17-C20	3.69	117.77	112.18
2	A	501	CHD	C10-C9-C8	3.64	115.90	111.84
2	A	501	CHD	C1-C10-C9	-3.55	105.83	111.34
2	A	501	CHD	C15-C14-C8	3.47	123.11	118.36
2	A	502	CHD	C18-C13-C12	3.46	112.52	109.06
5	B	502	PP9	C1B-C2B-C3B	-3.40	100.60	108.42
2	A	501	CHD	O3-C3-C4	3.35	116.51	109.84
2	A	502	CHD	C13-C17-C20	3.31	123.50	119.48
2	A	501	CHD	C1-C10-C5	3.19	112.32	107.75
5	B	502	PP9	C4C-NC-C1C	-3.18	104.18	108.82
2	A	501	CHD	C23-C22-C20	-3.16	108.56	114.46
2	B	501	CHD	C15-C14-C13	3.08	106.52	103.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CHD	C22-C20-C17	3.04	116.64	110.33
2	A	502	CHD	C13-C14-C8	3.00	118.51	114.72
2	A	501	CHD	C21-C20-C22	-2.97	105.74	110.34
5	B	502	PP9	CAD-CBD-CGD	-2.96	105.80	113.67
5	B	502	PP9	CAB-C3B-C2B	-2.95	118.83	128.43
2	A	501	CHD	C11-C9-C10	-2.95	110.71	113.70
2	B	501	CHD	C19-C10-C9	-2.95	107.21	111.18
5	B	502	PP9	CMD-C2D-C1D	2.93	130.01	124.73
2	B	501	CHD	C11-C9-C10	2.91	116.65	113.70
2	B	501	CHD	C23-C22-C20	2.76	119.62	114.46
2	A	502	CHD	C9-C10-C5	2.75	112.33	108.51
5	B	502	PP9	CMC-C2C-C3C	2.74	130.16	124.68
2	B	501	CHD	C6-C7-C8	2.73	114.48	111.50
2	B	501	CHD	C18-C13-C12	-2.71	106.34	109.06
2	A	502	CHD	C9-C11-C12	-2.70	110.77	114.29
2	A	502	CHD	C5-C4-C3	2.69	116.77	112.71
2	A	501	CHD	C19-C10-C5	-2.63	106.04	110.44
2	A	501	CHD	C15-C14-C13	-2.62	101.00	103.54
5	B	502	PP9	CAA-CBA-CGA	-2.57	106.92	113.83
2	A	502	CHD	C14-C8-C7	2.51	115.19	111.85
5	B	502	PP9	CMA-C3A-C2A	2.48	129.62	124.94
2	A	502	CHD	C17-C13-C14	-2.39	97.71	100.11
2	A	501	CHD	C5-C6-C7	2.35	117.19	114.40
5	B	502	PP9	O1D-CGD-CBD	-2.32	115.73	123.09
2	B	501	CHD	C16-C15-C14	-2.31	100.62	105.14
2	A	501	CHD	C14-C13-C12	2.30	109.52	107.42
2	B	501	CHD	C10-C9-C8	-2.27	109.31	111.84
2	B	501	CHD	C6-C5-C4	-2.15	108.77	111.23
2	B	501	CHD	C18-C13-C17	-2.10	107.91	111.20
2	A	502	CHD	C19-C10-C1	-2.06	105.02	108.31
2	B	501	CHD	C22-C23-C24	2.03	117.92	112.49
5	B	502	PP9	C4B-C3B-CAB	2.03	134.38	128.00
2	A	502	CHD	C19-C10-C9	-2.01	108.47	111.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	C1-C2-C3-O3
5	B	502	PP9	C1A-C2A-CAA-CBA
5	B	502	PP9	C3A-C2A-CAA-CBA
5	B	502	PP9	C2D-C3D-CAD-CBD

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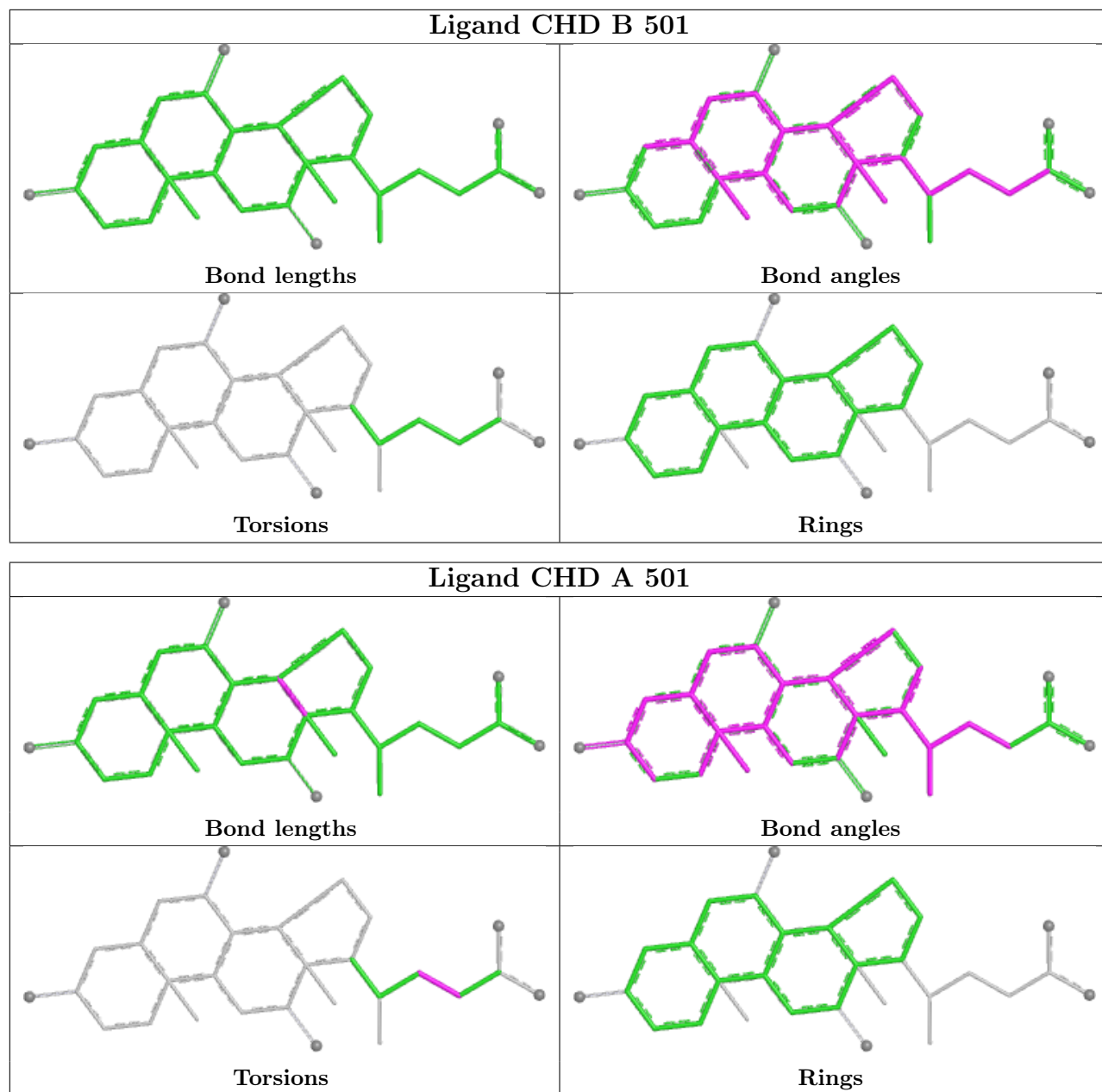
Mol	Chain	Res	Type	Atoms
5	B	502	PP9	C4D-C3D-CAD-CBD
3	A	503	GOL	O2-C2-C3-O3
5	B	502	PP9	CAA-CBA-CGA-O1A
5	B	502	PP9	CAA-CBA-CGA-O2A
2	A	501	CHD	C20-C22-C23-C24
5	B	502	PP9	CAD-CBD-CGD-O2D
2	A	502	CHD	C21-C20-C22-C23
5	B	502	PP9	CAD-CBD-CGD-O1D

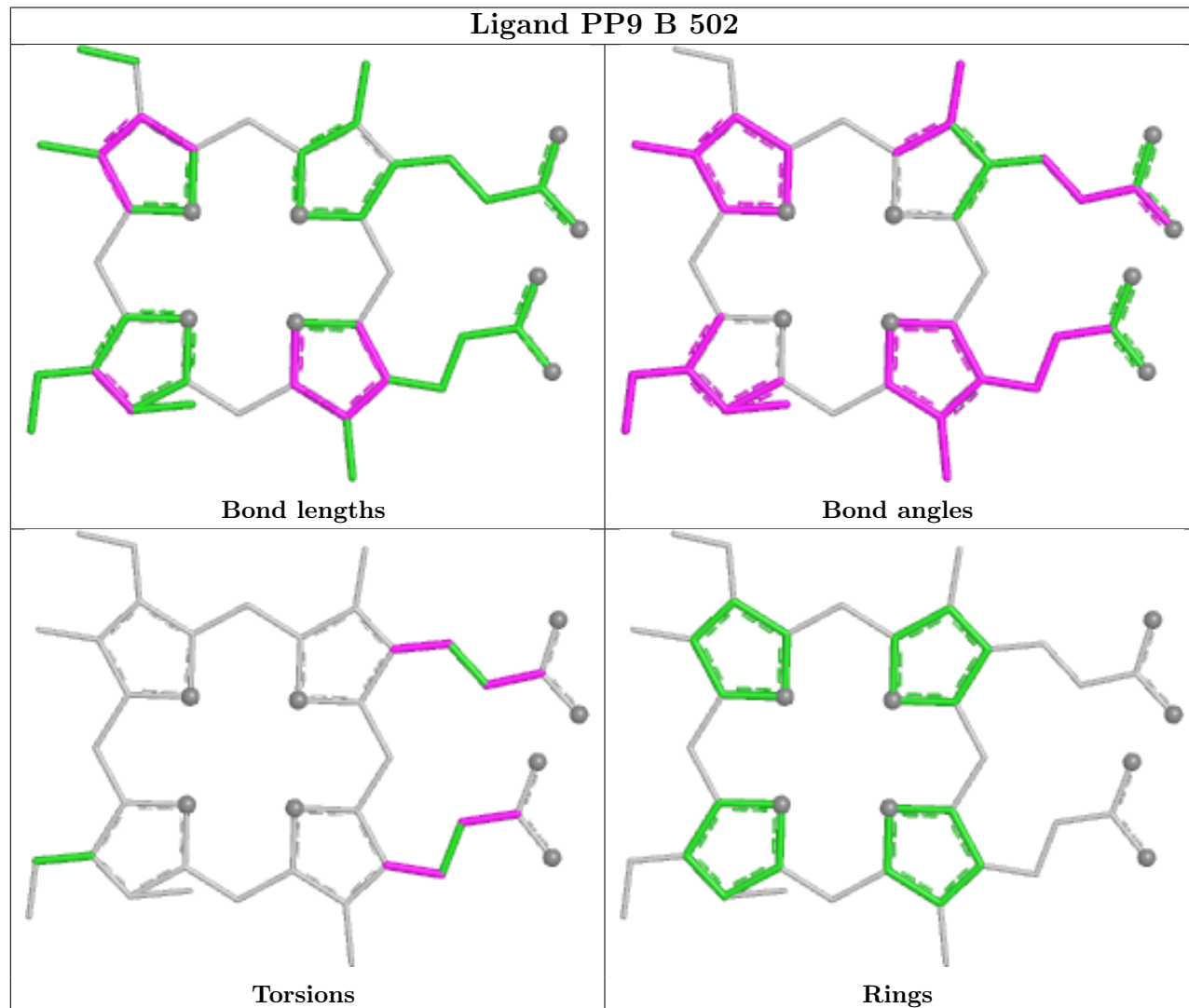
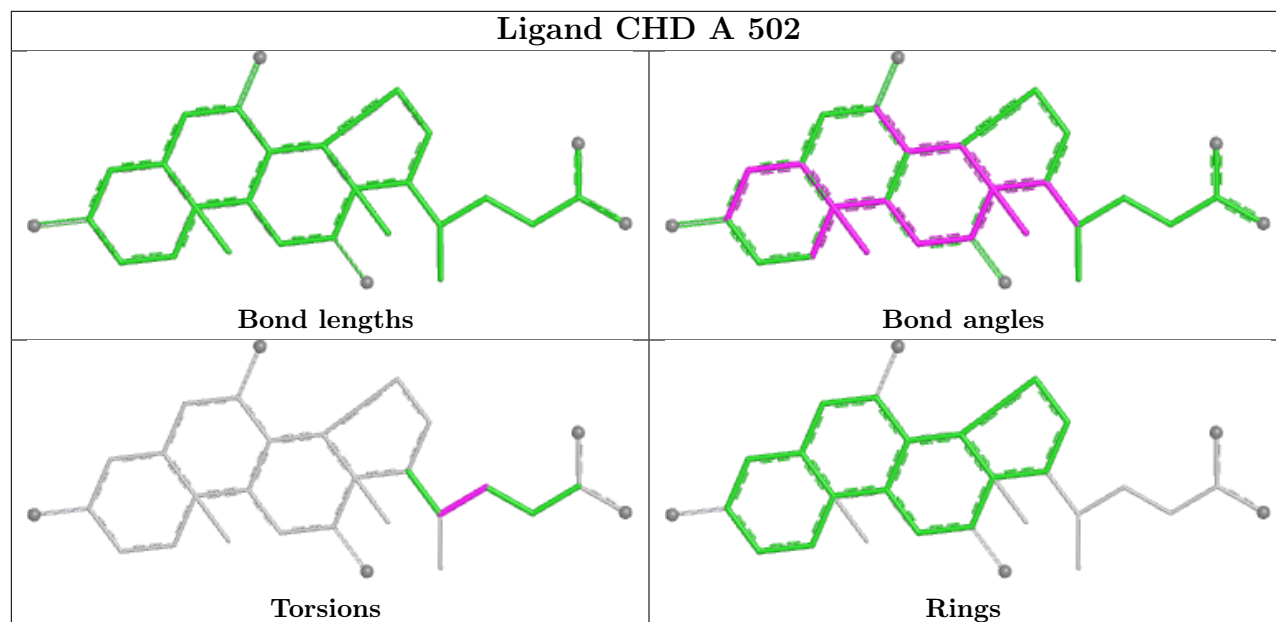
There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CHD	6	0
2	A	501	CHD	8	0
3	A	503	GOL	2	0
2	A	502	CHD	4	0
5	B	502	PP9	7	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	359/359 (100%)	-0.62	0 100 100	2, 13, 32, 39	0
1	B	359/359 (100%)	-0.59	2 (0%) 85 83	2, 12, 37, 44	1 (0%)
All	All	718/718 (100%)	-0.61	2 (0%) 90 88	2, 13, 34, 44	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	2.5
1	B	154	THR	2.4

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(Å ²)	Q<0.9
5	PP9	B	502	42/42	0.71	0.27	4,9,10,11	42
2	CHD	B	501	29/29	0.76	0.19	47,50,60,61	0
2	CHD	A	501	29/29	0.77	0.20	40,44,68,70	0

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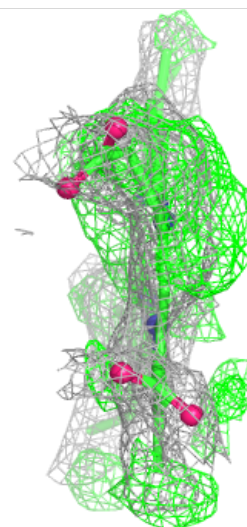
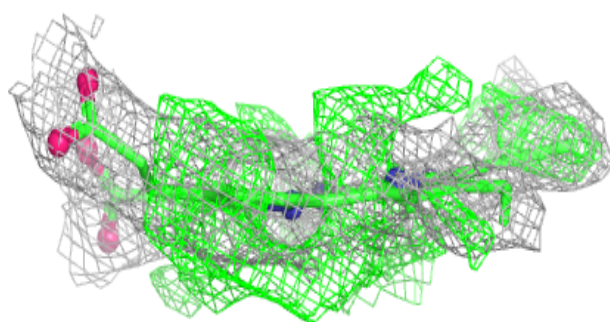
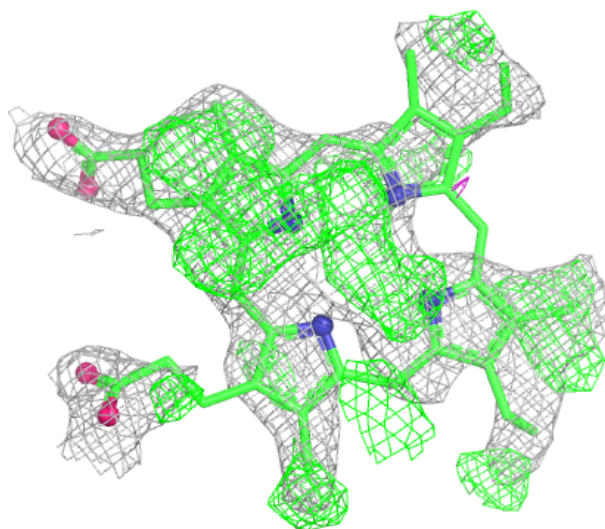
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CHD	A	502	29/29	0.91	0.09	21,24,27,27	0
3	GOL	A	503	6/6	0.93	0.23	2,2,2,2	6
4	FES	B	503	4/4	0.99	0.03	8,9,13,13	0
4	FES	A	504	4/4	0.99	0.02	7,8,10,12	0

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.

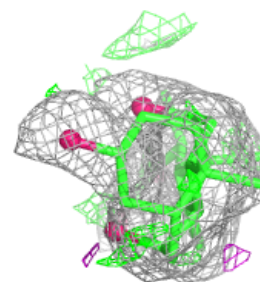
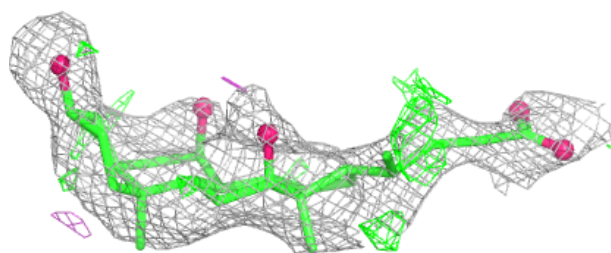
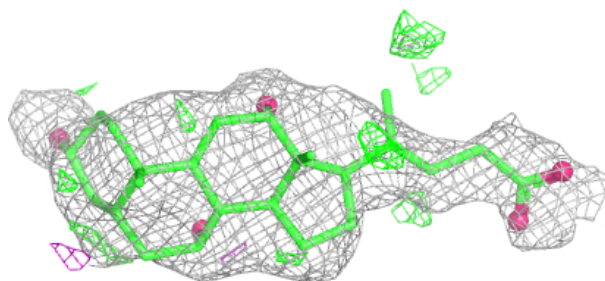
Electron density around PP9 B 502:

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

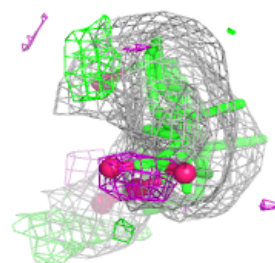
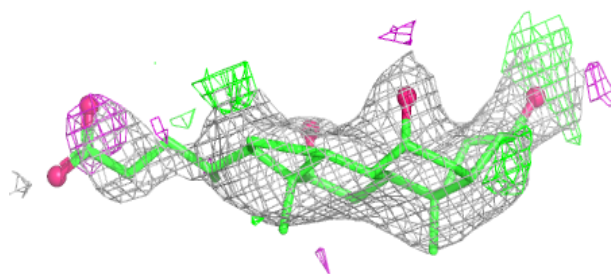
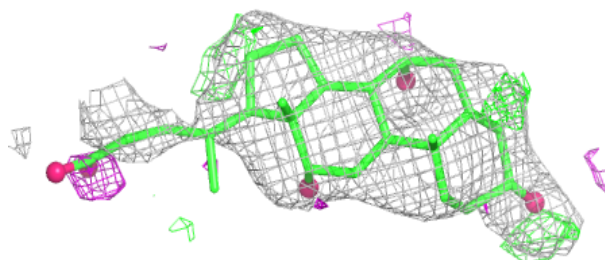


Electron density around CHD B 501:

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

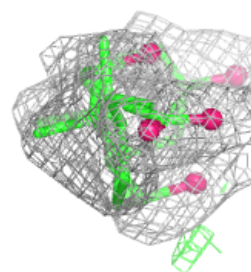
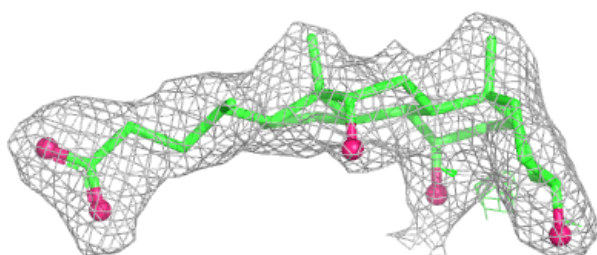
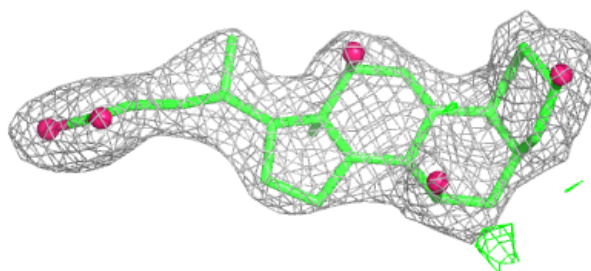
**Electron density around CHD A 501:**

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



Electron density around CHD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.