



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:31 AM UTC

PDB ID : 4F4D / pdb_00004f4d
Title : F337R variant of human ferrochelatase
Authors : Lanzilotta, W.N.; Medlock, A.E.; Dailey, T.E.; Dailey, H.A.
Deposited on : 2012-05-10
Resolution : 1.80 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

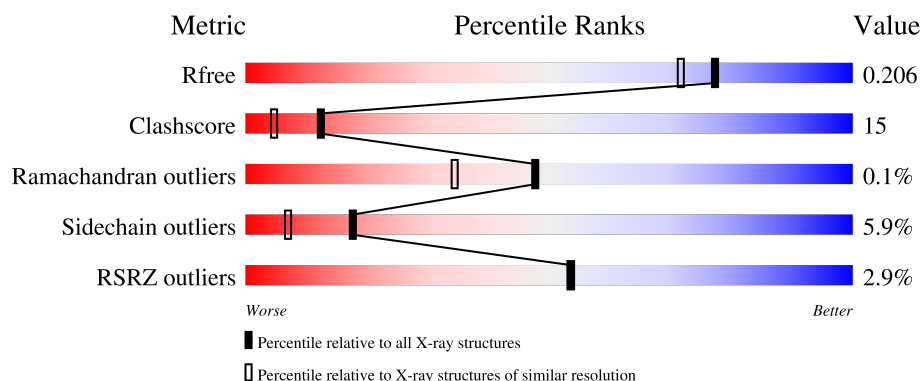
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	
1	B	359	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6787 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	17	0
			2982	1904	516	544	18			
1	B	359	Total	C	N	O	S	0	22	0
			3005	1921	519	543	22			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

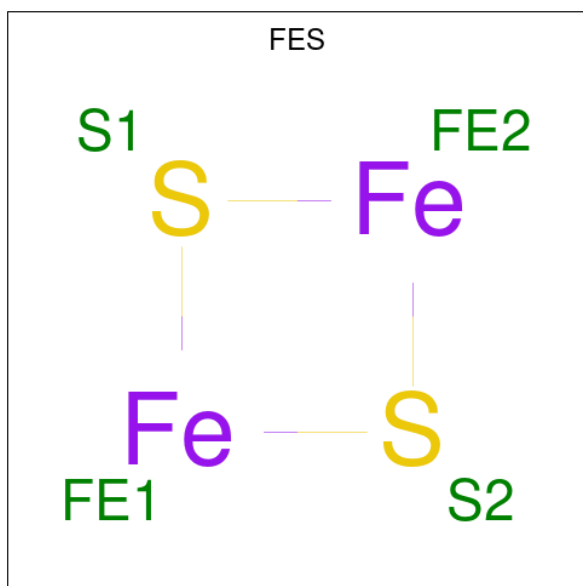
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



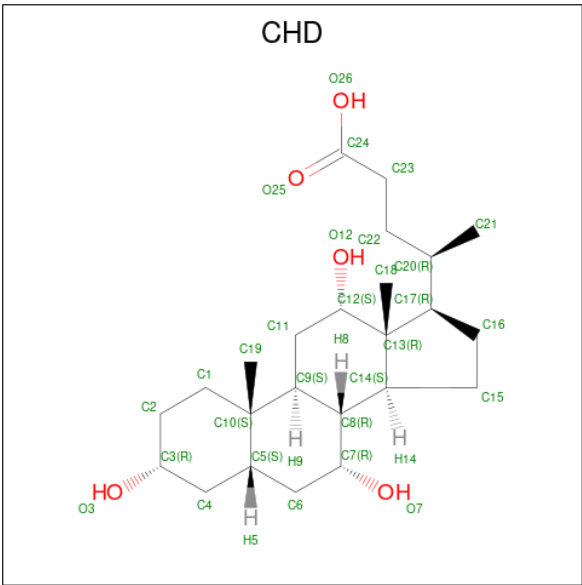
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		

- 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 CHOLIC ACID (CCD ID: CHD) (formula: $\text{C}_{24}\text{H}_{40}\text{O}_5$).



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

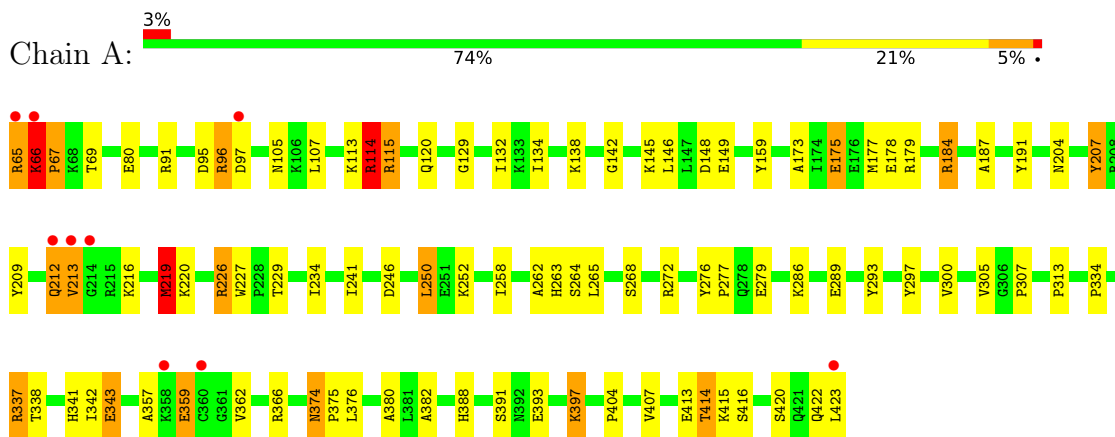
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	324	Total	O	0	0
			324	324		
6	B	280	Total	O	0	0
			280	280		

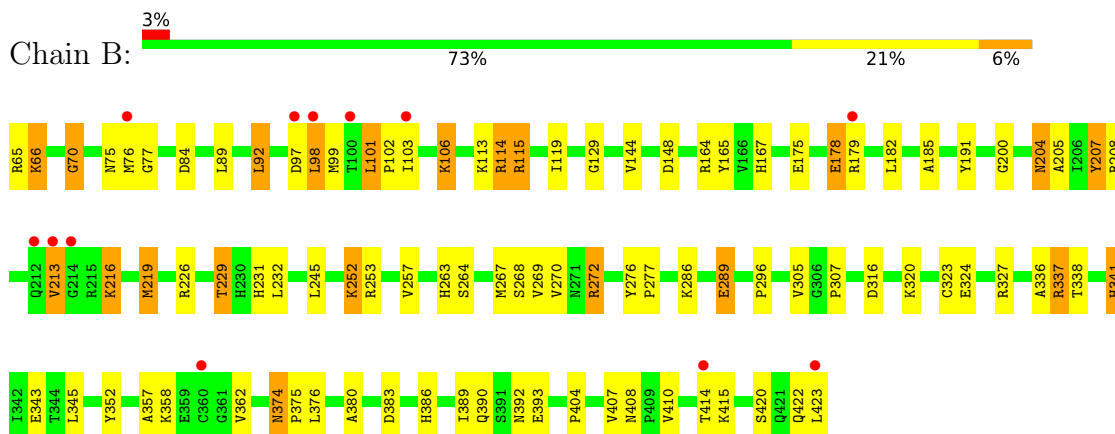
3 Residue-property plots [i](#)

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

- Molecule 1: Ferrochelatase, mitochondrial



- Molecule 1: Ferrochelatase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.21Å 93.51Å 111.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80 71.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 ((Not available)-1.80) 99.9 (71.76-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.177 , 0.207 0.175 , 0.206	Depositor DCC
R_{free} test set	4399 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	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	0.97	EDS
Total number of atoms	6787	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 59.86 % 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 1.6578e-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: CL, GOL, 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	1.67	27/3103 (0.9%)	1.37	10/4197 (0.2%)
1	B	1.64	21/3143 (0.7%)	1.35	12/4253 (0.3%)
All	All	1.66	48/6246 (0.8%)	1.36	22/8450 (0.3%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LYS	N-CA	12.94	1.64	1.46
1	B	129	GLY	N-CA	8.10	1.52	1.45
1	B	144	VAL	N-CA	7.55	1.55	1.46
1	A	307	PRO	CA-C	7.44	1.60	1.52
1	B	289[A]	GLU	C-O	7.44	1.32	1.24
1	B	289[B]	GLU	C-O	7.44	1.32	1.24
1	A	241	ILE	CA-CB	7.34	1.63	1.54
1	A	207	TYR	C-O	6.70	1.31	1.24
1	A	265	LEU	CA-C	6.68	1.59	1.52
1	B	245	LEU	N-CA	6.55	1.54	1.46
1	A	114	ARG	CG-CD	6.40	1.71	1.52
1	B	407	VAL	N-CA	6.18	1.52	1.46
1	B	380	ALA	CA-CB	6.17	1.62	1.53
1	A	120	GLN	N-CA	6.00	1.53	1.46
1	B	205	ALA	CA-CB	5.94	1.63	1.53
1	A	129	GLY	N-CA	5.94	1.52	1.45
1	B	70	GLY	N-CA	5.86	1.53	1.45
1	B	345	LEU	N-CA	5.86	1.53	1.46
1	A	380	ALA	CA-CB	5.72	1.62	1.53
1	B	204	ASN	C-O	5.69	1.31	1.24
1	A	397	LYS	CD-CE	-5.59	1.35	1.52
1	B	269	VAL	CA-C	5.58	1.59	1.52
1	A	66	LYS	C-N	5.57	1.40	1.33
1	A	382	ALA	CA-CB	5.57	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	420	SER	N-CA	5.55	1.53	1.46
1	A	246	ASP	N-CA	5.45	1.53	1.46
1	A	250	LEU	C-O	5.45	1.30	1.24
1	A	91	ARG	CZ-NH1	5.45	1.40	1.32
1	B	252	LYS	CG-CD	-5.42	1.36	1.52
1	A	262	ALA	CA-C	-5.37	1.46	1.52
1	B	389	ILE	CA-CB	-5.36	1.48	1.54
1	A	66	LYS	C-O	-5.34	1.17	1.24
1	A	366	ARG	CB-CG	5.31	1.68	1.52
1	A	134	ILE	CA-CB	5.29	1.60	1.54
1	A	416	SER	N-CA	5.29	1.52	1.46
1	B	207	TYR	C-O	5.28	1.30	1.24
1	A	159	TYR	CA-C	-5.26	1.45	1.52
1	B	167	HIS	CA-CB	5.26	1.61	1.52
1	A	148	ASP	N-CA	5.24	1.52	1.46
1	B	226	ARG	N-CA	5.24	1.52	1.46
1	B	148	ASP	N-CA	5.19	1.52	1.46
1	B	84	ASP	C-O	5.18	1.30	1.24
1	A	227	TRP	N-CA	5.17	1.53	1.46
1	A	175	GLU	N-CA	5.13	1.52	1.46
1	B	327	ARG	CA-CB	5.13	1.59	1.53
1	A	407	VAL	N-CA	5.04	1.51	1.46
1	A	420	SER	N-CA	5.01	1.52	1.46
1	A	67	PRO	N-CA	5.01	1.53	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	LYS	CA-C-N	-10.12	109.34	119.76
1	A	66	LYS	C-N-CA	-10.12	109.34	119.76
1	A	96	ARG	CA-C-N	-7.67	109.88	122.54
1	A	96	ARG	C-N-CA	-7.67	109.88	122.54
1	B	226	ARG	NE-CZ-NH1	7.31	128.81	121.50
1	B	178	GLU	CA-CB-CG	-6.51	101.08	114.10
1	A	97	ASP	CB-CA-C	6.46	120.87	110.09
1	B	92	LEU	CA-CB-CG	6.37	138.58	116.30
1	B	341	HIS	N-CA-C	-6.16	99.37	108.79
1	B	422	GLN	CA-C-N	5.85	132.24	121.70
1	B	422	GLN	C-N-CA	5.85	132.24	121.70
1	B	392	ASN	CB-CA-C	-5.79	102.27	111.48
1	B	200	GLY	N-CA-C	-5.75	105.83	112.73
1	A	219	MET	CG-SD-CE	-5.57	88.64	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ALA	N-CA-C	-5.41	98.47	107.99
1	A	226	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	B	213	VAL	N-CA-C	-5.15	106.01	113.07
1	B	66	LYS	CA-C-N	-5.12	114.67	119.85
1	B	66	LYS	C-N-CA	-5.12	114.67	119.85
1	B	164	ARG	CG-CD-NE	-5.08	100.83	112.00
1	A	191	TYR	CB-CA-C	-5.06	105.16	110.17
1	A	416	SER	CA-CB-OG	-5.04	101.02	111.10

There are no chirality outliers.

There are no planarity outliers.

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	2982	0	3044	87	1
1	B	3005	0	3083	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	15	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	87	0	117	12	0
5	B	87	0	117	12	0
6	A	324	0	0	17	1
6	B	280	0	0	21	4
All	All	6787	0	6376	193	5

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 15.

All (193) 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:65:ARG:CG	6:A:733:HOH:O	1.78	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334[B]:PRO:HG3	6:A:816:HOH:O	1.45	1.17
1:A:65:ARG:HG2	6:A:733:HOH:O	1.35	1.12
5:B:505:CHD:H22	6:B:852:HOH:O	1.49	1.12
1:B:323[B]:CYS:SG	1:B:362[B]:VAL:HG12	1.93	1.08
1:A:204:ASN:ND2	1:A:414[A]:THR:HG21	1.69	1.07
1:A:204:ASN:HD22	1:A:414[B]:THR:HG21	1.14	1.06
1:A:204:ASN:HD22	1:A:414[A]:THR:HG21	0.95	1.06
1:A:334[B]:PRO:HG2	6:A:663:HOH:O	1.54	1.05
1:B:204:ASN:HD22	1:B:414:THR:HG21	1.25	1.01
1:A:286[A]:LYS:NZ	6:A:726:HOH:O	1.95	1.00
1:B:208:ARG:NH2	1:B:410[A]:VAL:HG21	1.83	0.92
1:A:96:ARG:HH22	1:A:105:ASN:ND2	1.66	0.92
1:B:99:MET:HE3	1:B:101:LEU:HD21	1.52	0.91
1:B:272[A]:ARG:HD2	6:B:733:HOH:O	1.68	0.91
1:B:338:THR:HG21	6:B:802:HOH:O	1.70	0.90
1:B:76[A]:MET:HG2	1:B:191:TYR:OH	1.72	0.90
1:B:99:MET:CE	1:B:101:LEU:HD21	2.01	0.90
1:A:66:LYS:N	1:A:66:LYS:HD2	1.86	0.89
1:A:204:ASN:HD22	1:A:414[A]:THR:CG2	1.84	0.88
1:A:204:ASN:ND2	1:A:414[B]:THR:HG21	1.90	0.86
1:A:96:ARG:HH22	1:A:105:ASN:HD21	1.19	0.85
1:A:338:THR:HG21	6:A:699:HOH:O	1.77	0.84
1:A:234:ILE:HG13	1:A:286[B]:LYS:HE3	1.59	0.83
1:B:267:MET:HA	1:B:270[B]:VAL:HG12	1.60	0.83
1:B:204:ASN:ND2	1:B:414:THR:HG21	1.92	0.83
1:A:305[A]:VAL:HG21	5:A:504:CHD:H161	1.62	0.81
1:B:76[C]:MET:HG2	1:B:191:TYR:OH	1.82	0.79
3:A:502[B]:GOL:H11	1:B:277:PRO:HB2	1.66	0.78
1:B:182:LEU:HD12	1:B:219[A]:MET:HE1	1.66	0.78
1:B:286:LYS:NZ	6:B:831:HOH:O	2.18	0.75
1:B:357:ALA:HB1	1:B:362[B]:VAL:HG21	1.67	0.75
1:A:142:GLY:HA2	1:A:145[B]:LYS:HD3	1.68	0.75
1:A:204:ASN:ND2	1:A:414[A]:THR:CG2	2.47	0.75
1:B:208:ARG:HH21	1:B:410[A]:VAL:HG21	1.49	0.74
1:B:323[B]:CYS:SG	1:B:362[B]:VAL:CG1	2.75	0.72
1:A:145[B]:LYS:HE2	1:A:146:LEU:HG	1.71	0.71
1:A:220:LYS:HG3	6:A:793:HOH:O	1.89	0.71
1:B:383[B]:ASP:OD2	6:B:683:HOH:O	2.08	0.70
1:A:204:ASN:HA	1:A:414[B]:THR:HG21	1.73	0.70
1:A:65:ARG:HG3	6:A:733:HOH:O	1.63	0.70
5:A:504:CHD:O25	6:A:832:HOH:O	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HH11	1:A:343[B]:GLU:CD	2.02	0.68
1:A:209:TYR:O	1:A:212[A]:GLN:HG3	1.93	0.68
1:A:341:HIS:CE1	1:A:343[A]:GLU:HG2	2.29	0.68
5:B:505:CHD:O3	6:B:812:HOH:O	2.12	0.68
1:A:341:HIS:ND1	1:A:343[A]:GLU:HG2	2.09	0.68
1:B:114:ARG:CG	1:B:114:ARG:HH11	2.08	0.67
1:B:175:GLU:HG2	1:B:179[B]:ARG:NH1	2.09	0.67
1:B:204:ASN:HA	1:B:414:THR:HG21	1.76	0.67
1:A:96:ARG:NH2	1:A:105:ASN:ND2	2.41	0.66
1:A:66:LYS:HB2	1:A:67:PRO:HD2	1.78	0.66
1:B:114:ARG:HH11	1:B:114:ARG:HG3	1.60	0.66
5:B:505:CHD:C2	6:B:852:HOH:O	2.22	0.66
1:A:66:LYS:HD2	1:A:66:LYS:H	1.61	0.65
1:A:229:THR:HB	1:A:286[B]:LYS:HE2	1.77	0.65
1:A:357:ALA:HB1	1:A:362:VAL:HG11	1.77	0.65
1:B:75[A]:ASN:HD21	1:B:337[A]:ARG:HH22	1.43	0.65
1:B:103:ILE:HG23	1:B:106:LYS:HE2	1.78	0.64
1:B:115:ARG:NH1	5:B:505:CHD:O25	2.30	0.64
1:A:66:LYS:N	1:A:66:LYS:CD	2.61	0.64
1:A:277:PRO:HB2	3:A:502[A]:GOL:H31	1.79	0.64
1:B:76[B]:MET:HG3	1:B:165:TYR:HD1	1.63	0.64
1:B:374:ASN:HD22	1:B:376:LEU:H	1.47	0.63
1:B:76[C]:MET:HE3	6:B:761:HOH:O	1.99	0.62
1:B:374:ASN:ND2	1:B:376:LEU:H	1.97	0.62
1:B:76[C]:MET:HG2	6:B:761:HOH:O	1.98	0.62
1:B:341:HIS:ND1	1:B:343[B]:GLU:HG2	2.14	0.62
1:B:76[B]:MET:HG3	1:B:165:TYR:CD1	2.34	0.62
1:A:145[B]:LYS:HG2	1:A:146:LEU:N	2.15	0.62
1:A:337:ARG:NH1	1:A:343[B]:GLU:OE2	2.33	0.62
1:B:76[A]:MET:HG2	1:B:191:TYR:HH	1.66	0.61
1:B:185:ALA:HB2	1:B:219[A]:MET:HE2	1.83	0.60
5:A:505:CHD:H12	5:A:505:CHD:H212	1.84	0.60
1:B:272[B]:ARG:HG2	6:B:774:HOH:O	2.01	0.60
1:A:374:ASN:ND2	1:A:376:LEU:H	2.01	0.59
1:B:103:ILE:HG22	1:B:103:ILE:O	2.02	0.58
1:A:80:GLU:HG3	6:A:817:HOH:O	2.03	0.58
1:A:138[A]:LYS:NZ	6:A:864:HOH:O	2.35	0.58
1:A:115:ARG:HD2	5:A:505:CHD:H222	1.85	0.58
1:B:320:LYS:HE2	1:B:324:GLU:OE2	2.03	0.58
1:A:114:ARG:HH11	1:A:114:ARG:CB	2.16	0.58
1:A:207:TYR:HB3	1:A:414[B]:THR:HG22	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76[C]:MET:HG2	1:B:191:TYR:HH	1.69	0.57
1:A:334[B]:PRO:CG	6:A:816:HOH:O	2.24	0.57
1:A:178:GLU:HG2	1:A:219:MET:HE2	1.86	0.56
1:B:76[C]:MET:SD	6:B:761:HOH:O	2.58	0.56
1:B:98:LEU:HD11	5:B:505:CHD:H192	1.86	0.56
1:A:374:ASN:HD22	1:A:375:PRO:N	2.05	0.55
1:A:374:ASN:HD22	1:A:374:ASN:C	2.14	0.55
1:B:75[A]:ASN:ND2	1:B:337[A]:ARG:HH22	2.04	0.55
1:B:374:ASN:HD22	1:B:374:ASN:C	2.15	0.55
1:B:182:LEU:HB2	1:B:219[A]:MET:CE	2.36	0.55
1:B:267:MET:SD	1:B:270[B]:VAL:HG11	2.47	0.55
1:A:250:LEU:HD12	6:A:767:HOH:O	2.07	0.54
1:A:69:THR:HG23	1:A:184:ARG:HG2	1.90	0.54
1:A:391:SER:OG	1:A:393[B]:GLU:HG2	2.07	0.54
1:A:175:GLU:HG2	1:A:179[A]:ARG:NH1	2.22	0.54
1:B:99:MET:HE3	1:B:101:LEU:CD2	2.31	0.54
1:A:115:ARG:NH1	5:A:504:CHD:H221	2.23	0.54
1:A:115:ARG:NH1	5:A:504:CHD:C22	2.71	0.53
1:B:357:ALA:HB1	1:B:362[B]:VAL:CG2	2.37	0.53
1:B:89:LEU:HD11	1:B:119[A]:ILE:HD12	1.90	0.53
1:A:220:LYS:CG	6:A:793:HOH:O	2.53	0.53
1:B:305:VAL:HG21	5:B:505:CHD:H161	1.91	0.53
1:B:337[A]:ARG:NH2	6:B:770:HOH:O	2.42	0.52
1:B:257[A]:VAL:HG12	1:B:296:PRO:HG2	1.91	0.52
1:A:422:GLN:HG2	1:A:423:LEU:HG	1.91	0.52
1:A:268:SER:O	1:A:272[B]:ARG:HG3	2.08	0.52
1:A:145[B]:LYS:HG2	1:A:146:LEU:H	1.75	0.52
1:B:267:MET:CE	1:B:270[B]:VAL:HG11	2.40	0.51
1:A:204:ASN:HA	1:A:414[A]:THR:HG21	1.92	0.51
1:A:357:ALA:HB1	1:A:362:VAL:CG1	2.41	0.51
1:B:182:LEU:HB2	1:B:219[A]:MET:HE3	1.93	0.51
1:B:99:MET:HE2	1:B:101:LEU:HD21	1.86	0.51
1:A:374:ASN:HD22	1:A:376:LEU:H	1.58	0.50
1:B:268:SER:O	1:B:272[B]:ARG:HG3	2.11	0.50
1:B:207:TYR:HB3	1:B:414:THR:HG22	1.93	0.49
1:B:336:ALA:C	1:B:337[A]:ARG:HG2	2.37	0.49
1:B:393:GLU:CD	6:B:666:HOH:O	2.55	0.49
1:B:263:HIS:HD2	1:B:264:SER:O	1.95	0.49
1:B:341:HIS:CE1	1:B:343[B]:GLU:HG2	2.47	0.49
1:B:305:VAL:HG11	5:B:505:CHD:H232	1.94	0.49
1:B:89:LEU:HD21	1:B:119[A]:ILE:CD1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253[A]:ARG:NH1	6:B:678:HOH:O	2.46	0.49
1:B:263:HIS:HE1	6:B:795:HOH:O	1.95	0.49
1:A:114:ARG:CB	1:A:114:ARG:NH1	2.75	0.48
1:B:75[B]:ASN:ND2	1:B:77:GLY:H	2.11	0.48
1:B:97[B]:ASP:HB2	1:B:408:ASN:HD21	1.78	0.48
1:B:374:ASN:HD22	1:B:375:PRO:N	2.12	0.48
1:A:263:HIS:HD2	1:A:264:SER:O	1.96	0.48
1:B:216:LYS:N	1:B:216:LYS:HD2	2.28	0.48
1:B:76[C]:MET:HG3	1:B:77:GLY:H	1.79	0.48
1:A:66:LYS:HB2	1:A:67:PRO:CD	2.40	0.47
1:B:415:LYS:HD3	6:B:718:HOH:O	2.13	0.47
1:B:204:ASN:HA	1:B:414:THR:CG2	2.44	0.47
1:A:263:HIS:HE1	6:A:691:HOH:O	1.98	0.47
1:B:97[B]:ASP:HB2	1:B:408:ASN:ND2	2.30	0.47
1:A:173:ALA:O	1:A:177:MET:HG3	2.14	0.47
1:A:142:GLY:O	1:A:145[B]:LYS:HG2	2.14	0.46
1:A:95:ASP:OD1	1:A:95:ASP:C	2.58	0.46
1:B:76[C]:MET:CE	6:B:761:HOH:O	2.61	0.46
1:A:114:ARG:HH11	1:A:114:ARG:CG	2.29	0.46
5:B:505:CHD:H161	5:B:505:CHD:C23	2.45	0.46
1:B:76[C]:MET:HG3	1:B:77:GLY:N	2.30	0.46
1:B:103:ILE:O	1:B:103:ILE:CG2	2.63	0.46
1:A:138[B]:LYS:HG3	6:A:751:HOH:O	2.16	0.45
1:A:204:ASN:HA	1:A:414[B]:THR:CG2	2.42	0.45
1:A:212[A]:GLN:HG3	1:A:213:VAL:H	1.81	0.45
1:B:307:PRO:HD2	6:B:740:HOH:O	2.15	0.45
5:B:505:CHD:H17	5:B:505:CHD:H231	1.59	0.45
1:A:341:HIS:CE1	1:A:342:ILE:HG22	2.52	0.45
1:A:226:ARG:HD3	1:A:279:GLU:OE2	2.17	0.45
1:A:96:ARG:NH2	1:A:105:ASN:HD21	1.99	0.45
1:A:289[A]:GLU:HG2	1:A:293:TYR:OH	2.16	0.45
1:B:92:LEU:HD13	1:B:165:TYR:CD1	2.52	0.45
1:B:229[A]:THR:HG23	1:B:286:LYS:HG3	1.98	0.45
1:B:101:LEU:HA	1:B:102:PRO:HD2	1.82	0.44
5:A:505:CHD:H193	5:A:505:CHD:H111	1.80	0.44
1:B:410[A]:VAL:HG12	1:B:414:THR:HG23	1.99	0.44
1:B:219[A]:MET:HE3	1:B:219[A]:MET:HB3	1.55	0.44
1:A:142:GLY:O	1:A:145[B]:LYS:HE2	2.18	0.44
1:A:212[A]:GLN:HG3	1:A:213:VAL:N	2.33	0.44
1:A:115:ARG:HH11	5:A:504:CHD:H222	1.83	0.44
1:B:229[A]:THR:HG22	6:B:659:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289[A]:GLU:OE2	6:B:756:HOH:O	2.21	0.43
5:B:504:CHD:H212	5:B:504:CHD:H12	2.00	0.43
1:A:359:GLU:O	1:A:359:GLU:HG3	2.16	0.43
1:A:145[B]:LYS:CG	1:A:146:LEU:N	2.82	0.43
1:B:98:LEU:HD21	5:B:505:CHD:C19	2.48	0.43
1:B:231:HIS:CE1	1:B:232:LEU:HG	2.54	0.43
1:A:305[B]:VAL:HG21	5:A:504:CHD:H232	2.00	0.43
1:B:386:HIS:O	1:B:390:GLN:HG3	2.18	0.43
1:A:300:VAL:HG12	1:A:313:PRO:HG2	2.02	0.42
5:A:504:CHD:H231	5:A:504:CHD:H17	1.57	0.42
1:B:70:GLY:HA3	1:B:182:LEU:HD13	2.00	0.42
1:B:178:GLU:HG3	1:B:219[B]:MET:HE2	2.02	0.42
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.55	0.42
1:B:337[A]:ARG:HD2	6:B:742:HOH:O	2.19	0.42
1:B:98:LEU:HD21	5:B:505:CHD:H193	2.01	0.42
1:A:115:ARG:NH1	5:A:504:CHD:H222	2.35	0.42
1:A:207:TYR:CZ	1:A:413[A]:GLU:HB3	2.54	0.41
1:B:276:TYR:HB3	1:B:277:PRO:HD3	2.02	0.41
1:A:388:HIS:ND1	1:A:393[B]:GLU:HG3	2.35	0.41
5:A:505:CHD:H213	6:A:771:HOH:O	2.20	0.41
1:B:102:PRO:O	1:B:103:ILE:C	2.63	0.41
1:A:258:ILE:O	1:A:297:TYR:HA	2.20	0.41
1:A:276:TYR:HB3	1:A:277:PRO:HD3	2.03	0.40
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.87	0.40
1:A:132:ILE:HD11	1:A:341:HIS:CD2	2.56	0.40

All (5) 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)
6:A:695:HOH:O	6:A:707:HOH:O[3_555]	1.56	0.64
1:A:149[B]:GLU:OE1	6:B:787:HOH:O[4_455]	1.90	0.30
6:B:718:HOH:O	6:B:724:HOH:O[3_655]	2.04	0.16
6:B:851:HOH:O	6:B:866:HOH:O[3_645]	2.05	0.15
6:B:719:HOH:O	6:B:723:HOH:O[3_655]	2.10	0.10

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	374/359 (104%)	364 (97%)	9 (2%)	1 (0%)	36	25
1	B	380/359 (106%)	372 (98%)	8 (2%)	0	100	100
All	All	754/718 (105%)	736 (98%)	17 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS

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	341/324 (105%)	319 (94%)	22 (6%)	15	5
1	B	347/324 (107%)	324 (93%)	23 (7%)	15	5
All	All	688/648 (106%)	643 (94%)	45 (6%)	18	5

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	66	LYS
1	A	113	LYS
1	A	114	ARG
1	A	115	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	184	ARG
1	A	212[A]	GLN
1	A	212[B]	GLN
1	A	213	VAL
1	A	216	LYS
1	A	219	MET
1	A	252	LYS
1	A	337	ARG
1	A	343[A]	GLU
1	A	343[B]	GLU
1	A	359	GLU
1	A	374	ASN
1	A	397	LYS
1	A	404	PRO
1	A	414[A]	THR
1	A	414[B]	THR
1	A	415	LYS
1	B	65	ARG
1	B	66	LYS
1	B	98	LEU
1	B	101	LEU
1	B	106	LYS
1	B	113	LYS
1	B	114	ARG
1	B	115	ARG
1	B	213	VAL
1	B	216	LYS
1	B	219[A]	MET
1	B	219[B]	MET
1	B	229[A]	THR
1	B	229[B]	THR
1	B	252	LYS
1	B	272[A]	ARG
1	B	272[B]	ARG
1	B	337[A]	ARG
1	B	337[B]	ARG
1	B	358	LYS
1	B	374	ASN
1	B	404	PRO
1	B	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	153	ASN
1	A	204	ASN
1	A	231	HIS
1	A	235	GLN
1	A	295	ASN
1	A	329	ASN
1	A	354	GLN
1	A	374	ASN
1	B	120	GLN
1	B	153	ASN
1	B	204	ASN
1	B	231	HIS
1	B	235	GLN
1	B	314	GLN
1	B	329	ASN
1	B	354	GLN
1	B	374	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHD	B	504	-	32,32,32	0.77	0	51,51,51	1.90	13 (25%)
4	FES	B	502	1	0,4,4	-	-	-		
5	CHD	B	503	-	32,32,32	0.96	1 (3%)	51,51,51	2.03	11 (21%)
5	CHD	A	506	-	32,32,32	0.77	0	51,51,51	1.33	7 (13%)
3	GOL	A	502[A]	-	5,5,5	1.08	1 (20%)	5,5,5	2.57	1 (20%)
4	FES	A	503	1	0,4,4	-	-	-		
5	CHD	B	505	-	32,32,32	1.14	2 (6%)	51,51,51	2.78	26 (50%)
5	CHD	A	505	-	32,32,32	1.11	1 (3%)	51,51,51	2.79	25 (49%)
5	CHD	A	504	-	32,32,32	1.25	3 (9%)	51,51,51	2.22	26 (50%)
3	GOL	A	502[B]	-	5,5,5	0.60	0	5,5,5	1.73	2 (40%)

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
5	CHD	B	504	-	-	4/9/74/74	0/4/4/4
4	FES	B	502	1	-	-	0/1/1/1
5	CHD	B	503	-	-	3/9/74/74	0/4/4/4
5	CHD	A	506	-	-	4/9/74/74	0/4/4/4
3	GOL	A	502[A]	-	-	2/4/4/4	-
4	FES	A	503	1	-	-	0/1/1/1
5	CHD	B	505	-	-	4/9/74/74	0/4/4/4
5	CHD	A	505	-	-	3/9/74/74	0/4/4/4
5	CHD	A	504	-	-	9/9/74/74	0/4/4/4
3	GOL	A	502[B]	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	CHD	O12-C12	2.56	1.47	1.43
5	A	504	CHD	O12-C12	2.48	1.47	1.43
5	A	504	CHD	C1-C2	2.43	1.58	1.53
5	A	504	CHD	C23-C24	2.20	1.55	1.50
3	A	502[A]	GOL	O1-C1	2.16	1.51	1.42
5	B	505	CHD	C4-C5	2.10	1.57	1.53
5	A	505	CHD	C6-C7	2.07	1.56	1.52
5	B	503	CHD	O26-C24	-2.01	1.24	1.30

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	CHD	C9-C8-C7	-8.47	101.19	111.86
5	B	505	CHD	C5-C6-C7	-6.19	107.03	114.40
5	A	505	CHD	C11-C9-C10	-6.05	107.56	113.70
5	A	505	CHD	C19-C10-C9	-5.93	103.20	111.18
5	B	505	CHD	C9-C8-C7	-5.88	104.45	111.86
5	B	503	CHD	O3-C3-C4	-5.72	98.45	109.84
5	B	503	CHD	C6-C5-C4	-5.56	104.87	111.23
5	B	505	CHD	C15-C14-C13	5.23	108.61	103.54
3	A	502[A]	GOL	C3-C2-C1	5.21	130.89	111.80
5	B	503	CHD	C14-C13-C12	5.13	112.10	107.42
5	A	505	CHD	C14-C13-C12	4.93	111.92	107.42
5	B	505	CHD	C9-C11-C12	4.63	120.35	114.29
5	B	505	CHD	C1-C10-C5	4.58	114.31	107.75
5	B	504	CHD	C1-C10-C9	-4.57	104.24	111.34
5	A	504	CHD	C22-C23-C24	4.52	124.56	112.49
5	A	505	CHD	C17-C13-C12	-4.43	113.68	117.67
5	B	504	CHD	C22-C23-C24	-4.41	100.73	112.49
5	B	505	CHD	C23-C22-C20	-4.39	106.26	114.46
5	B	505	CHD	C9-C10-C5	4.31	114.50	108.51
5	A	505	CHD	C9-C10-C5	4.26	114.43	108.51
5	A	505	CHD	C14-C8-C7	4.23	117.46	111.85
5	B	503	CHD	C11-C9-C8	4.11	116.97	110.89
5	B	505	CHD	C11-C9-C10	4.07	117.83	113.70
5	B	504	CHD	C14-C13-C12	4.01	111.08	107.42
5	A	504	CHD	C14-C13-C12	3.97	111.05	107.42
5	B	505	CHD	O12-C12-C13	3.86	117.54	111.02
5	A	505	CHD	C5-C4-C3	3.84	118.51	112.71
5	B	505	CHD	C11-C9-C8	3.84	116.58	110.89
5	B	505	CHD	C14-C8-C9	-3.82	104.41	109.75
5	A	504	CHD	C5-C6-C7	3.77	118.89	114.40
5	B	505	CHD	C14-C13-C12	3.66	110.76	107.42
5	B	504	CHD	C21-C20-C17	3.64	118.35	112.88
5	A	506	CHD	C15-C14-C13	3.63	107.06	103.54
5	B	503	CHD	C15-C14-C13	3.57	107.00	103.54
5	A	505	CHD	C6-C7-C8	3.56	115.39	111.50
5	A	504	CHD	C6-C7-C8	-3.56	107.61	111.50
5	B	503	CHD	C1-C10-C5	3.53	112.81	107.75
5	B	505	CHD	C4-C5-C10	3.40	116.28	112.66
5	B	505	CHD	C6-C5-C10	3.40	116.28	112.66
5	B	503	CHD	C21-C20-C17	3.39	117.97	112.88
5	A	504	CHD	C6-C5-C4	3.30	114.99	111.23
5	B	504	CHD	C1-C10-C5	3.27	112.44	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	CHD	C15-C14-C8	-3.26	113.88	118.36
5	A	505	CHD	C5-C6-C7	3.22	118.23	114.40
5	A	505	CHD	C6-C5-C4	-3.20	107.57	111.23
5	B	505	CHD	C14-C8-C7	-3.18	107.64	111.85
5	B	504	CHD	C23-C22-C20	-3.17	108.54	114.46
5	B	505	CHD	C1-C10-C9	-3.16	106.43	111.34
5	A	504	CHD	C17-C13-C12	-3.15	114.83	117.67
5	A	505	CHD	C4-C5-C10	3.12	115.98	112.66
5	B	503	CHD	C17-C13-C14	-3.09	97.01	100.11
5	A	505	CHD	O12-C12-C13	3.01	116.11	111.02
5	A	504	CHD	C17-C13-C14	-3.01	97.10	100.11
5	A	504	CHD	C15-C14-C13	3.01	106.46	103.54
5	A	505	CHD	C23-C22-C20	3.00	120.06	114.46
5	B	505	CHD	C6-C7-C8	3.00	114.77	111.50
5	A	504	CHD	C11-C9-C10	-2.98	110.68	113.70
5	A	504	CHD	C13-C17-C20	2.95	123.06	119.48
5	A	505	CHD	C15-C14-C8	2.94	122.38	118.36
5	A	504	CHD	C21-C20-C22	-2.92	105.82	110.34
5	B	505	CHD	C18-C13-C17	-2.92	106.63	111.20
5	A	506	CHD	C16-C17-C13	2.89	106.34	103.54
5	A	505	CHD	C1-C10-C5	2.88	111.88	107.75
5	A	505	CHD	C13-C17-C20	-2.87	116.00	119.48
5	B	504	CHD	C11-C9-C8	2.87	115.14	110.89
5	A	504	CHD	C9-C8-C7	2.83	115.42	111.86
5	A	504	CHD	C9-C10-C5	-2.81	104.61	108.51
3	A	502[B]	GOL	O2-C2-C1	2.79	120.75	109.18
5	A	504	CHD	C15-C14-C8	-2.79	114.53	118.36
5	A	505	CHD	C11-C9-C8	2.78	115.00	110.89
5	B	505	CHD	C13-C14-C8	2.76	118.21	114.72
5	A	505	CHD	C15-C14-C13	-2.74	100.88	103.54
5	A	504	CHD	C11-C12-C13	-2.73	108.49	111.26
5	B	504	CHD	C16-C17-C20	2.70	116.27	112.18
5	A	504	CHD	C1-C10-C5	2.68	111.60	107.75
5	B	504	CHD	C11-C9-C10	-2.66	111.00	113.70
5	B	504	CHD	C13-C17-C20	-2.65	116.28	119.48
5	A	504	CHD	C16-C17-C13	-2.64	100.98	103.54
3	A	502[B]	GOL	O2-C2-C3	2.56	119.76	109.18
5	B	504	CHD	C6-C5-C4	-2.53	108.33	111.23
5	A	506	CHD	C10-C9-C8	2.53	114.66	111.84
5	A	504	CHD	C16-C15-C14	-2.47	100.30	105.14
5	A	504	CHD	C1-C10-C9	2.41	115.08	111.34
5	A	506	CHD	C6-C5-C4	-2.31	108.59	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	CHD	C18-C13-C12	2.29	111.35	109.06
5	B	505	CHD	O25-C24-C23	-2.29	115.83	123.09
5	A	504	CHD	O26-C24-C23	2.28	121.22	114.00
5	A	505	CHD	C22-C20-C17	2.26	115.02	110.33
5	A	505	CHD	C17-C13-C14	2.25	102.37	100.11
5	B	505	CHD	C17-C13-C12	2.21	119.65	117.67
5	B	505	CHD	C21-C20-C22	-2.21	106.92	110.34
5	A	504	CHD	C19-C10-C1	-2.21	104.80	108.31
5	A	506	CHD	C6-C7-C8	2.18	113.88	111.50
5	B	505	CHD	O3-C3-C4	2.18	114.18	109.84
5	B	503	CHD	C6-C5-C10	2.15	114.95	112.66
5	B	503	CHD	C9-C11-C12	2.15	117.10	114.29
5	A	504	CHD	O3-C3-C4	-2.15	105.57	109.84
5	A	506	CHD	C15-C14-C8	2.14	121.29	118.36
5	B	503	CHD	C2-C1-C10	2.12	116.32	112.74
5	A	505	CHD	C19-C10-C1	2.12	111.67	108.31
5	A	504	CHD	C19-C10-C5	-2.11	106.92	110.44
5	A	504	CHD	C23-C22-C20	-2.10	110.54	114.46
5	A	505	CHD	C9-C11-C12	2.09	117.03	114.29
5	B	504	CHD	C17-C13-C12	-2.08	115.79	117.67
5	A	506	CHD	C14-C13-C12	2.08	109.32	107.42
5	B	505	CHD	C19-C10-C9	-2.06	108.40	111.18
5	B	505	CHD	C18-C13-C12	2.06	111.12	109.06
5	A	505	CHD	C1-C10-C9	-2.05	108.16	111.34
5	A	504	CHD	C13-C14-C8	-2.04	112.13	114.72
5	B	504	CHD	C15-C16-C17	2.04	109.14	105.14
5	A	505	CHD	O3-C3-C4	-2.02	105.82	109.84

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	CHD	C17-C20-C22-C23
5	B	505	CHD	C17-C20-C22-C23
5	A	506	CHD	C17-C20-C22-C23
5	A	506	CHD	C21-C20-C22-C23
5	A	504	CHD	C16-C17-C20-C22
5	A	505	CHD	C17-C20-C22-C23
3	A	502[A]	GOL	O1-C1-C2-O2
5	B	504	CHD	C17-C20-C22-C23
5	B	504	CHD	C21-C20-C22-C23
5	B	505	CHD	C20-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	504	CHD	C13-C17-C20-C21
3	A	502[A]	GOL	C1-C2-C3-O3
3	A	502[B]	GOL	O2-C2-C3-O3
5	A	504	CHD	C16-C17-C20-C21
3	A	502[B]	GOL	O1-C1-C2-O2
5	A	504	CHD	C20-C22-C23-C24
5	A	504	CHD	C21-C20-C22-C23
5	A	504	CHD	C13-C17-C20-C22
5	A	504	CHD	C22-C23-C24-O25
5	B	504	CHD	C22-C23-C24-O26
5	B	504	CHD	C22-C23-C24-O25
5	A	506	CHD	C22-C23-C24-O25
5	A	504	CHD	C22-C23-C24-O26
5	A	505	CHD	C22-C23-C24-O25
5	A	506	CHD	C22-C23-C24-O26
5	A	505	CHD	C22-C23-C24-O26
5	B	505	CHD	C22-C23-C24-O26
5	B	503	CHD	C22-C23-C24-O25
5	B	505	CHD	C22-C23-C24-O25
5	B	503	CHD	C22-C23-C24-O26
5	B	503	CHD	C13-C17-C20-C21

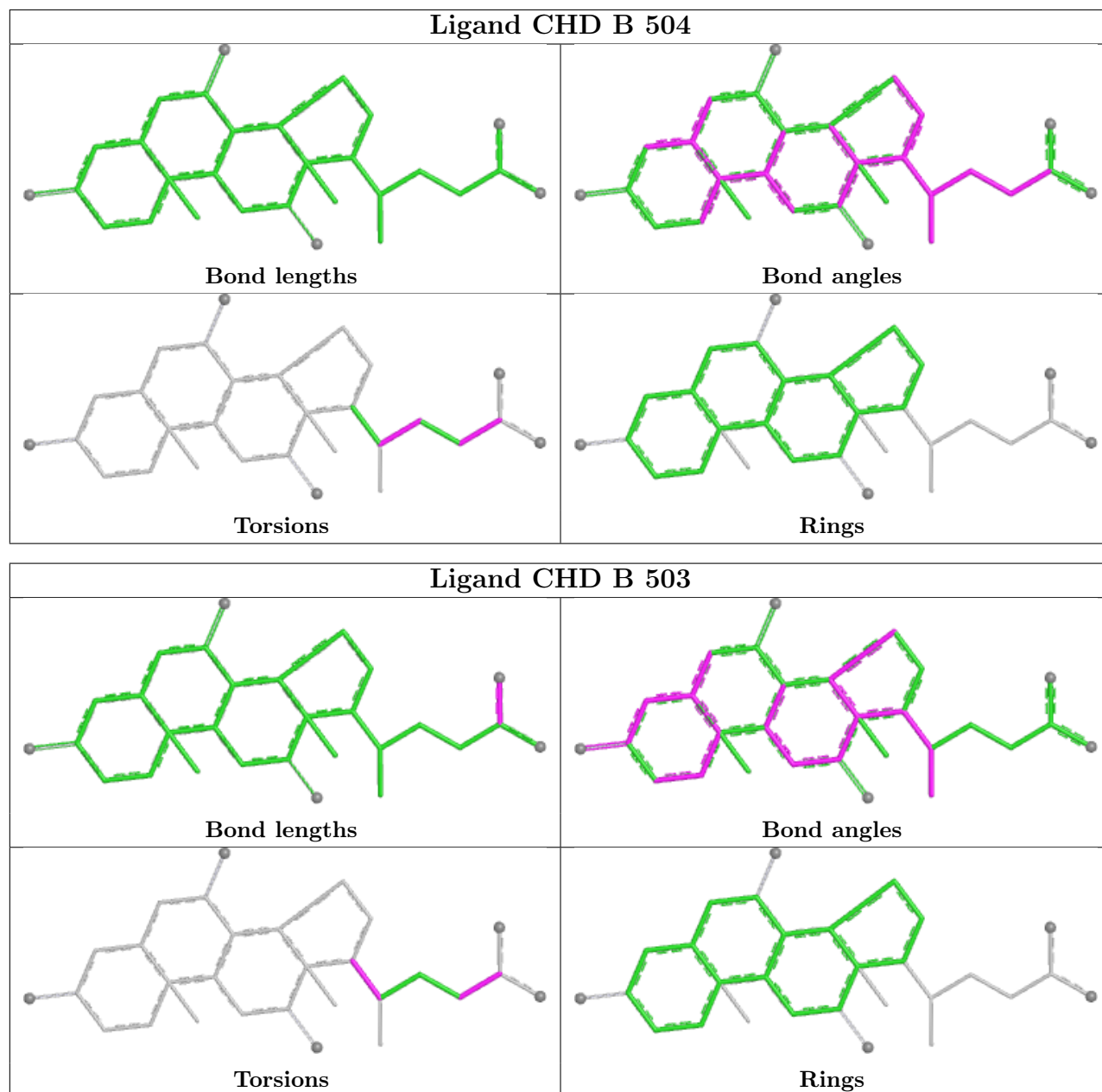
There are no ring outliers.

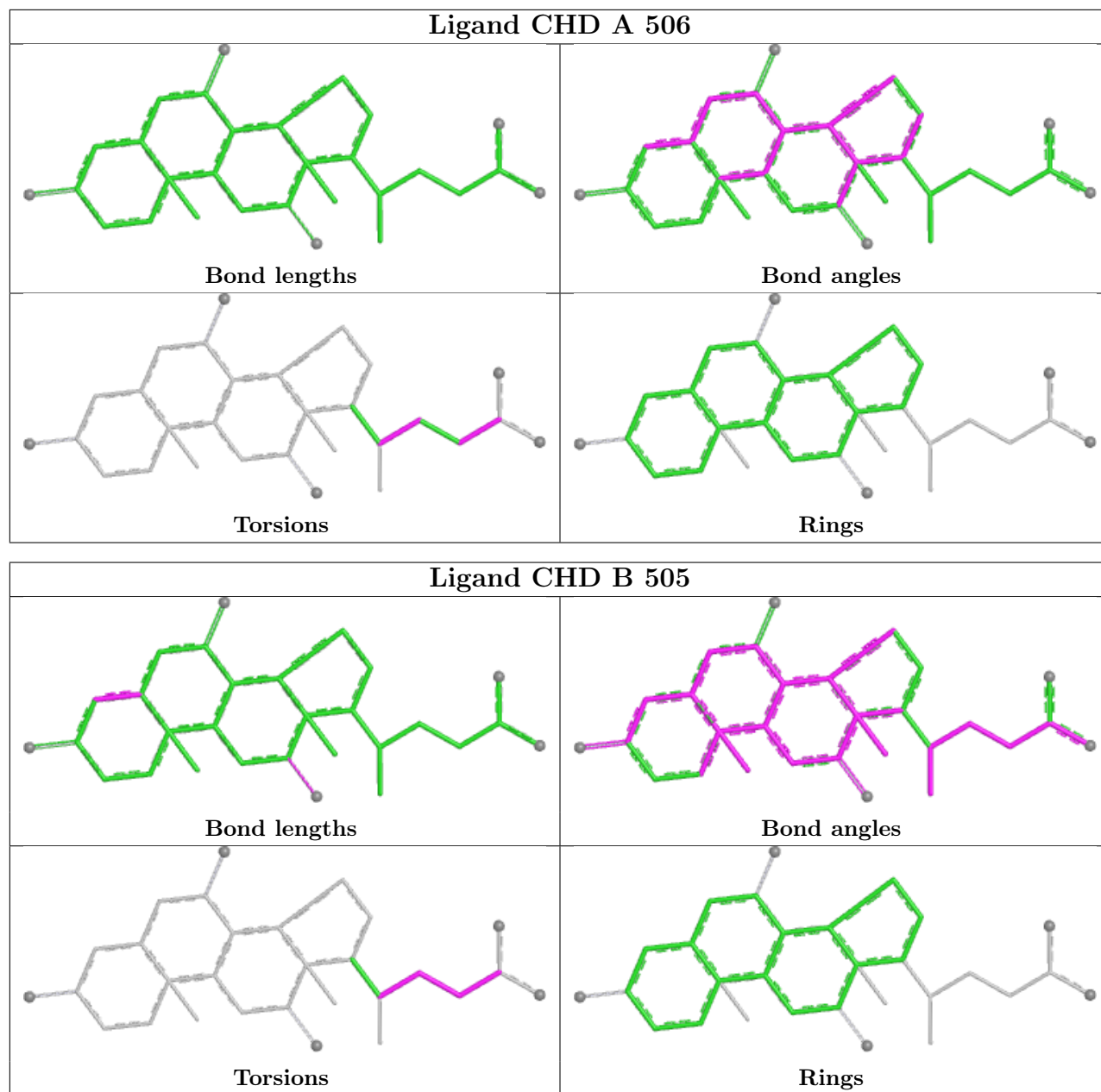
6 monomers are involved in 26 short contacts:

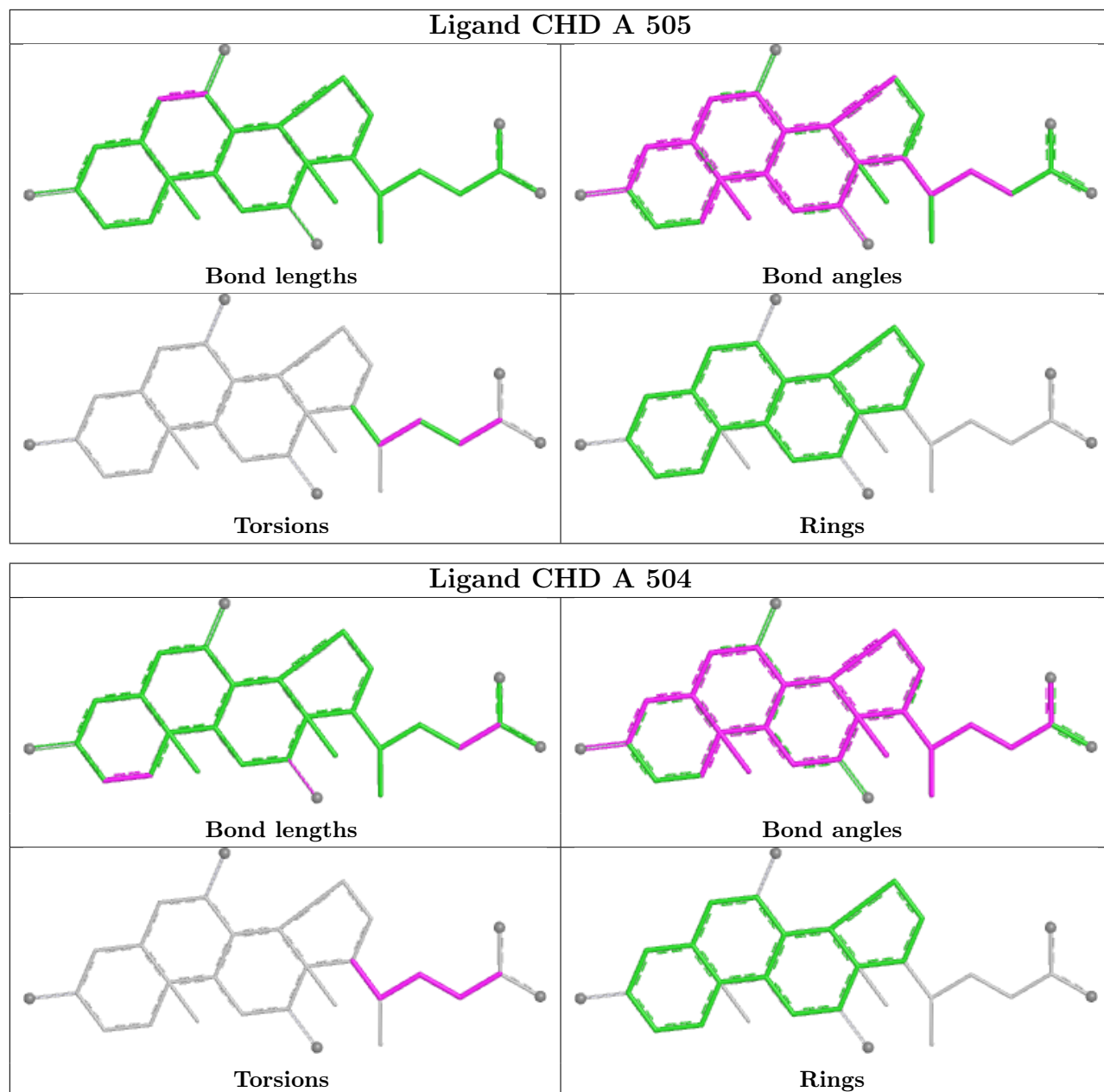
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	CHD	1	0
3	A	502[A]	GOL	1	0
5	B	505	CHD	11	0
5	A	505	CHD	4	0
5	A	504	CHD	8	0
3	A	502[B]	GOL	1	0

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	359/359 (100%)	-0.22	9 (2%) 58 58	9, 20, 39, 67	17 (4%)
1	B	359/359 (100%)	-0.24	12 (3%) 49 49	8, 20, 46, 59	22 (6%)
All	All	718/718 (100%)	-0.23	21 (2%) 53 53	8, 20, 41, 67	39 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ARG	6.8
1	A	423	LEU	3.8
1	B	213	VAL	3.5
1	B	423	LEU	3.4
1	A	213	VAL	3.4
1	B	98	LEU	3.2
1	A	66	LYS	3.0
1	B	214	GLY	2.8
1	B	103	ILE	2.8
1	A	360	CYS	2.7
1	B	414	THR	2.7
1	A	97	ASP	2.7
1	B	97[A]	ASP	2.6
1	A	212[A]	GLN	2.6
1	A	214	GLY	2.5
1	B	76[A]	MET	2.1
1	B	179[A]	ARG	2.1
1	B	360	CYS	2.1
1	B	100	THR	2.1
1	B	212	GLN	2.1
1	A	358	LYS	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](#)

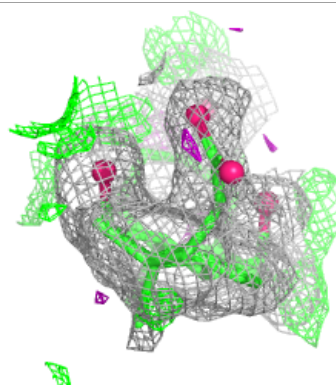
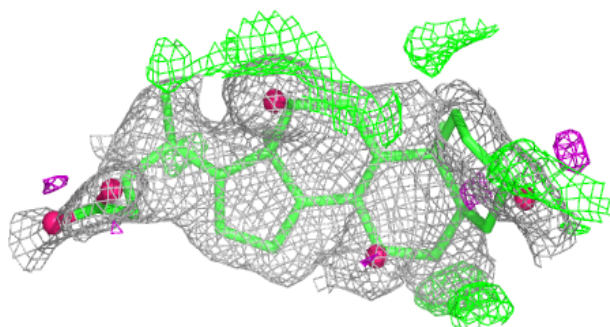
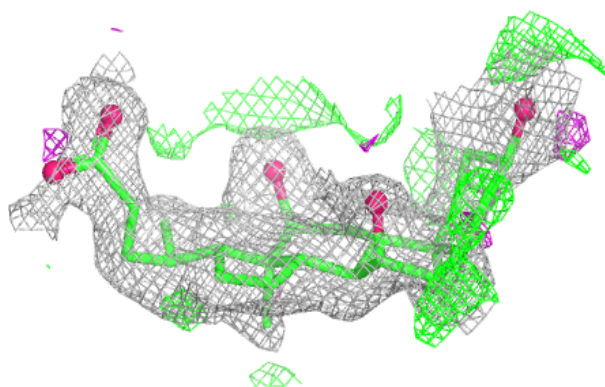
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	CHD	B	505	29/29	0.78	0.18	41,53,62,65	0
5	CHD	A	506	29/29	0.83	0.14	51,54,75,76	0
5	CHD	A	505	29/29	0.83	0.16	27,41,63,66	0
5	CHD	B	504	29/29	0.86	0.12	42,49,74,76	0
5	CHD	A	504	29/29	0.86	0.13	25,28,58,59	0
5	CHD	B	503	29/29	0.87	0.13	37,44,59,65	0
3	GOL	A	502[A]	6/6	0.93	0.09	11,13,19,23	6
3	GOL	A	502[B]	6/6	0.93	0.09	13,19,21,21	6
2	CL	B	501	1/1	0.98	0.04	24,24,24,24	0
2	CL	A	501	1/1	0.99	0.03	22,22,22,22	0
4	FES	A	503	4/4	0.99	0.03	16,16,17,18	0
4	FES	B	502	4/4	0.99	0.03	17,17,19,19	0

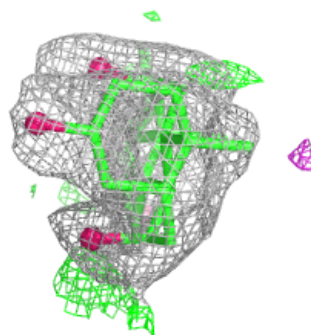
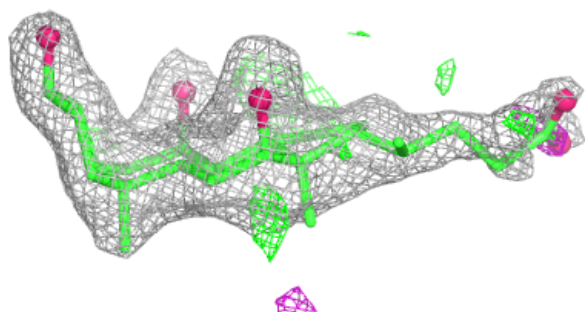
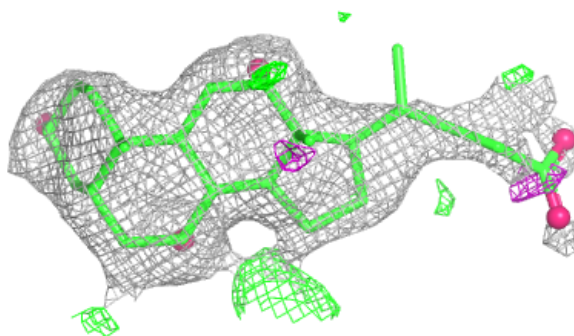
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD B 505:

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

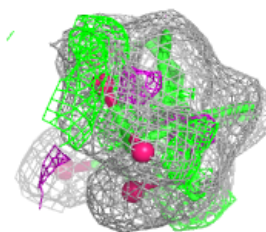
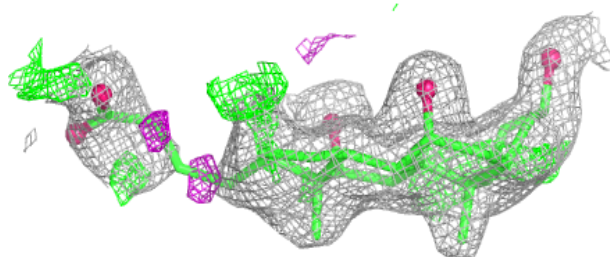
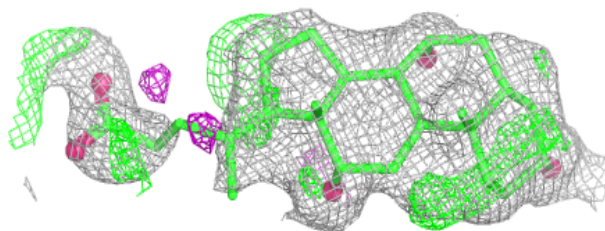
**Electron density around CHD A 506:**

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

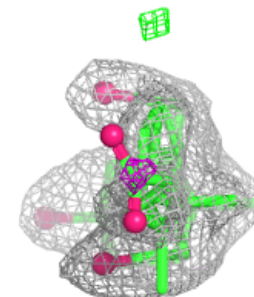
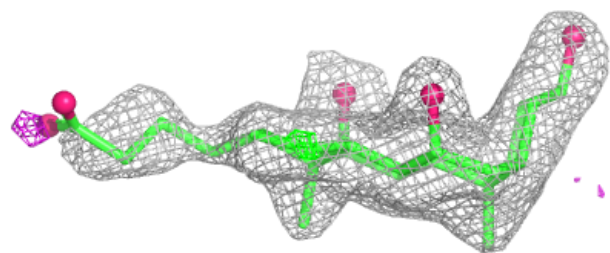


Electron density around CHD A 505:

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

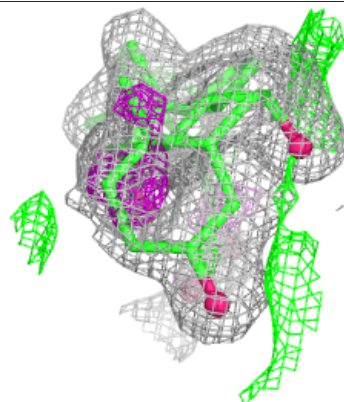
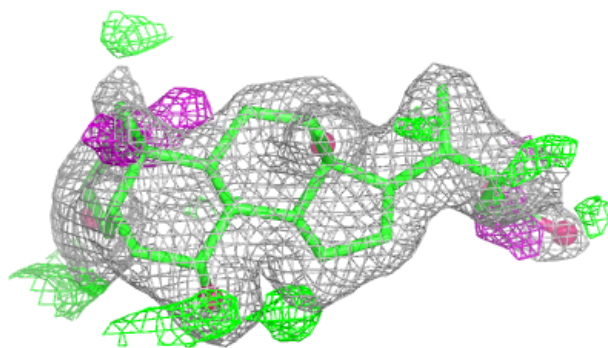
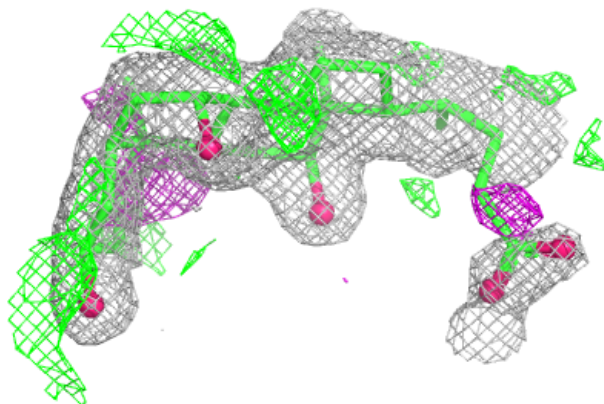
**Electron density around CHD B 504:**

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

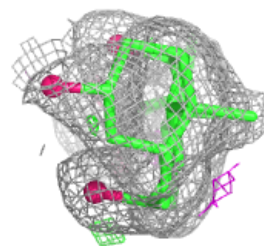
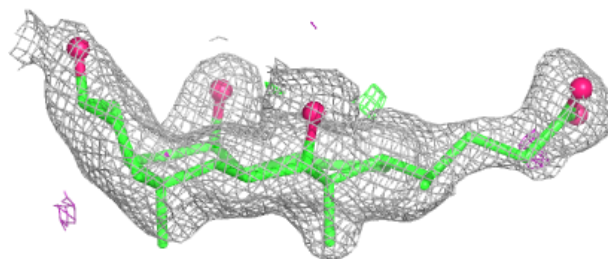
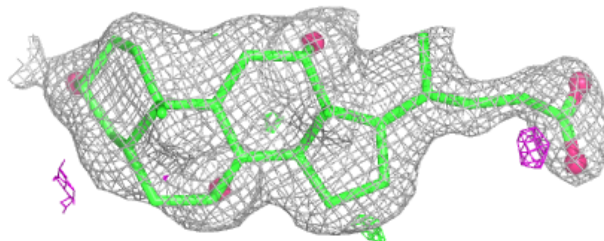


Electron density around CHD A 504:

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

**Electron density around CHD B 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.