



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:50 AM UTC

PDB ID : 2HRC / pdb_00002hrc
Title : 1.7 angstrom structure of human ferrochelatase variant R115L
Authors : Medlock, A.; Swartz, L.; Dailey, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2006-07-20
Resolution : 1.70 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

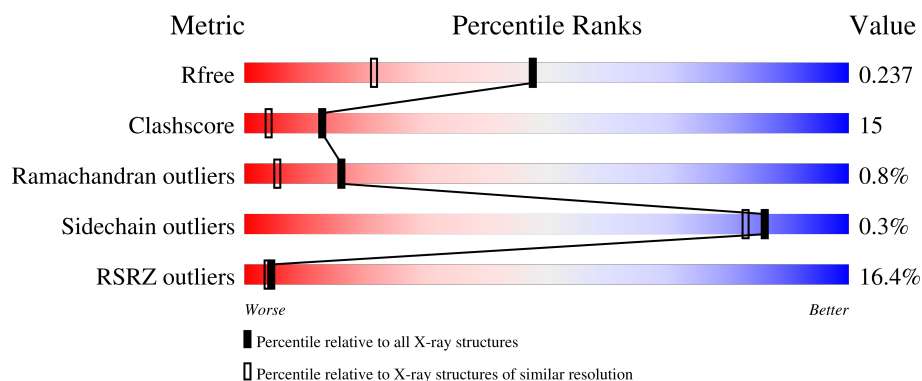
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	17% 70% 30%
1	B	359	16% 72% 27%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6923 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	21	0
			3057	1935	533	569	20			
1	B	359	Total	C	N	O	S	0	20	0
			3062	1939	537	567	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	engineered mutation	UNP P22830
B	615	LEU	ARG	engineered mutation	UNP P22830

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

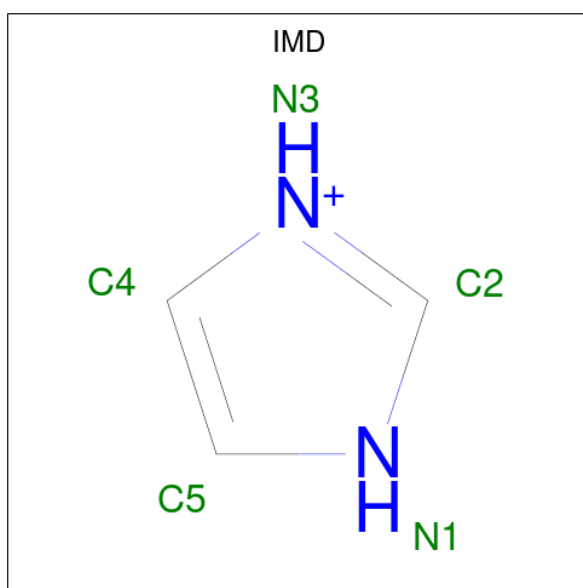
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



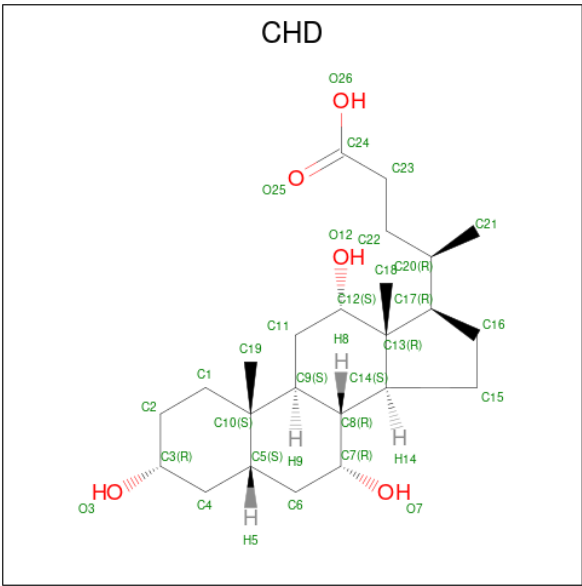
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

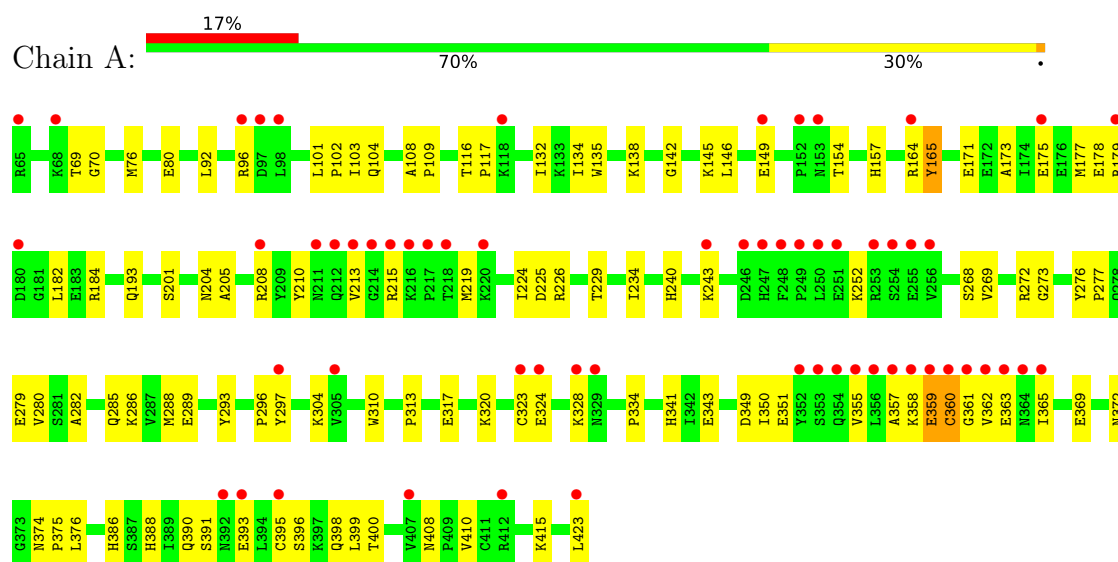
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	306	Total	O	0	0
			306	306		
7	B	298	Total	O	0	0
			298	298		

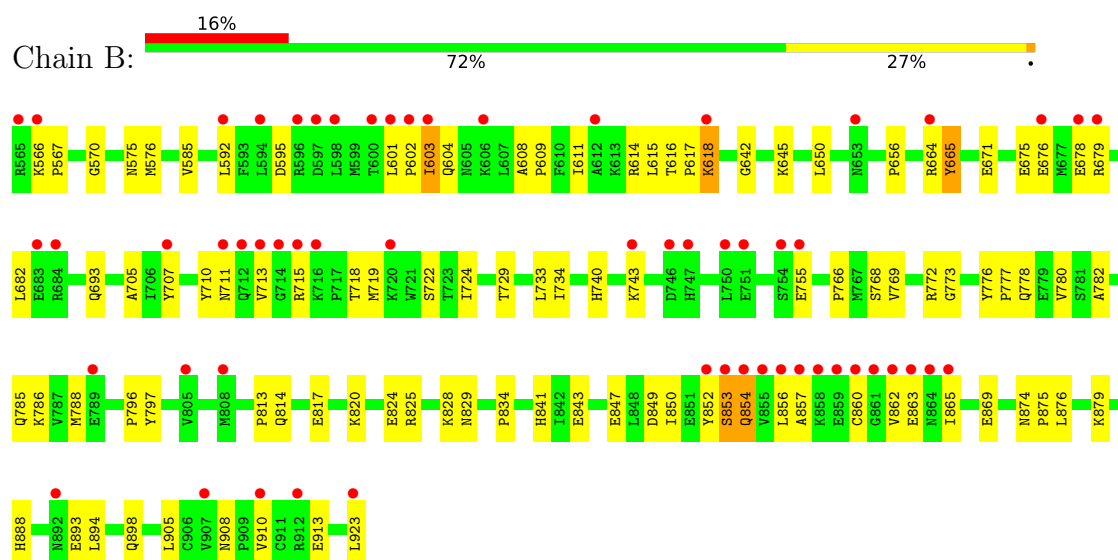
3 Residue-property plots

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	88.53Å 92.98Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.84 – 1.70 41.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.84-1.70) 99.6 (41.84-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.242 0.218 , 0.237	Depositor DCC
R_{free} test set	7294 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 54.37 % 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 3.6882e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/3127	0.82	6/4230 (0.1%)
1	B	0.33	0/3132	0.81	6/4234 (0.1%)
All	All	0.33	0/6259	0.82	12/8464 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	ILE	N-CA-C	-6.55	95.72	109.34
1	A	224	ILE	N-CA-C	-6.36	96.11	109.34
1	B	665	TYR	N-CA-C	5.95	120.59	112.91
1	A	349	ASP	N-CA-C	5.89	117.78	111.36
1	A	165	TYR	N-CA-C	5.67	120.22	112.91
1	B	849	ASP	N-CA-C	5.50	117.35	111.36
1	B	834	PRO	N-CA-C	-5.49	102.06	110.95
1	A	350	ILE	N-CA-C	5.32	116.48	111.48
1	A	334	PRO	N-CA-C	-5.29	102.38	110.95
1	B	585	VAL	N-CA-C	5.27	115.48	110.42
1	B	733	LEU	N-CA-C	-5.16	105.56	111.14
1	A	132	ILE	N-CA-C	5.11	115.73	110.36

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	3057	0	3025	91	0
1	B	3062	0	3047	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	5	0	5	0	0
4	B	5	0	5	1	0
5	A	87	0	117	1	0
5	B	87	0	117	3	0
6	A	6	0	8	3	0
7	A	306	0	0	5	0
7	B	298	0	0	11	0
All	All	6923	0	6324	192	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 15.

All (192) 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:B:664[A]:ARG:NH1	1:B:705:ALA:HB2	1.68	1.07
1:B:664[A]:ARG:HH11	1:B:705:ALA:HB2	1.26	1.00
1:A:164[A]:ARG:NH1	1:A:205:ALA:HB2	1.76	0.99
1:A:164[A]:ARG:HH11	1:A:205:ALA:HB2	1.29	0.96
1:A:398:GLN:HE22	1:B:797:TYR:H	1.17	0.93
1:A:297:TYR:H	1:B:898:GLN:HE22	1.15	0.89
1:A:323[B]:CYS:SG	1:A:362:VAL:HG12	2.18	0.84
1:B:814:GLN:HB2	1:B:817[B]:GLU:HG2	1.61	0.82
1:A:285[B]:GLN:HE21	1:B:778:GLN:HE22	1.27	0.80
1:B:650:LEU:HD11	1:B:879[B]:LYS:NZ	1.98	0.79
1:B:853:SER:O	1:B:854:GLN:HG3	1.83	0.77
1:A:324:GLU:HG2	1:A:360:CYS:SG	2.26	0.76
1:A:229:THR:HB	1:A:286:LYS:HE2	1.70	0.73
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.73	0.71
1:B:650:LEU:HD11	1:B:879[B]:LYS:HZ1	1.57	0.70
1:A:277:PRO:HB3	6:A:707:GOL:H2	1.75	0.69
1:B:602:PRO:C	1:B:603:ILE:HD13	2.18	0.68
1:B:664[A]:ARG:HG3	1:B:665:TYR:CE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:VAL:HG21	1:B:865:ILE:HG13	1.76	0.68
1:B:862:VAL:HG21	1:B:865:ILE:CG1	2.24	0.68
1:A:269:VAL:O	1:A:272[A]:ARG:HG2	1.96	0.65
1:B:608:ALA:HB3	1:B:609:PRO:HD3	1.77	0.65
1:A:175[A]:GLU:O	1:A:179[A]:ARG:HG3	1.96	0.65
1:A:285[B]:GLN:NE2	1:B:778:GLN:HE22	1.94	0.65
1:B:769:VAL:O	1:B:772[A]:ARG:HG2	1.97	0.64
1:A:297:TYR:N	1:B:898:GLN:HE22	1.94	0.64
1:A:285[A]:GLN:HG3	1:B:782:ALA:HB1	1.79	0.64
1:A:391:SER:OG	1:A:393[B]:GLU:HG2	1.97	0.63
1:A:142:GLY:O	1:A:145[B]:LYS:HG3	1.98	0.62
1:A:268:SER:O	1:A:272[B]:ARG:HG3	2.00	0.62
1:A:234:ILE:HG13	1:A:286:LYS:HE3	1.81	0.62
1:A:395[B]:CYS:SG	1:A:399:LEU:HD22	2.40	0.62
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.82	0.61
1:A:240:HIS:HD2	1:A:369:GLU:O	1.82	0.61
1:B:734:ILE:HG13	1:B:786[B]:LYS:HE3	1.82	0.61
1:B:820:LYS:O	1:B:824:GLU:HG3	2.00	0.61
1:A:374:ASN:C	1:A:374:ASN:HD22	2.09	0.60
1:B:722:SER:OG	1:B:888:HIS:HE1	1.85	0.60
1:B:853:SER:HB3	7:B:1858:HOH:O	2.02	0.59
1:A:351:GLU:O	1:A:355:VAL:HG23	2.02	0.59
1:B:874:ASN:HD22	1:B:875:PRO:N	2.00	0.59
1:B:611:ILE:HA	1:B:614:ARG:HG2	1.83	0.59
1:A:320:LYS:O	1:A:324:GLU:HG3	2.01	0.59
1:A:395[B]:CYS:SG	1:A:396:SER:N	2.75	0.59
1:A:395[B]:CYS:SG	1:A:399:LEU:CD2	2.91	0.58
1:B:740:HIS:HD2	1:B:869:GLU:O	1.86	0.58
1:B:768:SER:O	1:B:772[B]:ARG:HG3	2.04	0.58
1:A:398:GLN:HE22	1:B:797:TYR:N	1.95	0.58
1:A:164[A]:ARG:HG3	1:A:165:TYR:CE2	2.39	0.58
1:A:313:PRO:HG2	1:B:773:GLY:HA2	1.85	0.58
1:B:707:TYR:CE1	1:B:711[A]:ASN:ND2	2.72	0.58
1:A:178:GLU:HG2	1:A:219:MET:HE2	1.85	0.57
1:A:285[A]:GLN:OE1	1:B:786[A]:LYS:NZ	2.37	0.57
1:A:374:ASN:HD22	1:A:375:PRO:N	2.02	0.57
1:B:874:ASN:HD22	1:B:874:ASN:C	2.10	0.57
1:A:76:MET:HB2	1:A:164[B]:ARG:NH2	2.19	0.57
1:A:374:ASN:ND2	1:A:376:LEU:H	2.03	0.57
1:B:664[A]:ARG:HH12	1:B:705:ALA:HB2	1.66	0.56
1:A:273:GLY:HA2	1:B:813:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:LYS:NZ	1:B:618:LYS:HB2	2.21	0.56
1:B:857:ALA:HA	7:B:1765:HOH:O	2.05	0.55
1:B:566:LYS:HD2	1:B:567:PRO:HD2	1.89	0.55
1:B:841:HIS:CE1	1:B:843:GLU:HB2	2.42	0.55
1:B:862:VAL:HG21	1:B:865:ILE:HD11	1.89	0.55
1:B:879[B]:LYS:O	1:B:879[B]:LYS:HE3	2.07	0.54
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.89	0.54
1:A:101:LEU:HB2	1:A:104:GLN:HG3	1.90	0.53
1:A:388:HIS:ND1	1:A:393[B]:GLU:HG3	2.23	0.53
1:B:602:PRO:O	1:B:603:ILE:C	2.50	0.53
1:B:862:VAL:HG21	1:B:865:ILE:CD1	2.39	0.53
1:B:874:ASN:ND2	1:B:876:LEU:H	2.05	0.53
1:A:175[B]:GLU:HG2	1:A:179[B]:ARG:HH11	1.74	0.53
1:B:860:CYS:HB2	7:B:1765:HOH:O	2.09	0.52
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.75	0.52
1:B:575:ASN:HD22	1:B:576:MET:H	1.56	0.52
1:B:601:LEU:HB2	1:B:604:GLN:HG3	1.90	0.52
1:B:729:THR:HB	1:B:786[B]:LYS:HE2	1.90	0.52
1:B:676:GLU:HA	1:B:679[A]:ARG:HE	1.74	0.52
1:A:282:ALA:HB1	1:B:785:GLN:HG2	1.91	0.52
1:B:566:LYS:CD	1:B:567:PRO:HD2	2.40	0.52
1:B:828:LYS:HB3	1:B:863:GLU:H	1.74	0.52
1:B:642:GLY:HA2	1:B:645[B]:LYS:HD3	1.91	0.51
1:B:888:HIS:HD2	7:B:1818:HOH:O	1.92	0.51
1:A:395[B]:CYS:SG	1:A:399:LEU:CB	2.98	0.51
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.92	0.51
1:A:145[B]:LYS:HD2	1:A:146:LEU:HG	1.93	0.51
1:B:713:VAL:HG21	1:B:715[B]:ARG:HH21	1.77	0.50
1:B:675[B]:GLU:O	1:B:679[B]:ARG:HG3	2.11	0.50
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.76	0.50
1:A:213:VAL:HG13	1:A:215:ARG:HG2	1.94	0.50
1:A:395[B]:CYS:SG	1:A:399:LEU:HB3	2.51	0.50
1:B:615:LEU:HD22	1:B:618:LYS:HD2	1.94	0.50
1:A:102:PRO:O	1:A:103:ILE:C	2.53	0.50
1:A:204:ASN:O	1:A:208:ARG:HG3	2.12	0.50
1:B:841:HIS:HD2	7:B:1773:HOH:O	1.95	0.50
1:B:894:LEU:HD11	1:B:923:LEU:HD11	1.93	0.50
1:B:852:TYR:O	1:B:854:GLN:N	2.42	0.49
1:A:175[B]:GLU:O	1:A:179[B]:ARG:HG3	2.12	0.49
1:B:879[B]:LYS:HE3	1:B:879[B]:LYS:HA	1.94	0.49
1:B:678:GLU:OE1	1:B:719:MET:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASN:OD1	1:A:410:VAL:HG12	2.13	0.48
1:B:570:GLY:HA3	1:B:682:LEU:HD13	1.95	0.48
1:A:171:GLU:O	1:A:175[A]:GLU:HG3	2.13	0.48
1:B:576:MET:HB2	1:B:664[B]:ARG:NH2	2.29	0.48
1:B:788:MET:HG3	1:B:797:TYR:CE2	2.49	0.48
1:A:386:HIS:O	1:A:390:GLN:HG3	2.14	0.48
1:B:675[A]:GLU:O	1:B:679[A]:ARG:HG3	2.13	0.48
1:A:210:TYR:HA	1:A:213:VAL:HG12	1.96	0.47
1:A:92:LEU:C	1:A:92:LEU:HD23	2.39	0.47
1:A:252:LYS:HE3	7:A:1751:HOH:O	2.14	0.47
1:B:772[B]:ARG:HG2	7:B:1897:HOH:O	2.14	0.47
1:B:841:HIS:HE1	7:B:1844:HOH:O	1.97	0.47
1:B:908:ASN:CG	1:B:910:VAL:HG12	2.39	0.47
1:A:135:TRP:CZ3	1:A:372:ASN:HB3	2.50	0.47
1:A:175[B]:GLU:HG2	1:A:179[B]:ARG:NH1	2.30	0.47
1:A:243:LYS:HG3	7:A:1680:HOH:O	2.14	0.47
1:A:286:LYS:HD3	7:B:1734:HOH:O	2.15	0.47
1:A:149:GLU:HG2	7:A:1903:HOH:O	2.13	0.47
1:B:734:ILE:HG13	1:B:786[B]:LYS:CE	2.45	0.47
1:A:359:GLU:O	1:A:361:GLY:N	2.48	0.46
1:A:328:LYS:HB3	1:A:363:GLU:H	1.80	0.46
1:B:908:ASN:OD1	1:B:910:VAL:HG12	2.15	0.46
1:A:365:ILE:O	1:A:365:ILE:HG23	2.15	0.46
1:A:365:ILE:HD13	7:A:1822:HOH:O	2.16	0.46
1:A:116:THR:HB	1:A:117:PRO:HD3	1.97	0.46
1:A:134:ILE:CG2	1:A:138[B]:LYS:HE3	2.46	0.46
1:A:277:PRO:CB	6:A:707:GOL:H2	2.44	0.46
1:B:567:PRO:HA	1:B:656:PRO:HG2	1.97	0.46
1:B:615:LEU:HD21	5:B:1603:CHD:H232	1.98	0.46
1:B:755:GLU:OE2	1:B:829:ASN:HB2	2.16	0.46
5:B:1605:CHD:H212	5:B:1605:CHD:H12	1.98	0.46
1:A:80[B]:GLU:HG3	7:A:1642:HOH:O	2.15	0.45
1:B:592:LEU:HD23	1:B:592:LEU:C	2.42	0.45
1:A:142:GLY:O	1:A:145[B]:LYS:HE3	2.17	0.45
1:B:862:VAL:HG11	1:B:865:ILE:HD12	1.99	0.45
1:A:317[B]:GLU:OE2	1:B:905:LEU:HD13	2.16	0.44
1:A:70:GLY:HA3	1:A:182:LEU:HD13	1.99	0.44
1:B:879[B]:LYS:HE3	1:B:879[B]:LYS:CA	2.47	0.44
1:B:566:LYS:HG3	1:B:567:PRO:HD2	1.99	0.44
1:B:566:LYS:CG	1:B:567:PRO:HD2	2.47	0.44
1:B:850:ILE:HG23	1:B:854:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:GLN:C	7:B:1857:HOH:O	2.61	0.44
1:B:616:THR:HB	1:B:617:PRO:HD3	1.99	0.44
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.00	0.43
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.53	0.43
1:B:740:HIS:HA	1:B:743:LYS:HG2	2.00	0.43
1:A:289[B]:GLU:HG2	1:A:293:TYR:OH	2.18	0.43
1:A:296:PRO:HA	1:B:898:GLN:NE2	2.34	0.43
1:A:225:ASP:OD1	1:A:395[B]:CYS:SG	2.70	0.43
1:A:135:TRP:CE3	1:A:372:ASN:HB3	2.54	0.43
1:A:341:HIS:NE2	1:A:343:GLU:HB2	2.33	0.43
1:A:226:ARG:HD3	1:A:279:GLU:OE1	2.18	0.43
1:B:615:LEU:CD2	1:B:618:LYS:HD2	2.49	0.43
4:B:1602:IMD:H2	7:B:1670:HOH:O	2.19	0.43
1:B:595:ASP:CG	1:B:664[A]:ARG:HH21	2.26	0.42
1:B:862:VAL:CG2	1:B:865:ILE:HG13	2.47	0.42
1:A:96:ARG:HG2	1:A:96:ARG:NH1	2.33	0.42
1:A:398:GLN:NE2	1:B:796:PRO:HA	2.35	0.42
1:B:602:PRO:HB2	1:B:603:ILE:HD13	2.01	0.42
1:A:388:HIS:CE1	1:A:393[B]:GLU:HG3	2.54	0.42
1:B:679[B]:ARG:CZ	1:B:679[B]:ARG:HB3	2.49	0.42
1:B:825:ARG:HG3	1:B:825:ARG:NH1	2.34	0.42
1:A:297:TYR:CD1	1:A:297:TYR:C	2.98	0.42
1:A:69:THR:HG23	1:A:184:ARG:HD2	2.02	0.42
1:B:820:LYS:HB2	1:B:856:LEU:HD11	2.02	0.42
6:A:707:GOL:H31	1:B:777:PRO:HB3	2.02	0.41
1:B:618:LYS:NZ	1:B:618:LYS:CB	2.82	0.41
1:B:671:GLU:O	1:B:675[B]:GLU:HG3	2.20	0.41
1:B:713:VAL:HG21	1:B:715[B]:ARG:NH2	2.35	0.41
1:A:374:ASN:C	1:A:374:ASN:ND2	2.77	0.41
1:B:828:LYS:O	1:B:862:VAL:HG22	2.21	0.41
1:B:893[B]:GLU:CD	7:B:1818:HOH:O	2.63	0.41
1:A:400:THR:HA	1:A:415:LYS:HD2	2.02	0.41
1:B:874:ASN:C	1:B:874:ASN:ND2	2.79	0.41
1:B:603:ILE:HD13	1:B:603:ILE:N	2.36	0.41
1:A:164[A]:ARG:NH1	1:A:201:SER:O	2.54	0.41
1:A:173:ALA:O	1:A:177:MET:HG3	2.21	0.41
1:B:678:GLU:OE1	1:B:718:THR:OG1	2.33	0.41
1:A:304:LYS:HG3	1:A:310:TRP:CG	2.55	0.41
1:B:650:LEU:HD11	1:B:879[B]:LYS:HZ3	1.79	0.41
1:A:154:THR:OG1	1:A:157:HIS:CE1	2.74	0.41
1:A:208:ARG:NH1	1:A:208:ARG:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:PRO:CB	1:B:603:ILE:HD13	2.51	0.41
1:B:766:PRO:HG2	5:B:1603:CHD:H11	2.03	0.41
1:B:693:GLN:HG2	1:B:780:VAL:HA	2.02	0.40
1:B:713:VAL:O	1:B:715[B]:ARG:HG3	2.21	0.40
1:B:755:GLU:CD	1:B:829:ASN:HB2	2.46	0.40
1:B:847:GLU:OE2	1:B:852:TYR:OH	2.37	0.40
1:A:423:LEU:HD22	1:A:423:LEU:N	2.36	0.40
1:B:707:TYR:CZ	1:B:913[B]:GLU:HB3	2.56	0.40
5:A:701:CHD:H212	5:A:701:CHD:H12	2.02	0.40
1:B:879[B]:LYS:O	1:B:879[B]:LYS:CE	2.69	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	378/359 (105%)	365 (97%)	9 (2%)	4 (1%)	11	3
1	B	377/359 (105%)	365 (97%)	10 (3%)	2 (0%)	24	12
All	All	755/718 (105%)	730 (97%)	19 (2%)	6 (1%)	16	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	853	SER
1	B	854	GLN
1	A	357	ALA
1	A	358	LYS
1	A	360	CYS
1	A	359	GLU

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	343/324 (106%)	343 (100%)	0	100	100
1	B	344/324 (106%)	342 (99%)	2 (1%)	78	72
All	All	687/648 (106%)	685 (100%)	2 (0%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	603	ILE
1	B	618	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	120	GLN
1	A	157	HIS
1	A	240	HIS
1	A	374	ASN
1	A	390	GLN
1	A	398	GLN
1	A	421	GLN
1	B	575	ASN
1	B	605	ASN
1	B	620	GLN
1	B	740	HIS
1	B	814	GLN
1	B	829	ASN
1	B	841	HIS
1	B	854	GLN
1	B	864	ASN
1	B	874	ASN
1	B	888	HIS
1	B	898	GLN

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Mol	Chain	Res	Type
1	B	921	GLN
1	B	922	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 ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	A	702	-	32,32,32	2.19	12 (37%)	51,51,51	1.78	15 (29%)
5	CHD	A	701	-	32,32,32	2.22	16 (50%)	51,51,51	1.87	16 (31%)
5	CHD	A	703	-	32,32,32	2.20	15 (46%)	51,51,51	1.83	16 (31%)
4	IMD	B	1602	-	5,5,5	0.24	0	5,5,5	0.42	0
4	IMD	A	1601	-	5,5,5	0.28	0	5,5,5	0.42	0
6	GOL	A	707	-	5,5,5	0.22	0	5,5,5	0.24	0
5	CHD	B	1603	-	32,32,32	2.16	13 (40%)	51,51,51	1.81	16 (31%)
3	FES	B	1502	1	0,4,4	-	-	-	-	-
5	CHD	B	1604	-	32,32,32	2.21	14 (43%)	51,51,51	1.84	16 (31%)
3	FES	A	1501	1	0,4,4	-	-	-	-	-
5	CHD	B	1605	-	32,32,32	2.20	16 (50%)	51,51,51	1.89	17 (33%)

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	A	702	-	-	0/9/74/74	0/4/4/4
5	CHD	A	701	-	-	2/9/74/74	0/4/4/4
5	CHD	A	703	-	-	4/9/74/74	0/4/4/4
4	IMD	B	1602	-	-	-	0/1/1/1
6	GOL	A	707	-	-	2/4/4/4	-
4	IMD	A	1601	-	-	-	0/1/1/1
5	CHD	B	1603	-	-	3/9/74/74	0/4/4/4
3	FES	B	1502	1	-	-	0/1/1/1
5	CHD	B	1604	-	-	5/9/74/74	0/4/4/4
3	FES	A	1501	1	-	-	0/1/1/1
5	CHD	B	1605	-	-	3/9/74/74	0/4/4/4

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	CHD	O25-C24	4.69	1.37	1.22
5	B	1603	CHD	O25-C24	4.67	1.37	1.22
5	A	703	CHD	O25-C24	4.66	1.37	1.22
5	A	701	CHD	O25-C24	4.66	1.37	1.22
5	B	1604	CHD	O25-C24	4.63	1.37	1.22
5	B	1605	CHD	O25-C24	4.44	1.36	1.22
5	B	1604	CHD	C11-C9	4.03	1.60	1.53
5	B	1603	CHD	C11-C9	4.03	1.60	1.53
5	A	702	CHD	C11-C9	3.89	1.60	1.53
5	A	703	CHD	C11-C9	3.88	1.60	1.53
5	A	703	CHD	C16-C17	3.75	1.62	1.54
5	A	701	CHD	C11-C9	3.75	1.59	1.53
5	B	1604	CHD	C16-C17	3.73	1.62	1.54
5	A	702	CHD	C16-C17	3.72	1.62	1.54
5	B	1603	CHD	C16-C17	3.68	1.61	1.54
5	B	1605	CHD	C16-C17	3.40	1.61	1.54
5	A	701	CHD	C16-C17	3.35	1.61	1.54
5	B	1605	CHD	C11-C9	3.33	1.59	1.53
5	B	1604	CHD	C6-C5	3.27	1.59	1.53
5	A	703	CHD	C6-C5	3.24	1.59	1.53
5	B	1605	CHD	C6-C5	3.22	1.59	1.53
5	A	701	CHD	C10-C9	3.21	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1605	CHD	C10-C9	3.15	1.61	1.56
5	B	1603	CHD	C6-C5	3.14	1.58	1.53
5	A	701	CHD	C6-C5	3.13	1.58	1.53
5	A	702	CHD	C10-C9	3.11	1.61	1.56
5	A	703	CHD	C10-C9	3.07	1.61	1.56
5	B	1603	CHD	C10-C9	3.06	1.61	1.56
5	A	702	CHD	C6-C5	3.03	1.58	1.53
5	A	702	CHD	O12-C12	3.03	1.48	1.43
5	B	1604	CHD	C10-C9	3.00	1.61	1.56
5	B	1605	CHD	O12-C12	2.99	1.48	1.43
5	A	703	CHD	O12-C12	2.96	1.48	1.43
5	A	701	CHD	C18-C13	2.93	1.59	1.54
5	B	1604	CHD	O12-C12	2.92	1.48	1.43
5	B	1605	CHD	C18-C13	2.88	1.58	1.54
5	A	701	CHD	O12-C12	2.85	1.48	1.43
5	B	1603	CHD	O12-C12	2.82	1.48	1.43
5	A	702	CHD	O26-C24	-2.79	1.21	1.30
5	A	701	CHD	O26-C24	-2.77	1.21	1.30
5	B	1603	CHD	C18-C13	2.77	1.58	1.54
5	A	702	CHD	C18-C13	2.74	1.58	1.54
5	B	1604	CHD	C18-C13	2.74	1.58	1.54
5	B	1604	CHD	O26-C24	-2.70	1.21	1.30
5	A	703	CHD	C18-C13	2.70	1.58	1.54
5	B	1605	CHD	C8-C14	2.68	1.59	1.53
5	B	1603	CHD	O26-C24	-2.66	1.22	1.30
5	B	1605	CHD	O26-C24	-2.64	1.22	1.30
5	A	703	CHD	O26-C24	-2.62	1.22	1.30
5	B	1605	CHD	C22-C23	2.61	1.60	1.52
5	A	701	CHD	C8-C14	2.60	1.58	1.53
5	A	703	CHD	C13-C12	2.59	1.58	1.54
5	B	1605	CHD	C19-C10	2.57	1.58	1.54
5	A	703	CHD	C19-C10	2.57	1.58	1.54
5	B	1604	CHD	C19-C10	2.56	1.58	1.54
5	B	1604	CHD	C13-C12	2.55	1.58	1.54
5	A	701	CHD	C19-C10	2.55	1.58	1.54
5	A	702	CHD	C13-C12	2.54	1.58	1.54
5	B	1605	CHD	C13-C12	2.52	1.58	1.54
5	B	1604	CHD	C8-C7	2.52	1.58	1.53
5	A	701	CHD	C8-C7	2.48	1.58	1.53
5	A	701	CHD	C22-C23	2.38	1.60	1.52
5	A	702	CHD	C8-C14	2.34	1.58	1.53
5	B	1604	CHD	C8-C14	2.33	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	CHD	C13-C12	2.33	1.58	1.54
5	B	1605	CHD	C8-C7	2.33	1.57	1.53
5	B	1603	CHD	C13-C12	2.31	1.58	1.54
5	A	703	CHD	C8-C7	2.30	1.57	1.53
5	A	703	CHD	C8-C14	2.30	1.58	1.53
5	B	1603	CHD	C8-C7	2.28	1.57	1.53
5	A	701	CHD	C4-C3	2.25	1.55	1.52
5	A	702	CHD	C19-C10	2.22	1.58	1.54
5	B	1605	CHD	C20-C17	2.21	1.58	1.54
5	B	1604	CHD	O7-C7	2.21	1.48	1.43
5	B	1603	CHD	C8-C14	2.19	1.58	1.53
5	B	1605	CHD	O7-C7	2.18	1.47	1.43
5	B	1603	CHD	O7-C7	2.18	1.47	1.43
5	A	703	CHD	O7-C7	2.14	1.47	1.43
5	A	702	CHD	C8-C7	2.13	1.57	1.53
5	B	1605	CHD	C4-C3	2.12	1.55	1.52
5	B	1603	CHD	C19-C10	2.11	1.57	1.54
5	A	701	CHD	C20-C17	2.09	1.58	1.54
5	A	701	CHD	O7-C7	2.06	1.47	1.43
5	A	703	CHD	C4-C3	2.05	1.55	1.52
5	A	703	CHD	C8-C9	2.04	1.57	1.53
5	B	1604	CHD	C8-C9	2.03	1.57	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	CHD	O26-C24-C23	4.41	127.93	114.00
5	B	1605	CHD	C18-C13-C12	-4.33	104.73	109.06
5	A	701	CHD	C18-C13-C12	-4.32	104.73	109.06
5	B	1604	CHD	O26-C24-C23	4.22	127.34	114.00
5	A	703	CHD	O26-C24-C23	4.22	127.33	114.00
5	B	1603	CHD	O26-C24-C23	4.21	127.31	114.00
5	B	1605	CHD	O26-C24-C23	4.18	127.22	114.00
5	A	702	CHD	O26-C24-C23	4.05	126.79	114.00
5	B	1605	CHD	C17-C13-C12	4.02	121.28	117.67
5	A	701	CHD	C17-C13-C12	3.97	121.24	117.67
5	A	703	CHD	C18-C13-C12	-3.92	105.14	109.06
5	B	1604	CHD	C18-C13-C12	-3.87	105.18	109.06
5	A	702	CHD	C18-C13-C12	-3.72	105.33	109.06
5	A	701	CHD	C19-C10-C1	-3.69	102.45	108.31
5	B	1605	CHD	C16-C17-C13	-3.67	99.98	103.54
5	B	1603	CHD	C18-C13-C12	-3.66	105.39	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1604	CHD	C19-C10-C1	-3.65	102.51	108.31
5	B	1605	CHD	C19-C10-C1	-3.56	102.64	108.31
5	A	703	CHD	C19-C10-C1	-3.53	102.69	108.31
5	A	701	CHD	C16-C17-C13	-3.49	100.16	103.54
5	A	702	CHD	C19-C10-C1	-3.42	102.87	108.31
5	A	703	CHD	C17-C13-C14	3.27	103.39	100.11
5	B	1603	CHD	O12-C12-C13	-3.23	105.57	111.02
5	B	1603	CHD	C19-C10-C1	-3.21	103.19	108.31
5	A	701	CHD	O12-C12-C13	-3.20	105.62	111.02
5	B	1604	CHD	C17-C13-C14	3.18	103.30	100.11
5	A	702	CHD	C17-C13-C14	3.15	103.27	100.11
5	A	702	CHD	C17-C13-C12	3.13	120.48	117.67
5	A	703	CHD	O12-C12-C13	-3.11	105.77	111.02
5	B	1604	CHD	C17-C13-C12	3.07	120.43	117.67
5	A	703	CHD	C17-C13-C12	3.06	120.42	117.67
5	B	1604	CHD	O12-C12-C13	-3.02	105.92	111.02
5	B	1605	CHD	O12-C12-C13	-2.99	105.97	111.02
5	A	702	CHD	O12-C12-C13	-2.98	105.98	111.02
5	A	703	CHD	O25-C24-C23	-2.95	113.73	123.09
5	A	701	CHD	O25-C24-C23	-2.95	113.75	123.09
5	B	1604	CHD	O25-C24-C23	-2.90	113.89	123.09
5	B	1603	CHD	O25-C24-C23	-2.83	114.10	123.09
5	B	1603	CHD	C17-C13-C12	2.83	120.22	117.67
5	B	1605	CHD	C11-C9-C10	-2.80	110.86	113.70
5	B	1603	CHD	C17-C13-C14	2.76	102.88	100.11
5	B	1605	CHD	C17-C13-C14	2.68	102.80	100.11
5	B	1605	CHD	O25-C24-C23	-2.67	114.62	123.09
5	A	702	CHD	C6-C5-C10	-2.66	109.83	112.66
5	B	1603	CHD	C6-C5-C10	-2.64	109.86	112.66
5	B	1605	CHD	C1-C10-C5	2.59	111.46	107.75
5	B	1603	CHD	C9-C11-C12	-2.58	110.91	114.29
5	A	701	CHD	C17-C13-C14	2.58	102.70	100.11
5	B	1604	CHD	C6-C5-C10	-2.57	109.93	112.66
5	A	702	CHD	O25-C24-C23	-2.55	115.01	123.09
5	A	703	CHD	C6-C5-C10	-2.52	109.98	112.66
5	A	702	CHD	C1-C10-C5	2.52	111.36	107.75
5	A	702	CHD	C11-C9-C10	-2.50	111.17	113.70
5	A	701	CHD	C1-C10-C5	2.50	111.33	107.75
5	B	1603	CHD	C1-C10-C5	2.49	111.33	107.75
5	A	701	CHD	C11-C9-C10	-2.49	111.18	113.70
5	A	702	CHD	C6-C5-C4	2.48	114.06	111.23
5	B	1604	CHD	C11-C9-C10	-2.44	111.23	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1603	CHD	C16-C17-C13	-2.43	101.19	103.54
5	B	1605	CHD	C21-C20-C22	-2.41	106.60	110.34
5	B	1604	CHD	C11-C12-C13	2.41	113.72	111.26
5	B	1603	CHD	C11-C12-C13	2.41	113.72	111.26
5	B	1604	CHD	C1-C10-C5	2.41	111.21	107.75
5	A	703	CHD	C11-C12-C13	2.41	113.71	111.26
5	A	703	CHD	C9-C11-C12	-2.38	111.18	114.29
5	B	1604	CHD	C9-C11-C12	-2.38	111.19	114.29
5	A	703	CHD	C11-C9-C10	-2.37	111.30	113.70
5	A	703	CHD	C1-C10-C5	2.36	111.14	107.75
5	B	1603	CHD	C11-C9-C10	-2.36	111.31	113.70
5	B	1603	CHD	C6-C5-C4	2.35	113.91	111.23
5	A	703	CHD	C16-C17-C13	-2.32	101.29	103.54
5	A	702	CHD	C9-C8-C7	-2.31	108.95	111.86
5	B	1605	CHD	C6-C5-C4	2.30	113.85	111.23
5	B	1604	CHD	C6-C5-C4	2.28	113.83	111.23
5	B	1604	CHD	C16-C17-C13	-2.26	101.35	103.54
5	B	1604	CHD	C19-C10-C9	2.26	114.21	111.18
5	A	703	CHD	C19-C10-C9	2.25	114.21	111.18
5	A	702	CHD	C11-C12-C13	2.23	113.53	111.26
5	A	701	CHD	C6-C5-C10	-2.19	110.33	112.66
5	A	701	CHD	C6-C5-C4	2.18	113.72	111.23
5	B	1605	CHD	C6-C5-C10	-2.18	110.34	112.66
5	A	703	CHD	C6-C5-C4	2.15	113.68	111.23
5	A	702	CHD	C9-C11-C12	-2.14	111.49	114.29
5	A	701	CHD	C21-C20-C22	-2.13	107.04	110.34
5	B	1605	CHD	C11-C12-C13	2.13	113.43	111.26
5	A	701	CHD	C11-C12-C13	2.13	113.43	111.26
5	A	701	CHD	C19-C10-C9	2.12	114.03	111.18
5	B	1603	CHD	C9-C8-C7	-2.12	109.19	111.86
5	B	1605	CHD	C9-C11-C12	-2.11	111.53	114.29
5	A	701	CHD	C9-C11-C12	-2.10	111.55	114.29
5	A	703	CHD	C9-C8-C7	-2.08	109.24	111.86
5	B	1605	CHD	C9-C8-C7	-2.06	109.26	111.86
5	B	1603	CHD	C13-C17-C20	2.04	121.95	119.48
5	A	702	CHD	C16-C17-C13	-2.02	101.58	103.54
5	B	1604	CHD	C9-C8-C7	-2.02	109.31	111.86
5	B	1605	CHD	O26-C24-O25	-2.01	118.16	123.33

There are no chirality outliers.

All (19) torsion outliers are listed below:

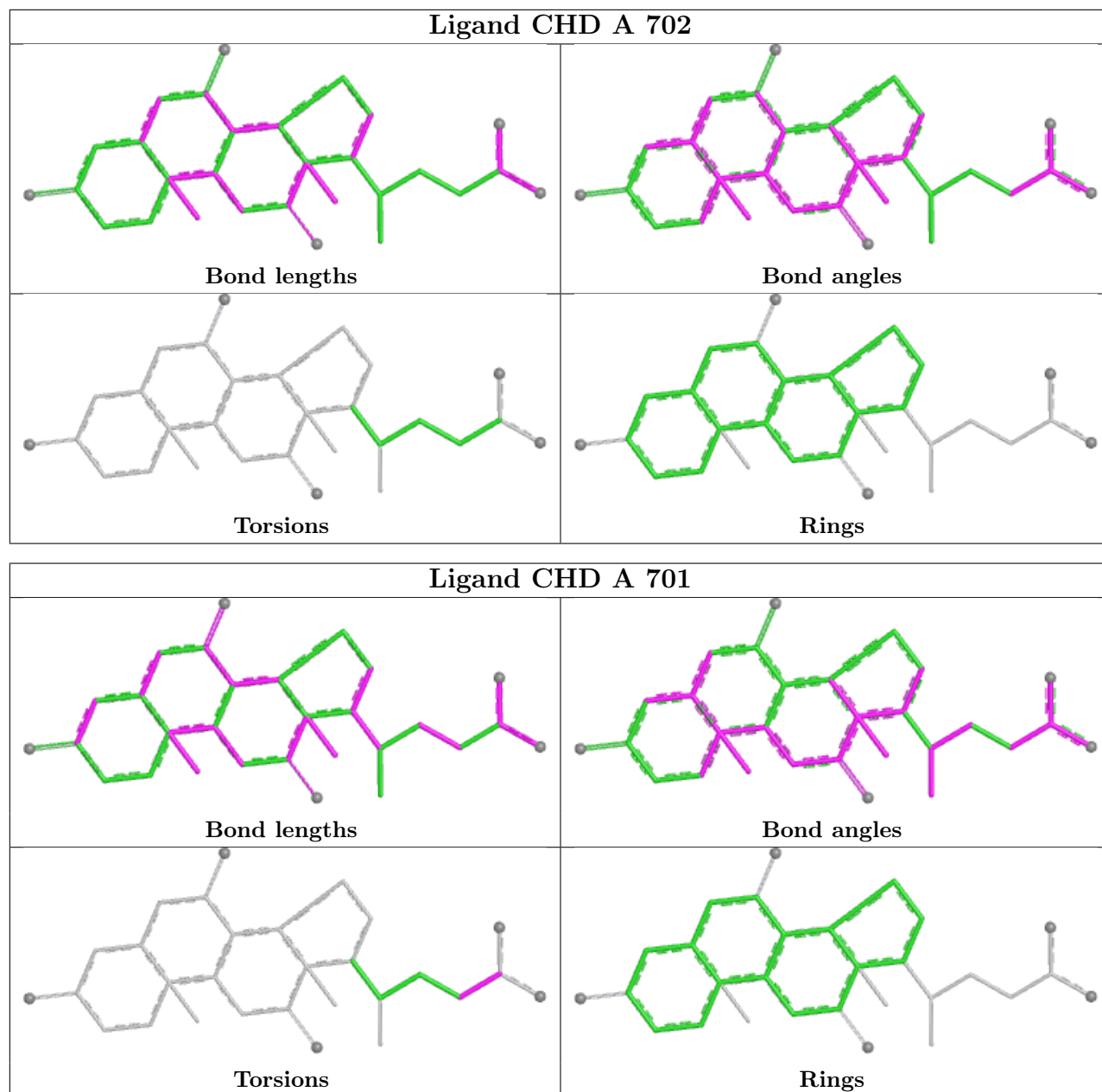
Mol	Chain	Res	Type	Atoms
5	B	1603	CHD	C20-C22-C23-C24
5	A	703	CHD	C21-C20-C22-C23
5	A	703	CHD	C17-C20-C22-C23
6	A	707	GOL	O1-C1-C2-O2
6	A	707	GOL	O1-C1-C2-C3
5	B	1604	CHD	C21-C20-C22-C23
5	B	1605	CHD	C20-C22-C23-C24
5	A	701	CHD	C22-C23-C24-O25
5	B	1605	CHD	C22-C23-C24-O25
5	B	1604	CHD	C17-C20-C22-C23
5	A	703	CHD	C22-C23-C24-O26
5	A	701	CHD	C22-C23-C24-O26
5	A	703	CHD	C22-C23-C24-O25
5	B	1605	CHD	C22-C23-C24-O26
5	B	1604	CHD	C22-C23-C24-O26
5	B	1603	CHD	C22-C23-C24-O26
5	B	1604	CHD	C22-C23-C24-O25
5	B	1604	CHD	C20-C22-C23-C24
5	B	1603	CHD	C22-C23-C24-O25

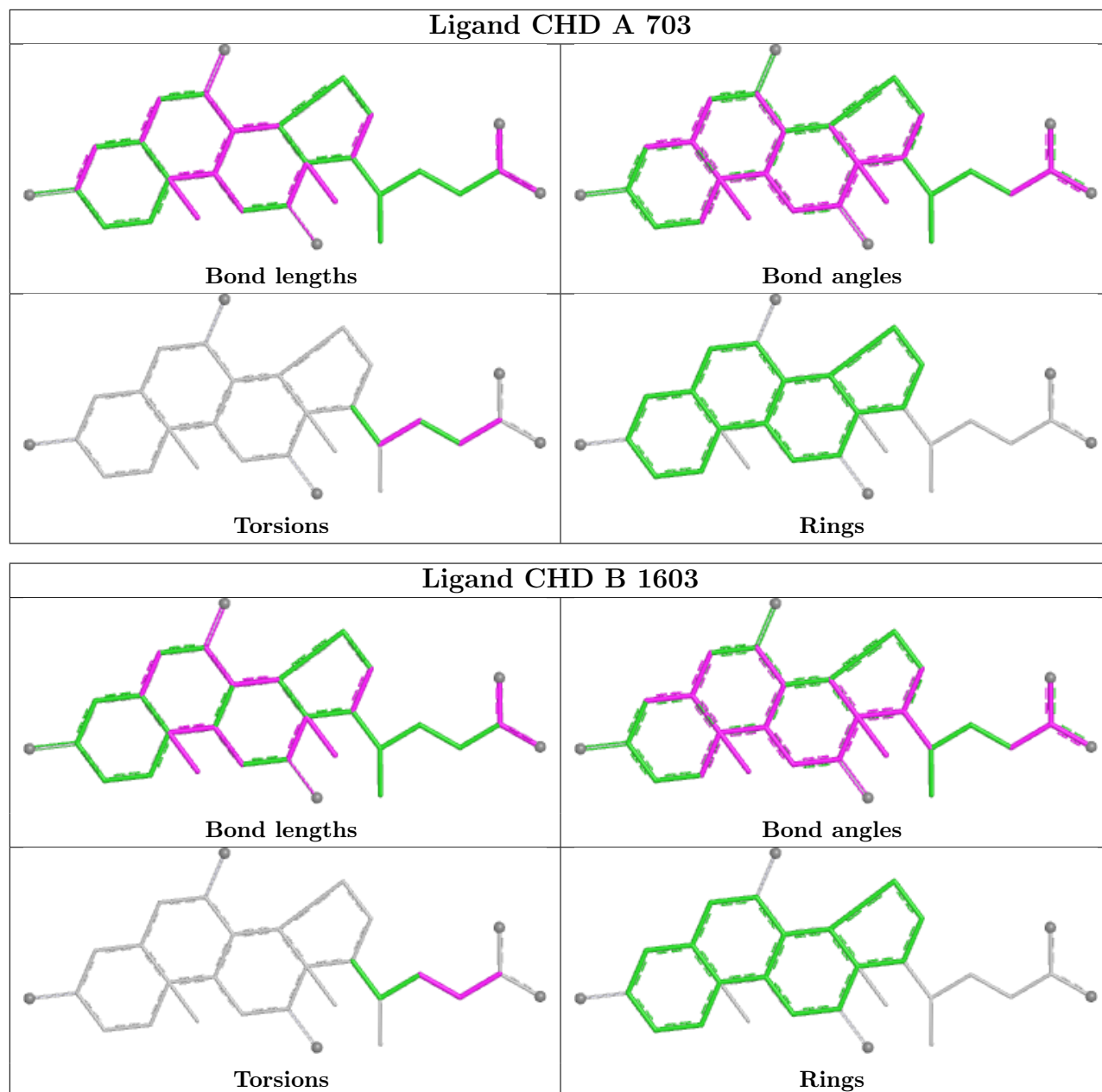
There are no ring outliers.

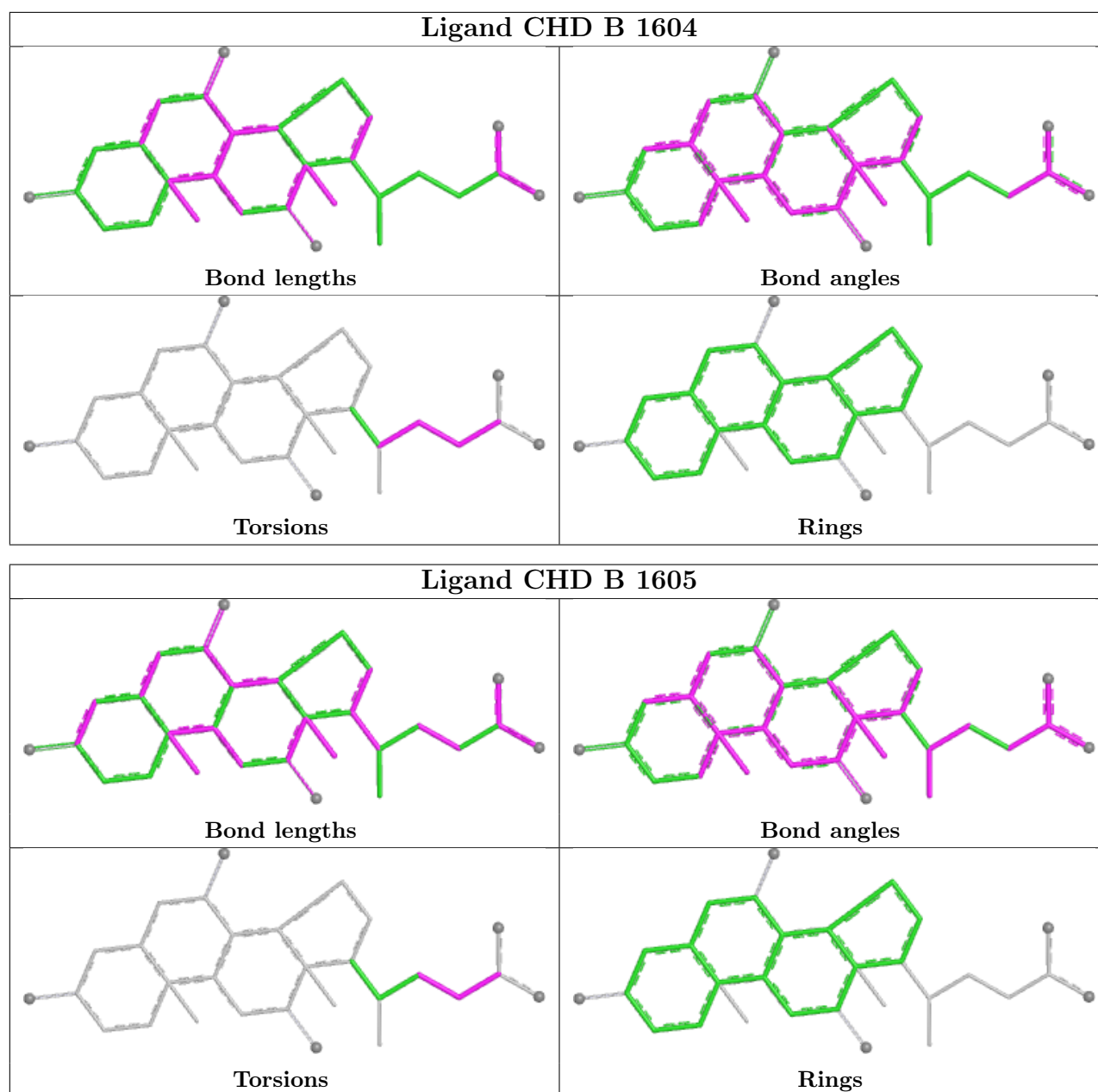
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	CHD	1	0
4	B	1602	IMD	1	0
6	A	707	GOL	3	0
5	B	1603	CHD	2	0
5	B	1605	CHD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/359 (100%)	1.00	60 (16%)  	6, 19, 33, 44	21 (5%)
1	B	359/359 (100%)	0.97	58 (16%)  	7, 18, 34, 43	20 (5%)
All	All	718/718 (100%)	0.98	118 (16%)  	6, 18, 34, 44	41 (5%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	CYS	12.9
1	B	857	ALA	11.0
1	B	855	VAL	10.4
1	B	860	CYS	10.3
1	B	853	SER	8.7
1	B	854	GLN	8.3
1	A	359	GLU	8.1
1	A	356	LEU	7.8
1	A	357	ALA	6.8
1	B	862	VAL	6.8
1	B	856	LEU	6.6
1	A	358	LYS	6.3
1	A	362	VAL	6.0
1	A	423	LEU	5.9
1	B	923	LEU	5.7
1	B	858	LYS	5.6
1	A	212	GLN	5.3
1	A	246	ASP	5.3
1	B	852	TYR	5.2
1	A	363	GLU	5.2
1	B	565	ARG	5.1
1	A	96	ARG	4.9
1	A	213	VAL	4.9
1	B	861	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	755	GLU	4.6
1	A	250	LEU	4.5
1	B	597	ASP	4.4
1	B	679[A]	ARG	4.3
1	A	243	LYS	4.2
1	A	253[A]	ARG	4.2
1	A	354	GLN	4.1
1	B	912	ARG	4.1
1	A	355	VAL	4.1
1	A	214	GLY	4.1
1	A	395[A]	CYS	3.9
1	B	907	VAL	3.9
1	B	865	ILE	3.9
1	A	353	SER	3.9
1	A	97	ASP	3.9
1	B	713	VAL	3.8
1	A	249	PRO	3.8
1	B	892	ASN	3.7
1	A	407	VAL	3.6
1	A	179[A]	ARG	3.6
1	B	596	ARG	3.5
1	A	153	ASN	3.5
1	A	364	ASN	3.5
1	B	715[A]	ARG	3.4
1	B	712	GLN	3.4
1	A	361	GLY	3.3
1	B	864	ASN	3.3
1	B	711[A]	ASN	3.3
1	B	566	LYS	3.3
1	A	393[A]	GLU	3.2
1	B	603	ILE	3.2
1	A	251	GLU	3.2
1	B	714	GLY	3.2
1	B	743	LYS	3.2
1	A	392	ASN	3.1
1	A	65	ARG	3.1
1	B	653	ASN	3.1
1	B	751	GLU	3.1
1	B	683	GLU	3.0
1	A	352	TYR	3.0
1	B	859	GLU	2.9
1	A	248	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	2.9
1	B	676	GLU	2.9
1	A	323[A]	CYS	2.8
1	A	220[A]	LYS	2.8
1	B	750	LEU	2.8
1	A	164[A]	ARG	2.7
1	B	863	GLU	2.7
1	A	412	ARG	2.7
1	A	247	HIS	2.7
1	B	808	MET	2.7
1	A	328	LYS	2.7
1	B	618	LYS	2.7
1	B	789[A]	GLU	2.6
1	A	365	ILE	2.6
1	A	254	SER	2.6
1	B	747	HIS	2.6
1	A	98	LEU	2.5
1	B	594	LEU	2.5
1	B	606	LYS	2.5
1	A	324	GLU	2.5
1	A	329	ASN	2.5
1	A	175[A]	GLU	2.5
1	A	211	ASN	2.4
1	A	297	TYR	2.4
1	A	180	ASP	2.4
1	B	684	ARG	2.4
1	A	216	LYS	2.3
1	B	716	LYS	2.3
1	A	118	LYS	2.3
1	A	218	THR	2.3
1	B	592	LEU	2.3
1	A	255	GLU	2.2
1	B	678	GLU	2.2
1	A	208	ARG	2.2
1	B	600	THR	2.2
1	B	602	PRO	2.2
1	A	68	LYS	2.2
1	B	707	TYR	2.2
1	A	152	PRO	2.2
1	A	305	VAL	2.1
1	B	612	ALA	2.1
1	B	598	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	601	LEU	2.1
1	A	217	PRO	2.1
1	A	215	ARG	2.1
1	B	664[A]	ARG	2.1
1	A	256	VAL	2.1
1	B	720	LYS	2.1
1	B	754	SER	2.1
1	B	746	ASP	2.1
1	B	805	VAL	2.0
1	B	910	VAL	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](#)

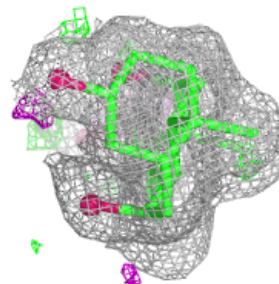
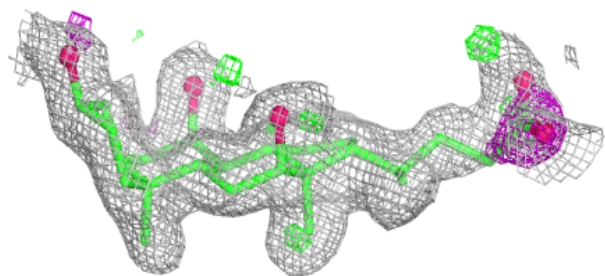
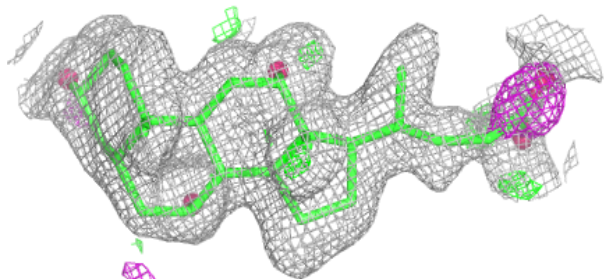
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	IMD	A	1601	5/5	0.64	0.20	37,37,37,37	0
4	IMD	B	1602	5/5	0.72	0.18	36,36,36,36	0
6	GOL	A	707	6/6	0.75	0.18	29,29,29,29	0
5	CHD	B	1603	29/29	0.78	0.17	33,33,36,36	0
5	CHD	A	703	29/29	0.79	0.17	35,35,36,37	0
5	CHD	B	1604	29/29	0.82	0.17	41,41,43,43	0
5	CHD	A	702	29/29	0.85	0.13	31,31,33,33	0
5	CHD	A	701	29/29	0.88	0.12	20,21,24,25	0
5	CHD	B	1605	29/29	0.90	0.10	20,21,25,26	0
2	CL	A	802	1/1	0.98	0.04	17,17,17,17	0
2	CL	B	924	1/1	0.99	0.04	18,18,18,18	0
3	FES	A	1501	4/4	0.99	0.04	15,16,16,17	0
3	FES	B	1502	4/4	0.99	0.05	16,16,16,17	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.

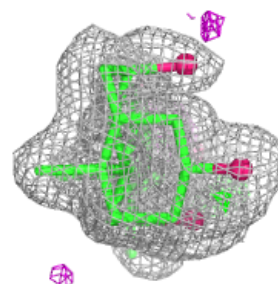
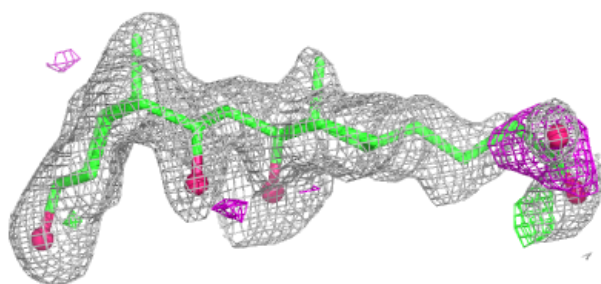
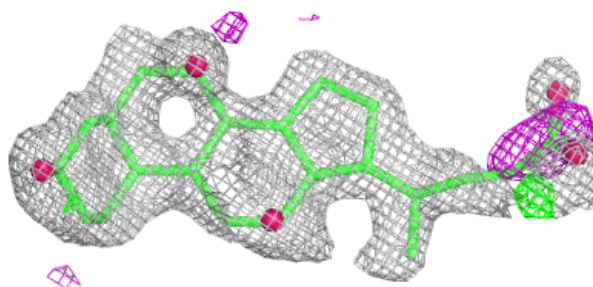
Electron density around CHD B 1603:

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

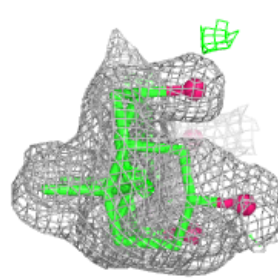
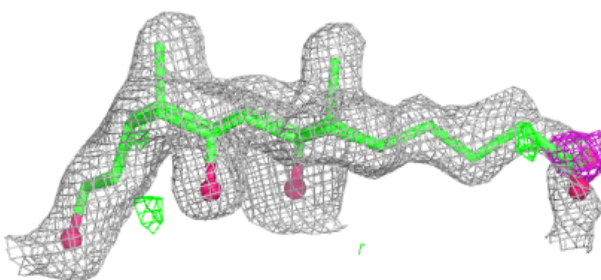
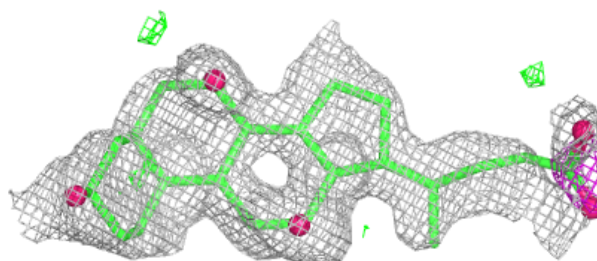


Electron density around CHD A 703:

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

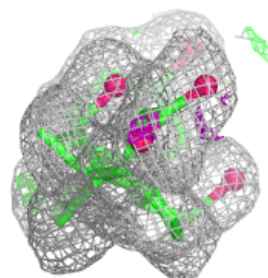
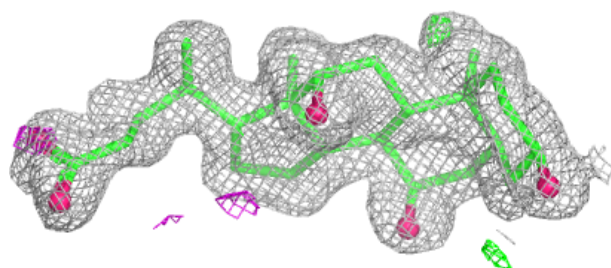
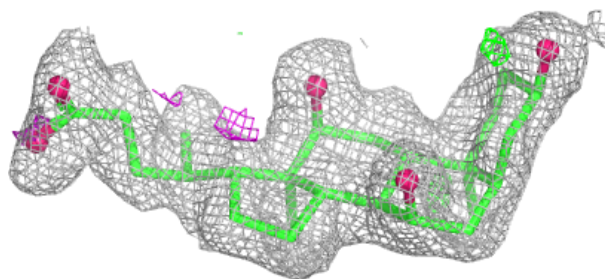
**Electron density around CHD B 1604:**

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

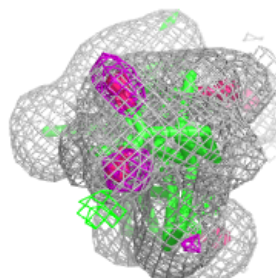
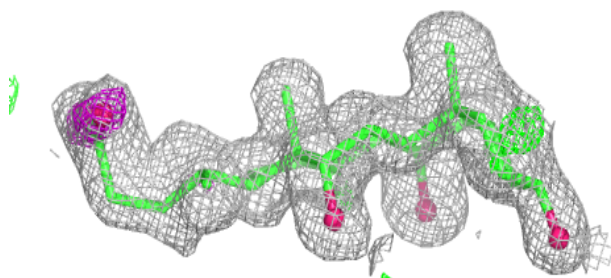
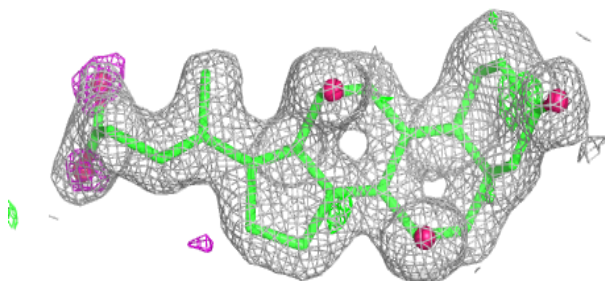


Electron density around CHD A 702:

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

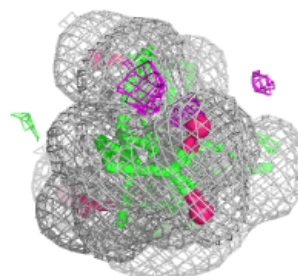
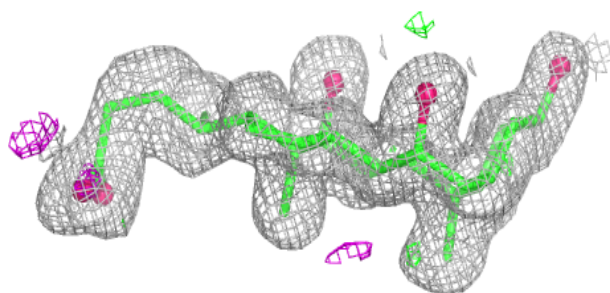
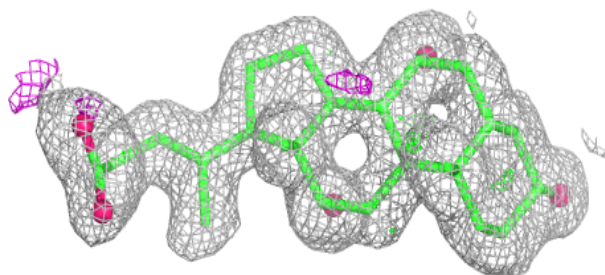
**Electron density around CHD A 701:**

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



Electron density around CHD B 1605:

$2mF_o-DF_c$ (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.