



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1TMX / pdb_00001tmx
Title : Crystal structure of hydroxyquinol 1,2-dioxygenase from Nocardioides Simplex 3E
Authors : Ferraroni, M.; Travkin, V.M.; Seifert, J.; Schlomann, M.; Golovleva, L.; Scoz-zafava, A.; Briganti, F.
Deposited on : 2004-06-11
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

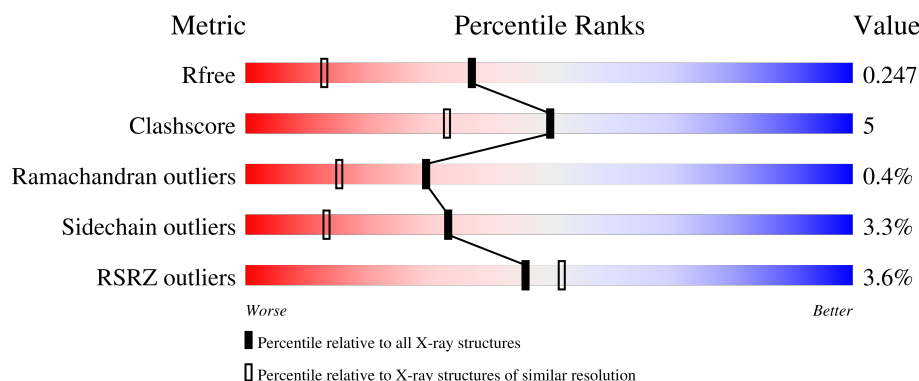
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	293	2% 90% 9% .
1	B	293	5% 86% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BEZ	A	881	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5359 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 hydroxyquinol 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	6	0
			2247	1410	396	434	7			
1	B	287	Total	C	N	O	S	0	0	0
			2174	1360	385	422	7			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

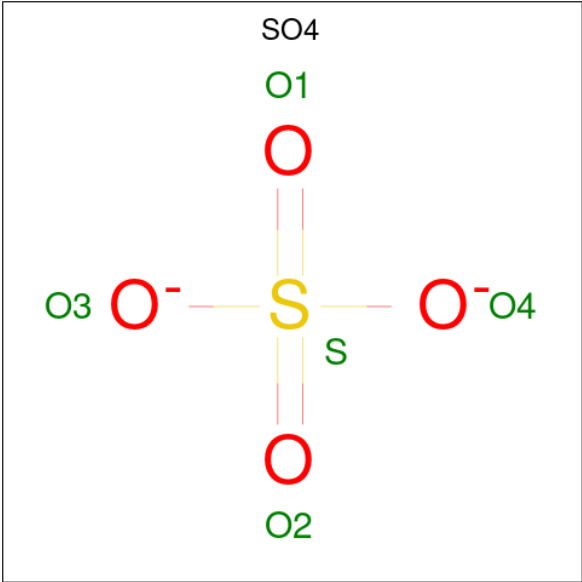
- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

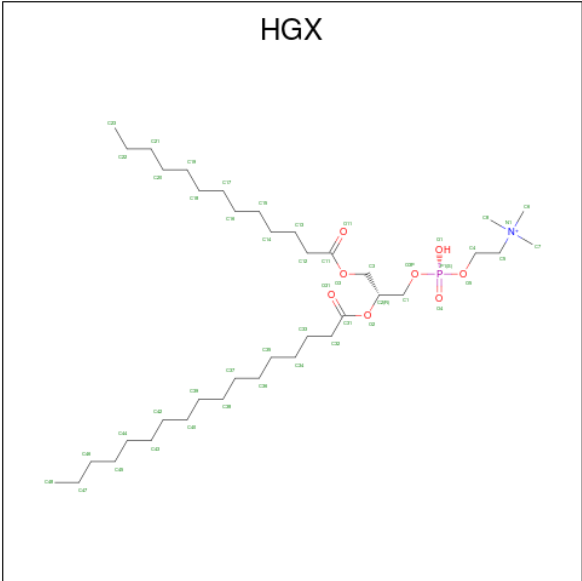
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1-HEPTADECANOYL-2-TRIDECANOYL-3-GLYCEROL-PHOSPHONYL CHOLINE (CCD ID: HGX) (formula: C₃₈H₇₇NO₈P).



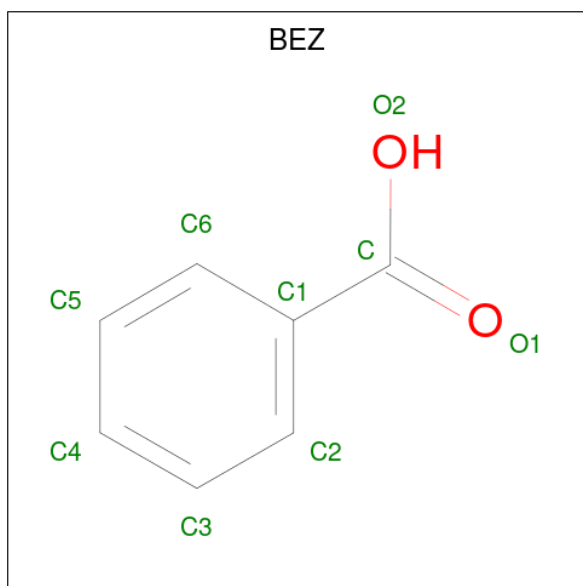
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	32	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			38	33	5		

- Molecule 7 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	7	2		
7	B	1	Total	C	O	0	0
			9	7	2		

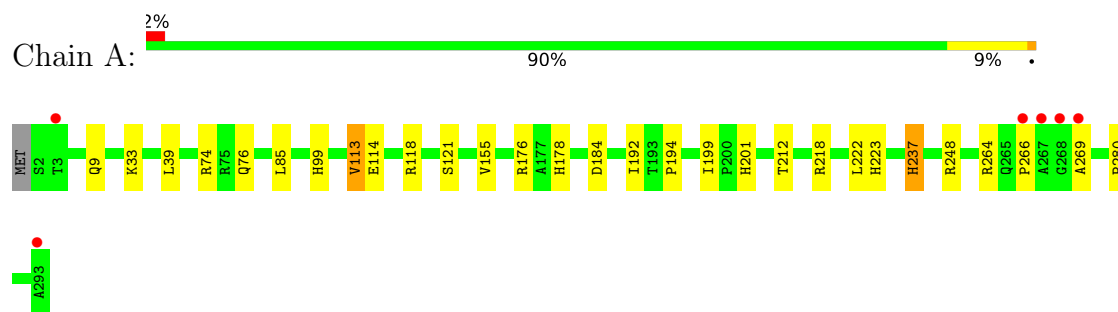
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	410	Total	O	0	0
			410	410		
8	B	421	Total	O	0	0
			421	421		

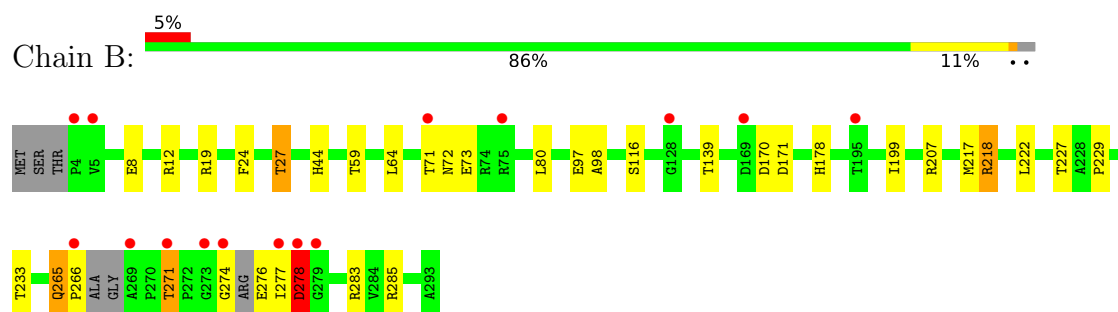
3 Residue-property plots [i](#)

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: hydroxyquinol 1,2-dioxygenase



- Molecule 1: hydroxyquinol 1,2-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.28Å 84.98Å 83.92Å 90.00° 92.84° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 20.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-1.75) 91.7 (20.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.193 , 0.247 0.194 , 0.247	Depositor DCC
R_{free} test set	3001 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k 0.002 for -h,l,k 0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5359	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, BEZ, CL, HGX, FE, CU

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	0.96	0/2330	1.01	0/3172
1	B	0.93	1/2227 (0.0%)	1.07	6/3028 (0.2%)
All	All	0.95	1/4557 (0.0%)	1.04	6/6200 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	MET	SD-CE	-7.10	1.61	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ASN	N-CA-C	11.84	126.16	110.53
1	B	19	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	B	278	ASP	N-CA-C	6.19	116.17	108.19
1	B	71	THR	N-CA-C	5.12	121.70	110.80
1	B	19	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	B	265	GLN	N-CA-C	5.06	121.00	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	278	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2247	0	2134	26	0
1	B	2174	0	2036	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	37	0	58	1	0
6	B	38	0	63	4	0
7	A	9	0	5	0	0
7	B	9	0	5	1	0
8	A	410	0	0	9	0
8	B	421	0	0	7	0
All	All	5359	0	4301	47	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 5.

All (47) 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:118[B]:ARG:HE	1:A:178:HIS:CE1	1.77	1.02
1:A:118[B]:ARG:HE	1:A:178:HIS:HE1	1.03	0.96
1:A:212:THR:HA	1:B:27:THR:HB	1.59	0.84
1:A:184:ASP:HB3	8:A:1037:HOH:O	1.79	0.83
1:A:184:ASP:OD1	8:A:1310:HOH:O	1.97	0.82
6:B:852:HGX:H31	8:B:1284:HOH:O	1.80	0.81
1:B:97:GLU:HG2	8:B:977:HOH:O	1.82	0.78
1:B:271:THR:HG21	1:B:276:GLU:N	2.02	0.75
1:A:194:PRO:HG3	1:A:222[B]:LEU:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118[B]:ARG:NE	1:A:178:HIS:CE1	2.57	0.71
1:A:264:ARG:HD2	1:A:280:PRO:HB2	1.76	0.67
1:A:218:ARG:HH22	1:A:237:HIS:HE1	1.43	0.66
1:B:229:PRO:HD2	8:B:1313:HOH:O	1.94	0.66
1:B:24:PHE:O	1:B:27:THR:HG23	1.96	0.66
1:B:274:GLY:O	1:B:276:GLU:N	2.31	0.64
1:B:207:ARG:NH1	8:B:1137:HOH:O	2.30	0.61
1:A:118[B]:ARG:NE	1:A:178:HIS:HE1	1.88	0.59
1:A:33:LYS:HD2	8:A:1214:HOH:O	2.03	0.59
1:A:266:PRO:HB3	8:A:1211:HOH:O	2.01	0.59
1:A:223:HIS:HA	1:A:237:HIS:HB3	1.84	0.59
1:A:155[A]:VAL:CG2	1:A:222[A]:LEU:HD11	2.33	0.59
1:B:8:GLU:CG	1:B:12:ARG:HH12	2.18	0.56
1:A:269:ALA:HA	8:A:1285:HOH:O	2.08	0.52
1:B:80:LEU:HD11	1:B:199:ILE:HD12	1.92	0.51
1:A:33:LYS:NZ	8:A:1214:HOH:O	2.43	0.51
1:A:194:PRO:HD3	1:A:222[B]:LEU:HD11	1.94	0.50
1:B:265:GLN:O	1:B:266:PRO:CB	2.62	0.48
1:A:39:LEU:HD11	6:B:852:HGX:H201	1.95	0.48
1:B:218:ARG:NH1	7:B:882:BEZ:O1	2.47	0.47
6:A:851:HGX:H192	6:B:852:HGX:H472	1.97	0.47
1:B:24:PHE:O	1:B:27:THR:CG2	2.61	0.46
1:A:85:LEU:O	1:B:44:HIS:HE1	1.98	0.46
1:B:59:THR:HG21	6:B:852:HGX:H2	1.97	0.46
1:B:139:THR:HG23	8:B:1020:HOH:O	2.14	0.46
1:A:9:GLN:HE21	1:B:98:ALA:H	1.62	0.46
1:B:278:ASP:HA	8:B:1272:HOH:O	2.15	0.46
1:A:155[A]:VAL:HG22	1:A:222[A]:LEU:HD11	1.96	0.46
1:A:9:GLN:NE2	1:B:98:ALA:H	2.14	0.46
1:A:33:LYS:CD	8:A:1214:HOH:O	2.61	0.45
1:A:113:VAL:HG13	1:A:176:ARG:CZ	2.49	0.42
1:A:199:ILE:O	1:A:201:HIS:HD2	2.02	0.42
1:A:99:HIS:HE1	8:A:1217:HOH:O	2.02	0.42
1:B:170:ASP:O	1:B:171:ASP:HB2	2.21	0.41
8:A:1207:HOH:O	1:B:12:ARG:HD2	2.21	0.41
1:B:116:SER:OG	1:B:178:HIS:HD2	2.03	0.41
1:B:283:ARG:NH1	8:B:1044:HOH:O	2.53	0.41
1:B:227:THR:HG22	1:B:233:THR:HG23	2.02	0.41

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	296/293 (101%)	291 (98%)	5 (2%)	0	100	100
1	B	281/293 (96%)	272 (97%)	7 (2%)	2 (1%)	18	7
All	All	577/586 (98%)	563 (98%)	12 (2%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	GLU
1	B	277	ILE

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	231/234 (99%)	223 (96%)	8 (4%)	32	12
1	B	221/234 (94%)	214 (97%)	7 (3%)	34	14
All	All	452/468 (97%)	437 (97%)	15 (3%)	33	13

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	76	GLN
1	A	113	VAL
1	A	114	GLU

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Mol	Chain	Res	Type
1	A	121	SER
1	A	192	ILE
1	A	237	HIS
1	A	248	ARG
1	B	27	THR
1	B	64	LEU
1	B	218	ARG
1	B	222	LEU
1	B	271	THR
1	B	278	ASP
1	B	285	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	90	GLN
1	A	95	ASN
1	A	178	HIS
1	A	201	HIS
1	A	237	HIS
1	B	10	GLN
1	B	44	HIS
1	B	90	GLN
1	B	96	ASN
1	B	146	ASN
1	B	178	HIS

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
6	HGX	A	851	-	36,36,47	1.13	2 (5%)	38,38,55	1.23	2 (5%)
7	BEZ	B	882	2	9,9,9	1.92	1 (11%)	11,11,11	1.97	4 (36%)
5	SO4	A	902	-	4,4,4	0.19	0	6,6,6	0.28	0
6	HGX	B	852	-	37,37,47	1.09	2 (5%)	39,39,55	1.26	4 (10%)
7	BEZ	A	881	2	9,9,9	1.76	1 (11%)	11,11,11	1.89	5 (45%)
5	SO4	B	901	-	4,4,4	0.40	0	6,6,6	0.41	0

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
7	BEZ	A	881	2	-	4/4/4/4	0/1/1/1
6	HGX	B	852	-	-	20/39/39/51	-
6	HGX	A	851	-	-	21/38/38/51	-
7	BEZ	B	882	2	-	4/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	882	BEZ	O1-C	5.53	1.38	1.22
6	A	851	HGX	O2-C31	4.83	1.47	1.34
7	A	881	BEZ	O1-C	4.62	1.36	1.22
6	B	852	HGX	O2-C31	4.48	1.46	1.34
6	A	851	HGX	O3-C11	4.15	1.45	1.33
6	B	852	HGX	O3-C11	4.12	1.45	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	851	HGX	O2-C31-C32	4.61	121.46	111.48
6	B	852	HGX	O2-C31-C32	4.57	121.37	111.48
7	B	882	BEZ	O2-C-C1	3.95	124.97	114.84
7	A	881	BEZ	C6-C1-C2	3.80	123.41	118.57
7	B	882	BEZ	O2-C-O1	-2.83	117.26	123.35
6	B	852	HGX	O3-C11-C12	2.66	119.96	111.83
6	A	851	HGX	O3-C11-C12	2.57	119.68	111.83
7	A	881	BEZ	C3-C2-C1	-2.54	117.87	120.36
7	A	881	BEZ	C5-C6-C1	-2.52	117.89	120.36
6	B	852	HGX	O2-C31-O31	-2.35	118.21	123.70
7	A	881	BEZ	O2-C-O1	-2.19	118.65	123.35
7	B	882	BEZ	C3-C2-C1	-2.10	118.30	120.36
7	A	881	BEZ	O2-C-C1	2.09	120.20	114.84
6	B	852	HGX	O3-C11-O11	-2.07	118.46	123.63
7	B	882	BEZ	C6-C1-C2	2.01	121.12	118.57

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	852	HGX	O11-C11-O3-C3
6	B	852	HGX	C12-C11-O3-C3
6	B	852	HGX	O31-C31-O2-C2
6	B	852	HGX	C32-C31-O2-C2
7	B	882	BEZ	O2-C-C1-C6
7	B	882	BEZ	O1-C-C1-C2
7	B	882	BEZ	O1-C-C1-C6
7	B	882	BEZ	O2-C-C1-C2
7	A	881	BEZ	O2-C-C1-C2
7	A	881	BEZ	O1-C-C1-C2
7	A	881	BEZ	O2-C-C1-C6
6	A	851	HGX	C12-C11-O3-C3
6	B	852	HGX	C11-C12-C13-C14
6	A	851	HGX	C31-C32-C33-C34
7	A	881	BEZ	O1-C-C1-C6
6	A	851	HGX	O11-C11-O3-C3
6	A	851	HGX	C37-C38-C39-C40
6	B	852	HGX	C12-C13-C14-C15
6	B	852	HGX	C43-C44-C45-C46
6	B	852	HGX	C37-C38-C39-C40
6	B	852	HGX	C14-C15-C16-C17
6	A	851	HGX	C40-C42-C43-C44
6	B	852	HGX	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
6	B	852	HGX	C32-C33-C34-C35
6	A	851	HGX	C38-C39-C40-C42
6	B	852	HGX	C13-C14-C15-C16
6	B	852	HGX	C42-C43-C44-C45
6	B	852	HGX	C45-C46-C47-C48
6	A	851	HGX	C42-C43-C44-C45
6	A	851	HGX	C19-C20-C21-C22
6	A	851	HGX	C45-C46-C47-C48
6	A	851	HGX	C12-C13-C14-C15
6	A	851	HGX	O2-C2-C3-O3
6	A	851	HGX	C16-C17-C18-C19
6	A	851	HGX	C33-C34-C35-C36
6	B	852	HGX	C15-C16-C17-C18
6	B	852	HGX	C35-C36-C37-C38
6	A	851	HGX	C39-C40-C42-C43
6	A	851	HGX	C35-C36-C37-C38
6	A	851	HGX	C1-C2-C3-O3
6	B	852	HGX	C36-C37-C38-C39
6	B	852	HGX	C38-C39-C40-C42
6	A	851	HGX	C44-C45-C46-C47
6	A	851	HGX	C32-C33-C34-C35
6	A	851	HGX	C36-C37-C38-C39
6	A	851	HGX	C11-C12-C13-C14
6	B	852	HGX	C17-C18-C19-C20
6	A	851	HGX	O2-C31-C32-C33
6	B	852	HGX	C16-C17-C18-C19

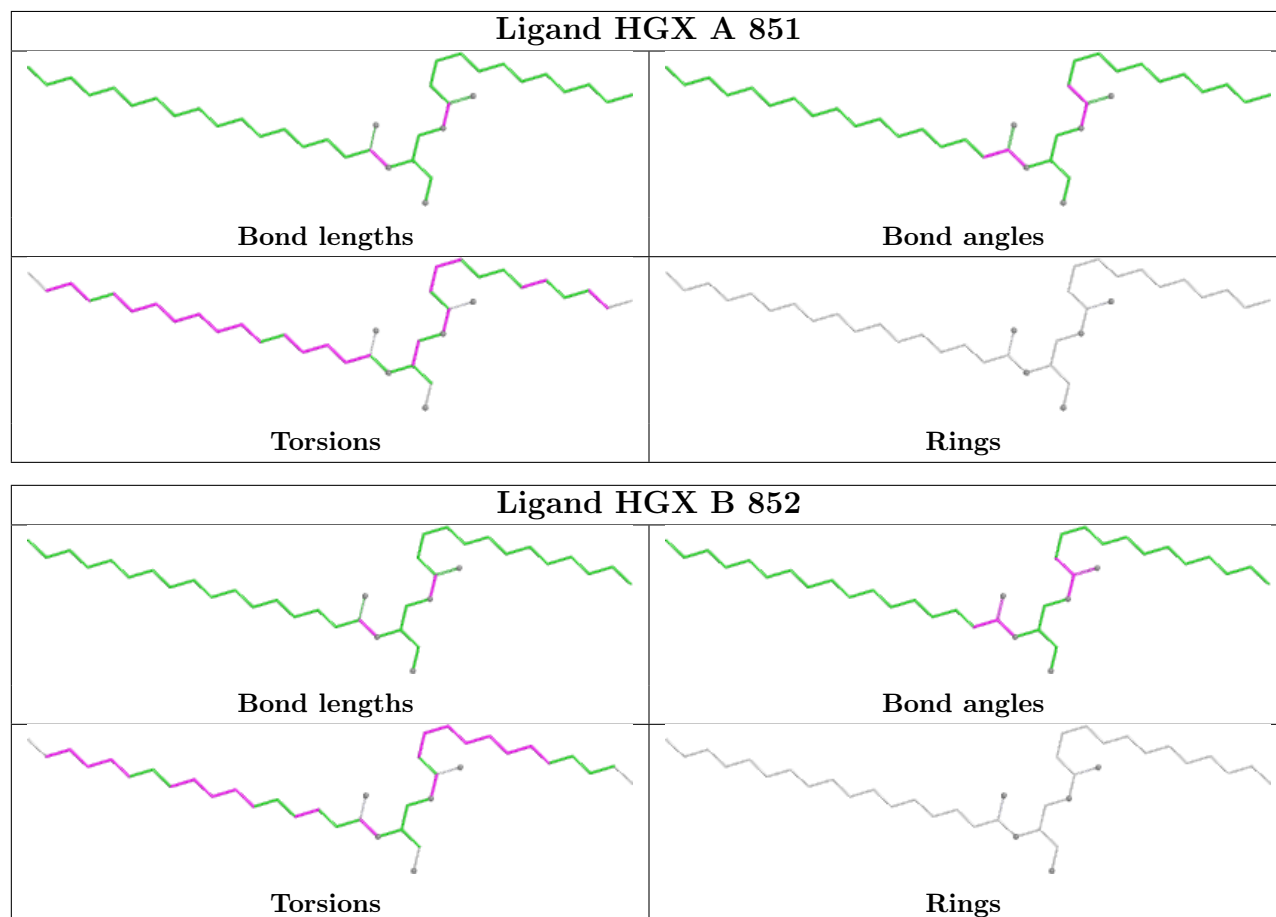
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	851	HGX	1	0
7	B	882	BEZ	1	0
6	B	852	HGX	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	292/293 (99%)	0.15	6 (2%) 63 70	13, 24, 41, 55	6 (2%)
1	B	287/293 (97%)	0.23	15 (5%) 33 37	16, 26, 49, 63	0
All	All	579/586 (98%)	0.19	21 (3%) 46 52	13, 25, 44, 63	6 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	THR	4.7
1	A	267	ALA	4.4
1	B	279	GLY	4.3
1	B	274	GLY	4.2
1	B	266	PRO	4.1
1	B	169	ASP	3.4
1	A	266	PRO	3.4
1	A	269	ALA	3.3
1	A	3	THR	3.0
1	B	273	GLY	2.9
1	A	268	GLY	2.9
1	B	75	ARG	2.6
1	B	269	ALA	2.6
1	B	277	ILE	2.6
1	B	278	ASP	2.5
1	B	4	PRO	2.5
1	B	195	THR	2.4
1	B	271	THR	2.2
1	A	293	ALA	2.2
1	B	128	GLY	2.1
1	B	5	VAL	2.1

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](#)

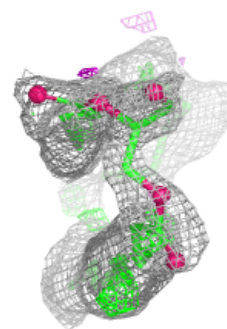
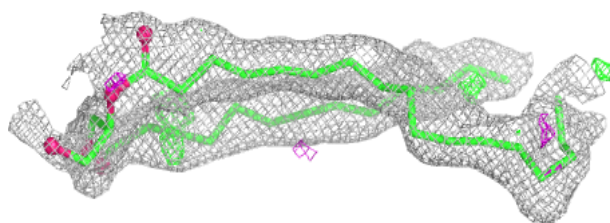
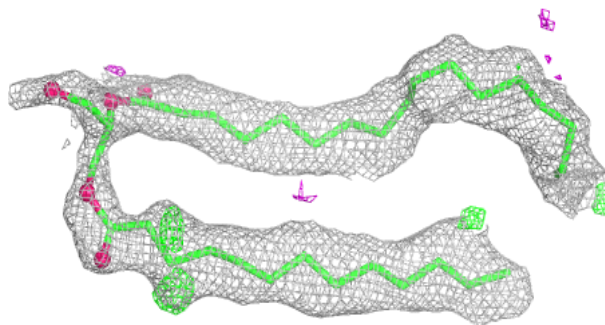
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	901	5/5	0.82	0.15	19,28,31,33	5
6	HGX	B	852	38/48	0.83	0.12	40,47,56,58	0
7	BEZ	B	882	9/9	0.83	0.15	25,27,29,30	9
6	HGX	A	851	37/48	0.86	0.10	32,40,48,52	0
7	BEZ	A	881	9/9	0.94	0.09	21,21,22,24	0
5	SO4	A	902	5/5	0.94	0.08	27,31,34,35	5
4	CL	A	891	1/1	0.98	0.12	23,23,23,23	1
2	FE	B	862	1/1	0.99	0.02	23,23,23,23	0
3	CU	A	871	1/1	1.00	0.05	23,23,23,23	0
2	FE	A	861	1/1	1.00	0.03	19,19,19,19	0

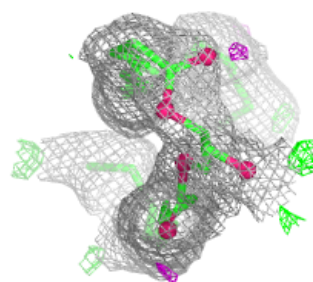
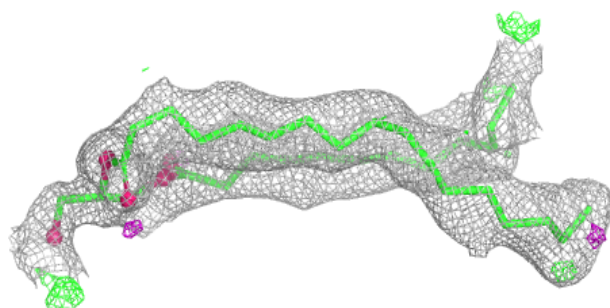
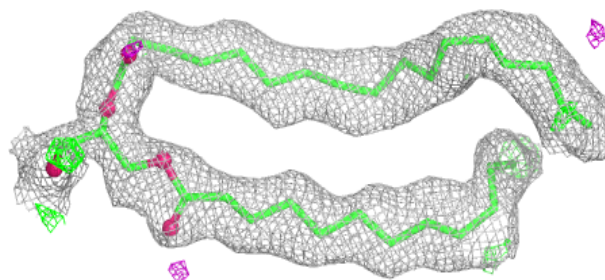
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HGX B 852:

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

**Electron density around HGX A 851:**

$2mF_o-DF_c$ (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.