



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:35 AM UTC

PDB ID : 2Z77 / pdb_00002z77
Title : X-ray crystal structure of RV0760c from Mycobacterium tuberculosis in complex with estradiol-17beta-hemisuccinate
Authors : Cherney, M.M.; Garen, C.R.; James, M.N.G.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2007-08-16
Resolution : 2.03 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:

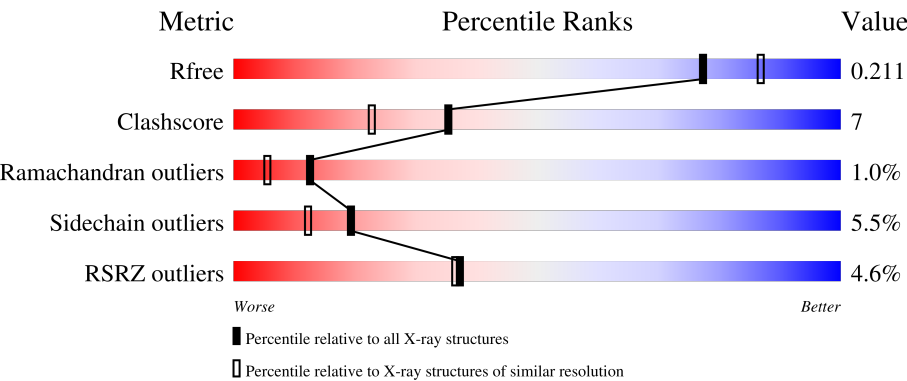
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	139	6% 73% 17% 6%
1	B	139	% 81% 12% 6%
1	C	139	% 81% 12% 6%
1	D	139	9% 73% 19% 6%

2 Entry composition [i](#)

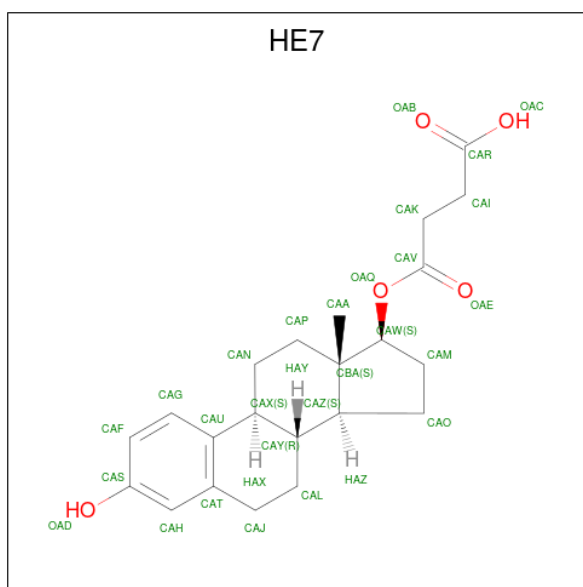
There are 5 unique types of molecules in this entry. The entry contains 4519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative steroid isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	1	0
			1027	644	177	200	6			
1	B	131	Total	C	N	O	S	0	0	0
			1008	634	172	196	6			
1	C	133	Total	C	N	O	S	0	2	0
			1030	647	177	199	7			
1	D	130	Total	C	N	O	S	0	0	0
			1001	630	171	194	6			

- Molecule 2 is 4-[(14beta,17alpha)-3-hydroxyestra-1,3,5(10)-trien-17-yl]oxy}-4-oxobutanoic acid (CCD ID: HE7) (formula: C₂₂H₂₈O₅).



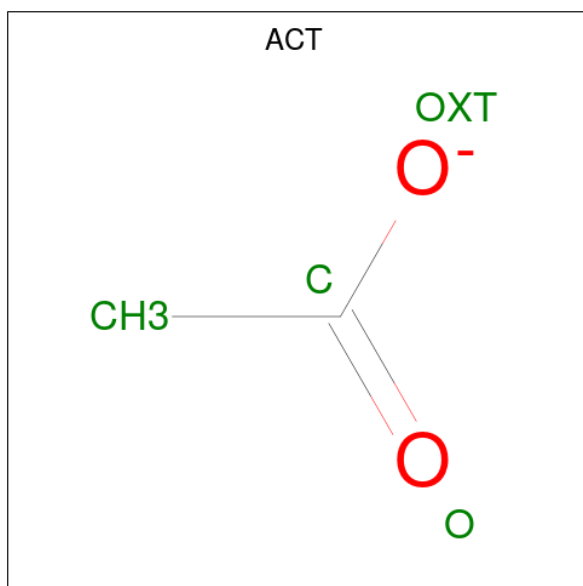
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	22	5		
2	B	1	Total	C	O	0	0
			27	22	5		

Continued on next page...

Continued from previous page...

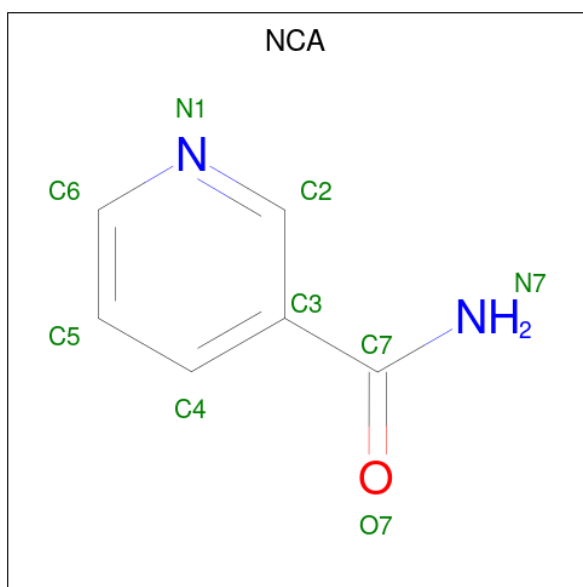
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			27	22	5		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is NICOTINAMIDE (CCD ID: NCA) (formula: $C_6H_6N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			9	6	2	1		

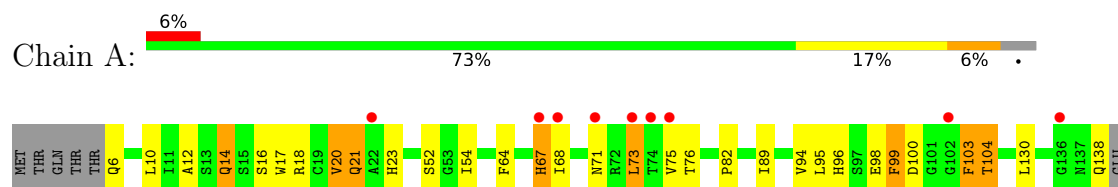
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	105	Total	O	0	0
			105	105		
5	C	104	Total	O	0	0
			104	104		
5	D	55	Total	O	0	0
			55	55		

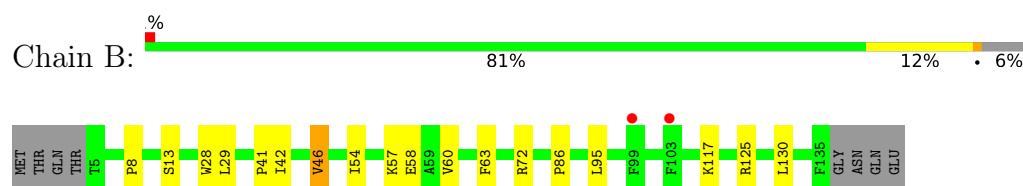
3 Residue-property plots [i](#)

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.

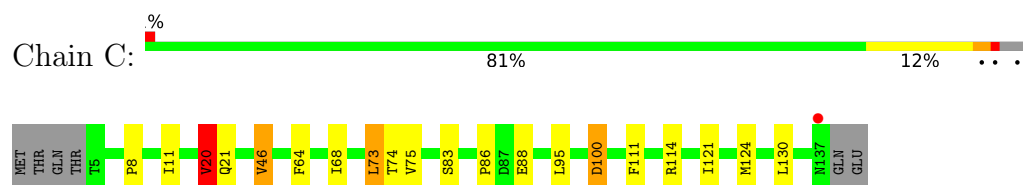
- Molecule 1: Putative steroid isomerase



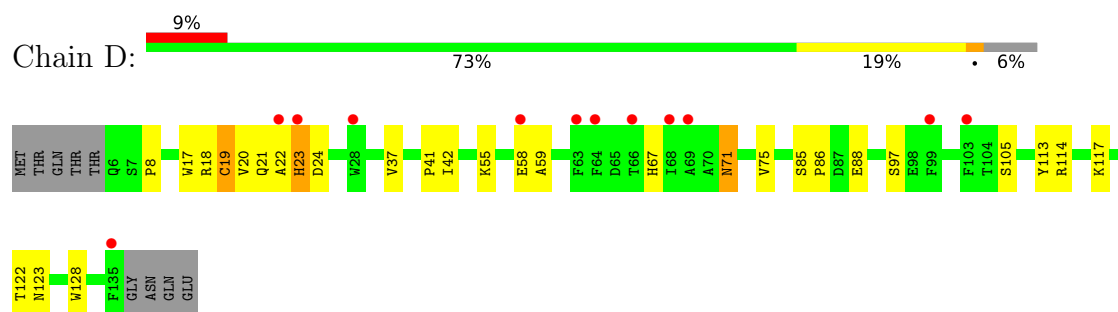
- Molecule 1: Putative steroid isomerase



- Molecule 1: Putative steroid isomerase



- Molecule 1: Putative steroid isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.91Å 66.43Å 80.30Å 90.00° 105.95° 90.00°	Depositor
Resolution (Å)	36.47 – 2.03 36.47 – 2.03	Depositor EDS
% Data completeness (in resolution range)	95.4 (36.47-2.03) 95.6 (36.47-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.277 (Not available) , 0.211	Depositor DCC
R_{free} test set	1760 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.9	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	0.95	EDS
Total number of atoms	4519	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 20.01 % 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 9.5424e-03. 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: HE7, ACT, NCA

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	1.13	2/1054 (0.2%)	1.25	6/1430 (0.4%)
1	B	1.13	0/1031	1.08	2/1400 (0.1%)
1	C	1.13	0/1062	1.10	1/1441 (0.1%)
1	D	0.84	0/1024	0.99	2/1390 (0.1%)
All	All	1.07	2/4171 (0.0%)	1.11	11/5661 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ASP	N-CA	5.21	1.52	1.45
1	A	54	ILE	CA-CB	5.03	1.59	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	PHE	CA-C-N	9.50	138.81	121.70
1	A	103	PHE	C-N-CA	9.50	138.81	121.70
1	A	67	HIS	N-CA-C	7.62	119.58	111.28
1	A	73	LEU	N-CA-C	7.57	119.86	109.11
1	A	103	PHE	O-C-N	-6.34	115.84	123.13
1	C	20	VAL	CB-CA-C	6.32	120.68	112.14
1	B	46	VAL	CB-CA-C	-5.63	104.54	112.14
1	B	13	SER	CB-CA-C	-5.10	102.87	110.88
1	D	85	SER	CA-C-N	-5.09	114.80	120.45
1	D	85	SER	C-N-CA	-5.09	114.80	120.45
1	A	12	ALA	N-CA-C	5.02	117.14	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1027	0	980	15	0
1	B	1008	0	966	11	0
1	C	1030	0	983	17	0
1	D	1001	0	959	19	0
2	A	27	0	26	0	0
2	B	27	0	27	3	0
2	C	27	0	26	3	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
4	D	9	0	6	1	0
5	A	91	0	0	2	0
5	B	105	0	0	0	0
5	C	104	0	0	1	0
5	D	55	0	0	0	0
All	All	4519	0	3979	60	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 7.

All (60) 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:D:58:GLU:HG3	1:D:59:ALA:H	1.23	1.01
1:C:20:VAL:HG22	1:C:68:ILE:HD13	1.68	0.76
1:D:58:GLU:HG3	1:D:59:ALA:N	2.00	0.76
1:C:46:VAL:HG23	5:C:403:HOH:O	1.85	0.75
1:C:20:VAL:HG13	1:C:73:LEU:CD1	2.19	0.73
1:D:22:ALA:O	1:D:23:HIS:HB2	1.90	0.72
1:C:21:GLN:NE2	1:C:75:VAL:H	1.94	0.66
1:C:46:VAL:HG21	2:C:200:HE7:OAD	1.97	0.64
1:A:18:ARG:NH1	5:A:253:HOH:O	2.31	0.63
1:B:130:LEU:O	1:C:46:VAL:HG13	2.00	0.62
1:D:88:GLU:HG2	1:D:114:ARG:HG3	1.81	0.62
1:C:121:ILE:HG21	1:C:124[B]:MET:HG3	1.82	0.61
1:B:95:LEU:HD23	2:B:200:HE7:HAF	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:C	1:A:95:LEU:HD12	2.30	0.57
1:A:98:GLU:HA	1:A:104:THR:H	1.71	0.55
1:D:97:SER:HB2	1:D:105:SER:OG	2.05	0.55
1:C:46:VAL:HG21	2:C:200:HE7:CAS	2.37	0.55
1:D:67:HIS:HA	1:D:71:ASN:OD1	2.08	0.54
2:B:200:HE7:OAC	2:C:200:HE7:HAH	2.07	0.54
1:D:18:ARG:C	1:D:20:VAL:H	2.16	0.53
1:B:95:LEU:HD23	2:B:200:HE7:CAF	2.38	0.53
1:C:8:PRO:HD2	1:C:86:PRO:HB2	1.92	0.52
1:A:95:LEU:HD12	1:A:95:LEU:N	2.26	0.51
1:A:71:ASN:HA	1:A:98:GLU:O	2.10	0.50
1:B:8:PRO:HD2	1:B:86:PRO:HB2	1.93	0.50
1:A:14:GLN:HG3	1:A:17:TRP:CZ3	2.48	0.49
1:D:71:ASN:C	1:D:71:ASN:HD22	2.21	0.49
1:D:113:TYR:OH	4:D:200:NCA:N7	2.46	0.48
1:C:88:GLU:HG2	1:C:114:ARG:HG3	1.96	0.48
1:C:111:PHE:CD1	1:C:124[A]:MET:HE1	2.48	0.48
1:A:6:GLN:HG2	1:A:10:LEU:HD23	1.96	0.47
1:B:130:LEU:O	1:C:46:VAL:CG1	2.62	0.47
1:C:100:ASP:OD2	1:C:100:ASP:N	2.48	0.47
1:C:83:SER:HB2	1:D:42:ILE:HB	1.97	0.46
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.67	0.46
1:D:17:TRP:O	1:D:21:GLN:NE2	2.49	0.46
1:A:16:SER:O	1:A:20:VAL:HG13	2.16	0.45
1:C:21:GLN:HE21	1:C:74:THR:HA	1.81	0.45
1:A:99:PHE:N	1:A:103:PHE:O	2.50	0.45
1:A:64:PHE:O	1:A:68:ILE:HG23	2.16	0.45
1:B:95:LEU:HD12	1:B:95:LEU:N	2.31	0.45
1:A:96:HIS:HB2	5:A:245:HOH:O	2.18	0.44
1:B:28:TRP:CZ3	1:B:60:VAL:HG12	2.53	0.44
1:D:17:TRP:CD1	1:D:75:VAL:HG11	2.53	0.44
1:A:82:PRO:HA	1:A:89:ILE:HG13	1.99	0.44
1:B:42:ILE:HD11	1:B:125:ARG:HB3	2.00	0.43
1:D:122:THR:OG1	1:D:123:ASN:ND2	2.52	0.43
1:A:18:ARG:HG2	1:A:21[B]:GLN:NE2	2.33	0.43
1:A:99:PHE:N	1:A:99:PHE:CD1	2.87	0.43
1:D:22:ALA:O	1:D:23:HIS:CB	2.64	0.43
1:D:37:VAL:HG22	1:D:55:LYS:HG2	2.01	0.43
1:D:41:PRO:HD3	1:D:128:TRP:CZ2	2.54	0.43
1:B:29:LEU:O	1:B:57:LYS:HE3	2.19	0.42
1:D:18:ARG:NH1	1:D:19:CYS:SG	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:HD13	1:B:63:PHE:CD1	2.55	0.42
1:D:8:PRO:HD2	1:D:86:PRO:HB2	2.01	0.42
1:D:58:GLU:CG	1:D:59:ALA:N	2.74	0.41
1:B:95:LEU:N	1:B:95:LEU:CD1	2.83	0.41
1:C:111:PHE:HD1	1:C:124[A]:MET:HE1	1.85	0.41
1:C:64:PHE:CD2	1:C:64:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	132/139 (95%)	124 (94%)	7 (5%)	1 (1%)	16	8
1	B	129/139 (93%)	127 (98%)	2 (2%)	0	100	100
1	C	133/139 (96%)	129 (97%)	3 (2%)	1 (1%)	16	8
1	D	128/139 (92%)	117 (91%)	8 (6%)	3 (2%)	5	1
All	All	522/556 (94%)	497 (95%)	20 (4%)	5 (1%)	12	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	ASP
1	D	23	HIS
1	D	24	ASP
1	A	104	THR
1	D	19	CYS

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	111/116 (96%)	99 (89%)	12 (11%)	6	2
1	B	109/116 (94%)	104 (95%)	5 (5%)	24	17
1	C	112/116 (97%)	106 (95%)	6 (5%)	20	13
1	D	108/116 (93%)	106 (98%)	2 (2%)	50	50
All	All	440/464 (95%)	415 (94%)	25 (6%)	19	11

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	20	VAL
1	A	21[A]	GLN
1	A	21[B]	GLN
1	A	23	HIS
1	A	52	SER
1	A	67	HIS
1	A	73	LEU
1	A	75	VAL
1	A	76	THR
1	A	99	PHE
1	A	138	GLN
1	B	41	PRO
1	B	46	VAL
1	B	58	GLU
1	B	72	ARG
1	B	117	LYS
1	C	11	ILE
1	C	20	VAL
1	C	46	VAL
1	C	73	LEU
1	C	95	LEU
1	C	130	LEU
1	D	71	ASN
1	D	117	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	23	HIS
1	A	138	GLN
1	B	6	GLN
1	B	14	GLN
1	B	123	ASN
1	C	21	GLN
1	C	137	ASN
1	D	67	HIS
1	D	123	ASN

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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HE7	B	200	-	30,30,30	1.69	3 (10%)	45,45,45	1.59	10 (22%)
2	HE7	A	200	-	30,30,30	1.77	3 (10%)	45,45,45	1.36	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	B	300	-	3,3,3	0.92	0	3,3,3	1.11	0
3	ACT	C	400	-	3,3,3	0.86	0	3,3,3	1.15	0
2	HE7	C	200	-	30,30,30	1.68	2 (6%)	45,45,45	1.53	8 (17%)
4	NCA	D	200	-	9,9,9	0.73	0	11,11,11	1.47	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HE7	A	200	-	-	5/9/49/49	0/4/4/4
2	HE7	B	200	-	-	1/9/49/49	0/4/4/4
4	NCA	D	200	-	-	0/4/4/4	0/1/1/1
2	HE7	C	200	-	-	2/9/49/49	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	200	HE7	OAE-CAV	8.01	1.46	1.22
2	B	200	HE7	OAE-CAV	7.09	1.43	1.22
2	C	200	HE7	OAE-CAV	6.76	1.42	1.22
2	C	200	HE7	OAQ-CAV	3.42	1.43	1.34
2	A	200	HE7	OAQ-CAV	3.06	1.42	1.34
2	B	200	HE7	OAQ-CAV	2.57	1.41	1.34
2	B	200	HE7	CAU-CAX	-2.27	1.49	1.52
2	A	200	HE7	CAU-CAX	-2.07	1.49	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	HE7	OAQ-CAV-OAE	-5.69	110.41	123.70
2	C	200	HE7	OAQ-CAV-OAE	-5.69	110.41	123.70
2	A	200	HE7	OAE-CAV-CAK	-3.49	110.14	123.78
2	A	200	HE7	OAQ-CAW-CAM	3.48	119.64	111.06
2	A	200	HE7	OAQ-CAV-OAE	-3.23	116.15	123.70
2	C	200	HE7	OAQ-CAW-CAM	3.18	118.88	111.06
4	D	200	NCA	C6-N1-C2	2.86	121.87	116.85
2	B	200	HE7	OAQ-CAV-CAK	-2.72	105.60	111.48
2	B	200	HE7	CAN-CAX-CAU	-2.63	109.91	113.84
2	C	200	HE7	OAE-CAV-CAK	-2.58	113.69	123.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200	HE7	CAJ-CAT-CAH	-2.50	114.98	119.91
2	B	200	HE7	CAJ-CAL-CAY	-2.47	106.48	110.61
2	A	200	HE7	CAL-CAY-CAX	-2.42	106.96	109.27
2	B	200	HE7	CAI-CAK-CAV	-2.37	106.41	113.44
2	C	200	HE7	CAO-CAZ-CBA	2.23	106.46	103.84
4	D	200	NCA	C3-C2-N1	-2.20	120.23	123.50
2	C	200	HE7	CAW-OAQ-CAV	2.18	122.01	118.03
2	C	200	HE7	CAJ-CAT-CAU	2.14	124.29	121.11
2	B	200	HE7	CAL-CAY-CAZ	2.13	115.61	112.08
2	B	200	HE7	OAE-CAV-CAK	-2.08	115.65	123.78
2	B	200	HE7	CAA-CBA-CAW	-2.06	106.79	109.84
2	B	200	HE7	CAN-CAX-CAY	-2.04	108.79	111.45
2	C	200	HE7	CAM-CAW-CBA	-2.03	103.14	105.18
2	B	200	HE7	CAP-CBA-CAZ	2.00	110.24	107.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	200	HE7	CAM-CAW-OAQ-CAV
2	A	200	HE7	CAR-CAI-CAK-CAV
2	A	200	HE7	OAE-CAV-OAQ-CAW
2	C	200	HE7	CAM-CAW-OAQ-CAV
2	B	200	HE7	OAE-CAV-OAQ-CAW
2	C	200	HE7	OAE-CAV-OAQ-CAW
2	A	200	HE7	CAK-CAI-CAR-OAB
2	A	200	HE7	CAK-CAI-CAR-OAC

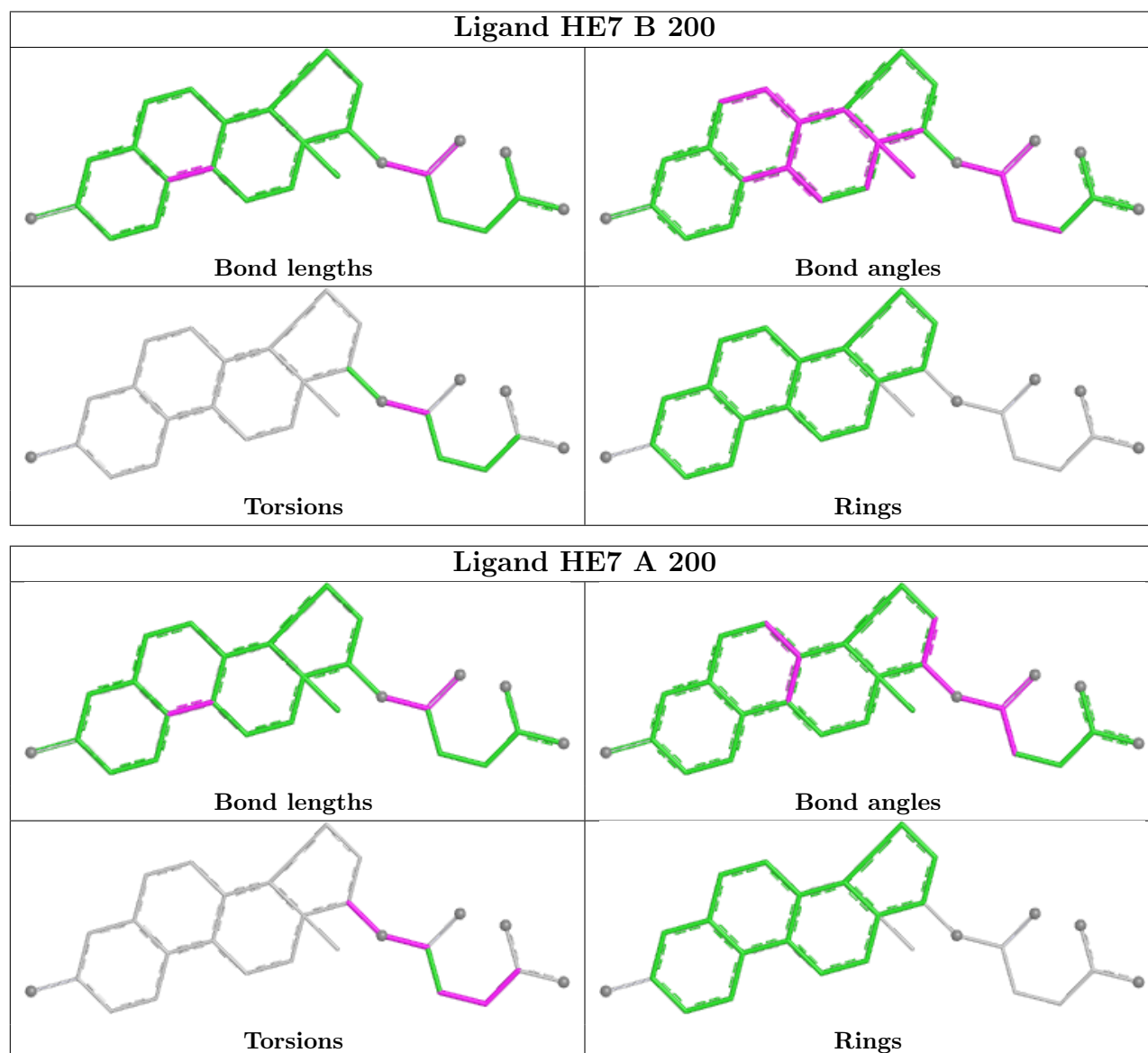
There are no ring outliers.

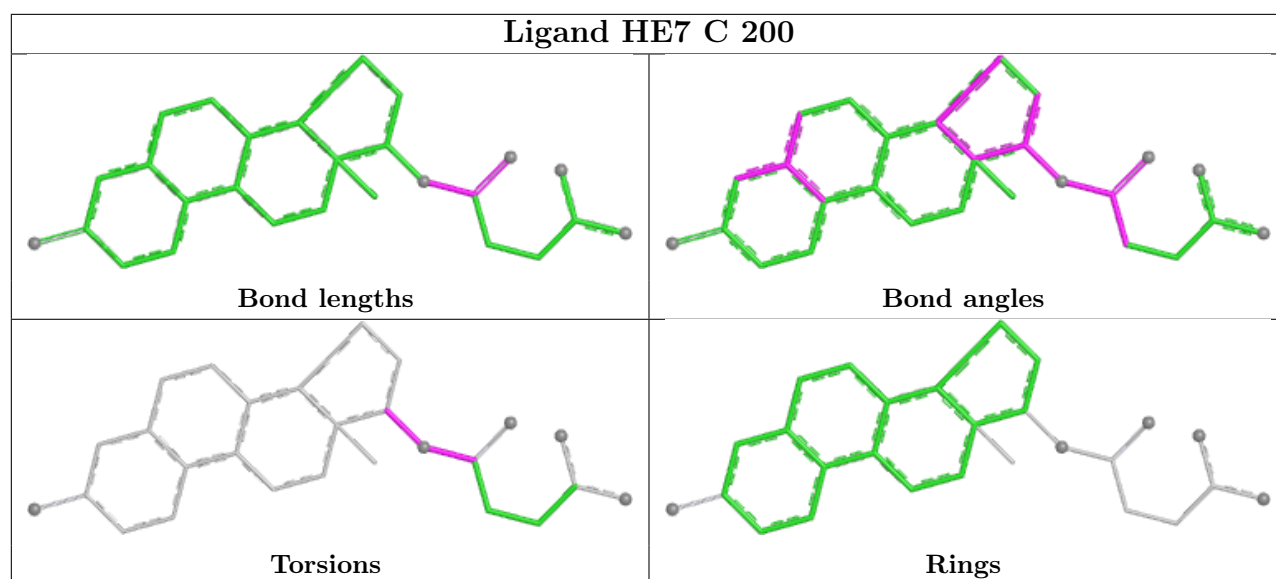
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200	HE7	3	0
2	C	200	HE7	3	0
4	D	200	NCA	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(Å²)	Q<0.9	
1	A	133/139 (95%)	0.15	9 (6%)	23	22	17, 30, 50, 60	1 (0%)
1	B	131/139 (94%)	-0.14	2 (1%)	72	72	15, 26, 49, 58	0
1	C	133/139 (95%)	-0.08	1 (0%)	82	83	16, 28, 43, 52	2 (1%)
1	D	130/139 (93%)	0.70	12 (9%)	14	13	26, 44, 73, 81	0
All	All	527/556 (94%)	0.16	24 (4%)	37	36	15, 30, 64, 81	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	ASN	4.4
1	D	135	PHE	4.0
1	D	69	ALA	3.4
1	A	73	LEU	3.3
1	A	102	GLY	3.2
1	D	23	HIS	2.9
1	A	74	THR	2.8
1	D	58	GLU	2.7
1	A	22	ALA	2.7
1	D	22	ALA	2.6
1	D	103	PHE	2.6
1	D	64	PHE	2.4
1	D	99	PHE	2.4
1	D	68	ILE	2.4
1	D	66	THR	2.4
1	D	28	TRP	2.3
1	A	67	HIS	2.3
1	D	63	PHE	2.2
1	A	71	ASN	2.2
1	A	75	VAL	2.2
1	A	68	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	99	PHE	2.1
1	B	103	PHE	2.1
1	A	136	GLY	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](#)

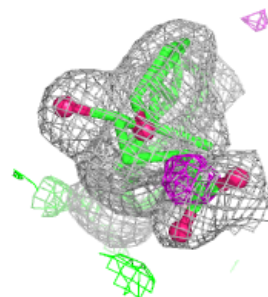
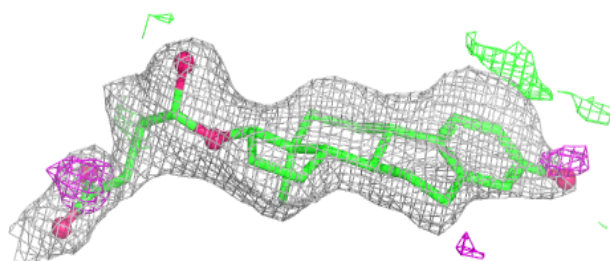
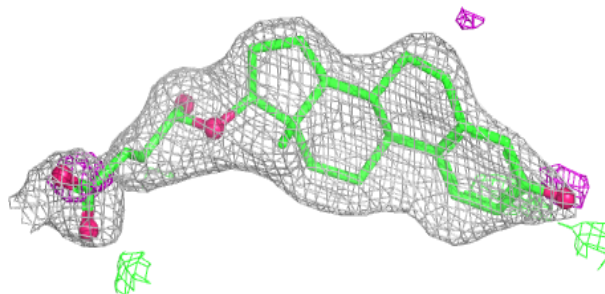
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACT	B	300	4/4	0.79	0.14	50,50,51,51	0
2	HE7	B	200	27/27	0.86	0.11	36,41,43,43	0
2	HE7	C	200	27/27	0.89	0.09	26,31,37,38	0
2	HE7	A	200	27/27	0.89	0.10	34,39,46,47	0
3	ACT	C	400	4/4	0.89	0.12	56,56,56,57	0
4	NCA	D	200	9/9	0.89	0.09	49,50,51,51	0

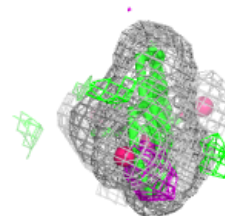
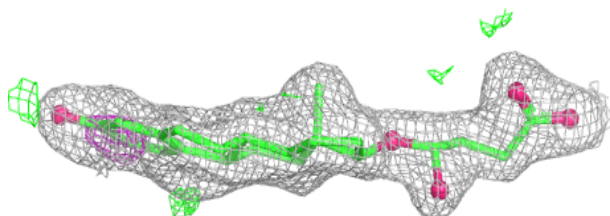
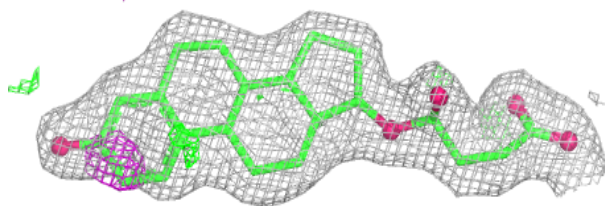
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HE7 B 200:

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

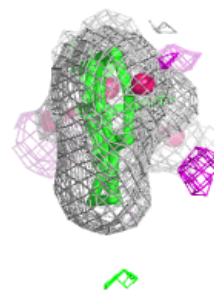
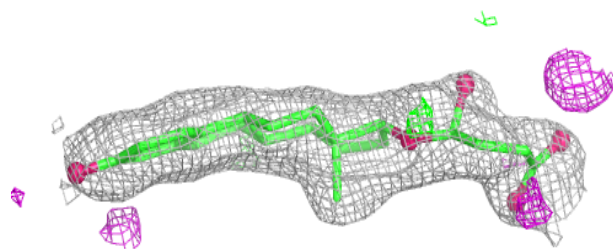
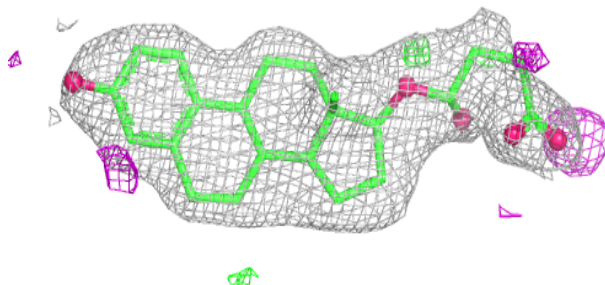
**Electron density around HE7 C 200:**

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



Electron density around HE7 A 200:

$2mF_o-DF_c$ (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.