



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 AM UTC

PDB ID : 4HT2 / pdb_00004ht2
Title : Crystal structure of human carbonic anhydrase isozyme XII with the inhibitor.
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2012-10-31
Resolution : 1.45 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

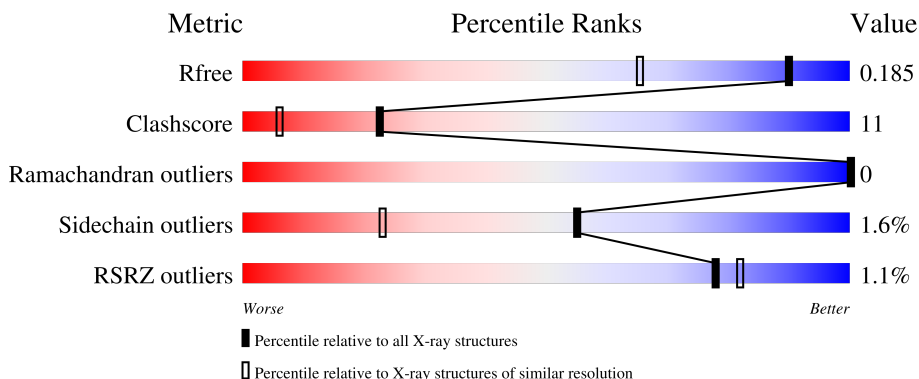
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


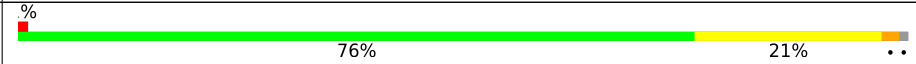
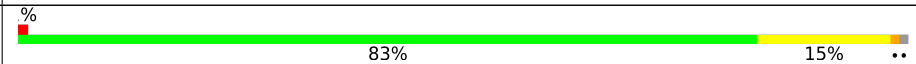

The reported resolution of this entry is 1.45 Å.

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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	263	 78% 19% ..
1	B	263	 76% 21% ..
1	C	263	 83% 15% ..
1	D	263	 81% 16% ..

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
4	PEG	A	303	-	-	X	-
4	PEG	B	303	-	-	X	-
4	PEG	D	303	-	-	X	-
5	EDO	A	304[B]	-	-	X	-
5	EDO	B	305	-	-	X	-
5	EDO	B	307	-	-	X	-
5	EDO	D	305[A]	-	-	X	-
5	EDO	D	306	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10435 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	Total 2220	C 1405	N 382	O 426	S 7	0	15	0
1	B	261	Total 2154	C 1366	N 365	O 415	S 8	0	7	0
1	C	261	Total 2191	C 1387	N 376	O 421	S 7	0	12	0
1	D	261	Total 2170	C 1377	N 370	O 415	S 8	0	9	0

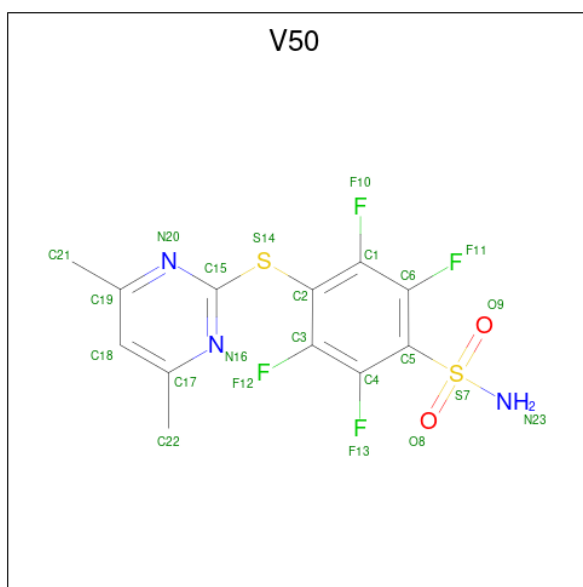
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O43570
B	1	MET	-	expression tag	UNP O43570
C	1	MET	-	expression tag	UNP O43570
D	1	MET	-	expression tag	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

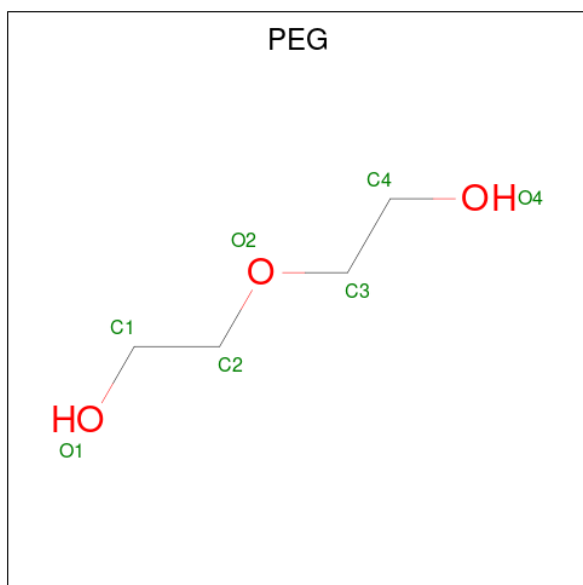
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is 4-[(4,6-dimethylpyrimidin-2-yl)thio]-2,3,5,6-tetrafluorobenzenesulfonamide (CCD ID: V50) (formula: C₁₂H₉F₄N₃O₂S₂).



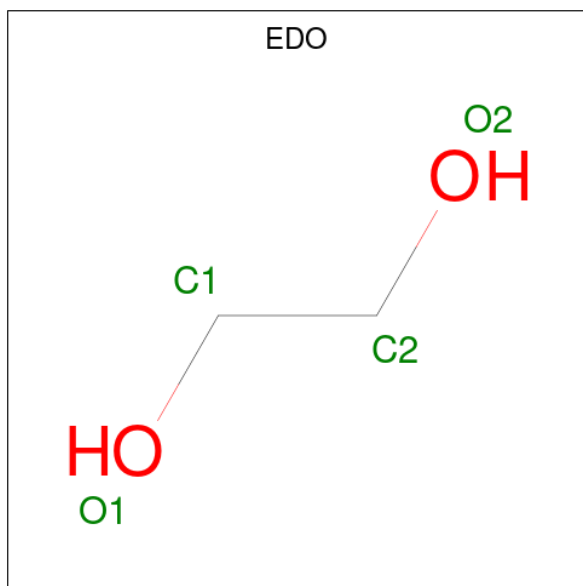
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	A	1	Total 46	C 24	F 8	N 6	O 4	S 4	0	1
3	B	1	Total 23	C 12	F 4	N 3	O 2	S 2	0	0
3	C	1	Total 23	C 12	F 4	N 3	O 2	S 2	0	0
3	D	1	Total 23	C 12	F 4	N 3	O 2	S 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	1
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

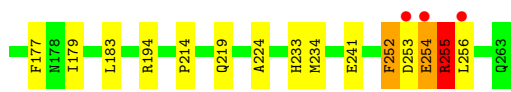
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 8 4 4	0	1
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	369	Total O 369 369	0	0
6	B	375	Total O 375 375	0	0
6	C	350	Total O 350 350	0	0
6	D	410	Total O 410 410	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.71Å 67.26Å 80.69Å 81.78° 84.01° 86.48°	Depositor
Resolution (Å)	26.50 – 1.45 26.50 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (26.50-1.45) 97.1 (26.50-1.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 1.45Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.188 0.148 , 0.185	Depositor DCC
R_{free} test set	16448 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtrriage
Anisotropy	0.243	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10435	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6825e-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: ZN, V50, PEG, EDO

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	1.68	14/2285 (0.6%)	1.37	10/3113 (0.3%)
1	B	1.85	27/2217 (1.2%)	1.42	7/3016 (0.2%)
1	C	1.72	17/2254 (0.8%)	1.38	6/3067 (0.2%)
1	D	1.72	18/2234 (0.8%)	1.42	7/3039 (0.2%)
All	All	1.74	76/8990 (0.8%)	1.39	30/12235 (0.2%)

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	D	0	1

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	THR	C-O	9.66	1.33	1.24
1	B	132	ALA	N-CA	9.36	1.58	1.46
1	B	200	PRO	CA-C	8.12	1.59	1.52
1	A	173	PHE	CA-C	-8.06	1.43	1.52
1	B	17	LYS	N-CA	7.89	1.55	1.46
1	B	256	LEU	CA-C	7.84	1.62	1.52
1	B	174	VAL	CA-C	7.80	1.58	1.52
1	C	19	TYR	CA-CB	7.58	1.61	1.53
1	B	186	ARG	C-O	7.14	1.32	1.23
1	A	67	SER	C-O	6.96	1.30	1.24
1	C	11	GLY	C-O	6.83	1.30	1.23
1	C	217	ILE	CA-C	6.82	1.60	1.52
1	D	140	ALA	N-CA	6.57	1.54	1.46
1	B	174	VAL	C-O	-6.38	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	ASP	N-CA	6.36	1.53	1.46
1	D	252	PHE	C-O	6.20	1.30	1.23
1	B	24	GLY	C-O	6.18	1.30	1.24
1	C	239	PRO	N-CA	6.12	1.54	1.47
1	A	258	TYR	N-CA	6.11	1.53	1.46
1	B	85	TYR	N-CA	6.10	1.53	1.46
1	D	98	ASN	CG-OD1	6.08	1.35	1.23
1	A	128	ASP	CA-C	6.06	1.59	1.52
1	C	24	GLY	C-O	6.04	1.29	1.24
1	B	49	GLN	N-CA	5.93	1.53	1.46
1	B	122	ASN	CA-C	5.91	1.60	1.52
1	D	38	GLN	N-CA	5.89	1.53	1.46
1	A	168	LYS	C-O	5.84	1.30	1.23
1	C	51	TYR	N-CA	5.84	1.53	1.46
1	D	43	LEU	N-CA	5.82	1.53	1.46
1	D	28	SER	N-CA	5.74	1.52	1.45
1	C	188	ALA	CA-CB	5.72	1.63	1.53
1	B	203	ASN	N-CA	5.72	1.53	1.45
1	C	252	PHE	CA-C	-5.71	1.48	1.53
1	A	17	LYS	C-O	5.70	1.30	1.24
1	A	245	ASN	N-CA	5.70	1.53	1.46
1	C	124	ASP	N-CA	5.66	1.53	1.46
1	C	109	GLY	C-O	5.63	1.32	1.24
1	B	224	ALA	CA-CB	5.55	1.62	1.53
1	C	227	THR	CA-CB	5.54	1.61	1.54
1	A	191	TYR	CA-C	-5.53	1.45	1.52
1	A	5	THR	C-O	5.52	1.30	1.24
1	B	137	GLU	N-CA	-5.51	1.38	1.46
1	D	8	GLY	N-CA	5.51	1.52	1.44
1	D	253	ASP	CA-C	-5.45	1.46	1.52
1	D	37	LEU	N-CA	5.41	1.52	1.45
1	B	43	LEU	C-O	-5.40	1.17	1.23
1	B	122	ASN	N-CA	5.37	1.53	1.46
1	D	183	LEU	N-CA	5.36	1.52	1.45
1	B	69	LYS	C-O	5.34	1.30	1.23
1	B	16	SER	N-CA	5.32	1.53	1.46
1	B	144	VAL	CA-CB	5.31	1.61	1.54
1	D	14	SER	N-CA	5.29	1.53	1.46
1	C	16	SER	CA-C	5.29	1.60	1.52
1	C	67	SER	C-O	5.27	1.29	1.23
1	C	175	PRO	C-O	5.25	1.29	1.23
1	D	114	ALA	N-CA	5.24	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	LEU	CA-C	5.24	1.58	1.52
1	D	177	PHE	CA-C	5.23	1.59	1.52
1	D	252	PHE	CA-C	-5.23	1.47	1.53
1	A	143	ALA	N-CA	5.23	1.52	1.46
1	B	179	ILE	CA-CB	-5.20	1.47	1.54
1	B	177	PHE	CA-C	5.19	1.59	1.52
1	D	241	GLU	C-O	5.15	1.29	1.23
1	B	252	PHE	CA-C	-5.15	1.48	1.53
1	D	24	GLY	C-O	5.12	1.28	1.24
1	B	87	ALA	N-CA	5.11	1.52	1.46
1	D	214	PRO	CA-CB	5.09	1.61	1.53
1	B	171	GLU	C-O	5.07	1.30	1.23
1	A	9	PRO	CA-CB	5.07	1.60	1.53
1	D	159	PHE	N-CA	5.05	1.52	1.46
1	C	225	LEU	N-CA	5.05	1.52	1.46
1	B	6	TYR	N-CA	5.04	1.52	1.46
1	A	247	ARG	CA-C	5.03	1.59	1.52
1	A	53	LEU	CA-C	5.02	1.59	1.52
1	B	109	GLY	C-O	5.02	1.31	1.24
1	C	160	SER	N-CA	5.02	1.52	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	ILE	O-C-N	7.43	128.92	122.16
1	C	199	THR	O-C-N	6.80	126.85	121.55
1	C	252	PHE	CB-CA-C	-6.52	102.51	111.51
1	C	199	THR	CA-C-N	-6.51	113.67	120.38
1	C	199	THR	C-N-CA	-6.51	113.67	120.38
1	D	254	GLU	CA-C-N	-6.29	109.41	122.75
1	D	254	GLU	C-N-CA	-6.29	109.41	122.75
1	A	234	MET	CA-C-N	-6.28	113.97	125.02
1	A	234	MET	C-N-CA	-6.28	113.97	125.02
1	B	158	ILE	N-CA-C	-6.03	105.94	111.67
1	B	138	GLY	N-CA-C	6.03	120.49	112.77
1	C	111	HIS	CB-CA-C	-6.01	99.94	109.80
1	A	260	SER	N-CA-C	-5.97	105.65	113.17
1	D	69	LYS	CG-CD-CE	-5.84	97.86	111.30
1	B	72	LEU	O-C-N	5.74	126.73	121.80
1	A	199[A]	THR	OG1-CB-CG2	5.63	120.56	109.30
1	A	199[B]	THR	OG1-CB-CG2	5.63	120.56	109.30
1	A	17	LYS	O-C-N	-5.56	116.08	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	SER	N-CA-C	-5.52	106.13	112.92
1	A	49	GLN	CA-CB-CG	-5.51	103.07	114.10
1	D	19	TYR	O-C-N	-5.33	116.57	121.37
1	D	255	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	C	119	VAL	O-C-N	5.25	128.93	122.95
1	B	84	ARG	CA-C-N	-5.10	115.54	122.93
1	B	84	ARG	C-N-CA	-5.10	115.54	122.93
1	A	109	GLY	CA-C-N	5.08	128.55	121.24
1	A	109	GLY	C-N-CA	5.08	128.55	121.24
1	D	255	ARG	CG-CD-NE	-5.08	100.83	112.00
1	B	122	ASN	O-C-N	5.01	129.28	122.57
1	A	69	LYS	CG-CD-CE	-5.01	99.78	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	255	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2220	0	2095	45	0
1	B	2154	0	2033	51	0
1	C	2191	0	2073	19	0
1	D	2170	0	2051	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	46	0	18	2	0
3	B	23	0	9	0	0
3	C	23	0	9	0	0
3	D	23	0	9	0	0
4	A	7	0	10	15	0
4	B	7	0	10	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	7	0	10	6	0
5	A	16	0	24	6	0
5	B	20	0	30	10	0
5	C	4	0	6	0	0
5	D	16	0	22	15	0
6	A	369	0	0	11	0
6	B	375	0	0	18	0
6	C	350	0	0	2	0
6	D	410	0	0	19	0
All	All	10435	0	8409	183	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 11.

All (183) 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:255:ARG:HB2	1:D:256[B]:LEU:CD2	1.67	1.23
1:A:64:ASN:HD22	4:A:303:PEG:H11	1.05	1.11
1:D:255:ARG:HB2	1:D:256[B]:LEU:HD22	1.12	1.11
1:A:64:ASN:ND2	4:A:303:PEG:H11	1.69	1.07
1:A:255[B]:ARG:NH2	6:A:468:HOH:O	1.88	1.04
1:D:134[A]:ASN:OD1	6:D:779:HOH:O	1.78	0.99
1:D:64:ASN:HD22	5:D:305[A]:EDO:H22	1.23	0.99
1:D:255:ARG:CB	1:D:256[B]:LEU:HD22	1.91	0.98
1:D:18:LYS:HD2	6:D:795:HOH:O	1.61	0.98
1:B:234[B]:MET:HE1	6:B:721:HOH:O	1.63	0.98
1:B:253[B]:ASP:O	6:B:653:HOH:O	1.82	0.97
1:A:137:GLU:HG3	6:A:737:HOH:O	1.67	0.95
1:B:253[B]:ASP:OD1	6:B:704:HOH:O	1.84	0.95
4:A:303:PEG:H32	5:A:304[B]:EDO:O1	1.67	0.95
1:B:89:GLN:HE22	1:B:91:HIS:HD1	1.07	0.93
1:A:69:LYS:NZ	4:A:303:PEG:H12	1.84	0.92
1:D:3[B]:LYS:N	6:D:600:HOH:O	2.03	0.91
1:A:64:ASN:HD22	4:A:303:PEG:C1	1.84	0.89
1:A:69:LYS:CE	4:A:303:PEG:H12	2.04	0.88
1:D:164:HIS:CD2	5:D:306:EDO:H21	2.13	0.83
1:C:164:HIS:HD2	6:C:590:HOH:O	1.60	0.83
1:A:254[B]:GLU:C	1:A:255[B]:ARG:HG3	2.03	0.83
4:B:303:PEG:H22	6:B:499:HOH:O	1.80	0.81
1:A:180:GLU:HG2	6:A:648:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161[B]:HIS:CD2	5:D:306:EDO:O2	2.36	0.79
1:D:252:PHE:CZ	1:D:255:ARG:HG3	2.18	0.79
1:D:255:ARG:HB2	1:D:256[B]:LEU:HD23	1.63	0.78
1:A:254[B]:GLU:O	1:A:255[B]:ARG:HG3	1.84	0.77
1:A:46:LEU:HD22	1:A:78[B]:ILE:CG2	2.15	0.77
1:C:46[A]:LEU:HD22	1:C:78[A]:ILE:HG21	1.66	0.76
1:D:64:ASN:ND2	5:D:305[A]:EDO:H22	2.01	0.76
1:C:110[A]:GLN:NE2	1:D:110:GLN:NE2	2.33	0.76
1:B:78[B]:ILE:HD11	1:B:81:LEU:HD12	1.67	0.75
1:A:69:LYS:HZ3	4:A:303:PEG:H12	1.51	0.75
1:D:64:ASN:HD22	5:D:305[A]:EDO:C2	2.00	0.75
1:B:255:ARG:C	1:B:256:LEU:HD23	2.11	0.74
1:B:89:GLN:NE2	1:B:91:HIS:HD1	1.85	0.74
1:D:255:ARG:NH2	6:D:608:HOH:O	2.21	0.74
1:B:255:ARG:O	1:B:256:LEU:HD22	1.89	0.72
1:A:46:LEU:HD22	1:A:78[B]:ILE:HG21	1.72	0.72
4:D:303:PEG:H32	6:D:786:HOH:O	1.87	0.72
1:A:234:MET:O	1:A:235:ASP:HB2	1.88	0.71
1:A:27:GLN:HE22	1:A:202:CYS:HB3	1.56	0.71
1:A:111[B]:HIS:CE1	6:A:634:HOH:O	2.43	0.70
3:A:302[C]:V50:N16	6:A:592:HOH:O	2.24	0.70
1:B:255:ARG:C	1:B:256:LEU:CD2	2.65	0.70
4:B:303:PEG:H32	6:B:499:HOH:O	1.90	0.70
1:D:164:HIS:NE2	5:D:306:EDO:H21	2.07	0.70
1:B:234[A]:MET:O	1:B:235[A]:ASP:OD1	2.11	0.69
1:D:64:ASN:HD22	5:D:305[B]:EDO:H12	1.58	0.68
1:B:69:LYS:NZ	5:B:305:EDO:H12	2.07	0.68
4:A:303:PEG:C3	5:A:304[B]:EDO:O1	2.40	0.68
1:B:233:HIS:HE1	6:B:714:HOH:O	1.75	0.67
1:C:47:GLU:HG3	1:C:79:GLN:OE1	1.94	0.67
1:D:3[B]:LYS:HG2	1:D:18:LYS:HZ1	1.60	0.67
1:A:147:GLU:HG3	1:A:216:GLN:HG2	1.76	0.67
1:B:69:LYS:HZ2	5:B:305:EDO:H12	1.59	0.66
1:A:110[A]:GLN:NE2	1:B:110:GLN:OE1	2.28	0.65
1:A:7:PHE:CE1	1:B:253[B]:ASP:OD2	2.49	0.65
1:D:161[A]:HIS:HA	5:D:306:EDO:H22	1.77	0.65
1:B:186:ARG:NH2	1:B:189[B]:GLU:OE2	2.30	0.64
1:C:110[A]:GLN:HE21	1:D:110:GLN:HE22	1.46	0.64
1:C:46[A]:LEU:HD22	1:C:78[A]:ILE:CG2	2.28	0.64
1:A:99:ASP:OD1	1:A:101:HIS:HD2	1.81	0.63
1:A:7:PHE:HE1	1:B:253[B]:ASP:OD2	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:SER:HB3	6:D:756:HOH:O	1.98	0.62
1:D:51:TYR:O	1:D:179[B]:ILE:HD12	1.98	0.62
1:D:161[A]:HIS:ND1	5:D:306:EDO:O2	2.29	0.61
1:D:179[B]:ILE:HD12	1:D:179[B]:ILE:H	1.66	0.61
1:B:27:GLN:NE2	1:B:247:ARG:HH12	2.00	0.60
1:D:161[A]:HIS:HD1	5:D:306:EDO:C2	2.13	0.60
1:B:69:LYS:NZ	5:B:305:EDO:C1	2.65	0.59
1:B:27:GLN:HE22	1:B:202:CYS:HB3	1.68	0.59
1:D:255:ARG:NH1	6:D:517:HOH:O	2.24	0.59
1:D:148[B]:MET:HE3	1:D:148[B]:MET:C	2.28	0.59
1:D:255:ARG:CA	1:D:256[B]:LEU:HD22	2.33	0.58
1:B:170:GLN:HE22	1:B:234[A]:MET:HE3	1.67	0.58
1:D:161[B]:HIS:HA	5:D:306:EDO:H22	1.83	0.58
5:D:305[A]:EDO:H12	6:D:665:HOH:O	2.03	0.58
1:A:27:GLN:NE2	1:A:247:ARG:HH12	2.01	0.58
1:B:185:GLU:HG2	6:B:634:HOH:O	2.03	0.58
4:A:303:PEG:H32	5:A:304[A]:EDO:H21	1.86	0.57
1:D:3[A]:LYS:HG3	1:D:18:LYS:HZ1	1.69	0.57
1:B:99:ASP:OD1	1:B:101:HIS:HD2	1.87	0.57
1:D:53:LEU:CD1	1:D:179[B]:ILE:HD11	2.34	0.57
1:A:79:GLN:NE2	6:A:525:HOH:O	2.36	0.57
1:A:78[B]:ILE:HD13	1:A:78[B]:ILE:N	2.20	0.57
1:D:255:ARG:HD2	6:D:444:HOH:O	2.04	0.57
3:A:302[C]:V50:S14	4:A:303:PEG:H41	2.44	0.56
1:B:255:ARG:O	1:B:256:LEU:CD2	2.54	0.56
1:A:51:TYR:OH	1:A:78[B]:ILE:HD11	2.06	0.56
1:B:83:SER:HA	5:B:307:EDO:H11	1.87	0.55
1:D:53:LEU:HG	1:D:179[B]:ILE:CD1	2.36	0.55
1:C:82[A]:GLN:HB2	6:C:584:HOH:O	2.06	0.55
1:D:99:ASP:OD1	1:D:101:HIS:HD2	1.88	0.55
1:A:197[A]:LEU:HD12	1:A:203[A]:ASN:OD1	2.07	0.54
4:B:303:PEG:C4	6:B:769:HOH:O	2.56	0.54
1:D:98:ASN:HB3	6:D:757:HOH:O	2.08	0.54
1:A:253:ASP:O	1:A:254[B]:GLU:HG2	2.07	0.54
1:D:255:ARG:HA	1:D:256[B]:LEU:HD22	1.90	0.53
1:A:234:MET:O	1:A:235:ASP:CB	2.54	0.53
1:A:199[B]:THR:HG21	4:A:303:PEG:O4	2.08	0.53
1:C:110[A]:GLN:NE2	1:D:110:GLN:HE21	2.04	0.53
1:D:233:HIS:HE1	6:D:676:HOH:O	1.91	0.53
1:A:254[B]:GLU:HG2	6:A:558:HOH:O	2.09	0.53
1:B:69:LYS:HD3	5:B:305:EDO:H11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234[A]:MET:O	1:B:235[A]:ASP:CG	2.53	0.52
1:D:53:LEU:HG	1:D:179[B]:ILE:HD11	1.92	0.52
1:B:27:GLN:HE21	1:B:247:ARG:HH12	1.57	0.52
4:B:303:PEG:C1	6:B:573:HOH:O	2.58	0.52
1:A:36[B]:ILE:HD12	1:A:252:PHE:CD2	2.45	0.52
1:C:110[A]:GLN:HE22	1:D:110:GLN:HE21	1.57	0.52
1:D:69:LYS:NZ	5:D:305[A]:EDO:H21	2.25	0.52
1:A:248:GLN:HE21	1:B:251:LYS:NZ	2.08	0.51
1:C:201:PRO:HG2	1:C:203[A]:ASN:OD1	2.11	0.51
1:D:53:LEU:HD11	1:D:179[B]:ILE:HD11	1.92	0.51
1:A:69:LYS:HE2	4:A:303:PEG:H12	1.89	0.50
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.93	0.50
1:A:220:GLU:OE1	6:A:716:HOH:O	2.20	0.50
1:D:148[A]:MET:SD	1:D:219:GLN:HB2	2.52	0.50
1:D:234:MET:HE3	6:D:508:HOH:O	2.10	0.50
1:B:185:GLU:CD	6:B:748:HOH:O	2.56	0.48
1:C:19:TYR:CD1	1:C:200:PRO:HB3	2.48	0.48
4:D:303:PEG:H41	6:D:551:HOH:O	2.13	0.48
1:A:254[B]:GLU:O	1:A:255[B]:ARG:CG	2.59	0.48
4:A:303:PEG:H32	5:A:304[B]:EDO:C1	2.42	0.48
1:D:161[B]:HIS:HD2	5:D:306:EDO:O2	1.94	0.48
1:B:254:GLU:HG3	6:B:702:HOH:O	2.14	0.47
1:A:27:GLN:HE21	1:A:247:ARG:HH12	1.62	0.47
1:A:111[A]:HIS:HE1	6:A:406:HOH:O	1.97	0.47
4:B:303:PEG:H42	6:B:769:HOH:O	2.15	0.47
1:C:52:ASN:HA	1:C:178:ASN:HA	1.97	0.47
1:D:53:LEU:CG	1:D:179[B]:ILE:HD11	2.44	0.47
4:D:303:PEG:H41	6:D:582:HOH:O	2.14	0.47
1:C:99:ASP:OD1	1:C:101:HIS:HD2	1.98	0.47
1:A:148:MET:HG3	1:A:219[B]:GLN:HE21	1.80	0.46
1:B:253[B]:ASP:CG	6:B:704:HOH:O	2.48	0.46
1:B:83:SER:CB	5:B:307:EDO:H11	2.46	0.46
1:B:185:GLU:O	1:B:186:ARG:C	2.59	0.46
1:A:49:GLN:OE1	1:A:77[A]:HIS:NE2	2.43	0.45
4:D:303:PEG:C3	6:D:786:HOH:O	2.55	0.45
1:C:147:GLU:HG3	1:C:216:GLN:HG2	1.99	0.45
1:B:69:LYS:HZ3	5:B:305:EDO:C1	2.30	0.44
1:B:124:ASP:HB3	5:B:307:EDO:H22	2.00	0.44
1:B:255:ARG:C	1:B:256:LEU:HD22	2.38	0.44
1:B:83:SER:HA	5:B:307:EDO:C1	2.48	0.43
1:D:224:ALA:CA	4:D:303:PEG:H12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:GLU:OE2	6:D:597:HOH:O	2.21	0.43
4:D:303:PEG:C4	6:D:551:HOH:O	2.65	0.43
1:A:33:HIS:O	1:A:36[A]:ILE:HG13	2.18	0.43
1:C:46[B]:LEU:HD12	1:C:46[B]:LEU:N	2.32	0.43
1:A:69:LYS:NZ	4:A:303:PEG:C1	2.71	0.43
1:A:147:GLU:CD	6:A:589:HOH:O	2.61	0.43
1:B:82:GLN:HG2	6:B:719:HOH:O	2.18	0.43
1:D:135:LYS:NZ	6:D:779:HOH:O	2.50	0.43
1:B:89:GLN:C	1:B:89:GLN:HE21	2.25	0.42
1:D:49:GLN:HE22	1:D:79:GLN:NE2	2.17	0.42
5:A:304[B]:EDO:H22	6:A:498:HOH:O	2.19	0.42
1:B:69:LYS:HZ2	5:B:305:EDO:C1	2.26	0.42
4:B:303:PEG:H12	6:B:573:HOH:O	2.19	0.42
1:A:36[A]:ILE:HD12	1:A:36[A]:ILE:C	2.45	0.42
1:B:78[B]:ILE:CD1	1:B:81:LEU:HD12	2.45	0.42
1:D:69:LYS:HD3	5:D:305[A]:EDO:H21	2.02	0.42
1:D:161[B]:HIS:HE1	6:D:530:HOH:O	2.02	0.42
1:A:19:TYR:CD1	1:A:200:PRO:HB3	2.55	0.41
1:B:79:GLN:HG3	1:B:80:GLY:N	2.36	0.41
1:D:148[B]:MET:HE2	1:D:148[B]:MET:HB3	1.96	0.41
1:D:255:ARG:HG3	1:D:256[B]:LEU:H	1.85	0.41
1:B:49:GLN:OE1	1:B:77:HIS:CD2	2.73	0.41
1:B:192:ARG:HD2	1:B:207:LEU:HD11	2.02	0.41
1:C:192:ARG:HD2	1:C:207:LEU:HD11	2.03	0.41
1:C:253:ASP:O	1:C:255[A]:ARG:HG3	2.21	0.41
1:B:185:GLU:HG2	6:B:748:HOH:O	2.20	0.40
1:B:185:GLU:CG	6:B:748:HOH:O	2.69	0.40
1:B:256:LEU:CD2	1:B:256:LEU:N	2.83	0.40
1:C:110[A]:GLN:HE22	1:D:110:GLN:NE2	2.13	0.40
1:D:255:ARG:HD2	1:D:255:ARG:HH11	1.55	0.40
1:A:49:GLN:HB2	1:A:77[A]:HIS:CD2	2.56	0.40
4:A:303:PEG:H21	5:A:304[A]:EDO:O1	2.21	0.40
1:B:170:GLN:HE22	1:B:234[A]:MET:CE	2.33	0.40
4:B:303:PEG:H11	6:B:573:HOH:O	2.20	0.40
1:B:60:LEU:HD11	1:B:171:GLU:HB3	2.02	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	274/263 (104%)	269 (98%)	5 (2%)	0	100	100
1	B	266/263 (101%)	258 (97%)	8 (3%)	0	100	100
1	C	271/263 (103%)	265 (98%)	6 (2%)	0	100	100
1	D	267/263 (102%)	262 (98%)	5 (2%)	0	100	100
All	All	1078/1052 (102%)	1054 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	248/235 (106%)	243 (98%)	5 (2%)	48	16
1	B	240/235 (102%)	237 (99%)	3 (1%)	61	31
1	C	245/235 (104%)	242 (99%)	3 (1%)	63	33
1	D	242/235 (103%)	238 (98%)	4 (2%)	53	21
All	All	975/940 (104%)	960 (98%)	15 (2%)	55	25

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

Mol	Chain	Res	Type
1	A	3	LYS
1	A	89	GLN

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Mol	Chain	Res	Type
1	A	137	GLU
1	A	156	ASP
1	A	194	ARG
1	B	89	GLN
1	B	156	ASP
1	B	256	LEU
1	C	25	LEU
1	C	89	GLN
1	C	156	ASP
1	D	89	GLN
1	D	156	ASP
1	D	194	ARG
1	D	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	64	ASN
1	A	66	HIS
1	A	101	HIS
1	A	233	HIS
1	A	248	GLN
1	A	250	GLN
1	B	13	ASN
1	B	27	GLN
1	B	56	ASN
1	B	89	GLN
1	B	111	HIS
1	B	170	GLN
1	B	233	HIS
1	C	164	HIS
1	C	250	GLN
1	D	13	ASN
1	D	79	GLN
1	D	110	GLN
1	D	111	HIS
1	D	233	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	EDO	A	304[B]	-	3,3,3	0.46	0	2,2,2	0.66	0
5	EDO	A	306	-	3,3,3	0.50	0	2,2,2	0.41	0
5	EDO	B	305	-	3,3,3	0.19	0	2,2,2	0.89	0
3	V50	C	302	2	24,24,24	1.74	6 (25%)	37,37,37	2.69	15 (40%)
5	EDO	A	304[A]	-	3,3,3	0.74	0	2,2,2	0.79	0
3	V50	A	302[C]	2	24,24,24	1.14	4 (16%)	37,37,37	2.81	15 (40%)
3	V50	D	302	2	24,24,24	1.17	1 (4%)	37,37,37	1.71	9 (24%)
5	EDO	D	306	-	3,3,3	1.19	1 (33%)	2,2,2	1.00	0
5	EDO	A	305	-	3,3,3	0.44	0	2,2,2	0.23	0
5	EDO	B	304	-	3,3,3	0.41	0	2,2,2	0.92	0
5	EDO	B	308	-	3,3,3	0.48	0	2,2,2	0.51	0
4	PEG	A	303	-	6,6,6	0.92	0	5,5,5	1.42	1 (20%)
5	EDO	B	306	-	3,3,3	0.88	0	2,2,2	0.11	0
3	V50	B	302	2	24,24,24	2.12	9 (37%)	37,37,37	2.32	13 (35%)
5	EDO	D	305[A]	-	3,3,3	1.01	0	2,2,2	0.86	0
5	EDO	B	307	-	3,3,3	0.27	0	2,2,2	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	305[B]	-	3,3,3	0.51	0	2,2,2	0.31	0
4	PEG	D	303	-	6,6,6	1.06	0	5,5,5	1.45	1 (20%)
5	EDO	D	304	-	3,3,3	0.55	0	2,2,2	0.69	0
5	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.55	0
4	PEG	B	303	-	6,6,6	0.99	0	5,5,5	1.50	1 (20%)
3	V50	A	302[B]	2	24,24,24	1.34	5 (20%)	37,37,37	2.18	12 (32%)

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	EDO	A	304[B]	-	-	1/1/1/1	-
5	EDO	A	306	-	-	1/1/1/1	-
5	EDO	B	305	-	-	0/1/1/1	-
3	V50	C	302	2	-	1/10/10/10	0/2/2/2
5	EDO	A	304[A]	-	-	1/1/1/1	-
3	V50	A	302[C]	2	-	1/10/10/10	0/2/2/2
3	V50	D	302	2	-	1/10/10/10	0/2/2/2
5	EDO	D	306	-	-	1/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	B	304	-	-	0/1/1/1	-
5	EDO	B	308	-	-	0/1/1/1	-
4	PEG	A	303	-	-	2/4/4/4	-
5	EDO	B	306	-	-	0/1/1/1	-
3	V50	B	302	2	-	1/10/10/10	0/2/2/2
5	EDO	D	305[A]	-	-	1/1/1/1	-
5	EDO	B	307	-	-	0/1/1/1	-
5	EDO	D	305[B]	-	-	1/1/1/1	-
4	PEG	D	303	-	-	3/4/4/4	-
5	EDO	D	304	-	-	0/1/1/1	-
5	EDO	C	303	-	-	0/1/1/1	-
4	PEG	B	303	-	-	3/4/4/4	-
3	V50	A	302[B]	2	-	3/10/10/10	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	V50	C5-S7	5.53	1.87	1.78
3	C	302	V50	C5-S7	4.07	1.85	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	V50	F11-C6	-3.85	1.29	1.34
3	B	302	V50	C15-S14	3.03	1.80	1.76
3	B	302	V50	C15-N20	-2.74	1.29	1.34
3	C	302	V50	F11-C6	-2.68	1.31	1.34
3	A	302[B]	V50	C1-C6	2.62	1.42	1.38
3	C	302	V50	C22-C17	2.61	1.56	1.50
3	C	302	V50	O9-S7	2.51	1.48	1.43
3	B	302	V50	C19-N20	2.44	1.39	1.34
3	B	302	V50	C15-N16	2.39	1.37	1.34
3	A	302[C]	V50	C4-C5	2.35	1.43	1.39
3	B	302	V50	C1-C6	2.32	1.41	1.38
3	A	302[B]	V50	C6-C5	2.22	1.43	1.39
3	A	302[B]	V50	C4-C5	2.20	1.43	1.39
3	B	302	V50	C4-C5	2.20	1.43	1.39
3	C	302	V50	F13-C4	2.16	1.38	1.34
3	D	302	V50	C2-C3	2.15	1.42	1.39
3	A	302[C]	V50	C3-C4	2.14	1.41	1.38
3	C	302	V50	C4-C5	2.14	1.43	1.39
3	A	302[B]	V50	F13-C4	-2.14	1.31	1.34
3	B	302	V50	C2-C1	-2.11	1.35	1.39
3	A	302[C]	V50	O9-S7	-2.10	1.40	1.43
3	A	302[C]	V50	O8-S7	2.10	1.47	1.43
5	D	306	EDO	O2-C2	-2.04	1.31	1.42
3	A	302[B]	V50	C15-S14	-2.01	1.73	1.76

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	V50	C6-C5-C4	-9.63	110.06	116.65
3	A	302[C]	V50	C6-C5-C4	-9.28	110.30	116.65
3	A	302[C]	V50	C17-C18-C19	-6.09	111.58	118.80
3	B	302	V50	C22-C17-N16	-5.88	107.67	116.56
3	A	302[B]	V50	C17-C18-C19	-5.77	111.96	118.80
3	C	302	V50	C17-C18-C19	-5.62	112.14	118.80
3	A	302[C]	V50	O9-S7-N23	5.62	115.45	107.35
3	B	302	V50	C18-C17-N16	5.13	128.66	121.50
3	B	302	V50	C15-N16-C17	-4.89	110.61	115.96
3	A	302[C]	V50	C22-C17-C18	-4.58	115.03	121.80
3	C	302	V50	C6-C5-S7	4.31	131.82	121.34
3	B	302	V50	C17-C18-C19	-4.30	113.70	118.80
3	A	302[C]	V50	C1-C6-C5	4.24	126.90	121.78
3	C	302	V50	C1-C6-C5	4.04	126.66	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	V50	O8-S7-N23	3.99	113.10	107.35
3	C	302	V50	O9-S7-N23	3.95	113.05	107.35
3	A	302[B]	V50	O9-S7-C5	-3.80	101.69	107.28
3	D	302	V50	C17-C18-C19	-3.78	114.32	118.80
3	A	302[B]	V50	C15-S14-C2	3.73	108.24	101.92
3	A	302[B]	V50	C3-C4-C5	-3.50	117.55	121.78
3	A	302[C]	V50	F11-C6-C1	-3.49	112.33	119.27
3	A	302[C]	V50	C18-C19-N20	3.48	126.36	121.50
3	A	302[B]	V50	C18-C19-N20	3.35	126.18	121.50
3	B	302	V50	C1-C6-C5	-3.28	117.81	121.78
3	C	302	V50	C18-C17-N16	3.24	126.03	121.50
3	A	302[C]	V50	C18-C17-N16	3.15	125.90	121.50
3	B	302	V50	F10-C1-C6	-3.12	113.07	119.27
3	C	302	V50	C3-C4-C5	3.07	125.49	121.78
3	A	302[B]	V50	F12-C3-C4	-3.07	113.16	119.27
3	A	302[C]	V50	O8-S7-N23	-3.07	102.93	107.35
3	A	302[B]	V50	C6-C5-S7	-3.04	113.96	121.34
3	B	302	V50	O9-S7-N23	3.01	111.69	107.35
3	D	302	V50	C18-C17-N16	2.98	125.66	121.50
3	A	302[C]	V50	F13-C4-C3	-2.96	113.38	119.27
4	A	303	PEG	O1-C1-C2	2.96	129.23	111.82
3	C	302	V50	C5-S7-N23	-2.89	103.06	108.26
3	D	302	V50	C4-C5-S7	2.89	128.37	121.34
3	A	302[B]	V50	C6-C5-C4	2.87	118.62	116.65
3	C	302	V50	O8-S7-N23	2.85	111.47	107.35
3	C	302	V50	F11-C6-C5	-2.84	115.66	120.76
3	B	302	V50	C15-S14-C2	2.82	106.69	101.92
3	A	302[B]	V50	C21-C19-N20	-2.72	112.44	116.56
3	A	302[C]	V50	C4-C5-S7	2.71	127.94	121.34
3	A	302[B]	V50	C18-C17-N16	2.68	125.24	121.50
4	B	303	PEG	C3-O2-C2	2.63	124.78	113.26
3	A	302[C]	V50	C15-S14-C2	2.61	106.33	101.92
4	D	303	PEG	C3-O2-C2	2.54	124.37	113.26
3	C	302	V50	C21-C19-N20	-2.51	112.77	116.56
3	A	302[B]	V50	O8-S7-O9	2.50	122.64	118.80
3	D	302	V50	F11-C6-C1	-2.50	114.31	119.27
3	A	302[C]	V50	O8-S7-C5	-2.48	103.64	107.28
3	D	302	V50	C15-S14-C2	2.46	106.09	101.92
3	B	302	V50	C6-C5-S7	2.41	127.21	121.34
3	C	302	V50	C18-C19-N20	2.41	124.87	121.50
3	B	302	V50	C4-C5-S7	-2.31	115.72	121.34
3	C	302	V50	C22-C17-C18	-2.29	118.42	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	V50	F13-C4-C3	-2.25	114.80	119.27
3	B	302	V50	F10-C1-C2	2.24	122.86	119.79
3	D	302	V50	O9-S7-C5	-2.21	104.03	107.28
3	D	302	V50	C6-C5-S7	-2.20	116.01	121.34
3	B	302	V50	O8-S7-N23	2.20	110.52	107.35
3	D	302	V50	F10-C1-C2	-2.17	116.81	119.79
3	A	302[B]	V50	C4-C5-S7	2.14	126.54	121.34
3	B	302	V50	O8-S7-C5	-2.11	104.17	107.28
3	A	302[C]	V50	C3-C4-C5	2.10	124.32	121.78
3	A	302[C]	V50	F12-C3-C2	-2.10	116.91	119.79
3	C	302	V50	C3-C2-S14	-2.04	118.01	121.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

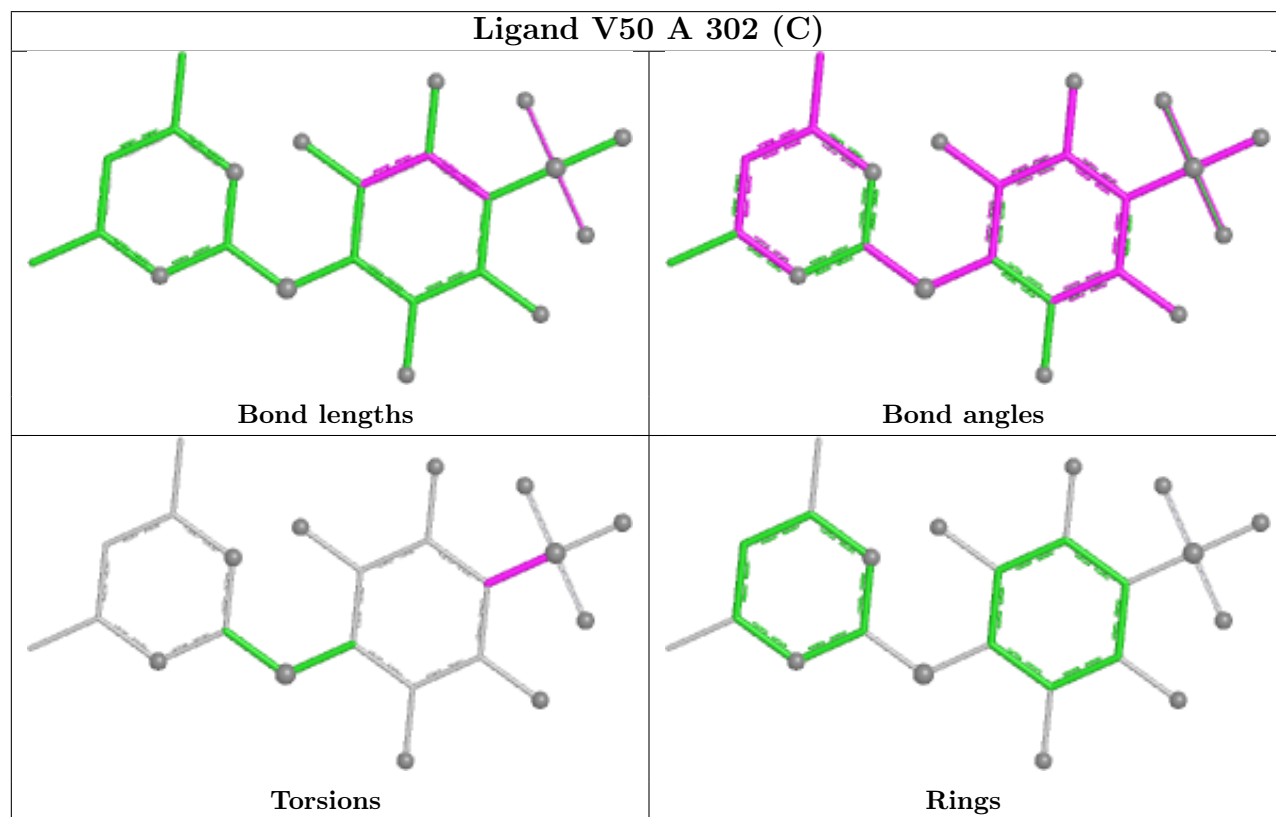
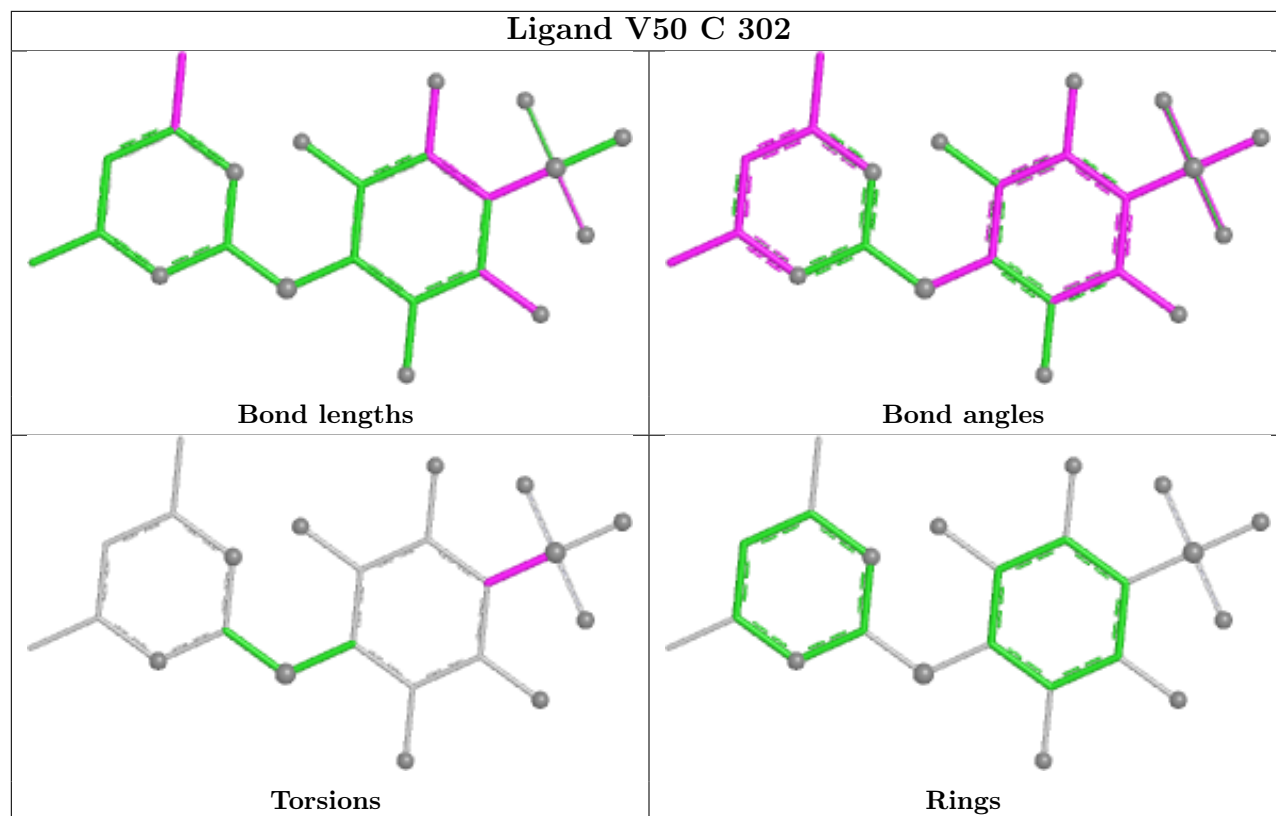
Mol	Chain	Res	Type	Atoms
3	A	302[B]	V50	C4-C5-S7-O9
3	A	302[B]	V50	C4-C5-S7-N23
4	B	303	PEG	O2-C3-C4-O4
4	D	303	PEG	O1-C1-C2-O2
4	A	303	PEG	O2-C3-C4-O4
4	B	303	PEG	O1-C1-C2-O2
5	A	304[A]	EDO	O1-C1-C2-O2
5	D	305[A]	EDO	O1-C1-C2-O2
5	D	306	EDO	O1-C1-C2-O2
3	B	302	V50	C6-C5-S7-N23
3	C	302	V50	C6-C5-S7-N23
3	D	302	V50	C4-C5-S7-N23
5	A	306	EDO	O1-C1-C2-O2
4	A	303	PEG	O1-C1-C2-O2
4	D	303	PEG	C1-C2-O2-C3
4	D	303	PEG	C4-C3-O2-C2
3	A	302[B]	V50	C6-C5-S7-O9
3	A	302[C]	V50	C4-C5-S7-N23
5	D	305[B]	EDO	O1-C1-C2-O2
5	A	304[B]	EDO	O1-C1-C2-O2
4	B	303	PEG	C1-C2-O2-C3

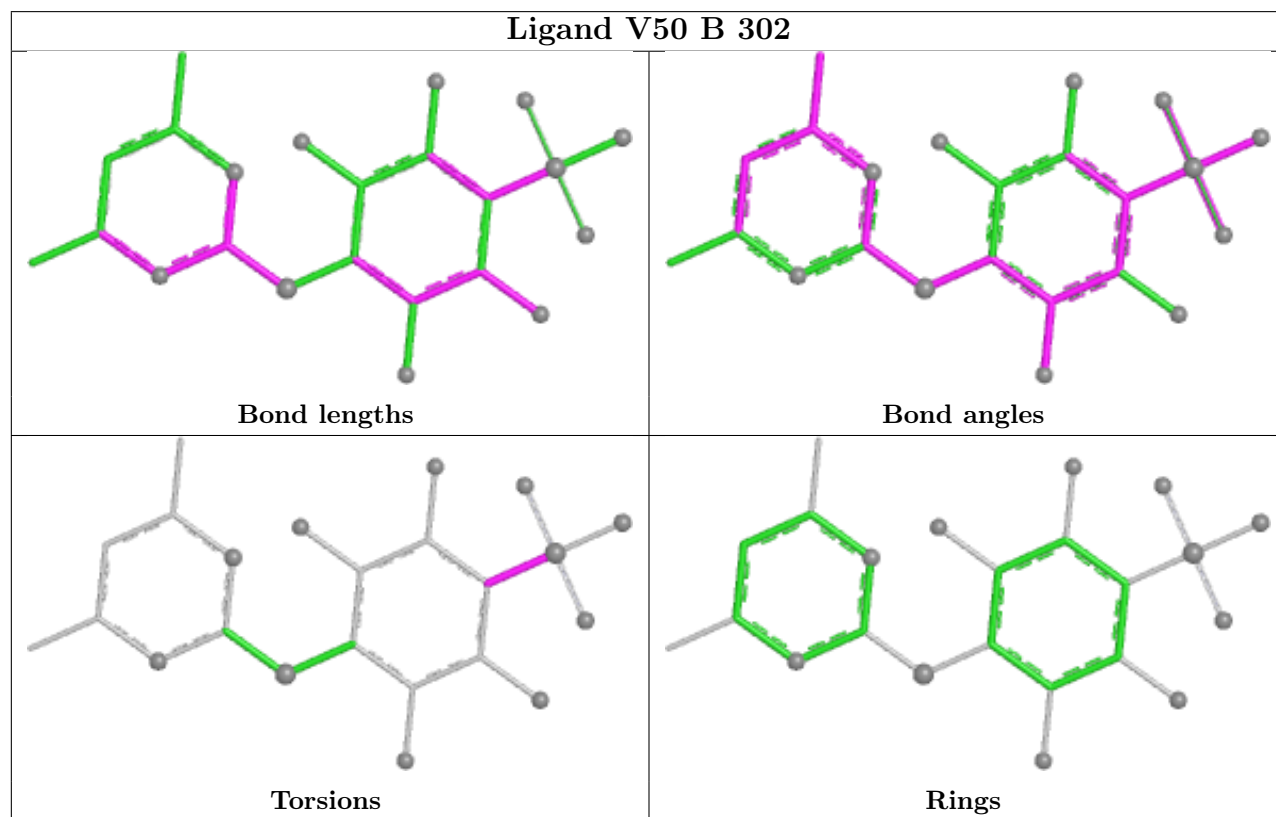
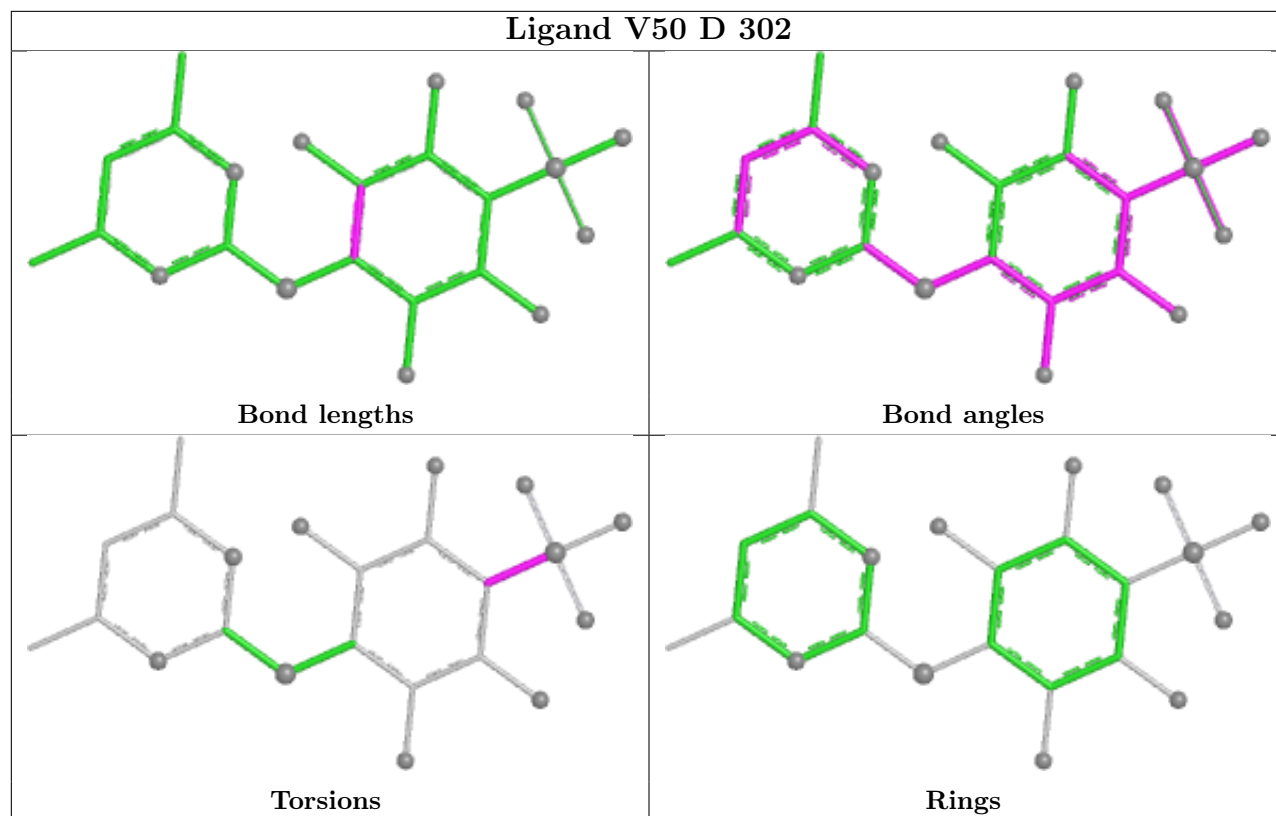
There are no ring outliers.

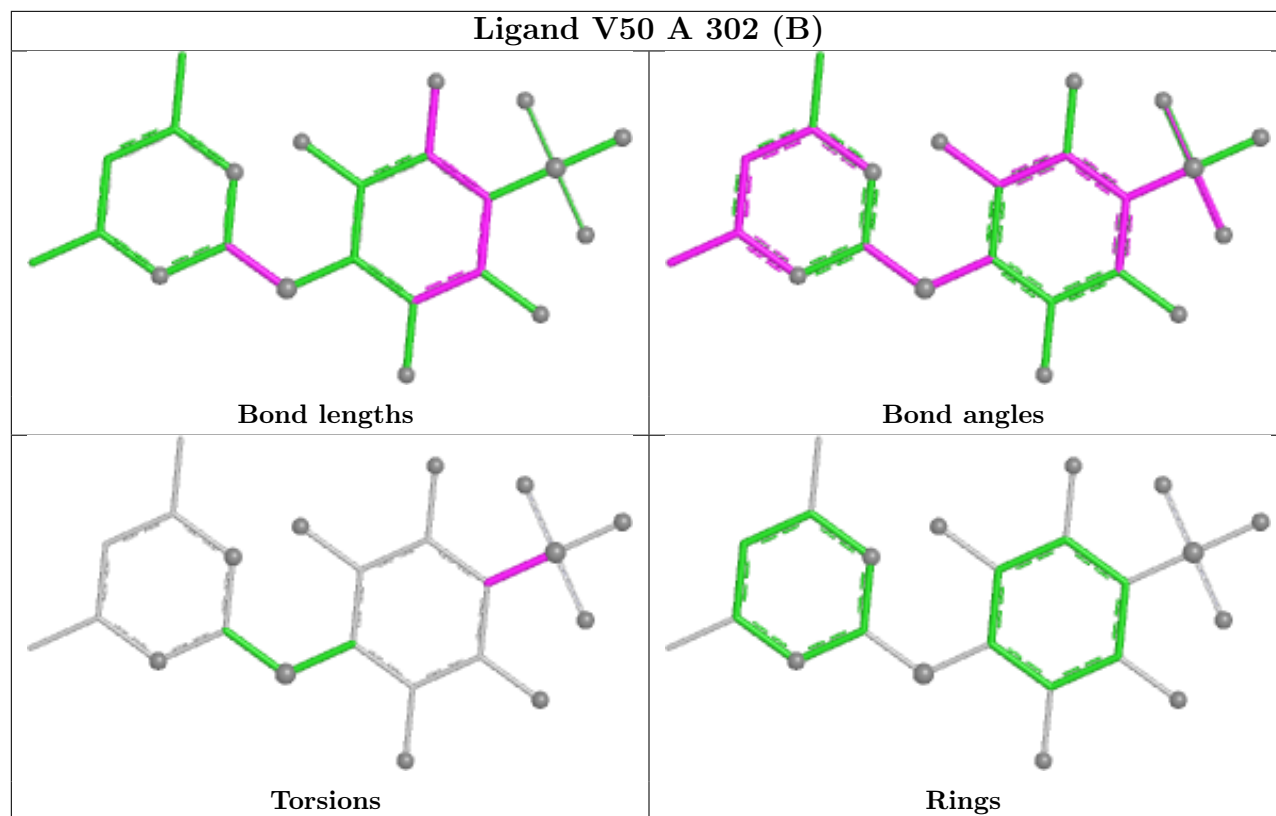
11 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304[B]	EDO	4	0
5	B	305	EDO	6	0
5	A	304[A]	EDO	2	0
3	A	302[C]	V50	2	0
5	D	306	EDO	8	0
4	A	303	PEG	15	0
5	D	305[A]	EDO	6	0
5	B	307	EDO	4	0
5	D	305[B]	EDO	1	0
4	D	303	PEG	6	0
4	B	303	PEG	7	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/263 (99%)	-0.48	3 (1%) 78 82	3, 9, 21, 36	17 (6%)
1	B	261/263 (99%)	-0.37	2 (0%) 82 86	5, 11, 21, 38	8 (3%)
1	C	261/263 (99%)	-0.45	3 (1%) 78 82	3, 10, 22, 36	13 (4%)
1	D	261/263 (99%)	-0.55	3 (1%) 78 82	4, 9, 17, 41	9 (3%)
All	All	1044/1052 (99%)	-0.46	11 (1%) 78 82	3, 10, 21, 41	47 (4%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	LYS	5.8
1	D	256[A]	LEU	4.4
1	B	254	GLU	4.3
1	A	237	PRO	3.2
1	D	254	GLU	2.8
1	D	253	ASP	2.7
1	A	3	LYS	2.4
1	C	237	PRO	2.3
1	C	235	ASP	2.2
1	A	135	LYS	2.2
1	B	253[A]	ASP	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

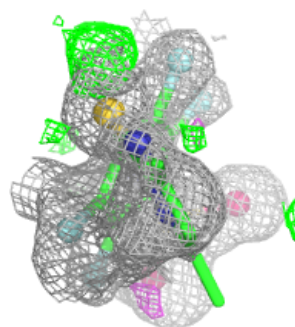
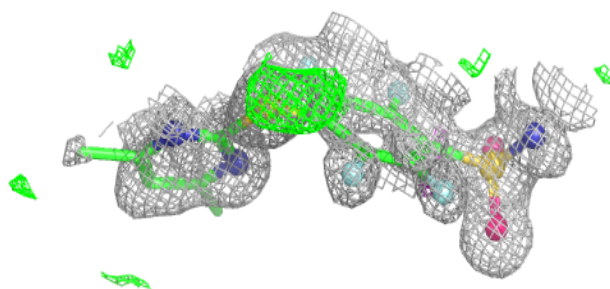
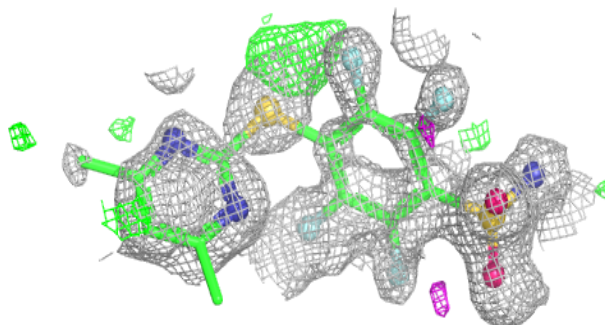
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	306	4/4	0.73	0.15	35,37,40,42	0
5	EDO	B	307	4/4	0.78	0.14	25,35,36,37	0
4	PEG	A	303	7/7	0.79	0.14	23,27,33,38	0
5	EDO	D	306	4/4	0.83	0.20	14,21,29,34	0
5	EDO	A	304[B]	4/4	0.87	0.12	11,17,19,22	4
5	EDO	D	305[A]	4/4	0.87	0.10	8,13,17,17	4
5	EDO	D	305[B]	4/4	0.87	0.10	13,20,21,22	4
5	EDO	A	304[A]	4/4	0.87	0.12	9,12,15,20	4
4	PEG	B	303	7/7	0.89	0.09	19,25,31,32	0
5	EDO	B	305	4/4	0.89	0.14	18,22,31,32	0
5	EDO	C	303	4/4	0.90	0.12	22,23,23,24	0
4	PEG	D	303	7/7	0.90	0.12	17,21,36,38	0
5	EDO	D	304	4/4	0.92	0.12	18,19,19,20	0
5	EDO	B	308	4/4	0.93	0.10	21,29,31,33	0
5	EDO	B	304	4/4	0.96	0.10	15,18,19,20	0
3	V50	A	302[C]	23/23	0.97	0.06	6,11,18,19	23
5	EDO	A	305	4/4	0.97	0.05	10,14,14,17	0
3	V50	C	302	23/23	0.97	0.07	6,12,21,23	0
3	V50	A	302[B]	23/23	0.97	0.06	3,8,11,13	23
5	EDO	B	306	4/4	0.98	0.05	10,11,12,12	0
3	V50	B	302	23/23	0.98	0.05	7,9,15,16	0
3	V50	D	302	23/23	0.99	0.04	5,9,13,17	0
2	ZN	C	301	1/1	1.00	0.01	5,5,5,5	0
2	ZN	D	301	1/1	1.00	0.01	4,4,4,4	0
2	ZN	A	301	1/1	1.00	0.01	5,5,5,5	0
2	ZN	B	301	1/1	1.00	0.01	5,5,5,5	0

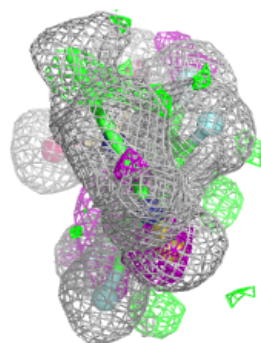
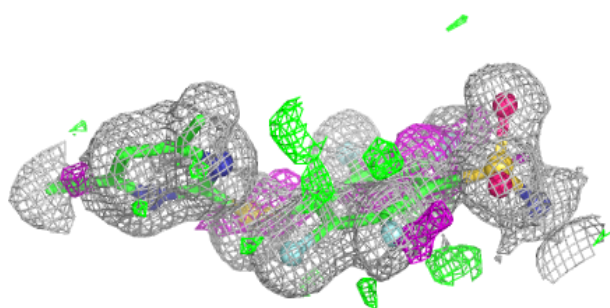
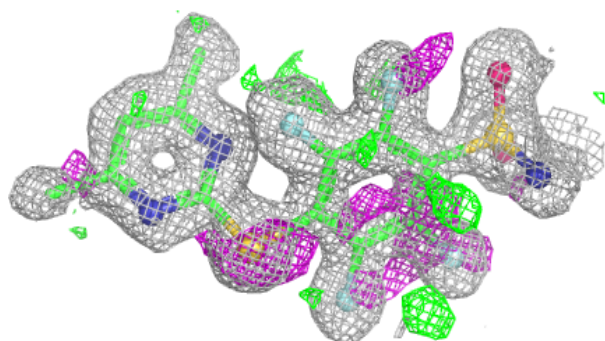
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V50 A 302 (C):

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

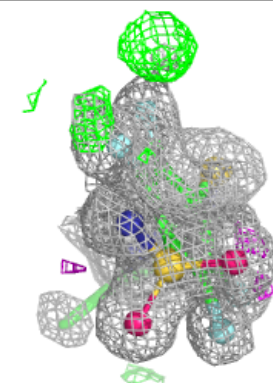
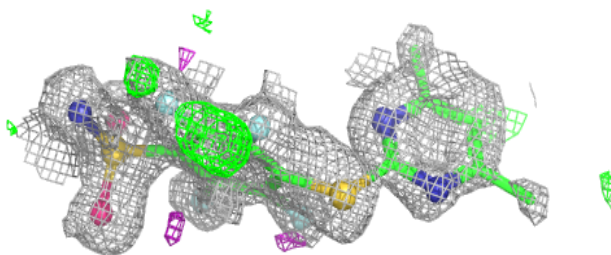
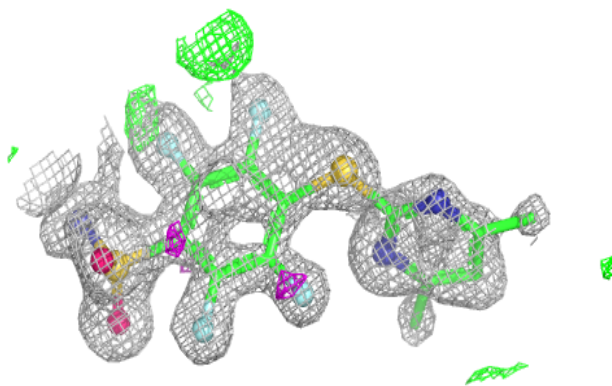
**Electron density around V50 C 302:**

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

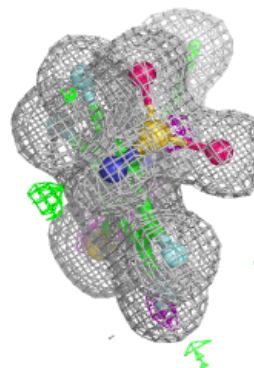
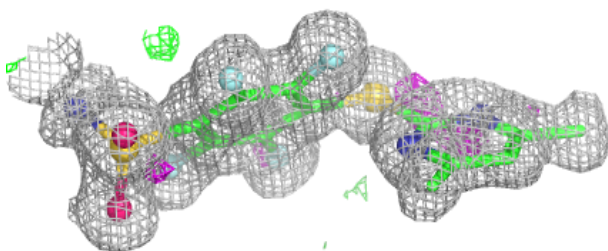
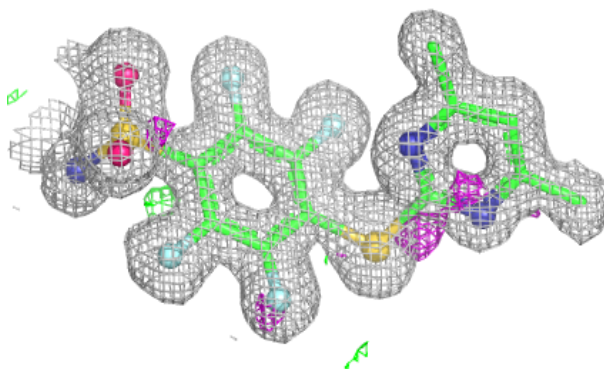


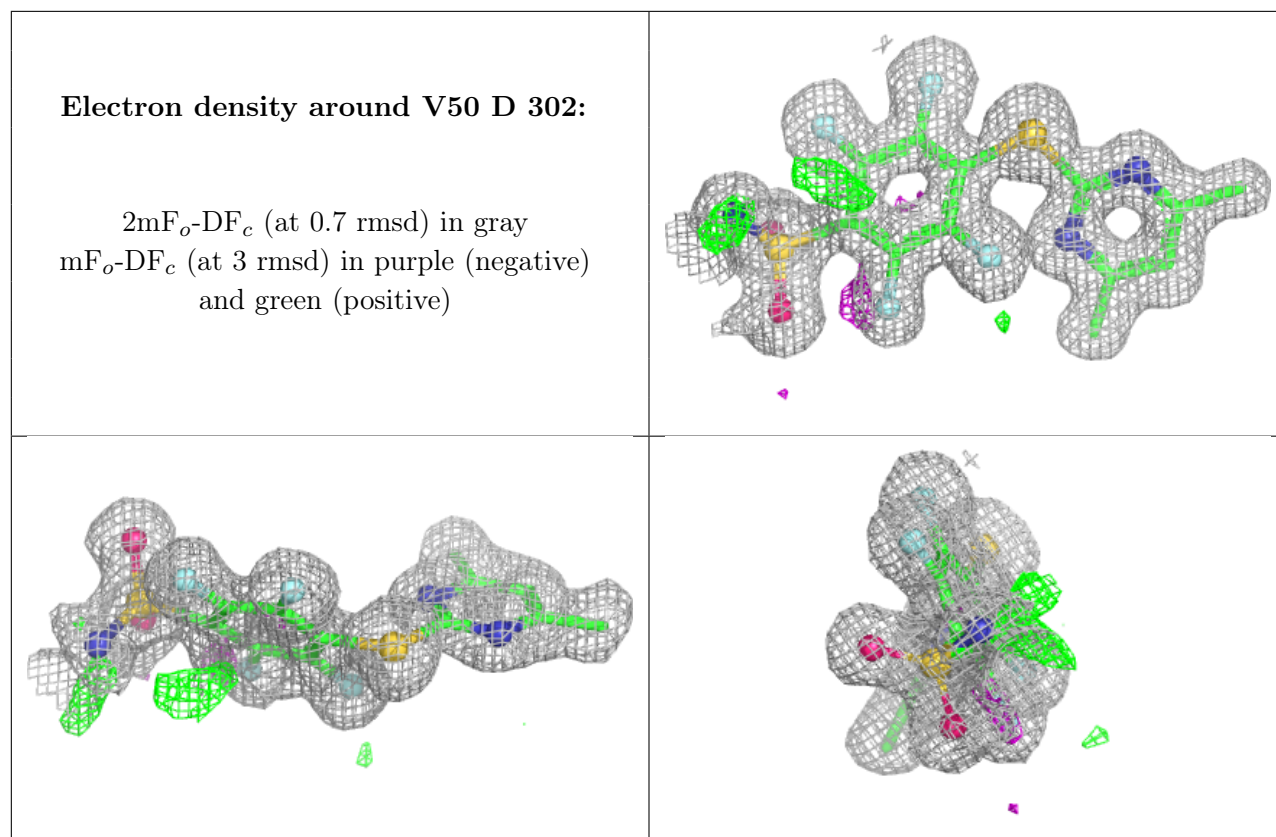
Electron density around V50 A 302 (B):

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

**Electron density around V50 B 302:**

$2mF_o-DF_c$ (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.