



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:15 AM UTC

PDB ID : 4KP5 / pdb_00004kp5
Title : Crystal structure of catalytic domain of human carbonic anhydrase isozyme XII with 2-Chloro-4-[(pyrimidin-2-ylsulfanyl)acetyl]benzenesulfonamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2013-05-13
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

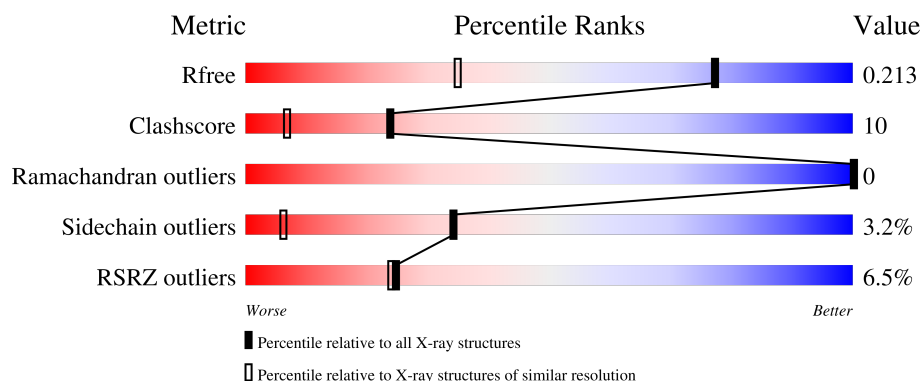
1 Overall quality at a glance

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	2% 80% 17% ..
1	B	263	3% 77% 19% ..
1	C	263	20% 63% 29% 7% .
1	D	263	2% 83% 15% ..

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
5	SO4	C	303	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10072 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
1	A	261	Total	C	N	O	S	0	10	0
			2187	1386	374	420	7			
1	B	261	Total	C	N	O	S	0	7	0
			2154	1365	368	413	8			
1	C	260	Total	C	N	O	S	0	16	0
			2223	1414	380	419	10			
1	D	260	Total	C	N	O	S	0	12	0
			2185	1383	370	424	8			

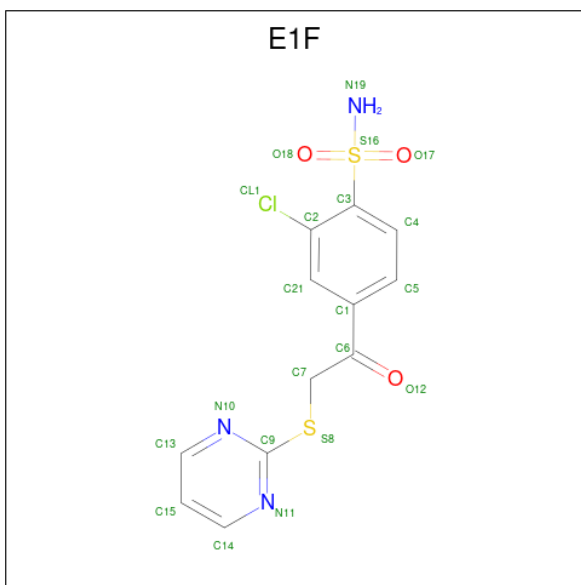
There are 4 discrepancies between the modelled and reference sequences:

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	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-chloro-4-[(pyrimidin-2-ylsulfanyl)acetyl]benzenesulfonamide (CCD ID: E1F) (formula: C₁₂H₁₀ClN₃O₃S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 12	Cl 1	N 3	O 3	S 2	0	0
3	B	1	Total 21	C 12	Cl 1	N 3	O 3	S 2	0	0
3	C	1	Total 21	C 12	Cl 1	N 3	O 3	S 2	0	0
3	D	1	Total 21	C 12	Cl 1	N 3	O 3	S 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	328	Total O 328 328	0	0
6	B	331	Total O 331 331	0	0
6	C	226	Total O 226 226	0	0

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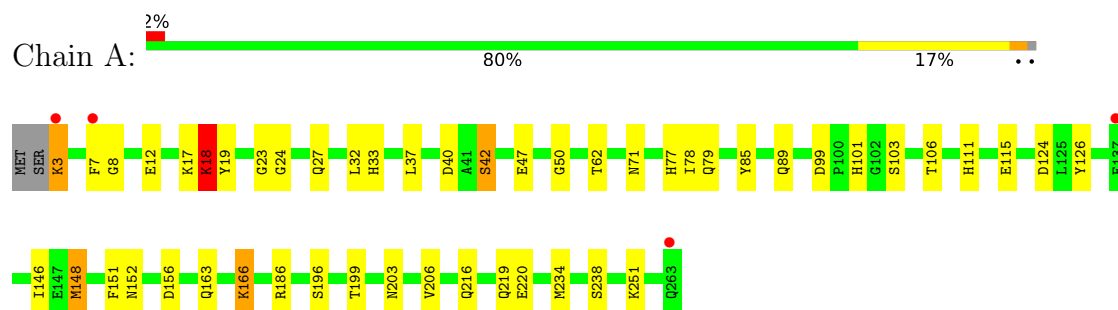
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	321	Total 321	O 321	0	0

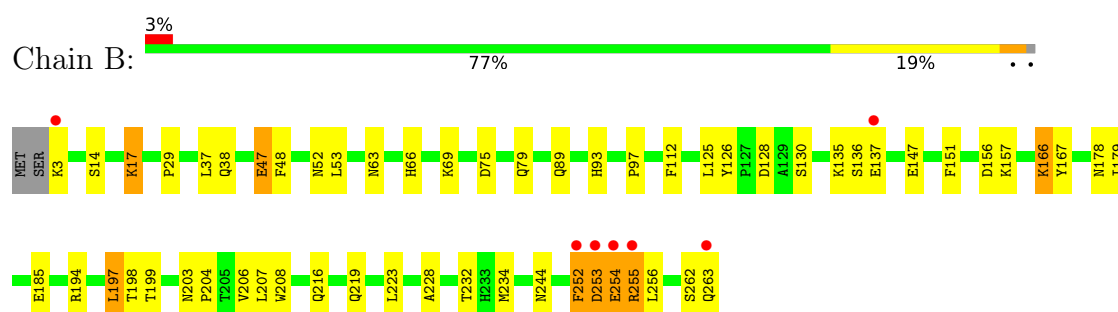
3 Residue-property plots [i](#)

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.

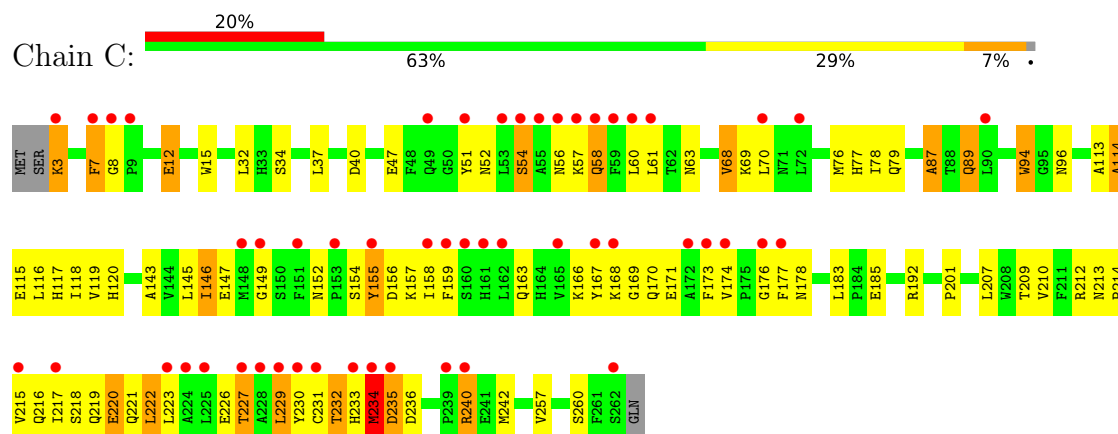
• Molecule 1: Carbonic anhydrase 12



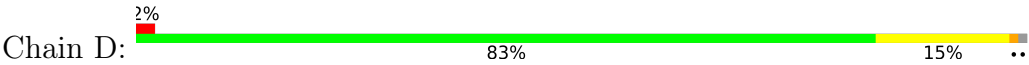
• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.30Å 74.16Å 91.39Å 90.00° 108.81° 90.00°	Depositor
Resolution (Å)	73.13 – 1.45 73.13 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.3 (73.13-1.45) 97.3 (73.13-1.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.02 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.216 0.175 , 0.213	Depositor DCC
R_{free} test set	16774 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10072	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 52.62 % 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 4.7385e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, E1F, 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	21/2250 (0.9%)	1.43	11/3057 (0.4%)
1	B	1.82	25/2218 (1.1%)	1.52	15/3019 (0.5%)
1	C	1.77	31/2287 (1.4%)	1.51	24/3107 (0.8%)
1	D	1.75	21/2248 (0.9%)	1.48	9/3058 (0.3%)
All	All	1.76	98/9003 (1.1%)	1.49	59/12241 (0.5%)

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	ARG	CA-C	10.61	1.66	1.52
1	C	78	ILE	CA-CB	9.87	1.66	1.54
1	B	37	LEU	N-CA	9.10	1.57	1.46
1	C	146	ILE	N-CA	8.87	1.57	1.46
1	C	257	VAL	CA-CB	-8.06	1.44	1.54
1	B	53	LEU	CA-C	7.89	1.63	1.52
1	C	115	GLU	CA-C	7.73	1.62	1.52
1	B	204	PRO	CA-CB	7.62	1.58	1.53
1	C	152	ASN	C-O	7.54	1.31	1.25
1	D	83	SER	N-CA	7.38	1.55	1.45
1	B	228	ALA	CA-CB	-7.29	1.41	1.53
1	C	221	GLN	C-O	7.28	1.32	1.24
1	D	86	SER	CA-C	7.22	1.61	1.52
1	C	63	ASN	N-CA	-7.14	1.37	1.46
1	C	37	LEU	C-O	7.05	1.32	1.23
1	A	23	GLY	CA-C	-7.04	1.44	1.51
1	C	114	ALA	C-O	-6.85	1.16	1.23
1	C	96	ASN	N-CA	6.82	1.52	1.45
1	D	23	GLY	C-O	6.82	1.30	1.24
1	D	47	GLU	C-O	6.70	1.32	1.24
1	C	227	THR	CA-CB	6.61	1.64	1.53
1	A	151	PHE	C-O	6.53	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	PRO	N-CA	6.44	1.52	1.47
1	A	126	TYR	CA-C	6.40	1.58	1.52
1	C	220	GLU	CA-C	-6.36	1.44	1.52
1	A	27	GLN	N-CA	6.36	1.53	1.46
1	C	118	ILE	CA-CB	-6.35	1.46	1.53
1	C	77	HIS	N-CA	6.32	1.53	1.46
1	D	232	THR	N-CA	6.31	1.53	1.45
1	A	251	LYS	C-O	6.30	1.31	1.23
1	C	118	ILE	C-O	6.26	1.31	1.24
1	D	199	THR	N-CA	6.25	1.50	1.45
1	A	32	LEU	CA-CB	6.16	1.60	1.52
1	A	78	ILE	CA-CB	6.16	1.61	1.54
1	D	21	SER	N-CA	6.16	1.54	1.46
1	C	209	THR	C-O	6.09	1.30	1.24
1	B	179	ILE	N-CA	6.08	1.54	1.46
1	B	38	GLN	CA-CB	-6.05	1.43	1.53
1	C	115	GLU	C-O	5.97	1.31	1.23
1	D	173	PHE	CA-C	-5.96	1.45	1.52
1	A	220	GLU	N-CA	-5.93	1.39	1.46
1	B	17	LYS	C-O	5.93	1.31	1.24
1	C	117	HIS	N-CA	5.91	1.53	1.46
1	D	83	SER	C-O	5.84	1.31	1.23
1	D	81	LEU	C-O	-5.81	1.17	1.23
1	B	14	SER	N-CA	5.79	1.53	1.45
1	A	50	GLY	N-CA	-5.77	1.37	1.45
1	C	120	HIS	N-CA	5.73	1.52	1.45
1	B	47	GLU	CA-C	5.71	1.59	1.52
1	C	116	LEU	C-O	5.71	1.30	1.24
1	D	17	LYS	C-O	5.71	1.31	1.24
1	A	37	LEU	N-CA	5.70	1.53	1.46
1	C	155	TYR	C-O	5.70	1.31	1.24
1	B	93	HIS	N-CA	5.67	1.53	1.46
1	D	255	ARG	C-O	5.67	1.31	1.23
1	D	93	HIS	N-CA	5.64	1.53	1.46
1	A	146	ILE	C-O	-5.64	1.18	1.24
1	C	185	GLU	C-O	5.59	1.30	1.23
1	B	66	HIS	N-CA	5.56	1.53	1.46
1	C	40	ASP	CA-C	5.56	1.58	1.52
1	B	206	VAL	CA-CB	5.55	1.60	1.54
1	B	197	LEU	N-CA	5.53	1.52	1.46
1	B	199	THR	N-CA	5.53	1.51	1.45
1	D	189	GLU	CA-C	5.52	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	HIS	CA-C	-5.47	1.45	1.52
1	C	32	LEU	CA-CB	5.46	1.60	1.53
1	C	94	TRP	CA-CB	5.42	1.62	1.53
1	B	256	LEU	CA-C	5.41	1.59	1.52
1	B	63	ASN	CA-C	-5.41	1.46	1.52
1	A	203	ASN	CA-C	-5.40	1.47	1.53
1	D	188	ALA	CA-C	5.38	1.60	1.52
1	C	119	VAL	CA-CB	-5.38	1.47	1.54
1	A	106	THR	N-CA	5.35	1.52	1.45
1	B	3	LYS	N-CA	5.35	1.56	1.46
1	C	217	ILE	C-O	5.29	1.29	1.24
1	B	112	PHE	N-CA	-5.26	1.39	1.45
1	B	151	PHE	C-N	5.26	1.39	1.33
1	C	34	SER	CA-C	-5.25	1.45	1.52
1	B	244	ASN	C-O	-5.24	1.17	1.23
1	C	215	VAL	N-CA	5.23	1.54	1.45
1	B	198	THR	C-N	5.20	1.40	1.33
1	A	37	LEU	C-O	5.18	1.30	1.23
1	A	50	GLY	CA-C	5.18	1.58	1.51
1	D	116	LEU	N-CA	5.17	1.52	1.46
1	D	217	ILE	C-O	5.17	1.29	1.23
1	A	106	THR	CA-C	-5.16	1.46	1.52
1	D	190	TYR	CA-C	-5.16	1.46	1.52
1	C	232	THR	C-O	5.14	1.30	1.23
1	A	77	HIS	CA-C	-5.09	1.46	1.52
1	D	48	PHE	C-O	-5.08	1.18	1.23
1	A	85	TYR	C-O	5.08	1.29	1.24
1	D	122	ASN	N-CA	5.06	1.53	1.46
1	C	68	VAL	CA-CB	5.06	1.60	1.54
1	A	115	GLU	C-O	5.06	1.30	1.23
1	A	152	ASN	CA-CB	5.04	1.60	1.53
1	A	196	SER	CA-C	5.02	1.59	1.52
1	D	206	VAL	C-O	-5.01	1.18	1.24
1	B	69	LYS	N-CA	5.00	1.52	1.45

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ALA	N-CA-C	11.07	124.73	111.33
1	C	234	MET	N-CA-C	8.75	122.94	111.75
1	B	206	VAL	N-CA-C	8.31	119.81	108.17
1	D	206	VAL	O-C-N	7.18	130.72	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	N-CA-C	-6.80	103.95	111.36
1	D	84	ARG	CB-CG-CD	6.64	126.58	111.30
1	B	253	ASP	N-CA-C	6.54	120.48	108.58
1	A	8	GLY	CA-C-N	6.42	126.11	119.56
1	A	8	GLY	C-N-CA	6.42	126.11	119.56
1	C	87	ALA	N-CA-C	6.29	118.90	110.35
1	C	222	LEU	N-CA-C	6.24	117.74	111.07
1	C	143	ALA	CA-C-O	6.23	127.09	120.36
1	C	7	PHE	N-CA-C	6.16	116.14	108.19
1	C	116	LEU	CA-C-O	-6.12	114.22	120.71
1	C	220	GLU	N-CA-CB	6.00	119.04	110.16
1	A	12	GLU	N-CA-C	5.99	118.59	111.71
1	A	199	THR	O-C-N	5.96	126.41	121.35
1	C	235	ASP	N-CA-C	-5.91	104.29	112.03
1	C	236	ASP	N-CA-C	-5.88	102.34	109.57
1	A	206	VAL	N-CA-C	5.87	116.39	108.17
1	C	77	HIS	N-CA-C	5.84	117.72	108.79
1	C	94	TRP	O-C-N	5.74	129.64	122.92
1	B	262	SER	O-C-N	5.63	128.99	122.17
1	B	157	LYS	N-CA-C	-5.59	105.71	112.54
1	C	229	LEU	N-CA-C	5.55	118.75	110.14
1	C	210	VAL	CA-C-N	-5.55	112.23	120.94
1	C	210	VAL	C-N-CA	-5.55	112.23	120.94
1	C	222	LEU	CA-C-O	5.50	126.60	120.82
1	D	252	PHE	N-CA-C	5.50	119.25	112.54
1	D	187	THR	N-CA-C	5.49	119.08	112.38
1	A	18[A]	LYS	N-CA-C	5.46	119.94	113.28
1	A	18[B]	LYS	N-CA-C	5.46	119.94	113.28
1	C	96	ASN	CA-C-N	-5.46	114.05	119.56
1	C	96	ASN	C-N-CA	-5.46	114.05	119.56
1	C	157	LYS	N-CA-C	-5.43	105.53	111.82
1	B	126	TYR	CA-C-N	5.40	125.02	119.56
1	B	126	TYR	C-N-CA	5.40	125.02	119.56
1	D	154	SER	N-CA-C	-5.38	104.84	111.40
1	B	208	TRP	CA-C-O	-5.33	114.61	120.69
1	B	252	PHE	CA-C-N	-5.32	113.65	122.32
1	B	252	PHE	C-N-CA	-5.32	113.65	122.32
1	C	183	LEU	N-CA-CB	5.29	116.43	110.03
1	D	192	ARG	CD-NE-CZ	5.29	131.80	124.40
1	D	133	SER	N-CA-C	5.28	117.78	111.71
1	C	260	SER	N-CA-C	-5.24	106.86	113.20
1	D	98	ASN	CA-C-N	-5.23	117.68	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	98	ASN	C-N-CA	-5.23	117.68	122.28
1	B	223	LEU	CA-C-O	-5.20	115.03	120.55
1	C	145	LEU	O-C-N	5.16	129.10	123.01
1	C	12	GLU	CB-CG-CD	-5.16	103.83	112.60
1	A	32	LEU	CA-C-N	-5.13	114.18	122.81
1	A	32	LEU	C-N-CA	-5.13	114.18	122.81
1	B	48	PHE	O-C-N	5.10	129.55	123.13
1	C	214	PRO	CA-C-O	-5.09	115.81	122.12
1	B	166[A]	LYS	CA-C-N	-5.03	114.36	122.81
1	B	166[A]	LYS	C-N-CA	-5.03	114.36	122.81
1	B	166[B]	LYS	CA-C-N	-5.03	114.36	122.81
1	B	166[B]	LYS	C-N-CA	-5.03	114.36	122.81
1	A	24	GLY	O-C-N	5.00	127.92	122.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2187	0	2073	43	0
1	B	2154	0	2033	40	0
1	C	2223	0	2118	86	0
1	D	2185	0	2055	13	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	21	0	9	0	0
3	B	21	0	9	0	0
3	C	21	0	9	2	0
3	D	21	0	9	0	0
4	A	8	0	12	0	0
4	B	8	0	12	0	0
4	D	8	0	12	3	0
5	C	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	328	0	0	12	0
6	B	331	0	0	5	0
6	C	226	0	0	8	0
6	D	321	0	0	5	0
All	All	10072	0	8351	174	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 10.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166[B]:LYS:HE2	6:D:700:HOH:O	1.30	1.30
1:D:75:ASP:HB3	6:D:669:HOH:O	1.43	1.17
1:A:3[B]:LYS:HE2	1:A:18[B]:LYS:HZ3	1.09	1.13
1:A:71[B]:ASN:OD1	6:A:711:HOH:O	1.63	1.11
1:A:3[B]:LYS:HE2	1:A:18[B]:LYS:NZ	1.65	1.10
1:B:253:ASP:HA	6:B:583:HOH:O	1.51	1.07
1:B:137:GLU:HB3	1:B:194:ARG:HH12	0.94	1.07
1:C:51:TYR:HA	1:C:76[B]:MET:HE3	1.31	1.06
1:C:168[A]:LYS:HB2	1:C:231[A]:CYS:O	1.56	1.04
1:B:136:SER:O	1:B:137:GLU:HG2	1.60	1.00
1:A:7:PHE:CE1	1:B:253:ASP:HB3	1.97	0.99
1:B:185:GLU:HG2	6:B:721:HOH:O	1.61	0.98
1:B:137:GLU:HB3	1:B:194:ARG:NH1	1.78	0.98
1:C:94:TRP:CZ2	1:C:242[B]:MET:HE3	1.99	0.96
1:B:252:PHE:CZ	1:B:255:ARG:HB2	2.02	0.95
1:C:94:TRP:CH2	1:C:242[B]:MET:HE3	2.03	0.94
1:A:3[A]:LYS:HD2	6:A:694:HOH:O	1.67	0.93
1:B:137:GLU:CB	1:B:194:ARG:HH12	1.80	0.93
1:D:163:GLN:OE1	1:D:166[A]:LYS:HD2	1.70	0.92
1:B:252:PHE:CE1	1:B:255:ARG:HB2	2.05	0.91
1:C:58:GLN:N	1:C:58:GLN:OE1	2.07	0.88
1:B:252:PHE:CZ	1:B:255:ARG:CB	2.59	0.85
1:A:7:PHE:HE1	1:B:253:ASP:HB3	1.33	0.85
1:D:47:GLU:HB2	1:D:79[B]:GLN:HG3	1.60	0.83
1:C:177:PHE:HA	6:C:599:HOH:O	1.79	0.83
1:A:163:GLN:HG3	6:A:675:HOH:O	1.79	0.82
1:C:7:PHE:HD1	1:C:8:GLY:N	1.78	0.81
1:C:94:TRP:CZ2	1:C:242[B]:MET:CE	2.64	0.81
1:C:51:TYR:HA	1:C:76[B]:MET:CE	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LEU:HD12	1:C:242[B]:MET:CE	2.11	0.80
1:A:40:ASP:OD1	1:A:42:SER:HB3	1.83	0.79
1:A:3[B]:LYS:O	1:A:3[B]:LYS:HD3	1.83	0.78
1:A:148:MET:SD	1:A:219:GLN:CA	2.71	0.78
1:C:7:PHE:CD1	1:C:8:GLY:N	2.53	0.77
1:C:231[B]:CYS:SG	1:C:240:ARG:HD2	2.24	0.76
1:B:166[A]:LYS:HE2	6:D:700:HOH:O	1.85	0.76
1:C:94:TRP:CH2	1:C:242[B]:MET:CE	2.70	0.74
1:A:148:MET:SD	1:A:219:GLN:N	2.61	0.73
1:A:3[B]:LYS:HD3	1:A:3[B]:LYS:C	2.14	0.73
1:D:47:GLU:HB3	1:D:79[B]:GLN:HE21	1.54	0.72
1:C:218:SER:HB2	5:C:303:SO4:O1	1.90	0.71
1:C:229:LEU:HD12	1:C:242[B]:MET:HE2	1.73	0.70
1:C:192:ARG:HD2	1:C:207[B]:LEU:HD21	1.74	0.70
1:A:148:MET:SD	1:A:219:GLN:HA	2.32	0.69
1:C:219:GLN:HE21	1:C:223:LEU:HD22	1.56	0.69
1:C:232:THR:HG23	1:C:240:ARG:HG3	1.73	0.69
1:A:163:GLN:CG	6:A:675:HOH:O	2.39	0.67
1:C:51:TYR:CD2	1:C:76[B]:MET:HE2	2.29	0.67
1:C:229:LEU:HD12	1:C:242[B]:MET:HE1	1.76	0.67
1:C:51:TYR:CG	1:C:76[B]:MET:HE2	2.30	0.67
1:A:7:PHE:CE1	1:B:253:ASP:CB	2.76	0.66
1:B:252:PHE:CE1	1:B:255:ARG:CB	2.76	0.65
1:A:18[B]:LYS:HD2	1:A:19:TYR:CZ	2.32	0.65
1:C:167:TYR:CD2	1:C:234:MET:HG2	2.32	0.65
1:C:219:GLN:NE2	1:C:223:LEU:HD22	2.12	0.64
1:A:47:GLU:CD	1:A:79:GLN:HE21	2.06	0.64
1:B:136:SER:C	1:B:137:GLU:HG2	2.22	0.64
1:B:252:PHE:CZ	1:B:255:ARG:HB3	2.33	0.64
1:C:192:ARG:CD	1:C:207[B]:LEU:HD21	2.29	0.63
1:D:163:GLN:HB2	6:D:688:HOH:O	1.99	0.63
1:A:166[B]:LYS:HE2	6:A:555:HOH:O	2.00	0.61
1:A:163:GLN:O	1:A:166[A]:LYS:HG3	2.01	0.61
1:A:7:PHE:CD1	1:B:253:ASP:HB3	2.36	0.60
1:A:216:GLN:HG3	6:A:593:HOH:O	2.02	0.59
1:C:69[A]:LYS:HD2	6:C:473:HOH:O	2.02	0.59
1:A:7:PHE:HE1	1:B:253:ASP:CB	2.09	0.59
1:C:7:PHE:CD1	1:C:7:PHE:C	2.81	0.59
1:A:148:MET:SD	1:A:219:GLN:HB3	2.43	0.59
1:C:69[B]:LYS:HE2	6:C:473:HOH:O	2.03	0.58
1:B:135:LYS:NZ	6:B:698:HOH:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212[A]:ARG:HH11	1:C:213:ASN:HD21	1.50	0.58
1:C:61[B]:LEU:CD2	1:C:70:LEU:HD13	2.34	0.58
1:C:170:GLN:HE22	1:C:234:MET:HE3	1.68	0.57
1:B:252:PHE:CE2	1:B:255:ARG:HB2	2.37	0.57
1:C:61[B]:LEU:HG	1:C:174:VAL:HG23	1.86	0.57
1:C:229:LEU:HB2	1:C:242[A]:MET:HB3	1.87	0.57
1:A:3[B]:LYS:HE2	1:A:18[B]:LYS:HZ1	1.62	0.57
1:D:47:GLU:CB	1:D:79[B]:GLN:HE21	2.17	0.57
1:C:219:GLN:HB3	5:C:303:SO4:O2	2.06	0.55
1:C:69[B]:LYS:NZ	6:C:582:HOH:O	2.39	0.55
1:C:54:SER:HB2	1:C:56:ASN:HB2	1.89	0.55
1:C:229:LEU:HB2	1:C:242[A]:MET:CB	2.37	0.55
1:B:128:ASP:OD2	1:B:130[A]:SER:HB2	2.07	0.54
1:C:8:GLY:HA2	1:D:25:LEU:HD21	1.90	0.54
1:B:252:PHE:CE2	1:B:255:ARG:C	2.85	0.54
1:C:207[B]:LEU:C	1:C:207[B]:LEU:HD23	2.32	0.54
1:A:148:MET:HE3	1:A:148:MET:C	2.31	0.54
1:C:167:TYR:CG	1:C:234:MET:HA	2.43	0.54
1:C:94:TRP:HH2	1:C:242[B]:MET:CE	2.21	0.54
1:C:7:PHE:HE2	1:C:240:ARG:HH11	1.57	0.53
1:B:252:PHE:CE1	1:B:255:ARG:NE	2.78	0.52
1:A:18[A]:LYS:HG2	6:A:642:HOH:O	2.10	0.52
1:B:167:TYR:CE2	1:B:234[B]:MET:HG3	2.44	0.52
1:C:232:THR:CG2	1:C:240:ARG:HG3	2.40	0.52
1:C:229:LEU:C	1:C:230:TYR:CD2	2.88	0.52
1:C:94:TRP:HZ2	1:C:242[B]:MET:CE	2.18	0.51
1:B:47:GLU:HB2	1:B:79:GLN:HB3	1.93	0.51
1:C:230:TYR:HA	1:C:240:ARG:O	2.11	0.51
1:C:230:TYR:CD2	1:C:230:TYR:N	2.78	0.51
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.92	0.51
1:A:148:MET:SD	1:A:219:GLN:CB	2.99	0.51
1:C:158[B]:ILE:N	1:C:158[B]:ILE:HD12	2.26	0.51
1:C:168[B]:LYS:HD3	1:C:169:GLY:N	2.26	0.51
1:C:94:TRP:CZ2	1:C:242[A]:MET:HG2	2.46	0.50
1:A:18[B]:LYS:HD2	1:A:19:TYR:CE2	2.47	0.50
1:C:154:SER:N	6:C:572:HOH:O	2.28	0.50
1:C:212[A]:ARG:NH1	1:C:213:ASN:HD21	2.09	0.49
1:B:234[B]:MET:HE3	6:D:549:HOH:O	2.12	0.49
1:C:76[A]:MET:HB3	1:C:87:ALA:HB3	1.95	0.49
1:B:252:PHE:CD1	1:B:255:ARG:HB2	2.45	0.49
1:A:7:PHE:CD1	1:B:253:ASP:CB	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:OE1	6:A:707:HOH:O	2.20	0.48
1:C:54:SER:O	1:C:176:GLY:HA3	2.13	0.48
1:A:3[B]:LYS:C	1:A:3[B]:LYS:CD	2.85	0.48
1:C:3[B]:LYS:O	1:C:3[B]:LYS:CG	2.61	0.48
1:C:58:GLN:HG2	1:C:173:PHE:CD1	2.48	0.48
1:C:154:SER:OG	6:C:593:HOH:O	2.20	0.48
1:B:252:PHE:CE2	1:B:255:ARG:O	2.66	0.47
1:C:114:ALA:HB3	1:C:146:ILE:HB	1.95	0.47
1:C:149:GLY:HA3	1:C:216:GLN:OE1	2.14	0.47
1:C:3[B]:LYS:O	1:C:3[B]:LYS:HG3	2.14	0.47
1:A:18[B]:LYS:O	1:A:18[B]:LYS:HD3	2.16	0.46
1:C:61[B]:LEU:HD23	1:C:70:LEU:HD13	1.97	0.46
1:A:3[B]:LYS:HD2	1:A:19:TYR:OH	2.16	0.46
1:D:43:LEU:HA	4:D:304:EDO:H12	1.97	0.46
1:C:220:GLU:O	1:C:220:GLU:HG3	2.15	0.46
1:A:17[B]:LYS:HG2	1:B:17:LYS:HG2	1.96	0.45
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.80	0.45
1:A:99:ASP:OD1	1:A:101:HIS:HD2	1.99	0.45
1:C:54:SER:C	1:C:56:ASN:N	2.75	0.45
1:C:233[A]:HIS:CG	1:C:234:MET:N	2.78	0.45
1:D:192:ARG:HD2	1:D:207:LEU:HD11	1.99	0.45
1:C:61[A]:LEU:HD11	1:C:68:VAL:HG22	1.99	0.44
1:C:54:SER:C	1:C:56:ASN:H	2.25	0.44
1:C:94:TRP:HZ2	1:C:242[B]:MET:HE2	1.80	0.44
1:A:148:MET:HE3	1:A:148:MET:HB3	1.46	0.44
1:C:201:PRO:CD	3:C:302:E1F:H1	2.47	0.44
1:D:253:ASP:O	1:D:254:GLU:HB2	2.17	0.44
1:C:60:LEU:HD11	1:C:171:GLU:HB3	2.00	0.44
1:C:52:ASN:HA	1:C:178:ASN:HA	2.00	0.43
1:C:219:GLN:HG2	6:C:589:HOH:O	2.16	0.43
1:A:103:SER:O	1:A:111:HIS:HD2	2.02	0.43
1:C:155:TYR:HB3	1:C:159:PHE:CE2	2.52	0.43
1:C:147:GLU:O	1:C:216:GLN:HA	2.18	0.43
1:A:163:GLN:HG3	6:A:608:HOH:O	2.18	0.43
1:A:163:GLN:OE1	6:A:582:HOH:O	2.20	0.43
1:B:219:GLN:HE21	1:B:219:GLN:HB3	1.68	0.43
1:C:163:GLN:OE1	1:C:166:LYS:HD2	2.17	0.43
1:B:147:GLU:HG3	1:B:216:GLN:HG2	2.01	0.43
1:B:52:ASN:HA	1:B:178:ASN:HA	2.00	0.42
1:B:252:PHE:O	1:B:254:GLU:N	2.51	0.42
1:C:192:ARG:CD	1:C:207[B]:LEU:CD2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234[B]:MET:HB3	1:D:234[B]:MET:HE2	1.64	0.42
1:C:7:PHE:HD1	1:C:8:GLY:CA	2.32	0.42
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.93	0.42
1:D:80:GLY:O	4:D:304:EDO:H21	2.19	0.42
1:C:69[A]:LYS:HG3	1:C:89:GLN:HB2	2.02	0.42
1:B:253:ASP:O	1:B:254:GLU:HB2	2.18	0.41
1:C:12:GLU:HA	1:C:15:TRP:CE2	2.55	0.41
1:C:149:GLY:O	1:C:218:SER:HA	2.20	0.41
1:C:61[B]:LEU:HD23	1:C:70:LEU:CD1	2.51	0.41
1:C:94:TRP:CZ2	1:C:242[B]:MET:HE2	2.53	0.41
1:A:234:MET:HE2	1:A:234:MET:HB3	1.70	0.41
1:B:197:LEU:HD13	1:B:203[A]:ASN:HB2	2.02	0.41
1:A:62[A]:THR:HG21	6:A:600:HOH:O	2.20	0.40
1:C:201:PRO:HD2	3:C:302:E1F:H1	2.02	0.40
1:C:3[A]:LYS:O	6:C:551:HOH:O	2.22	0.40
1:A:33:HIS:HE1	6:A:607:HOH:O	2.04	0.40
1:B:166[B]:LYS:CB	6:B:487:HOH:O	2.69	0.40
1:C:222:LEU:O	1:C:226:GLU:HG3	2.21	0.40
1:C:223:LEU:O	1:C:227:THR:OG1	2.32	0.40
1:B:253:ASP:CG	6:B:583:HOH:O	2.64	0.40
1:D:44:THR:O	4:D:304:EDO:H22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/263 (102%)	266 (99%)	3 (1%)	0	100	100
1	B	266/263 (101%)	258 (97%)	8 (3%)	0	100	100
1	C	273/263 (104%)	256 (94%)	17 (6%)	0	100	100
1	D	270/263 (103%)	264 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1078/1052 (102%)	1044 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	244/235 (104%)	233 (96%)	11 (4%)	24	2
1	B	240/235 (102%)	231 (96%)	9 (4%)	29	4
1	C	248/235 (106%)	238 (96%)	10 (4%)	28	3
1	D	244/235 (104%)	240 (98%)	4 (2%)	55	23
All	All	976/940 (104%)	942 (96%)	34 (4%)	34	5

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3[A]	LYS
1	A	3[B]	LYS
1	A	18[A]	LYS
1	A	18[B]	LYS
1	A	42	SER
1	A	89	GLN
1	A	148	MET
1	A	156	ASP
1	A	166[A]	LYS
1	A	166[B]	LYS
1	A	238	SER
1	B	29	PRO
1	B	75	ASP
1	B	89	GLN
1	B	97	PRO
1	B	125	LEU
1	B	156	ASP

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Mol	Chain	Res	Type
1	B	232	THR
1	B	254	GLU
1	B	263	GLN
1	C	3[A]	LYS
1	C	3[B]	LYS
1	C	54	SER
1	C	57	LYS
1	C	58	GLN
1	C	89	GLN
1	C	156	ASP
1	C	234	MET
1	C	235	ASP
1	C	240	ARG
1	D	69	LYS
1	D	75	ASP
1	D	89	GLN
1	D	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	33	HIS
1	A	56	ASN
1	A	58	GLN
1	A	79	GLN
1	A	110	GLN
1	A	111	HIS
1	A	163	GLN
1	A	213	ASN
1	B	79	GLN
1	B	110	GLN
1	B	219	GLN
1	B	250	GLN
1	C	13	ASN
1	C	38	GLN
1	C	49	GLN
1	C	110	GLN
1	C	170	GLN
1	C	213	ASN
1	C	219	GLN
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	110	GLN
1	D	213	ASN
1	D	219	GLN
1	D	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	B	304	-	3,3,3	1.11	0	2,2,2	0.35	0
4	EDO	B	303	-	3,3,3	1.37	0	2,2,2	0.80	0
3	E1F	B	302	2	22,22,22	2.78	10 (45%)	31,31,31	2.65	12 (38%)
5	SO4	C	303	-	4,4,4	0.30	0	6,6,6	0.34	0
4	EDO	A	304	-	3,3,3	0.83	0	2,2,2	0.66	0
3	E1F	C	302	2	22,22,22	2.13	5 (22%)	31,31,31	2.27	12 (38%)
4	EDO	A	303	-	3,3,3	0.95	0	2,2,2	0.32	0
4	EDO	D	303	-	3,3,3	0.85	0	2,2,2	0.95	0
4	EDO	D	304	-	3,3,3	0.62	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	E1F	D	302	2	22,22,22	2.08	3 (13%)	31,31,31	2.63	17 (54%)
3	E1F	A	302	2	22,22,22	2.57	9 (40%)	31,31,31	2.81	15 (48%)

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
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
3	E1F	B	302	2	-	0/15/15/15	0/2/2/2
4	EDO	A	304	-	-	0/1/1/1	-
3	E1F	C	302	2	-	2/15/15/15	0/2/2/2
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	D	303	-	-	1/1/1/1	-
4	EDO	D	304	-	-	0/1/1/1	-
3	E1F	D	302	2	-	1/15/15/15	0/2/2/2
3	E1F	A	302	2	-	1/15/15/15	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	E1F	C3-S16	8.40	1.88	1.77
3	D	302	E1F	C3-S16	7.53	1.87	1.77
3	C	302	E1F	O17-S16	6.70	1.55	1.43
3	A	302	E1F	O17-S16	5.85	1.54	1.43
3	A	302	E1F	O18-S16	5.07	1.52	1.43
3	C	302	E1F	C3-S16	5.05	1.84	1.77
3	B	302	E1F	C9-N10	4.13	1.41	1.33
3	A	302	E1F	C4-C5	4.03	1.45	1.38
3	A	302	E1F	C21-C2	3.71	1.44	1.38
3	A	302	E1F	C3-S16	3.63	1.82	1.77
3	B	302	E1F	C4-C3	3.63	1.43	1.39
3	B	302	E1F	C7-S8	3.60	1.89	1.80
3	B	302	E1F	C21-C1	-3.51	1.34	1.39
3	D	302	E1F	O18-S16	3.49	1.49	1.43
3	A	302	E1F	C2-CL1	-3.47	1.65	1.73
3	B	302	E1F	C9-S8	3.18	1.82	1.75
3	A	302	E1F	C7-S8	3.12	1.87	1.80
3	D	302	E1F	O17-S16	2.61	1.48	1.43
3	B	302	E1F	C21-C2	2.52	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	E1F	C7-S8	2.45	1.86	1.80
3	C	302	E1F	C9-N10	2.32	1.37	1.33
3	A	302	E1F	C9-N11	2.28	1.37	1.33
3	B	302	E1F	C4-C5	2.25	1.42	1.38
3	B	302	E1F	C9-N11	2.23	1.37	1.33
3	C	302	E1F	C9-N11	2.22	1.37	1.33
3	A	302	E1F	C9-N10	2.13	1.37	1.33
3	B	302	E1F	O18-S16	2.03	1.47	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	E1F	C4-C3-C2	6.62	123.79	119.05
3	A	302	E1F	O12-C6-C1	-5.81	112.96	120.73
3	C	302	E1F	O18-S16-N19	5.54	115.34	107.35
3	D	302	E1F	C13-N10-C9	5.38	122.90	114.96
3	C	302	E1F	C7-S8-C9	-5.37	94.76	101.65
3	B	302	E1F	C13-N10-C9	5.35	122.85	114.96
3	B	302	E1F	C21-C2-C3	-5.22	116.31	121.36
3	A	302	E1F	O12-C6-C7	5.04	128.26	120.41
3	B	302	E1F	C5-C1-C21	5.02	125.05	119.25
3	C	302	E1F	O12-C6-C1	-4.86	114.22	120.73
3	D	302	E1F	C4-C3-C2	4.68	122.40	119.05
3	A	302	E1F	C21-C2-C3	-4.67	116.84	121.36
3	B	302	E1F	C4-C3-C2	4.63	122.36	119.05
3	B	302	E1F	N10-C9-N11	-4.48	119.68	126.86
3	D	302	E1F	C15-C13-N10	-4.29	116.63	123.42
3	A	302	E1F	N10-C9-N11	-4.25	120.05	126.86
3	A	302	E1F	C14-N11-C9	4.05	120.93	114.96
3	B	302	E1F	C15-C13-N10	-4.03	117.04	123.42
3	D	302	E1F	C14-C15-C13	3.76	121.51	116.63
3	D	302	E1F	C2-C3-S16	-3.66	119.08	123.47
3	C	302	E1F	O12-C6-C7	3.57	125.97	120.41
3	B	302	E1F	O18-S16-N19	3.54	112.45	107.35
3	B	302	E1F	C4-C5-C1	-3.42	117.14	120.80
3	D	302	E1F	N10-C9-N11	-3.41	121.39	126.86
3	C	302	E1F	C13-N10-C9	3.41	119.99	114.96
3	D	302	E1F	O17-S16-N19	3.37	112.21	107.35
3	B	302	E1F	C2-C3-S16	-3.27	119.54	123.47
3	A	302	E1F	C7-S8-C9	-3.26	97.47	101.65
3	D	302	E1F	C15-C14-N11	-3.21	118.33	123.42
3	D	302	E1F	C7-S8-C9	3.18	105.74	101.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	E1F	O12-C6-C1	-3.03	116.68	120.73
3	B	302	E1F	O18-S16-C3	-2.97	102.94	107.26
3	A	302	E1F	C4-C3-S16	-2.96	113.49	117.52
3	D	302	E1F	O18-S16-N19	2.87	111.49	107.35
3	D	302	E1F	C14-N11-C9	2.85	119.17	114.96
3	A	302	E1F	O18-S16-N19	2.84	111.44	107.35
3	D	302	E1F	C5-C4-C3	-2.81	115.79	119.97
3	B	302	E1F	C21-C1-C6	-2.71	114.28	120.18
3	A	302	E1F	C3-C2-CL1	2.70	123.47	121.52
3	D	302	E1F	C3-C2-CL1	2.62	123.41	121.52
3	A	302	E1F	C5-C4-C3	-2.60	116.09	119.97
3	A	302	E1F	C13-N10-C9	2.54	118.71	114.96
3	A	302	E1F	C21-C1-C6	-2.53	114.68	120.18
3	B	302	E1F	C14-N11-C9	2.48	118.62	114.96
3	C	302	E1F	C15-C13-N10	-2.46	119.52	123.42
3	C	302	E1F	C2-C3-S16	-2.37	120.62	123.47
3	C	302	E1F	O17-S16-N19	-2.35	103.96	107.35
3	D	302	E1F	O17-S16-C3	-2.30	103.92	107.26
3	D	302	E1F	O12-C6-C7	2.28	123.96	120.41
3	A	302	E1F	O17-S16-O18	-2.24	115.34	118.80
3	D	302	E1F	C5-C1-C21	2.24	121.84	119.25
3	C	302	E1F	C4-C3-S16	2.20	120.52	117.52
3	A	302	E1F	O17-S16-N19	2.19	110.51	107.35
3	C	302	E1F	N10-C9-N11	-2.17	123.38	126.86
3	C	302	E1F	O17-S16-C3	-2.10	104.20	107.26
3	C	302	E1F	C14-C15-C13	2.04	119.28	116.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

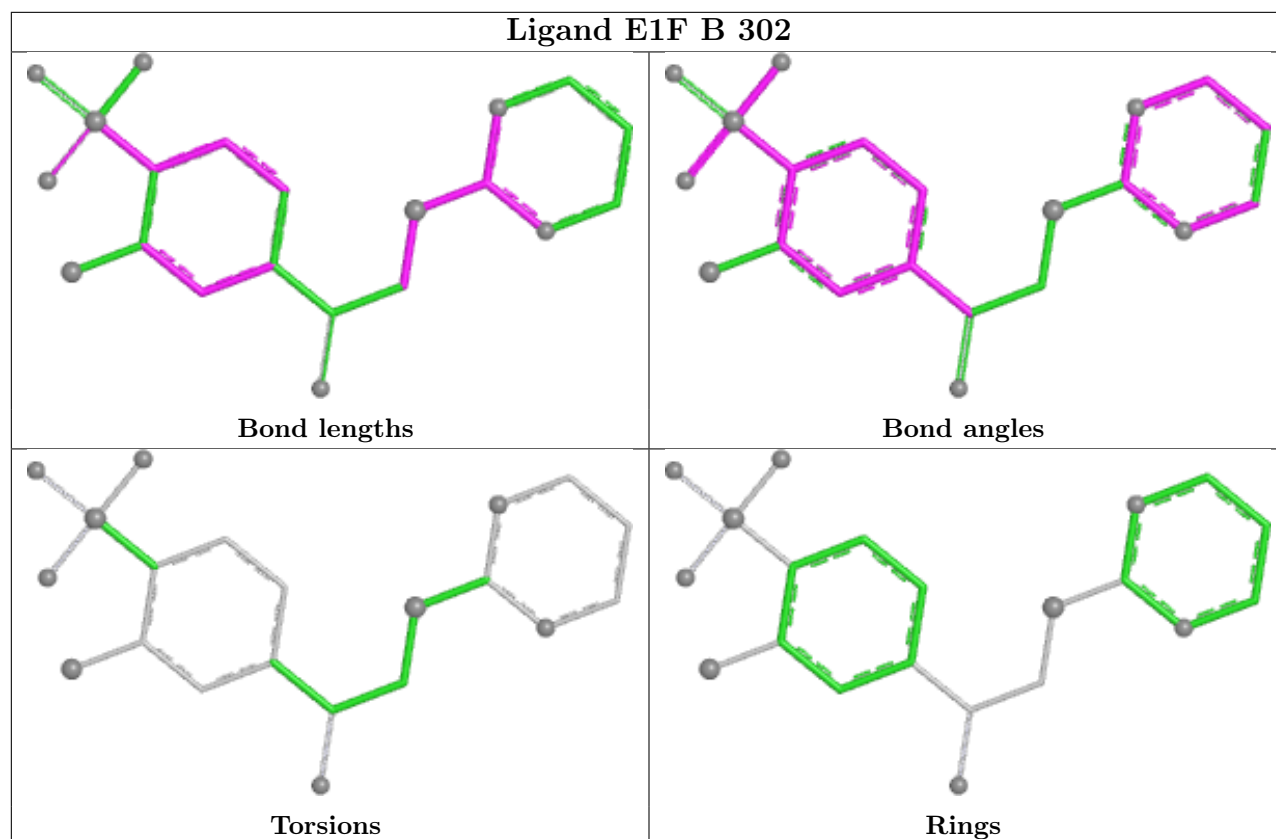
Mol	Chain	Res	Type	Atoms
4	B	304	EDO	O1-C1-C2-O2
3	C	302	E1F	C4-C3-S16-O17
4	A	303	EDO	O1-C1-C2-O2
4	D	303	EDO	O1-C1-C2-O2
3	A	302	E1F	C2-C3-S16-N19
3	D	302	E1F	C2-C3-S16-N19
4	B	303	EDO	O1-C1-C2-O2
3	C	302	E1F	C2-C3-S16-N19

There are no ring outliers.

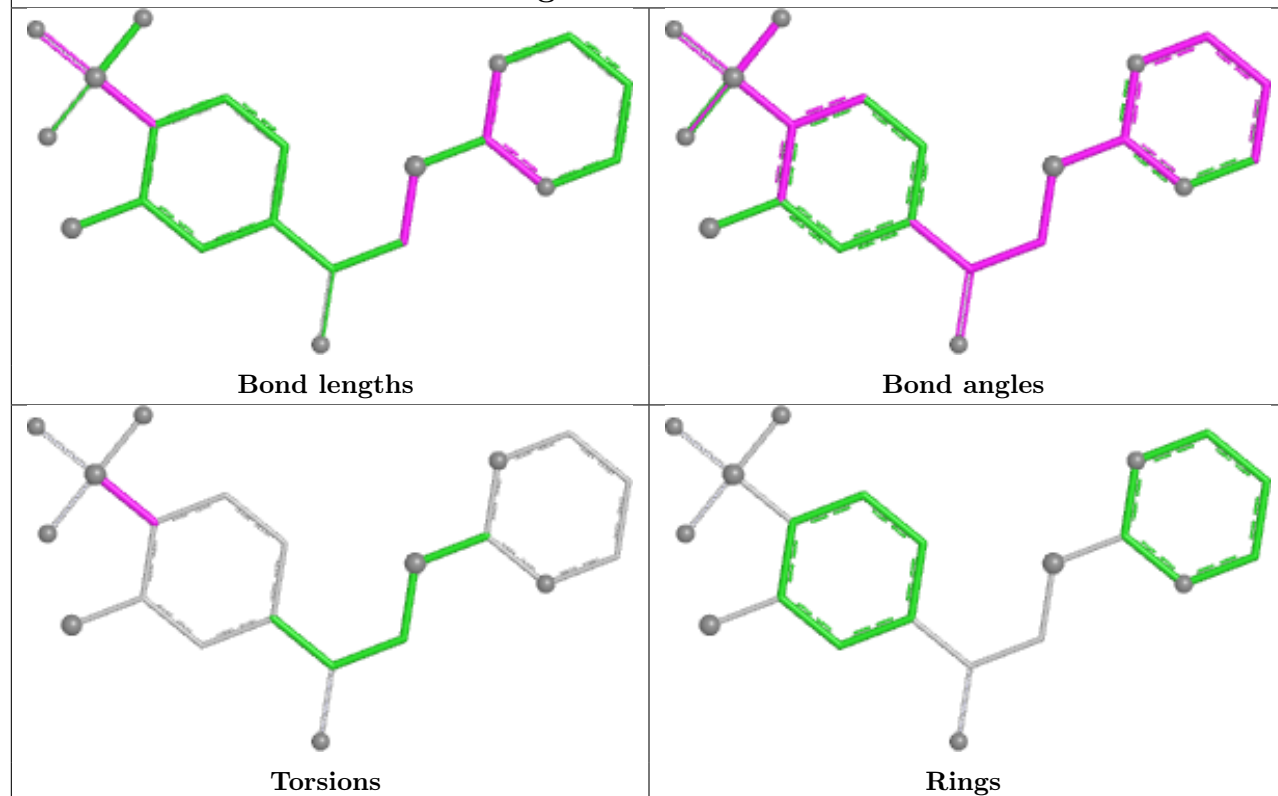
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	303	SO4	2	0
3	C	302	E1F	2	0
4	D	304	EDO	3	0

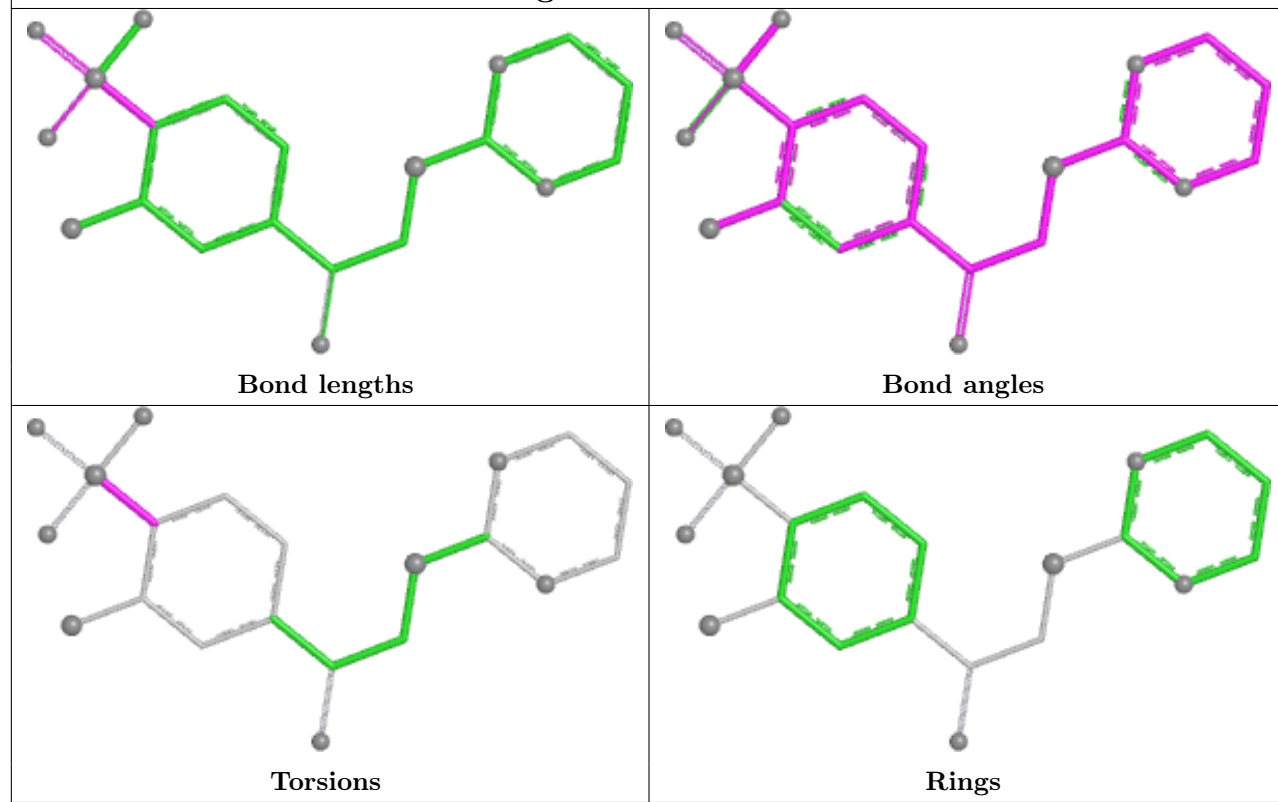
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

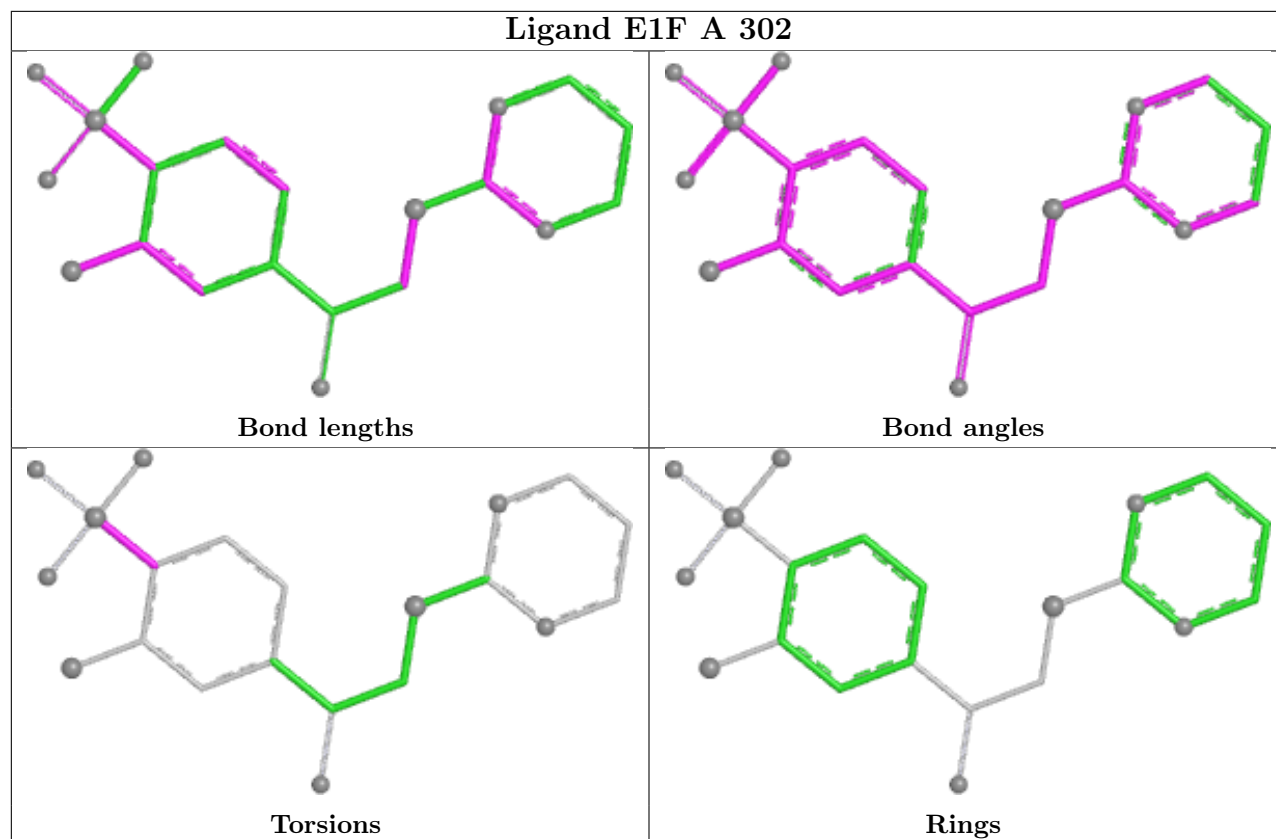


Ligand E1F C 302



Ligand E1F D 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/263 (99%)	-0.09	4 (1%) 72 75	3, 13, 25, 39	10 (3%)
1	B	261/263 (99%)	-0.13	7 (2%) 56 58	5, 11, 24, 35	7 (2%)
1	C	260/263 (98%)	0.93	52 (20%) 3 3	5, 19, 36, 47	16 (6%)
1	D	260/263 (98%)	-0.19	5 (1%) 66 68	6, 12, 22, 31	12 (4%)
All	All	1042/1052 (99%)	0.13	68 (6%) 25 24	3, 13, 29, 47	45 (4%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	7.3
1	B	253	ASP	5.9
1	B	252	PHE	4.5
1	C	233[A]	HIS	4.5
1	C	228	ALA	4.4
1	C	7	PHE	4.3
1	C	158[A]	ILE	4.1
1	C	3[A]	LYS	4.0
1	B	254	GLU	3.9
1	A	3[A]	LYS	3.7
1	C	159	PHE	3.6
1	A	7	PHE	3.6
1	C	230	TYR	3.4
1	C	234	MET	3.4
1	C	167	TYR	3.4
1	C	173	PHE	3.3
1	C	174	VAL	3.2
1	C	177	PHE	3.1
1	C	54	SER	2.9
1	C	172	ALA	2.9
1	C	56	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	58	GLN	2.9
1	C	149	GLY	2.9
1	C	231[A]	CYS	2.8
1	C	57	LYS	2.8
1	C	151	PHE	2.7
1	C	8	GLY	2.7
1	D	253	ASP	2.6
1	B	137	GLU	2.6
1	C	162	LEU	2.6
1	C	160	SER	2.6
1	C	155	TYR	2.6
1	C	168[A]	LYS	2.6
1	C	224	ALA	2.5
1	B	263	GLN	2.5
1	D	252	PHE	2.5
1	B	3	LYS	2.5
1	C	217	ILE	2.5
1	D	80	GLY	2.5
1	C	229	LEU	2.4
1	C	165	VAL	2.4
1	C	215	VAL	2.4
1	C	53	LEU	2.4
1	C	61[A]	LEU	2.3
1	C	225	LEU	2.3
1	C	9	PRO	2.3
1	C	262	SER	2.3
1	C	59	PHE	2.3
1	C	153	PRO	2.3
1	C	240	ARG	2.2
1	C	70	LEU	2.2
1	C	223	LEU	2.2
1	C	176	GLY	2.2
1	B	255	ARG	2.2
1	D	98	ASN	2.2
1	C	148	MET	2.2
1	C	90	LEU	2.1
1	C	239	PRO	2.1
1	C	227	THR	2.1
1	A	137	GLU	2.1
1	C	161	HIS	2.1
1	C	235	ASP	2.1
1	C	49	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	51	TYR	2.0
1	A	263	GLN	2.0
1	C	60	LEU	2.0
1	C	72	LEU	2.0
1	D	262	SER	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.

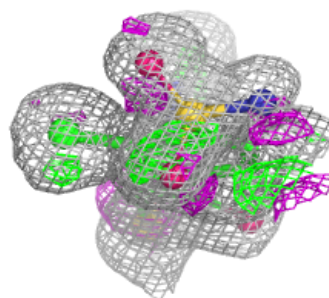
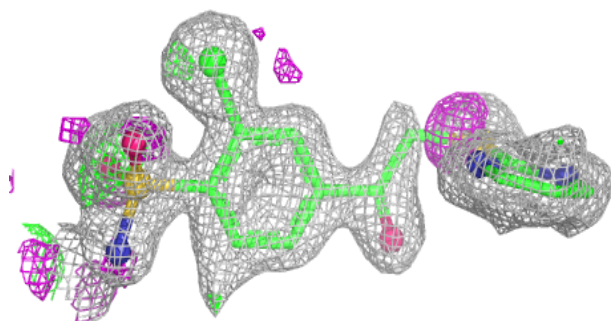
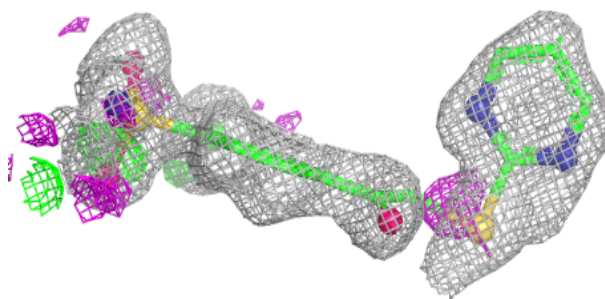
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	303	5/5	0.69	0.13	64,64,67,67	0
4	EDO	D	304	4/4	0.82	0.14	25,26,30,32	0
4	EDO	B	304	4/4	0.89	0.12	15,19,24,24	0
4	EDO	B	303	4/4	0.91	0.12	14,18,24,26	0
4	EDO	D	303	4/4	0.92	0.13	21,21,23,25	0
4	EDO	A	303	4/4	0.93	0.11	19,23,26,26	0
4	EDO	A	304	4/4	0.94	0.08	22,22,23,23	0
3	E1F	C	302	21/21	0.96	0.09	9,19,32,33	0
2	ZN	C	301	1/1	0.97	0.03	12,12,12,12	0
3	E1F	A	302	21/21	0.98	0.08	7,14,31,33	0
3	E1F	D	302	21/21	0.98	0.06	7,13,22,23	0
3	E1F	B	302	21/21	0.98	0.08	5,13,32,34	0
2	ZN	D	301	1/1	1.00	0.01	7,7,7,7	0
2	ZN	B	301	1/1	1.00	0.02	5,5,5,5	0
2	ZN	A	301	1/1	1.00	0.01	7,7,7,7	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.

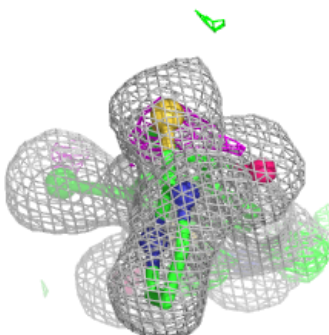
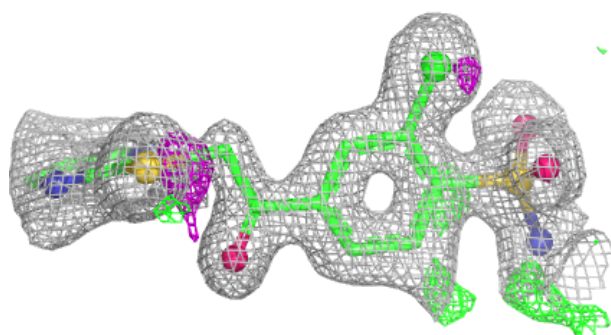
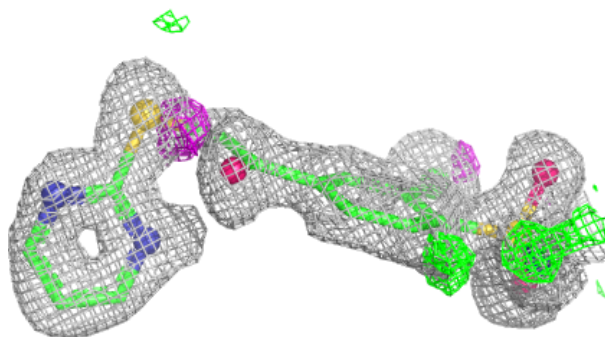
Electron density around E1F C 302:

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



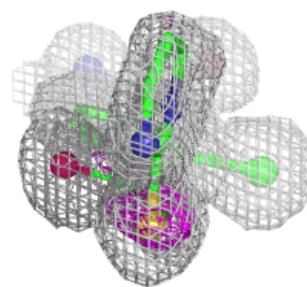
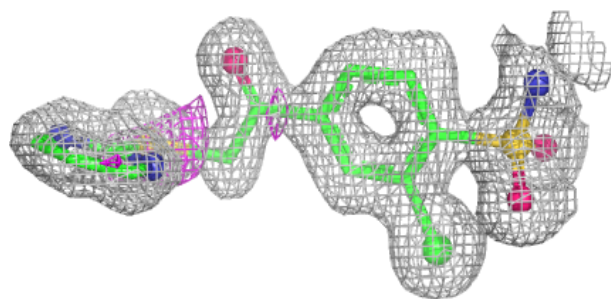
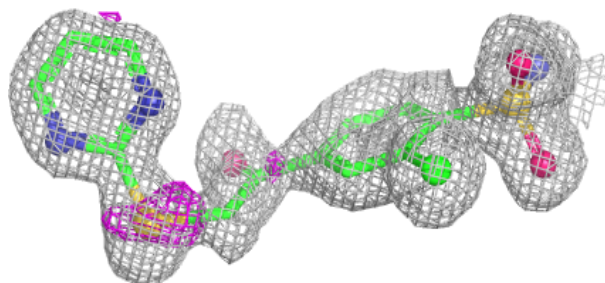
Electron density around E1F A 302:

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

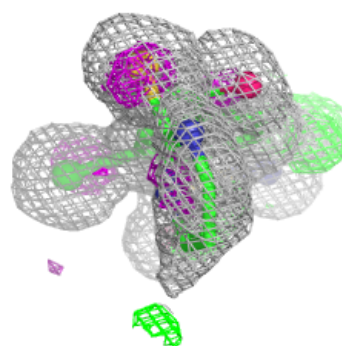
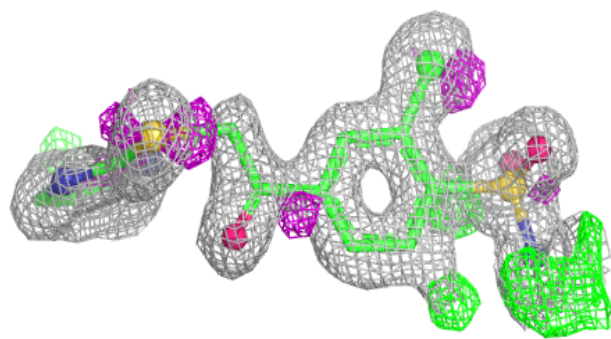
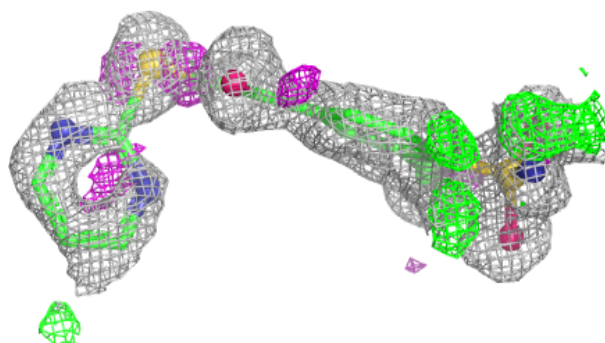


Electron density around E1F D 302:

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

**Electron density around E1F 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.