



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 AM UTC

PDB ID : 4HW2 / pdb_00004hw2
Title : Discovery of potent Mcl-1 inhibitors using fragment-based methods and structure-based design
Authors : Zhao, B.
Deposited on : 2012-11-07
Resolution : 2.80 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:

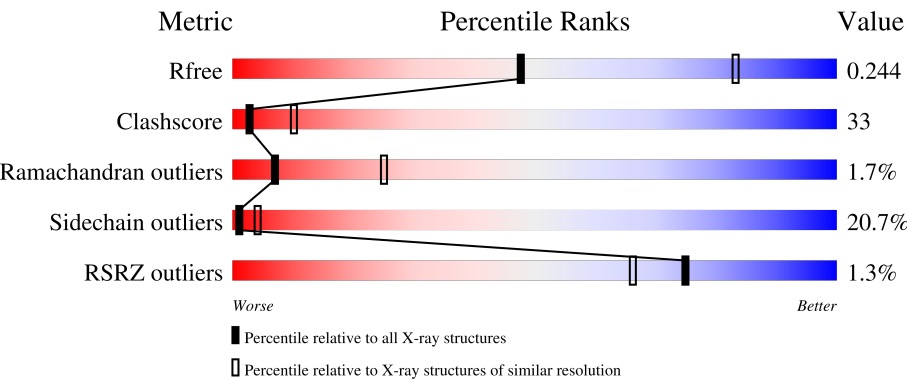
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.80 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.



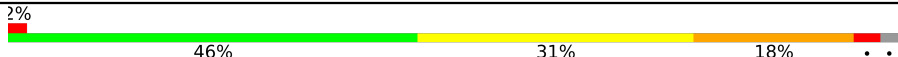
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	153	2% 46%40%9%..
1	B	153	2% 48%35%14%..
1	C	153	43%37%16%..
1	D	153	2% 57%32%10%. .
1	E	153	48%39%9%..

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Mol	Chain	Length	Quality of chain
1	F	153	

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
2	19H	C	400	-	X	-	-
2	19H	D	400	-	X	-	-
2	19H	E	400	-	X	-	-
2	19H	F	400	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7376 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.

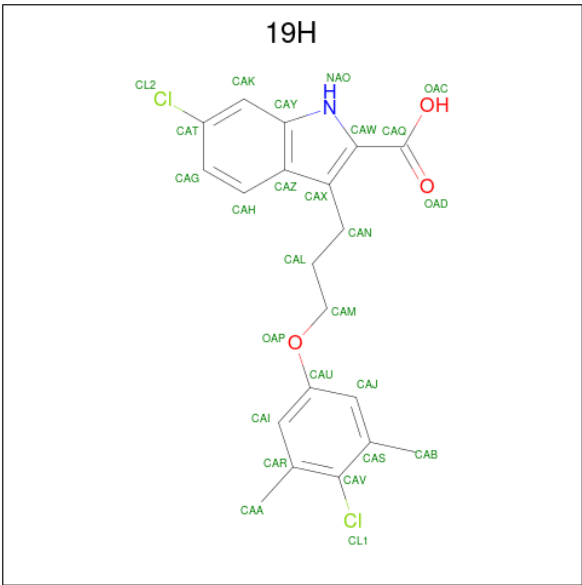
- Molecule 1 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1186	745	217	221	3			
1	B	151	Total	C	N	O	S	0	0	0
			1212	761	224	223	4			
1	C	150	Total	C	N	O	S	0	0	0
			1185	745	218	218	4			
1	D	151	Total	C	N	O	S	0	0	0
			1203	757	221	221	4			
1	E	151	Total	C	N	O	S	0	0	0
			1209	760	224	221	4			
1	F	150	Total	C	N	O	S	0	0	0
			1191	747	218	222	4			

There are 6 discrepancies between the modelled and reference sequences:

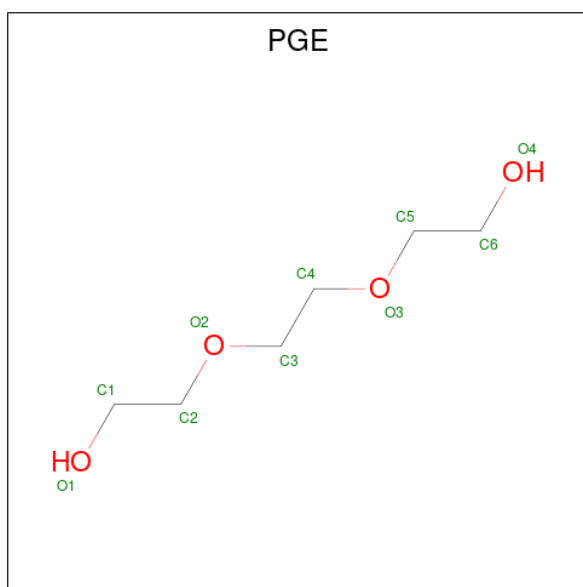
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q07820
B	171	GLY	-	expression tag	UNP Q07820
C	171	GLY	-	expression tag	UNP Q07820
D	171	GLY	-	expression tag	UNP Q07820
E	171	GLY	-	expression tag	UNP Q07820
F	171	GLY	-	expression tag	UNP Q07820

- Molecule 2 is 6-chloro-3-[3-(4-chloro-3,5-dimethylphenoxy)propyl]-1H-indole-2-carboxylic acid (CCD ID: 19H) (formula: C₂₀H₁₉Cl₂NO₃).



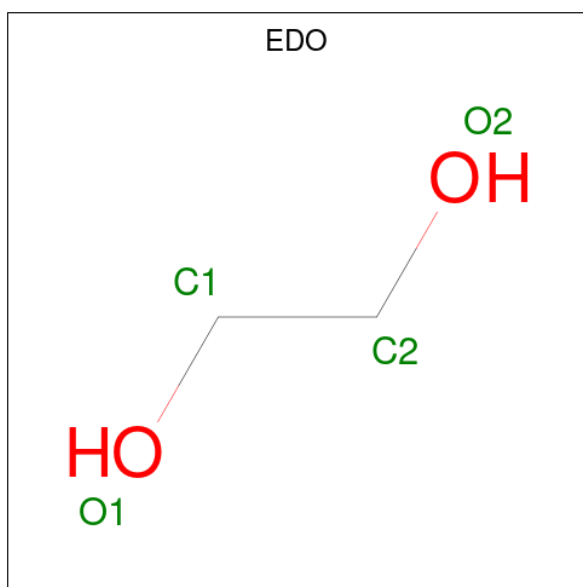
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	B	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	C	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	D	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	E	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	F	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

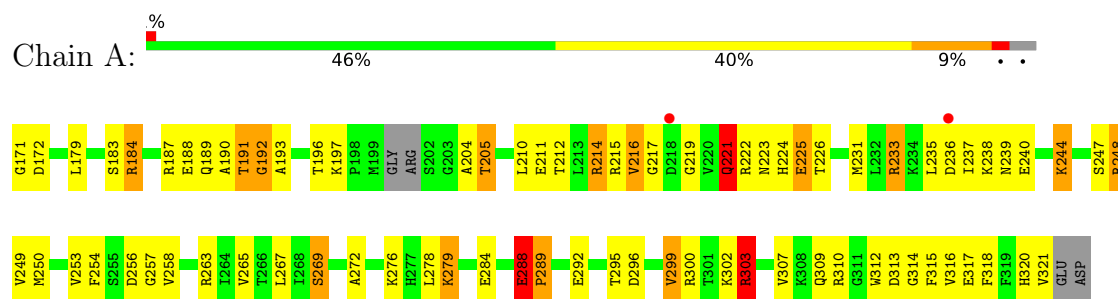


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

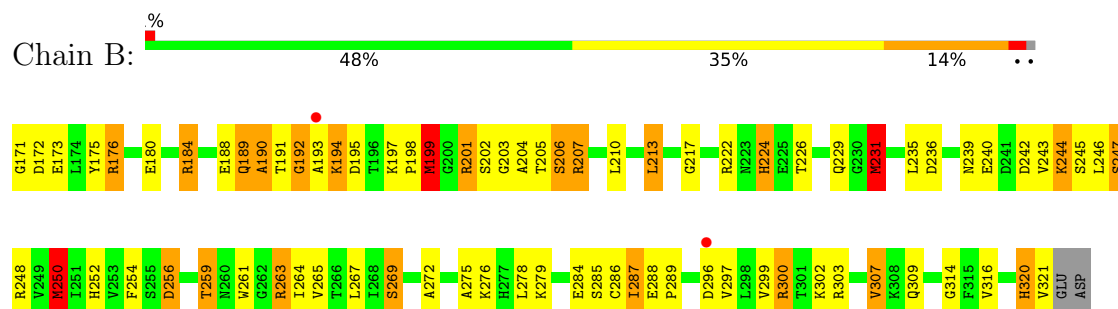
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

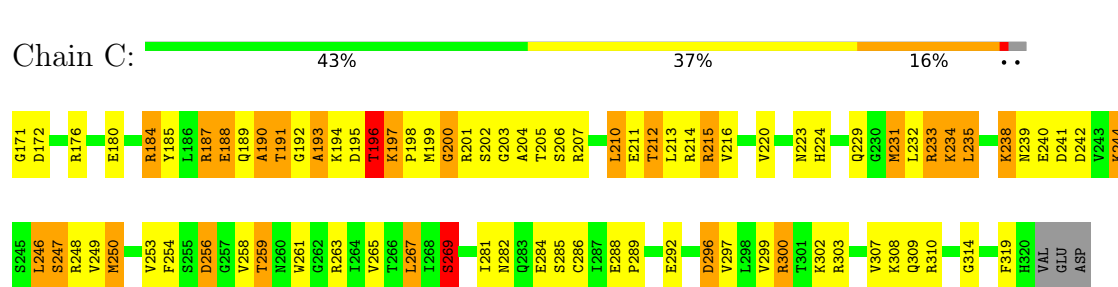
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



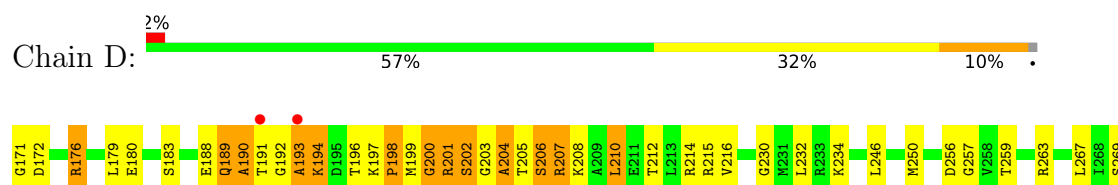
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

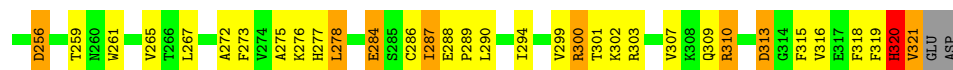
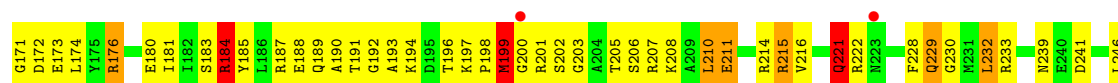


• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

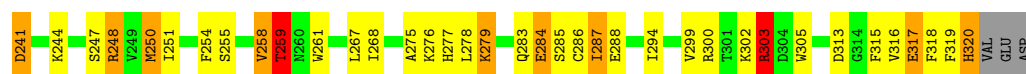




- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.00Å 134.33Å 62.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 97.2 (30.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.217 , 0.245 0.219 , 0.244	Depositor DCC
R_{free} test set	2491 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.3	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	0.93	EDS
Total number of atoms	7376	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 19H, 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	1.63	9/1205 (0.7%)	1.27	13/1623 (0.8%)
1	B	1.57	8/1232 (0.6%)	1.24	10/1656 (0.6%)
1	C	1.47	5/1205 (0.4%)	1.26	7/1623 (0.4%)
1	D	1.02	1/1223 (0.1%)	1.11	6/1645 (0.4%)
1	E	1.22	3/1229 (0.2%)	1.21	10/1652 (0.6%)
1	F	1.17	5/1211 (0.4%)	1.23	8/1631 (0.5%)
All	All	1.36	31/7305 (0.4%)	1.22	54/9830 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	2
All	All	0	4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	250	MET	SD-CE	-7.59	1.60	1.79
1	B	252	HIS	CE1-NE2	-6.94	1.25	1.32
1	B	250	MET	SD-CE	-6.50	1.63	1.79
1	F	226	THR	CB-OG1	-6.15	1.33	1.43
1	B	252	HIS	CG-ND1	-6.11	1.31	1.38
1	E	233	ARG	CZ-NH2	-6.11	1.25	1.33
1	A	193	ALA	CA-C	-6.07	1.44	1.52
1	B	231	MET	SD-CE	-6.04	1.64	1.79
1	C	231	MET	SD-CE	-6.03	1.64	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	GLN	CD-OE1	-5.80	1.12	1.23
1	B	300	ARG	CZ-NH2	-5.80	1.25	1.33
1	A	288	GLU	C-O	-5.62	1.19	1.24
1	F	300	ARG	CZ-NH2	-5.57	1.26	1.33
1	A	233	ARG	CZ-NH2	-5.50	1.26	1.33
1	E	221	GLN	CD-NE2	-5.44	1.21	1.33
1	C	193	ALA	CA-C	-5.40	1.46	1.52
1	B	224	HIS	CE1-NE2	-5.38	1.27	1.32
1	F	184	ARG	CZ-NH1	-5.28	1.25	1.32
1	A	250	MET	SD-CE	-5.27	1.66	1.79
1	C	269	SER	C-O	-5.25	1.17	1.24
1	B	229	GLN	CD-OE1	-5.23	1.13	1.23
1	A	320	HIS	CA-C	-5.18	1.46	1.52
1	E	233	ARG	CD-NE	-5.17	1.39	1.46
1	B	224	HIS	CG-ND1	-5.17	1.32	1.38
1	C	300	ARG	CZ-NH2	-5.15	1.26	1.33
1	A	233	ARG	CZ-NH1	-5.15	1.25	1.32
1	D	300	ARG	CZ-NH2	-5.13	1.26	1.33
1	A	184	ARG	CZ-NH1	-5.08	1.25	1.32
1	F	229	GLN	CD-OE1	-5.06	1.14	1.23
1	C	263	ARG	CZ-NH1	-5.04	1.25	1.32
1	A	197	LYS	C-N	5.02	1.40	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	ARG	N-CA-C	-11.31	99.30	113.55
1	C	190	ALA	N-CA-C	-10.67	96.77	110.53
1	F	204	ALA	N-CA-C	-10.13	99.63	112.90
1	F	237	ILE	N-CA-C	8.76	120.25	109.30
1	E	200	GLY	N-CA-C	8.68	133.76	113.18
1	B	254	PHE	N-CA-C	8.23	121.37	111.82
1	A	254	PHE	N-CA-C	8.07	121.18	111.82
1	F	215	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	A	257	GLY	N-CA-C	8.03	124.60	110.95
1	B	246	LEU	N-CA-C	7.90	122.18	112.54
1	E	300	ARG	N-CA-C	7.77	119.54	111.14
1	C	194	LYS	N-CA-C	-7.39	97.77	109.23
1	D	198	PRO	N-CA-C	7.35	123.46	113.98
1	B	204	ALA	N-CA-C	-7.14	103.58	111.36
1	D	201	ARG	N-CA-C	7.10	120.86	111.28
1	E	222	ARG	N-CA-C	7.00	118.70	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	313	ASP	N-CA-C	-7.00	103.65	111.28
1	B	190	ALA	N-CA-C	-6.76	101.81	110.53
1	A	204	ALA	N-CA-C	-6.73	104.94	113.02
1	D	190	ALA	N-CA-C	-6.66	101.93	110.53
1	E	320	HIS	N-CA-C	6.61	118.17	110.97
1	E	192	GLY	N-CA-C	6.59	123.10	113.48
1	C	193	ALA	N-CA-C	6.54	119.24	110.35
1	C	235	LEU	N-CA-C	6.49	118.43	111.36
1	B	320	HIS	N-CA-C	6.46	118.02	110.97
1	A	205	THR	N-CA-C	-6.45	104.33	111.82
1	D	204	ALA	N-CA-C	-6.42	103.53	112.45
1	A	217	GLY	N-CA-C	6.34	120.89	112.77
1	D	202	SER	N-CA-C	-6.34	103.43	111.92
1	D	257	GLY	N-CA-C	6.34	122.52	110.86
1	F	254	PHE	N-CA-C	6.29	121.14	112.90
1	F	239	ASN	N-CA-C	6.22	118.23	108.96
1	C	196	THR	N-CA-C	-6.13	104.28	110.97
1	F	303	ARG	N-CA-C	6.11	117.60	111.07
1	B	199	MET	N-CA-C	6.04	118.99	107.75
1	B	194	LYS	N-CA-CB	6.04	120.77	110.50
1	A	197	LYS	CA-C-N	-5.96	113.64	119.78
1	A	197	LYS	C-N-CA	-5.96	113.64	119.78
1	A	303	ARG	N-CA-C	5.95	117.44	111.07
1	A	223	ASN	N-CA-C	5.74	118.48	111.82
1	B	195	ASP	N-CA-C	5.67	117.97	108.73
1	B	247	SER	N-CA-C	5.63	117.42	111.28
1	F	241	ASP	N-CA-C	-5.53	105.65	112.90
1	C	246	LEU	N-CA-C	5.52	119.74	112.89
1	A	192	GLY	N-CA-C	-5.45	104.26	112.60
1	E	230	GLY	N-CA-C	-5.32	106.06	112.49
1	A	225	GLU	N-CA-C	5.25	117.00	111.28
1	C	191	THR	CB-CA-C	-5.25	99.97	110.42
1	E	184	ARG	N-CA-C	5.18	116.73	111.14
1	F	268	ILE	N-CA-C	5.17	115.94	110.72
1	A	247	SER	N-CA-C	5.13	116.87	111.28
1	E	199	MET	N-CA-C	-5.11	101.99	109.81
1	A	239	ASN	N-CA-C	5.04	115.97	108.86
1	B	264	ILE	N-CA-C	5.03	115.80	110.72

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	248	ARG	Sidechain
1	C	215	ARG	Sidechain
1	F	176	ARG	Sidechain
1	F	215	ARG	Sidechain

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	1186	0	1177	60	0
1	B	1212	0	1223	69	0
1	C	1185	0	1177	84	0
1	D	1203	0	1210	59	0
1	E	1209	0	1221	93	0
1	F	1191	0	1181	122	0
2	A	26	0	18	1	0
2	B	26	0	18	0	0
2	C	26	0	18	5	0
2	D	26	0	18	1	0
2	E	26	0	18	1	0
2	F	26	0	18	1	0
3	A	10	0	14	4	0
3	B	20	0	28	2	0
4	B	4	0	6	1	0
All	All	7376	0	7345	483	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 33.

All (483) 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:171:GLY:HA2	1:B:303:ARG:NH2	1.42	1.31
1:D:193:ALA:CB	1:D:194:LYS:HA	1.50	1.31
1:C:171:GLY:HA2	1:C:303:ARG:NH2	1.50	1.27
1:D:193:ALA:HB1	1:D:194:LYS:CA	1.70	1.21
1:E:318:PHE:HD2	1:E:319:PHE:CE1	1.59	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:GLY:CA	1:F:303:ARG:HH12	1.58	1.13
1:B:193:ALA:HB1	1:B:194:LYS:HB3	1.21	1.12
1:F:258:VAL:HG13	1:F:259:THR:H	1.08	1.11
1:E:318:PHE:CD2	1:E:319:PHE:HE1	1.68	1.10
1:C:191:THR:HG21	1:C:193:ALA:HB2	1.20	1.09
1:F:211:GLU:HA	1:F:211:GLU:OE1	1.52	1.08
1:F:189:GLN:HA	1:F:189:GLN:NE2	1.67	1.07
1:F:250:MET:HE1	1:F:294:ILE:HA	1.35	1.07
1:B:173:GLU:CD	1:B:201:ARG:HD3	1.79	1.06
1:B:203:GLY:O	1:B:207:ARG:HG3	1.56	1.06
1:C:191:THR:HG22	1:C:193:ALA:N	1.72	1.05
1:F:171:GLY:HA2	1:F:303:ARG:NH1	1.73	1.04
1:B:171:GLY:CA	1:B:303:ARG:HH22	1.70	1.03
1:F:258:VAL:HG13	1:F:259:THR:N	1.67	1.03
1:B:250:MET:HE2	1:B:297:VAL:HG21	1.41	1.03
1:F:189:GLN:HA	1:F:189:GLN:HE21	1.15	1.03
1:F:313:ASP:O	1:F:316:VAL:HG12	1.59	1.01
1:F:171:GLY:CA	1:F:303:ARG:NH1	2.23	1.00
1:B:171:GLY:HA2	1:B:303:ARG:HH22	0.90	0.98
1:C:171:GLY:CA	1:C:303:ARG:HH22	1.76	0.98
1:E:171:GLY:CA	1:E:303:ARG:NH2	2.26	0.97
1:F:258:VAL:O	1:F:259:THR:HB	1.62	0.97
1:C:171:GLY:CA	1:C:303:ARG:NH2	2.28	0.96
1:D:171:GLY:HA3	1:D:303:ARG:NH2	1.82	0.95
1:F:171:GLY:HA3	1:F:303:ARG:HH12	1.31	0.94
1:B:250:MET:CE	1:B:297:VAL:HG21	1.97	0.94
1:F:191:THR:HG22	1:F:279:LYS:HE2	1.49	0.94
1:A:224:HIS:CE1	3:A:402:PGE:H1	2.02	0.93
1:E:318:PHE:CD2	1:E:319:PHE:CE1	2.50	0.93
1:C:184:ARG:HH12	1:C:195:ASP:CB	1.81	0.92
1:E:171:GLY:HA3	1:E:303:ARG:NH2	1.82	0.92
1:A:171:GLY:HA3	1:A:303:ARG:HH22	1.34	0.92
1:A:224:HIS:NE2	3:A:402:PGE:H1	1.84	0.92
1:E:278:LEU:HD23	1:E:286:CYS:HB2	1.52	0.92
1:D:320:HIS:O	1:D:321:VAL:HG12	1.67	0.92
1:F:196:THR:O	1:F:197:LYS:O	1.87	0.92
1:F:320:HIS:O	1:F:320:HIS:ND1	2.02	0.92
1:C:191:THR:HG22	1:C:192:GLY:N	1.85	0.91
1:F:201:ARG:O	1:F:202:SER:OG	1.86	0.91
1:B:171:GLY:CA	1:B:303:ARG:NH2	2.29	0.91
1:F:259:THR:OG1	1:F:302:LYS:HE3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLU:OE2	1:B:201:ARG:HD3	1.70	0.91
1:C:190:ALA:O	1:C:191:THR:HB	1.67	0.91
1:C:171:GLY:HA2	1:C:303:ARG:HH22	1.08	0.90
1:F:236:ASP:OD1	1:F:236:ASP:O	1.90	0.90
1:C:202:SER:O	1:C:205:THR:HG22	1.70	0.90
1:A:187:ARG:O	1:A:191:THR:HG22	1.72	0.90
1:F:212:THR:HG23	1:F:215:ARG:NH2	1.88	0.89
1:E:278:LEU:CD2	1:E:286:CYS:HB2	2.03	0.89
1:F:171:GLY:HA2	1:F:303:ARG:HH12	1.31	0.89
1:F:199:MET:HE3	1:F:207:ARG:HD2	1.56	0.88
1:E:216:VAL:HG21	1:E:319:PHE:HD2	1.36	0.87
1:A:313:ASP:O	1:A:317:GLU:HG2	1.74	0.87
1:F:258:VAL:CG1	1:F:259:THR:H	1.66	0.86
1:C:191:THR:HG22	1:C:193:ALA:H	1.35	0.86
1:F:199:MET:HE3	1:F:207:ARG:CD	2.05	0.86
1:E:171:GLY:HA2	1:E:303:ARG:NH2	1.89	0.85
1:E:171:GLY:CA	1:E:303:ARG:HH22	1.89	0.85
1:C:229:GLN:O	1:C:229:GLN:NE2	2.10	0.84
1:F:212:THR:HG23	1:F:215:ARG:HH21	1.42	0.84
1:C:288:GLU:O	1:C:292:GLU:HG3	1.78	0.84
1:C:250:MET:HE3	1:C:297:VAL:HG21	1.59	0.83
1:F:221:GLN:O	1:F:225:GLU:HG2	1.79	0.83
1:D:193:ALA:HB1	1:D:194:LYS:HA	0.86	0.83
1:B:224:HIS:HA	4:B:404:EDO:H22	1.60	0.82
1:E:171:GLY:HA3	1:E:303:ARG:HH22	1.41	0.81
1:D:188:GLU:HG3	1:D:193:ALA:HB3	1.62	0.81
1:A:196:THR:CG2	1:C:284:GLU:OE2	2.28	0.80
1:C:191:THR:HG21	1:C:193:ALA:CB	2.07	0.80
1:E:318:PHE:HD2	1:E:319:PHE:HE1	0.87	0.80
1:A:303:ARG:O	1:A:307:VAL:HG23	1.80	0.80
1:C:191:THR:CG2	1:C:193:ALA:HB2	2.10	0.80
1:F:171:GLY:HA3	1:F:303:ARG:NH1	1.93	0.80
1:E:229:GLN:HE21	1:E:229:GLN:C	1.90	0.80
1:F:258:VAL:HG22	1:F:259:THR:N	1.96	0.79
1:A:196:THR:HG21	1:C:284:GLU:OE2	1.83	0.79
1:E:232:LEU:HD12	1:E:232:LEU:O	1.81	0.79
1:F:222:ARG:NH1	1:F:223:ASN:OD1	2.16	0.79
1:F:248:ARG:HG3	1:F:248:ARG:HH11	1.47	0.79
1:C:184:ARG:NH1	1:C:195:ASP:CB	2.46	0.79
1:F:258:VAL:CG1	1:F:259:THR:N	2.33	0.79
1:B:197:LYS:HG2	1:B:198:PRO:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:CA	1:A:303:ARG:HH22	1.97	0.78
1:B:193:ALA:HB1	1:B:194:LYS:CB	2.10	0.78
1:F:259:THR:HG22	1:F:305:TRP:CE2	2.19	0.77
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.49	0.77
1:C:196:THR:O	1:C:197:LYS:CB	2.30	0.77
1:F:211:GLU:OE1	1:F:211:GLU:CA	2.30	0.76
1:F:187:ARG:HA	1:F:190:ALA:HB3	1.67	0.76
1:E:216:VAL:HG21	1:E:319:PHE:CD2	2.21	0.76
1:F:259:THR:HG21	1:F:305:TRP:CD2	2.21	0.75
1:C:216:VAL:HG12	1:C:265:VAL:HG11	1.67	0.75
1:F:191:THR:HG22	1:F:279:LYS:CE	2.15	0.75
1:F:199:MET:HE1	1:F:210:LEU:HD12	1.69	0.74
1:F:279:LYS:HB2	1:F:284:GLU:OE2	1.87	0.74
1:F:239:ASN:HB3	1:F:283:GLN:OE1	1.88	0.74
1:E:313:ASP:O	1:E:316:VAL:HG12	1.88	0.73
1:A:295:THR:O	1:A:299:VAL:HG23	1.87	0.73
1:B:173:GLU:OE2	1:B:176:ARG:NH2	2.21	0.73
1:F:199:MET:O	1:F:199:MET:HG3	1.87	0.73
1:B:189:GLN:HG2	1:B:272:ALA:HB1	1.69	0.72
1:E:318:PHE:C	1:E:319:PHE:HD1	1.97	0.72
1:B:261:TRP:O	1:B:265:VAL:HG23	1.89	0.72
1:E:321:VAL:HG12	1:E:321:VAL:O	1.88	0.72
1:B:303:ARG:O	1:B:307:VAL:HG23	1.89	0.72
1:C:212:THR:HG23	1:C:215:ARG:HH12	1.55	0.72
1:F:191:THR:OG1	1:F:192:GLY:N	2.15	0.72
1:F:196:THR:OG1	1:F:197:LYS:N	2.20	0.72
1:B:189:GLN:CG	1:B:272:ALA:HB1	2.20	0.71
1:E:299:VAL:O	1:E:303:ARG:HB2	1.91	0.71
1:F:184:ARG:NH2	1:F:195:ASP:HB2	2.05	0.71
1:F:259:THR:CG2	1:F:305:TRP:CE2	2.73	0.71
1:B:171:GLY:HA3	1:B:175:TYR:HB2	1.73	0.71
1:C:191:THR:CG2	1:C:192:GLY:N	2.53	0.71
1:F:201:ARG:C	1:F:202:SER:HG	1.93	0.71
1:B:250:MET:CE	1:B:297:VAL:CG2	2.69	0.70
1:B:321:VAL:HG12	1:B:321:VAL:O	1.90	0.70
1:F:279:LYS:CB	1:F:284:GLU:OE2	2.39	0.70
1:A:171:GLY:HA3	1:A:303:ARG:NH2	2.07	0.70
1:E:205:THR:HG21	1:E:313:ASP:OD1	1.91	0.70
1:E:184:ARG:NH2	1:E:197:LYS:O	2.25	0.70
1:D:171:GLY:CA	1:D:303:ARG:NH2	2.54	0.69
1:E:229:GLN:NE2	1:E:229:GLN:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG12	2:A:401:19H:H9	1.75	0.69
1:D:321:VAL:O	1:D:321:VAL:HG13	1.92	0.69
1:F:196:THR:O	1:F:197:LYS:C	2.34	0.69
1:A:235:LEU:O	1:A:236:ASP:HB2	1.91	0.69
1:B:224:HIS:HE2	3:B:403:PGE:H12	1.57	0.69
1:F:258:VAL:O	1:F:259:THR:CB	2.39	0.69
1:F:232:LEU:HD21	1:F:277:HIS:CG	2.27	0.69
1:E:320:HIS:O	1:E:321:VAL:HB	1.92	0.69
1:E:259:THR:CG2	1:E:302:LYS:HZ3	2.06	0.68
1:A:299:VAL:HG12	1:A:303:ARG:HH21	1.57	0.68
1:F:248:ARG:HH11	1:F:248:ARG:CG	2.06	0.68
1:C:296:ASP:O	1:C:300:ARG:HB2	1.93	0.68
1:C:191:THR:CG2	1:C:193:ALA:N	2.53	0.68
1:D:278:LEU:HD23	1:D:287:ILE:HD13	1.74	0.68
1:E:181:ILE:HG23	1:E:210:LEU:HD12	1.74	0.67
1:F:186:LEU:O	1:F:190:ALA:HB2	1.95	0.67
1:D:212:THR:O	1:D:216:VAL:HG22	1.94	0.67
1:E:199:MET:HB2	1:E:203:GLY:HA3	1.77	0.67
1:D:232:LEU:HD11	1:D:277:HIS:CD2	2.30	0.66
1:E:229:GLN:HE21	1:E:229:GLN:CA	2.05	0.66
1:B:180:GLU:HG2	1:B:199:MET:HE3	1.77	0.66
1:B:256:ASP:O	1:B:263:ARG:NH2	2.29	0.66
1:F:212:THR:HG21	1:F:319:PHE:HB2	1.78	0.66
1:C:265:VAL:O	1:C:269:SER:HB2	1.96	0.66
1:D:193:ALA:CB	1:D:194:LYS:CA	2.40	0.66
1:D:246:LEU:HD13	2:D:400:19H:CL1	2.32	0.66
1:B:184:ARG:O	1:B:188:GLU:HG3	1.96	0.66
1:C:190:ALA:O	1:C:191:THR:CB	2.42	0.66
1:E:185:TYR:CZ	1:E:189:GLN:NE2	2.65	0.65
1:C:241:ASP:HA	1:C:244:LYS:HD3	1.77	0.65
1:C:191:THR:CG2	1:C:193:ALA:H	2.05	0.65
1:E:185:TYR:HE1	1:E:214:ARG:HA	1.61	0.65
1:C:188:GLU:OE2	1:C:214:ARG:NE	2.29	0.65
1:B:207:ARG:HH11	1:B:207:ARG:HB2	1.61	0.64
1:D:317:GLU:HG2	1:D:317:GLU:O	1.95	0.64
1:F:259:THR:CG2	1:F:305:TRP:CD2	2.79	0.64
1:A:190:ALA:O	1:A:191:THR:HG22	1.97	0.64
1:F:240:GLU:O	1:F:244:LYS:HG3	1.97	0.64
1:D:189:GLN:HG3	1:D:276:LYS:NZ	2.12	0.64
1:D:203:GLY:HA2	1:D:206:SER:HB2	1.80	0.64
1:F:183:SER:O	1:F:187:ARG:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HH11	1:A:248:ARG:CG	2.11	0.63
1:A:219:GLY:O	1:A:222:ARG:HB3	1.98	0.63
1:C:250:MET:HE3	1:C:297:VAL:CG2	2.29	0.63
1:F:221:GLN:OE1	1:F:276:LYS:NZ	2.31	0.62
1:E:232:LEU:HD21	1:E:277:HIS:CD2	2.34	0.62
1:A:299:VAL:CG1	1:A:303:ARG:HH21	2.13	0.62
1:B:265:VAL:O	1:B:269:SER:HB2	1.98	0.62
1:E:290:LEU:O	1:E:294:ILE:HG13	2.00	0.61
1:E:191:THR:HG22	1:E:191:THR:O	2.00	0.61
1:F:236:ASP:O	1:F:236:ASP:CG	2.43	0.61
1:A:189:GLN:HG2	1:A:272:ALA:HB1	1.82	0.61
1:D:298:LEU:HD11	1:D:306:LEU:HD11	1.82	0.61
1:A:279:LYS:HG2	1:A:284:GLU:HG2	1.83	0.61
1:C:239:ASN:HD22	1:C:241:ASP:HB2	1.66	0.61
1:D:171:GLY:HA3	1:D:303:ARG:HH22	1.65	0.61
1:F:216:VAL:HG11	1:F:319:PHE:CD1	2.35	0.61
1:A:299:VAL:CG1	1:A:303:ARG:NH2	2.64	0.61
1:F:184:ARG:CZ	1:F:199:MET:HE2	2.31	0.61
1:B:288:GLU:HB3	1:B:289:PRO:HD3	1.83	0.60
1:A:171:GLY:CA	1:A:303:ARG:NH2	2.62	0.60
1:D:256:ASP:O	1:D:263:ARG:NH2	2.25	0.60
1:E:286:CYS:C	1:E:289:PRO:HD2	2.27	0.60
1:D:197:LYS:HG2	1:D:198:PRO:HD2	1.84	0.60
1:F:188:GLU:CD	1:F:214:ARG:HE	2.09	0.60
1:C:215:ARG:NH2	1:C:319:PHE:O	2.34	0.60
1:B:256:ASP:OD1	1:B:256:ASP:N	2.27	0.60
1:D:180:GLU:OE2	1:D:199:MET:HG2	2.01	0.60
1:A:196:THR:HG23	1:C:284:GLU:OE2	2.00	0.59
1:A:309:GLN:O	1:A:310:ARG:HB2	2.00	0.59
1:B:203:GLY:HA2	1:B:206:SER:HB2	1.83	0.59
1:B:296:ASP:O	1:B:300:ARG:HB2	2.02	0.59
1:E:232:LEU:HD21	1:E:277:HIS:CG	2.37	0.59
1:B:180:GLU:O	1:B:184:ARG:HG2	2.03	0.59
1:E:318:PHE:HD2	1:E:319:PHE:CD1	2.15	0.59
1:F:258:VAL:CG2	1:F:259:THR:N	2.54	0.59
1:E:301:THR:O	1:E:302:LYS:HD3	2.02	0.59
1:E:211:GLU:OE1	1:E:214:ARG:NH1	2.36	0.59
1:F:284:GLU:OE1	1:F:284:GLU:N	2.36	0.58
1:C:247:SER:HA	1:C:250:MET:HE2	1.84	0.58
1:D:193:ALA:HB3	1:D:194:LYS:HA	1.69	0.58
1:E:301:THR:C	1:E:302:LYS:HD3	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:MET:HE1	1:F:210:LEU:CD1	2.33	0.58
1:F:313:ASP:O	1:F:316:VAL:CG1	2.46	0.58
1:E:278:LEU:CD2	1:E:286:CYS:CB	2.81	0.58
1:E:221:GLN:CD	1:E:276:LYS:HZ3	2.12	0.58
1:A:212:THR:OG1	1:A:316:VAL:HG13	2.03	0.57
1:B:173:GLU:OE1	1:B:201:ARG:HD3	2.05	0.57
1:C:212:THR:CG2	1:C:215:ARG:HH12	2.17	0.57
1:D:176:ARG:HH12	1:D:201:ARG:CB	2.17	0.57
1:E:259:THR:HG23	1:E:302:LYS:NZ	2.20	0.57
1:E:321:VAL:O	1:E:321:VAL:CG1	2.51	0.57
1:F:189:GLN:HE21	1:F:189:GLN:CA	2.03	0.57
1:A:183:SER:OG	1:A:187:ARG:NH1	2.37	0.57
1:E:239:ASN:OD1	1:E:239:ASN:N	2.37	0.57
1:C:202:SER:O	1:C:205:THR:CG2	2.47	0.57
1:E:232:LEU:HD12	1:E:232:LEU:C	2.29	0.57
1:D:216:VAL:HG11	1:D:319:PHE:CD1	2.38	0.57
1:A:188:GLU:CD	1:A:214:ARG:HE	2.13	0.57
1:B:197:LYS:CG	1:B:198:PRO:HD2	2.34	0.57
1:F:190:ALA:O	1:F:279:LYS:HD2	2.04	0.57
1:A:240:GLU:HG3	1:A:244:LYS:HE3	1.85	0.56
1:A:212:THR:O	1:A:216:VAL:HG13	2.05	0.56
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.70	0.56
1:D:197:LYS:CG	1:D:198:PRO:HD2	2.36	0.56
1:B:180:GLU:OE2	1:B:199:MET:HG3	2.04	0.56
1:C:212:THR:HG23	1:C:215:ARG:NH1	2.18	0.56
1:F:275:ALA:HB1	1:F:287:ILE:HD13	1.86	0.56
1:B:320:HIS:O	1:B:321:VAL:HB	2.05	0.56
1:C:197:LYS:N	1:C:198:PRO:HD3	2.20	0.56
1:A:221:GLN:NE2	1:A:276:LYS:HE3	2.21	0.56
1:C:187:ARG:HH11	1:C:187:ARG:CG	2.18	0.56
1:D:320:HIS:O	1:D:321:VAL:CG1	2.48	0.55
1:A:211:GLU:HG3	1:A:212:THR:N	2.19	0.55
1:A:299:VAL:HG12	1:A:303:ARG:NH2	2.20	0.55
1:A:188:GLU:OE2	1:A:214:ARG:NE	2.40	0.55
1:D:288:GLU:HB3	1:D:289:PRO:HD3	1.89	0.55
1:E:215:ARG:HG2	1:E:216:VAL:N	2.21	0.55
1:E:228:PHE:HB3	1:E:273:PHE:HD2	1.71	0.55
1:B:309:GLN:O	1:B:314:GLY:HA3	2.07	0.55
1:E:228:PHE:HB3	1:E:273:PHE:CD2	2.42	0.55
1:C:212:THR:CG2	1:C:215:ARG:NH1	2.69	0.55
1:F:284:GLU:C	1:F:286:CYS:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:HH11	1:B:207:ARG:CB	2.19	0.55
1:D:204:ALA:HA	1:D:207:ARG:NH2	2.22	0.55
1:F:189:GLN:HG3	1:F:276:LYS:HE3	1.88	0.55
1:F:191:THR:HG22	1:F:279:LYS:NZ	2.21	0.54
1:F:191:THR:HG1	1:F:192:GLY:H	1.48	0.54
1:F:318:PHE:HD2	1:F:319:PHE:CE2	2.24	0.54
1:D:179:LEU:O	1:D:183:SER:HB3	2.08	0.54
1:F:284:GLU:O	1:F:285:SER:C	2.45	0.54
1:F:211:GLU:OE1	1:F:214:ARG:HB2	2.07	0.54
1:C:261:TRP:O	1:C:265:VAL:HG23	2.07	0.54
1:E:208:LYS:HB3	1:E:316:VAL:HG21	1.89	0.54
1:C:188:GLU:HA	1:C:193:ALA:HB3	1.90	0.54
1:E:185:TYR:CE1	1:E:189:GLN:NE2	2.76	0.54
1:E:259:THR:HG23	1:E:302:LYS:HZ3	1.73	0.54
1:C:233:ARG:HG3	1:C:234:LYS:N	2.23	0.54
1:D:212:THR:CG2	1:D:319:PHE:HB2	2.38	0.53
1:E:173:GLU:OE2	1:E:176:ARG:NH2	2.42	0.53
1:E:199:MET:SD	1:E:206:SER:HB3	2.48	0.53
1:F:211:GLU:OE1	1:F:214:ARG:HD2	2.08	0.53
1:C:286:CYS:C	1:C:289:PRO:HD2	2.33	0.53
1:C:187:ARG:HH11	1:C:187:ARG:HG2	1.71	0.53
1:B:180:GLU:HG2	1:B:199:MET:CE	2.39	0.53
1:C:250:MET:O	1:C:253:VAL:HG12	2.08	0.53
1:C:256:ASP:OD1	1:C:256:ASP:N	2.28	0.53
1:F:176:ARG:NH1	1:F:201:ARG:CB	2.72	0.53
1:F:284:GLU:O	1:F:286:CYS:N	2.41	0.53
1:B:240:GLU:O	1:B:244:LYS:HG2	2.09	0.52
1:C:309:GLN:O	1:C:314:GLY:HA3	2.09	0.52
1:D:171:GLY:CA	1:D:303:ARG:HH22	2.20	0.52
1:E:183:SER:OG	1:E:187:ARG:NH2	2.41	0.52
1:F:258:VAL:HG22	1:F:259:THR:O	2.09	0.52
1:A:190:ALA:HB2	1:A:276:LYS:HA	1.91	0.52
1:D:288:GLU:OE1	1:D:288:GLU:HA	2.10	0.52
1:D:192:GLY:O	1:D:193:ALA:O	2.27	0.52
1:D:197:LYS:CG	1:D:198:PRO:CD	2.88	0.52
1:E:319:PHE:CD1	1:E:319:PHE:N	2.74	0.52
1:F:187:ARG:HA	1:F:190:ALA:CB	2.37	0.52
1:F:299:VAL:O	1:F:303:ARG:CB	2.58	0.52
1:A:265:VAL:O	1:A:269:SER:OG	2.25	0.52
1:D:275:ALA:HB1	1:D:287:ILE:HD12	1.92	0.52
1:E:189:GLN:HG2	1:E:272:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:VAL:HG13	1:F:317:GLU:N	2.24	0.52
1:C:187:ARG:CG	1:C:187:ARG:NH1	2.73	0.52
1:D:204:ALA:HA	1:D:207:ARG:CZ	2.40	0.52
1:D:180:GLU:OE2	1:D:199:MET:HA	2.10	0.51
1:A:224:HIS:CE1	3:A:402:PGE:C1	2.88	0.51
1:F:239:ASN:O	1:F:241:ASP:N	2.44	0.51
1:B:203:GLY:O	1:B:207:ARG:CG	2.45	0.51
1:C:197:LYS:N	1:C:198:PRO:CD	2.73	0.51
1:D:215:ARG:HG2	1:D:216:VAL:N	2.26	0.51
1:D:180:GLU:CD	1:D:199:MET:HG2	2.36	0.51
1:E:199:MET:SD	1:E:206:SER:CB	2.98	0.51
1:F:215:ARG:HH22	1:F:319:PHE:HB3	1.76	0.51
1:C:210:LEU:O	1:C:214:ARG:HG3	2.11	0.51
1:D:299:VAL:O	1:D:303:ARG:HB2	2.11	0.51
1:E:216:VAL:HG12	1:E:265:VAL:HG11	1.92	0.51
1:F:212:THR:CG2	1:F:319:PHE:HB2	2.41	0.50
1:F:278:LEU:HD13	1:F:286:CYS:HB2	1.93	0.50
1:B:213:LEU:O	1:B:217:GLY:N	2.41	0.50
1:B:197:LYS:HG2	1:B:198:PRO:CD	2.38	0.50
1:D:189:GLN:HG3	1:D:276:LYS:HZ3	1.75	0.50
1:E:221:GLN:HE22	1:E:276:LYS:NZ	2.10	0.50
1:A:224:HIS:CD2	3:A:402:PGE:H1	2.47	0.50
1:F:258:VAL:CG2	1:F:259:THR:H	2.12	0.50
1:F:215:ARG:NH2	1:F:319:PHE:O	2.45	0.50
1:C:267:LEU:HD12	2:C:400:19H:H10	1.92	0.50
1:E:185:TYR:HE2	1:E:272:ALA:HB2	1.77	0.49
1:B:259:THR:HG23	1:B:302:LYS:HE3	1.95	0.49
1:C:216:VAL:O	1:C:220:VAL:HG23	2.13	0.49
1:F:250:MET:CE	1:F:294:ILE:HA	2.25	0.49
1:E:278:LEU:HD21	1:E:286:CYS:CB	2.43	0.49
1:C:185:TYR:O	1:C:189:GLN:HG2	2.13	0.49
1:C:253:VAL:HG13	2:C:400:19H:H11	1.94	0.49
1:A:191:THR:HG23	1:A:192:GLY:O	2.12	0.49
1:C:180:GLU:O	1:C:184:ARG:HB2	2.13	0.49
1:B:176:ARG:HH12	1:B:201:ARG:H	1.61	0.49
1:B:272:ALA:O	1:B:276:LYS:HG3	2.13	0.49
1:A:256:ASP:O	1:A:263:ARG:NH2	2.46	0.48
1:C:238:LYS:HE2	1:C:239:ASN:OD1	2.12	0.48
1:A:248:ARG:CG	1:A:248:ARG:NH1	2.73	0.48
1:F:211:GLU:OE1	1:F:214:ARG:NH1	2.40	0.48
1:B:191:THR:O	1:B:193:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASP:OD1	1:C:242:ASP:N	2.46	0.48
1:F:279:LYS:HA	1:F:284:GLU:OE2	2.14	0.48
1:A:240:GLU:O	1:A:244:LYS:HD2	2.11	0.48
1:A:299:VAL:O	1:A:303:ARG:HB2	2.13	0.48
1:B:299:VAL:O	1:B:303:ARG:HB2	2.14	0.48
1:E:278:LEU:HD21	1:E:286:CYS:HB2	1.91	0.48
1:E:203:GLY:HA2	1:E:206:SER:HB2	1.96	0.48
1:C:171:GLY:HA2	1:C:303:ARG:CZ	2.33	0.48
1:D:193:ALA:HB1	1:D:194:LYS:C	2.33	0.48
1:B:189:GLN:HG2	1:B:272:ALA:CB	2.41	0.48
1:C:203:GLY:HA2	1:C:206:SER:HB2	1.96	0.48
1:D:189:GLN:CG	1:D:276:LYS:NZ	2.77	0.48
1:B:250:MET:HE2	1:B:297:VAL:CG2	2.27	0.47
1:E:261:TRP:CZ3	1:E:315:PHE:HB2	2.48	0.47
1:F:299:VAL:O	1:F:303:ARG:HB3	2.14	0.47
1:A:187:ARG:O	1:A:191:THR:CG2	2.56	0.47
1:C:215:ARG:NH1	1:C:319:PHE:HB3	2.29	0.47
1:E:284:GLU:O	1:E:287:ILE:HG13	2.13	0.47
1:F:212:THR:O	1:F:216:VAL:HG13	2.13	0.47
1:C:253:VAL:HG11	2:C:400:19H:H12	1.96	0.47
1:A:184:ARG:O	1:A:188:GLU:HB2	2.15	0.47
1:E:216:VAL:HG11	1:E:319:PHE:CE2	2.49	0.47
1:D:190:ALA:O	1:D:192:GLY:N	2.44	0.46
1:E:275:ALA:HB1	1:E:287:ILE:HD13	1.97	0.46
1:B:275:ALA:HB1	1:B:287:ILE:HD13	1.97	0.46
1:D:189:GLN:HG3	1:D:276:LYS:HZ1	1.79	0.46
1:E:259:THR:CG2	1:E:302:LYS:NZ	2.75	0.46
1:F:186:LEU:O	1:F:190:ALA:CB	2.62	0.46
1:F:258:VAL:HG22	1:F:259:THR:H	1.70	0.46
1:D:189:GLN:CG	1:D:276:LYS:HZ1	2.29	0.46
1:E:221:GLN:NE2	1:E:276:LYS:HZ3	2.13	0.46
1:F:238:LYS:HB3	1:F:238:LYS:HE2	1.63	0.46
1:C:253:VAL:CG1	2:C:400:19H:H11	2.45	0.46
1:F:259:THR:HG22	1:F:305:TRP:NE1	2.31	0.46
1:B:243:VAL:HG21	1:B:286:CYS:HB3	1.98	0.46
1:C:239:ASN:ND2	1:C:241:ASP:HB2	2.31	0.46
1:B:184:ARG:HB2	1:B:210:LEU:HD11	1.98	0.45
1:E:185:TYR:CE2	1:E:272:ALA:HB2	2.51	0.45
1:E:197:LYS:HG3	1:E:198:PRO:HD2	1.98	0.45
1:E:215:ARG:CG	1:E:216:VAL:N	2.79	0.45
1:B:173:GLU:OE2	1:B:176:ARG:CZ	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:GLN:NE2	1:E:229:GLN:CA	2.71	0.45
1:B:231:MET:O	1:B:235:LEU:HG	2.16	0.45
1:E:261:TRP:O	1:E:265:VAL:HG23	2.16	0.45
1:B:192:GLY:O	1:B:193:ALA:HB3	2.16	0.45
1:E:318:PHE:C	1:E:319:PHE:CD1	2.86	0.45
1:F:236:ASP:OD1	1:F:236:ASP:C	2.56	0.45
1:F:248:ARG:CG	1:F:248:ARG:NH1	2.71	0.45
1:F:261:TRP:CE3	1:F:315:PHE:HD1	2.34	0.45
1:C:204:ALA:O	1:C:207:ARG:HB2	2.17	0.45
1:C:216:VAL:CG1	1:C:265:VAL:HG11	2.42	0.45
1:D:210:LEU:HD13	1:D:210:LEU:HA	1.49	0.45
1:F:259:THR:HG21	1:F:305:TRP:CG	2.50	0.45
1:E:187:ARG:O	1:E:190:ALA:O	2.35	0.45
1:C:191:THR:CG2	1:C:193:ALA:CB	2.83	0.45
1:D:199:MET:O	1:D:200:GLY:O	2.35	0.45
1:D:232:LEU:HD23	1:D:273:PHE:HE1	1.82	0.45
1:E:256:ASP:OD1	1:E:256:ASP:C	2.59	0.45
1:F:284:GLU:C	1:F:286:CYS:H	2.24	0.45
1:B:207:ARG:HB2	1:B:207:ARG:NH1	2.30	0.45
1:C:244:LYS:HB2	1:C:244:LYS:NZ	2.32	0.45
1:C:199:MET:O	1:C:200:GLY:O	2.36	0.44
1:A:196:THR:HG21	1:C:284:GLU:CD	2.41	0.44
1:B:231:MET:HE3	1:B:231:MET:HB2	1.85	0.44
1:A:171:GLY:HA2	1:A:303:ARG:NH2	2.32	0.44
1:D:321:VAL:O	1:D:321:VAL:CG1	2.62	0.44
1:E:211:GLU:OE1	1:E:211:GLU:HA	2.17	0.44
1:B:201:ARG:CG	1:B:202:SER:N	2.80	0.44
1:D:309:GLN:O	1:D:314:GLY:HA3	2.17	0.44
1:D:250:MET:HE3	1:D:250:MET:HB2	1.89	0.44
1:E:207:ARG:NH2	2:F:400:19H:OAD	2.51	0.44
1:F:318:PHE:CD2	1:F:319:PHE:CE2	3.05	0.44
1:B:191:THR:HG22	1:B:279:LYS:HD2	2.00	0.43
1:E:210:LEU:O	1:E:214:ARG:HB2	2.18	0.43
1:F:189:GLN:NE2	1:F:189:GLN:CA	2.54	0.43
1:F:235:LEU:HD23	1:F:235:LEU:HA	1.79	0.43
1:C:235:LEU:HD22	1:C:246:LEU:HD21	1.99	0.43
1:F:184:ARG:O	1:F:188:GLU:HB2	2.18	0.43
1:A:190:ALA:CB	1:A:276:LYS:HA	2.48	0.43
1:D:232:LEU:HD21	1:D:277:HIS:HB2	1.99	0.43
1:F:226:THR:HG22	1:F:227:ALA:N	2.31	0.43
1:B:191:THR:O	1:B:191:THR:OG1	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:VAL:O	1:F:303:ARG:HB2	2.19	0.43
1:B:224:HIS:NE2	3:B:403:PGE:H12	2.29	0.43
1:B:189:GLN:HG3	1:B:276:LYS:HE3	2.01	0.43
1:B:288:GLU:OE1	1:B:288:GLU:HA	2.18	0.43
1:F:187:ARG:CA	1:F:190:ALA:HB3	2.43	0.43
1:F:208:LYS:H	1:F:208:LYS:HG2	1.63	0.43
1:B:191:THR:HG22	1:B:284:GLU:OE2	2.19	0.43
1:D:230:GLY:O	1:D:234:LYS:HG3	2.19	0.43
1:C:223:ASN:C	1:C:224:HIS:ND1	2.77	0.43
1:C:244:LYS:NZ	1:C:244:LYS:CB	2.81	0.43
1:D:197:LYS:HG3	1:D:198:PRO:CD	2.47	0.42
1:F:317:GLU:O	1:F:320:HIS:CD2	2.72	0.42
1:A:318:PHE:O	1:A:318:PHE:CD2	2.72	0.42
1:F:175:TYR:CD2	1:F:175:TYR:C	2.97	0.42
1:A:240:GLU:O	1:A:244:LYS:CD	2.68	0.42
1:E:185:TYR:CE1	1:E:214:ARG:HA	2.49	0.42
1:F:316:VAL:CG1	1:F:317:GLU:N	2.82	0.42
1:A:221:GLN:HE21	1:A:276:LYS:HE3	1.85	0.42
1:F:279:LYS:CA	1:F:284:GLU:OE2	2.67	0.42
1:B:239:ASN:O	1:B:242:ASP:HB2	2.19	0.42
1:C:254:PHE:CD2	2:C:400:19H:H8	2.54	0.42
1:F:222:ARG:CG	1:F:222:ARG:HH11	2.32	0.42
1:F:232:LEU:HD21	1:F:277:HIS:CB	2.50	0.42
1:A:299:VAL:HG11	1:A:303:ARG:NH2	2.34	0.42
1:A:312:TRP:O	1:A:315:PHE:HB3	2.20	0.42
1:C:202:SER:OG	1:C:205:THR:CG2	2.68	0.42
1:E:320:HIS:ND1	1:E:320:HIS:N	2.68	0.42
1:E:188:GLU:HG2	1:E:193:ALA:O	2.19	0.42
1:F:251:ILE:O	1:F:255:SER:HB2	2.20	0.42
1:D:171:GLY:N	1:D:303:ARG:NH2	2.68	0.42
1:F:171:GLY:HA3	1:F:175:TYR:HB2	2.01	0.42
1:A:179:LEU:O	1:A:183:SER:HB3	2.20	0.42
1:B:188:GLU:HG2	1:B:194:LYS:HA	2.02	0.42
1:C:259:THR:HG23	1:C:302:LYS:HE3	2.02	0.42
1:E:246:LEU:HD13	2:E:400:19H:CL1	2.57	0.42
1:E:273:PHE:CD1	1:E:273:PHE:C	2.97	0.42
1:A:309:GLN:O	1:A:314:GLY:HA3	2.19	0.41
1:D:171:GLY:HA3	1:D:303:ARG:CZ	2.46	0.41
1:E:174:LEU:HD12	1:E:174:LEU:HA	1.89	0.41
1:E:176:ARG:HE	1:E:176:ARG:HB3	1.60	0.41
1:E:310:ARG:O	1:E:313:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ARG:O	1:F:202:SER:CB	2.67	0.41
1:A:231:MET:O	1:A:235:LEU:HG	2.21	0.41
1:F:184:ARG:NH2	1:F:199:MET:HE2	2.35	0.41
1:F:186:LEU:O	1:F:190:ALA:N	2.53	0.41
1:A:300:ARG:HH11	1:A:300:ARG:HD3	1.71	0.41
1:B:176:ARG:HE	1:B:176:ARG:HB3	1.59	0.41
1:B:190:ALA:O	1:B:191:THR:C	2.63	0.41
1:F:214:ARG:O	1:F:218:ASP:OD2	2.38	0.41
1:A:190:ALA:O	1:A:191:THR:CB	2.69	0.41
1:C:254:PHE:O	1:C:254:PHE:CG	2.73	0.41
1:E:300:ARG:NH1	1:E:300:ARG:HG2	2.35	0.41
1:C:224:HIS:ND1	1:C:224:HIS:N	2.67	0.41
1:C:299:VAL:O	1:C:303:ARG:HB2	2.21	0.41
1:E:318:PHE:CD2	1:E:319:PHE:CD1	3.00	0.41
1:D:176:ARG:NH1	1:D:201:ARG:CB	2.84	0.40
1:E:199:MET:SD	1:E:206:SER:HB2	2.60	0.40
1:C:229:GLN:NE2	1:C:229:GLN:C	2.75	0.40
1:C:299:VAL:CG1	1:C:303:ARG:HH21	2.34	0.40
1:E:284:GLU:C	1:E:286:CYS:N	2.79	0.40
1:E:221:GLN:HE21	1:E:221:GLN:HB3	1.54	0.40
1:F:279:LYS:HA	1:F:284:GLU:CD	2.46	0.40
1:A:256:ASP:O	1:A:263:ARG:NH1	2.54	0.40
1:A:288:GLU:CB	1:A:289:PRO:HD3	2.51	0.40
1:C:215:ARG:CZ	1:C:319:PHE:O	2.69	0.40
1:E:180:GLU:O	1:E:184:ARG:HB2	2.20	0.40
1:D:286:CYS:C	1:D:289:PRO:HD2	2.46	0.40
1:F:199:MET:HE3	1:F:207:ARG:NE	2.35	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	145/153 (95%)	142 (98%)	2 (1%)	1 (1%)	18	47
1	B	149/153 (97%)	144 (97%)	4 (3%)	1 (1%)	18	47
1	C	148/153 (97%)	140 (95%)	5 (3%)	3 (2%)	6	21
1	D	149/153 (97%)	139 (93%)	6 (4%)	4 (3%)	4	15
1	E	149/153 (97%)	140 (94%)	9 (6%)	0	100	100
1	F	148/153 (97%)	135 (91%)	7 (5%)	6 (4%)	2	8
All	All	888/918 (97%)	840 (95%)	33 (4%)	15 (2%)	7	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	GLY
1	C	197	LYS
1	C	200	GLY
1	D	193	ALA
1	F	197	LYS
1	F	202	SER
1	F	240	GLU
1	F	259	THR
1	D	200	GLY
1	D	318	PHE
1	A	191	THR
1	C	201	ARG
1	D	172	ASP
1	F	258	VAL
1	F	192	GLY

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	127/133 (96%)	99 (78%)	28 (22%)	1	3
1	B	131/133 (98%)	103 (79%)	28 (21%)	1	4
1	C	125/133 (94%)	92 (74%)	33 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	129/133 (97%)	111 (86%)	18 (14%)	3	12
1	E	130/133 (98%)	105 (81%)	25 (19%)	1	5
1	F	127/133 (96%)	100 (79%)	27 (21%)	1	4
All	All	769/798 (96%)	610 (79%)	159 (21%)	1	4

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	205	THR
1	A	210	LEU
1	A	214	ARG
1	A	215	ARG
1	A	216	VAL
1	A	221	GLN
1	A	225	GLU
1	A	226	THR
1	A	233	ARG
1	A	237	ILE
1	A	238	LYS
1	A	244	LYS
1	A	248	ARG
1	A	249	VAL
1	A	258	VAL
1	A	267	LEU
1	A	269	SER
1	A	278	LEU
1	A	279	LYS
1	A	288	GLU
1	A	289	PRO
1	A	292	GLU
1	A	296	ASP
1	A	299	VAL
1	A	302	LYS
1	A	303	ARG
1	A	321	VAL
1	B	172	ASP
1	B	176	ARG
1	B	184	ARG
1	B	189	GLN
1	B	199	MET

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Mol	Chain	Res	Type
1	B	201	ARG
1	B	205	THR
1	B	206	SER
1	B	207	ARG
1	B	213	LEU
1	B	222	ARG
1	B	226	THR
1	B	231	MET
1	B	236	ASP
1	B	244	LYS
1	B	245	SER
1	B	247	SER
1	B	250	MET
1	B	256	ASP
1	B	259	THR
1	B	263	ARG
1	B	267	LEU
1	B	269	SER
1	B	278	LEU
1	B	285	SER
1	B	287	ILE
1	B	307	VAL
1	B	316	VAL
1	C	172	ASP
1	C	176	ARG
1	C	184	ARG
1	C	187	ARG
1	C	188	GLU
1	C	196	THR
1	C	210	LEU
1	C	211	GLU
1	C	212	THR
1	C	213	LEU
1	C	231	MET
1	C	232	LEU
1	C	233	ARG
1	C	234	LYS
1	C	238	LYS
1	C	240	GLU
1	C	244	LYS
1	C	247	SER
1	C	248	ARG

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Mol	Chain	Res	Type
1	C	249	VAL
1	C	250	MET
1	C	256	ASP
1	C	258	VAL
1	C	259	THR
1	C	267	LEU
1	C	269	SER
1	C	281	ILE
1	C	282	ASN
1	C	285	SER
1	C	296	ASP
1	C	307	VAL
1	C	308	LYS
1	C	310	ARG
1	D	176	ARG
1	D	189	GLN
1	D	191	THR
1	D	194	LYS
1	D	196	THR
1	D	202	SER
1	D	205	THR
1	D	206	SER
1	D	207	ARG
1	D	208	LYS
1	D	210	LEU
1	D	214	ARG
1	D	259	THR
1	D	267	LEU
1	D	269	SER
1	D	278	LEU
1	D	307	VAL
1	D	317	GLU
1	E	172	ASP
1	E	176	ARG
1	E	184	ARG
1	E	194	LYS
1	E	196	THR
1	E	199	MET
1	E	202	SER
1	E	210	LEU
1	E	211	GLU
1	E	215	ARG

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Mol	Chain	Res	Type
1	E	221	GLN
1	E	229	GLN
1	E	232	LEU
1	E	241	ASP
1	E	256	ASP
1	E	267	LEU
1	E	278	LEU
1	E	284	GLU
1	E	287	ILE
1	E	288	GLU
1	E	307	VAL
1	E	309	GLN
1	E	310	ARG
1	E	320	HIS
1	E	321	VAL
1	F	172	ASP
1	F	176	ARG
1	F	183	SER
1	F	187	ARG
1	F	189	GLN
1	F	195	ASP
1	F	199	MET
1	F	207	ARG
1	F	208	LYS
1	F	210	LEU
1	F	211	GLU
1	F	214	ARG
1	F	215	ARG
1	F	222	ARG
1	F	226	THR
1	F	238	LYS
1	F	247	SER
1	F	248	ARG
1	F	259	THR
1	F	267	LEU
1	F	279	LYS
1	F	284	GLU
1	F	287	ILE
1	F	288	GLU
1	F	303	ARG
1	F	317	GLU
1	F	320	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	309	GLN
1	B	177	GLN
1	C	260	ASN
1	C	277	HIS
1	C	309	GLN
1	D	224	HIS
1	D	239	ASN
1	D	277	HIS
1	D	309	GLN
1	E	177	GLN
1	E	189	GLN
1	E	229	GLN
1	F	189	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 ⓘ

10 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
3	PGE	A	402	-	9,9,9	0.68	0	8,8,8	0.73	0
3	PGE	B	403	-	9,9,9	0.70	0	8,8,8	0.98	0
2	19H	F	400	-	28,28,28	4.74	13 (46%)	39,40,40	3.24	15 (38%)
4	EDO	B	404	-	3,3,3	0.59	0	2,2,2	0.35	0
3	PGE	B	402	-	9,9,9	0.71	0	8,8,8	0.66	0
2	19H	C	400	-	28,28,28	4.77	14 (50%)	39,40,40	3.29	20 (51%)
2	19H	A	401	-	28,28,28	4.73	14 (50%)	39,40,40	3.13	12 (30%)
2	19H	B	401	-	28,28,28	4.74	13 (46%)	39,40,40	3.37	15 (38%)
2	19H	E	400	-	28,28,28	4.75	14 (50%)	39,40,40	3.32	16 (41%)
2	19H	D	400	-	28,28,28	4.66	14 (50%)	39,40,40	3.51	16 (41%)

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
3	PGE	A	402	-	-	4/7/7/7	-
3	PGE	B	403	-	-	4/7/7/7	-
2	19H	F	400	-	-	6/11/11/11	0/3/3/3
4	EDO	B	404	-	-	0/1/1/1	-
3	PGE	B	402	-	-	3/7/7/7	-
2	19H	C	400	-	-	8/11/11/11	0/3/3/3
2	19H	A	401	-	-	5/11/11/11	0/3/3/3
2	19H	B	401	-	-	1/11/11/11	0/3/3/3
2	19H	E	400	-	-	4/11/11/11	0/3/3/3
2	19H	D	400	-	-	4/11/11/11	0/3/3/3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	19H	CAW-CAQ	-13.41	1.27	1.48
2	C	400	19H	CAW-CAQ	-13.28	1.28	1.48
2	F	400	19H	CAW-CAQ	-13.18	1.28	1.48
2	B	401	19H	CAW-CAQ	-13.17	1.28	1.48
2	E	400	19H	CAW-CAQ	-13.16	1.28	1.48
2	D	400	19H	CAW-CAQ	-12.99	1.28	1.48
2	C	400	19H	CAB-CAS	-10.77	1.30	1.51
2	B	401	19H	CAB-CAS	-10.57	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	19H	CAA-CAR	-10.54	1.31	1.51
2	F	400	19H	CAB-CAS	-10.53	1.31	1.51
2	A	401	19H	CAB-CAS	-10.33	1.31	1.51
2	F	400	19H	CAA-CAR	-10.33	1.31	1.51
2	C	400	19H	CAA-CAR	-10.29	1.31	1.51
2	E	400	19H	CAB-CAS	-10.28	1.31	1.51
2	A	401	19H	CAA-CAR	-10.18	1.31	1.51
2	E	400	19H	CAA-CAR	-10.11	1.32	1.51
2	D	400	19H	CAA-CAR	-10.10	1.32	1.51
2	D	400	19H	CAB-CAS	-10.06	1.32	1.51
2	E	400	19H	CAN-CAX	6.94	1.61	1.51
2	E	400	19H	CAZ-CAX	-6.87	1.31	1.44
2	D	400	19H	CAZ-CAX	-6.82	1.31	1.44
2	D	400	19H	CAN-CAX	6.68	1.61	1.51
2	F	400	19H	CAZ-CAX	-6.62	1.32	1.44
2	F	400	19H	CAN-CAX	6.55	1.61	1.51
2	B	401	19H	CAZ-CAX	-6.50	1.32	1.44
2	C	400	19H	CAZ-CAX	-6.48	1.32	1.44
2	C	400	19H	CAN-CAX	6.43	1.61	1.51
2	B	401	19H	CAN-CAX	6.31	1.60	1.51
2	A	401	19H	CAN-CAX	6.27	1.60	1.51
2	A	401	19H	CAZ-CAX	-6.12	1.33	1.44
2	A	401	19H	CAZ-CAY	-6.10	1.33	1.41
2	E	400	19H	CAZ-CAY	-5.73	1.34	1.41
2	F	400	19H	CAZ-CAY	-5.63	1.34	1.41
2	C	400	19H	CAZ-CAY	-5.61	1.34	1.41
2	A	401	19H	CAK-CAY	-5.54	1.30	1.39
2	B	401	19H	CAK-CAY	-5.53	1.30	1.39
2	C	400	19H	CAK-CAY	-5.53	1.30	1.39
2	D	400	19H	CAZ-CAY	-5.45	1.34	1.41
2	F	400	19H	CAK-CAY	-5.39	1.31	1.39
2	B	401	19H	CAZ-CAY	-5.39	1.34	1.41
2	C	400	19H	CAH-CAZ	-5.38	1.31	1.39
2	B	401	19H	CAH-CAZ	-5.32	1.31	1.39
2	E	400	19H	CAK-CAY	-5.28	1.31	1.39
2	E	400	19H	CAH-CAZ	-5.17	1.32	1.39
2	F	400	19H	CAH-CAZ	-5.11	1.32	1.39
2	D	400	19H	CAK-CAY	-5.11	1.31	1.39
2	E	400	19H	CAW-CAX	-5.11	1.30	1.38
2	A	401	19H	CAH-CAZ	-5.07	1.32	1.39
2	D	400	19H	CAH-CAZ	-4.97	1.32	1.39
2	A	401	19H	CAW-CAX	-4.96	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	19H	CAW-CAX	-4.88	1.31	1.38
2	C	400	19H	CAW-CAX	-4.80	1.31	1.38
2	F	400	19H	CAW-CAX	-4.76	1.31	1.38
2	B	401	19H	CAW-CAX	-4.57	1.31	1.38
2	E	400	19H	OAD-CAQ	2.88	1.29	1.22
2	A	401	19H	OAD-CAQ	2.84	1.29	1.22
2	F	400	19H	OAD-CAQ	2.83	1.29	1.22
2	D	400	19H	OAD-CAQ	2.83	1.29	1.22
2	B	401	19H	OAD-CAQ	2.82	1.29	1.22
2	C	400	19H	OAD-CAQ	2.75	1.29	1.22
2	B	401	19H	CAI-CAR	2.71	1.43	1.39
2	A	401	19H	CAI-CAR	2.68	1.43	1.39
2	B	401	19H	CAH-CAG	2.59	1.43	1.38
2	D	400	19H	CAJ-CAS	2.55	1.43	1.39
2	C	400	19H	CAH-CAG	2.48	1.42	1.38
2	A	401	19H	CAH-CAG	2.43	1.42	1.38
2	F	400	19H	CAH-CAG	2.40	1.42	1.38
2	D	400	19H	CAI-CAR	2.35	1.42	1.39
2	E	400	19H	CAH-CAG	2.35	1.42	1.38
2	D	400	19H	CAH-CAG	2.35	1.42	1.38
2	C	400	19H	CAJ-CAS	2.34	1.42	1.39
2	A	401	19H	CAJ-CAS	2.33	1.42	1.39
2	E	400	19H	CAJ-CAS	2.28	1.42	1.39
2	B	401	19H	CAJ-CAS	2.27	1.42	1.39
2	F	400	19H	CAJ-CAS	2.22	1.42	1.39
2	C	400	19H	OAP-CAU	-2.21	1.32	1.37
2	E	400	19H	CAI-CAR	2.19	1.42	1.39
2	E	400	19H	OAP-CAU	-2.12	1.32	1.37
2	A	401	19H	OAP-CAU	-2.12	1.32	1.37
2	F	400	19H	CAI-CAR	2.11	1.42	1.39
2	D	400	19H	OAP-CAU	-2.10	1.32	1.37
2	C	400	19H	CAI-CAR	2.04	1.42	1.39

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	19H	CAX-CAW-NAO	-12.70	98.12	109.59
2	B	401	19H	CAX-CAW-NAO	-12.45	98.34	109.59
2	E	400	19H	CAX-CAW-NAO	-12.23	98.54	109.59
2	C	400	19H	CAX-CAW-NAO	-11.73	98.99	109.59
2	F	400	19H	CAX-CAW-NAO	-11.72	99.00	109.59
2	A	401	19H	CAX-CAW-NAO	-11.28	99.39	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	19H	CAZ-CAX-CAW	10.43	118.89	106.79
2	B	401	19H	CAZ-CAX-CAW	10.41	118.86	106.79
2	D	400	19H	CAZ-CAX-CAW	10.30	118.73	106.79
2	C	400	19H	CAZ-CAX-CAW	10.13	118.53	106.79
2	F	400	19H	CAZ-CAX-CAW	9.89	118.26	106.79
2	A	401	19H	CAZ-CAX-CAW	9.74	118.08	106.79
2	B	401	19H	OAC-CAQ-OAD	-6.12	109.33	123.90
2	D	400	19H	OAC-CAQ-OAD	-5.98	109.67	123.90
2	A	401	19H	OAC-CAQ-OAD	-5.97	109.68	123.90
2	A	401	19H	OAC-CAQ-CAW	5.92	126.12	116.73
2	C	400	19H	OAC-CAQ-OAD	-5.72	110.29	123.90
2	E	400	19H	OAC-CAQ-OAD	-5.66	110.41	123.90
2	F	400	19H	OAC-CAQ-OAD	-5.63	110.49	123.90
2	C	400	19H	OAC-CAQ-CAW	5.22	125.01	116.73
2	F	400	19H	OAC-CAQ-CAW	4.95	124.58	116.73
2	D	400	19H	CAK-CAT-CL2	4.66	125.02	119.17
2	D	400	19H	OAC-CAQ-CAW	4.62	124.06	116.73
2	E	400	19H	OAC-CAQ-CAW	4.55	123.94	116.73
2	B	401	19H	OAC-CAQ-CAW	4.27	123.51	116.73
2	D	400	19H	CAG-CAT-CAK	-4.09	116.18	121.53
2	B	401	19H	OAD-CAQ-CAW	4.00	127.16	120.20
2	F	400	19H	CAG-CAT-CAK	-3.92	116.40	121.53
2	B	401	19H	CAG-CAT-CAK	-3.84	116.51	121.53
2	D	400	19H	CAY-NAO-CAW	3.77	113.14	109.00
2	C	400	19H	CAG-CAT-CAK	-3.64	116.77	121.53
2	F	400	19H	CAA-CAR-CAI	3.56	125.85	119.57
2	E	400	19H	CAK-CAT-CL2	3.55	123.61	119.17
2	D	400	19H	OAD-CAQ-CAW	3.48	126.26	120.20
2	D	400	19H	CAQ-CAW-NAO	3.44	125.50	121.22
2	A	401	19H	CAG-CAT-CAK	-3.42	117.06	121.53
2	B	401	19H	CAB-CAS-CAJ	3.39	125.54	119.57
2	B	401	19H	CAY-NAO-CAW	3.29	112.61	109.00
2	D	400	19H	CAZ-CAY-NAO	-3.15	104.68	108.23
2	E	400	19H	CAQ-CAW-NAO	3.12	125.10	121.22
2	E	400	19H	OAD-CAQ-CAW	3.10	125.60	120.20
2	C	400	19H	CAK-CAT-CL2	3.07	123.03	119.17
2	E	400	19H	CAG-CAT-CAK	-3.00	117.61	121.53
2	B	401	19H	CAK-CAT-CL2	3.00	122.93	119.17
2	E	400	19H	CAY-NAO-CAW	2.92	112.21	109.00
2	E	400	19H	CAU-CAJ-CAS	2.90	123.66	120.61
2	D	400	19H	CAA-CAR-CAI	2.89	124.67	119.57
2	F	400	19H	CAY-NAO-CAW	2.81	112.08	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	19H	CAB-CAS-CAJ	2.80	124.51	119.57
2	C	400	19H	CAU-CAI-CAR	2.78	123.53	120.61
2	F	400	19H	OAD-CAQ-CAW	2.72	124.93	120.20
2	B	401	19H	CAH-CAZ-CAX	2.65	138.25	133.73
2	C	400	19H	CAH-CAG-CAT	-2.63	116.59	119.24
2	D	400	19H	CAU-CAJ-CAS	2.63	123.38	120.61
2	E	400	19H	CAH-CAG-CAT	-2.62	116.61	119.24
2	C	400	19H	CAY-NAO-CAW	2.61	111.86	109.00
2	C	400	19H	OAD-CAQ-CAW	2.57	124.68	120.20
2	C	400	19H	CAM-OAP-CAU	-2.56	111.28	117.93
2	C	400	19H	CAQ-CAW-NAO	2.52	124.35	121.22
2	B	401	19H	CAZ-CAY-NAO	-2.49	105.42	108.23
2	F	400	19H	CAK-CAT-CL2	2.48	122.28	119.17
2	F	400	19H	CAQ-CAW-CAX	2.47	138.13	130.58
2	F	400	19H	CAH-CAZ-CAX	2.47	137.94	133.73
2	C	400	19H	CAN-CAL-CAM	2.47	117.28	112.33
2	A	401	19H	CAL-CAN-CAX	2.45	117.16	113.30
2	D	400	19H	CAY-CAK-CAT	2.44	122.81	118.48
2	B	401	19H	CAQ-CAW-CAX	2.41	137.95	130.58
2	B	401	19H	CAH-CAG-CAT	-2.41	116.82	119.24
2	C	400	19H	CAU-CAJ-CAS	2.40	123.14	120.61
2	E	400	19H	CAZ-CAY-NAO	-2.40	105.53	108.23
2	A	401	19H	CAH-CAZ-CAX	2.39	137.81	133.73
2	F	400	19H	CAU-CAI-CAR	2.38	123.11	120.61
2	C	400	19H	CAY-CAZ-CAX	-2.35	104.70	106.84
2	A	401	19H	CAY-NAO-CAW	2.32	111.55	109.00
2	B	401	19H	CAY-CAZ-CAX	-2.29	104.76	106.84
2	A	401	19H	OAD-CAQ-CAW	2.29	124.18	120.20
2	A	401	19H	CAH-CAG-CAT	-2.28	116.95	119.24
2	C	400	19H	OAP-CAM-CAL	2.26	116.61	108.30
2	A	401	19H	CAY-CAZ-CAX	-2.21	104.83	106.84
2	E	400	19H	CAY-CAZ-CAX	-2.21	104.83	106.84
2	D	400	19H	CAU-CAI-CAR	2.19	122.92	120.61
2	F	400	19H	CAY-CAZ-CAX	-2.19	104.84	106.84
2	F	400	19H	CAZ-CAY-NAO	-2.16	105.80	108.23
2	C	400	19H	CAY-CAK-CAT	2.13	122.25	118.48
2	A	401	19H	CAQ-CAW-CAX	2.13	137.09	130.58
2	C	400	19H	CAH-CAZ-CAX	2.10	137.30	133.73
2	D	400	19H	CAH-CAG-CAT	-2.07	117.15	119.24
2	F	400	19H	CAB-CAS-CAJ	2.07	123.22	119.57
2	C	400	19H	CAZ-CAY-NAO	-2.06	105.91	108.23
2	E	400	19H	CAA-CAR-CAI	2.06	123.20	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	19H	CAY-CAK-CAT	2.05	122.11	118.48
2	E	400	19H	CAN-CAL-CAM	2.02	116.38	112.33
2	C	400	19H	CAJ-CAU-CAI	-2.01	117.92	120.98
2	D	400	19H	CAN-CAL-CAM	2.01	116.35	112.33

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	19H	OAC-CAQ-CAW-NAO
2	A	401	19H	OAC-CAQ-CAW-CAX
2	A	401	19H	OAD-CAQ-CAW-NAO
2	C	400	19H	OAC-CAQ-CAW-NAO
2	C	400	19H	OAC-CAQ-CAW-CAX
2	C	400	19H	OAD-CAQ-CAW-NAO
2	C	400	19H	OAD-CAQ-CAW-CAX
2	D	400	19H	OAC-CAQ-CAW-NAO
2	D	400	19H	OAC-CAQ-CAW-CAX
2	D	400	19H	OAD-CAQ-CAW-NAO
2	D	400	19H	OAD-CAQ-CAW-CAX
3	B	403	PGE	O2-C3-C4-O3
2	A	401	19H	OAD-CAQ-CAW-CAX
2	E	400	19H	OAD-CAQ-CAW-NAO
3	A	402	PGE	O1-C1-C2-O2
3	B	403	PGE	O1-C1-C2-O2
2	C	400	19H	CAN-CAL-CAM-OAP
2	C	400	19H	CAI-CAU-OAP-CAM
3	A	402	PGE	O3-C5-C6-O4
3	B	402	PGE	C4-C3-O2-C2
2	C	400	19H	CAJ-CAU-OAP-CAM
2	E	400	19H	OAD-CAQ-CAW-CAX
2	E	400	19H	OAC-CAQ-CAW-NAO
2	F	400	19H	OAC-CAQ-CAW-NAO
2	F	400	19H	OAD-CAQ-CAW-NAO
3	B	403	PGE	C3-C4-O3-C5
3	B	402	PGE	O2-C3-C4-O3
3	B	402	PGE	C1-C2-O2-C3
2	E	400	19H	OAC-CAQ-CAW-CAX
2	F	400	19H	OAC-CAQ-CAW-CAX
2	F	400	19H	CAI-CAU-OAP-CAM
3	B	403	PGE	C6-C5-O3-C4
2	F	400	19H	OAD-CAQ-CAW-CAX

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Mol	Chain	Res	Type	Atoms
3	A	402	PGE	C4-C3-O2-C2
2	A	401	19H	CAI-CAU-OAP-CAM
3	A	402	PGE	C1-C2-O2-C3
2	B	401	19H	CAI-CAU-OAP-CAM
2	C	400	19H	CAM-CAL-CAN-CAX
2	F	400	19H	CAJ-CAU-OAP-CAM

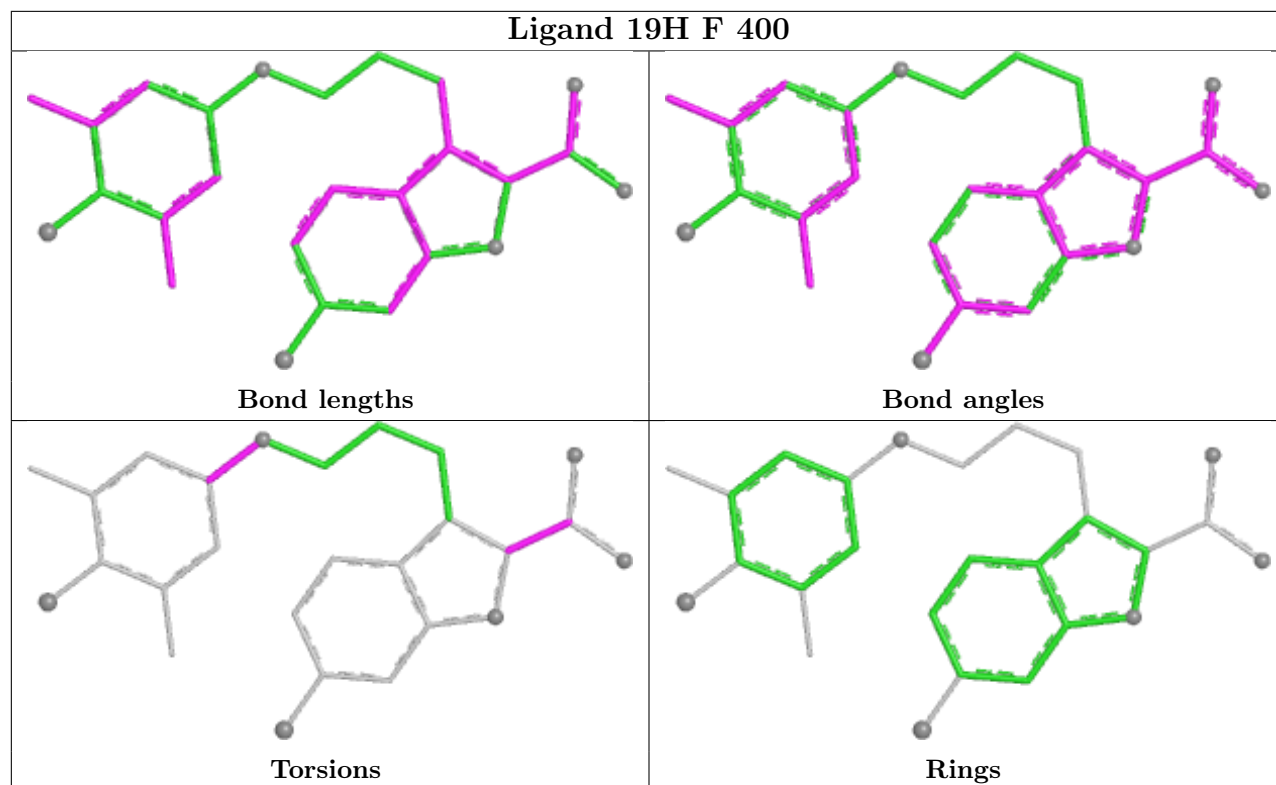
There are no ring outliers.

8 monomers are involved in 16 short contacts:

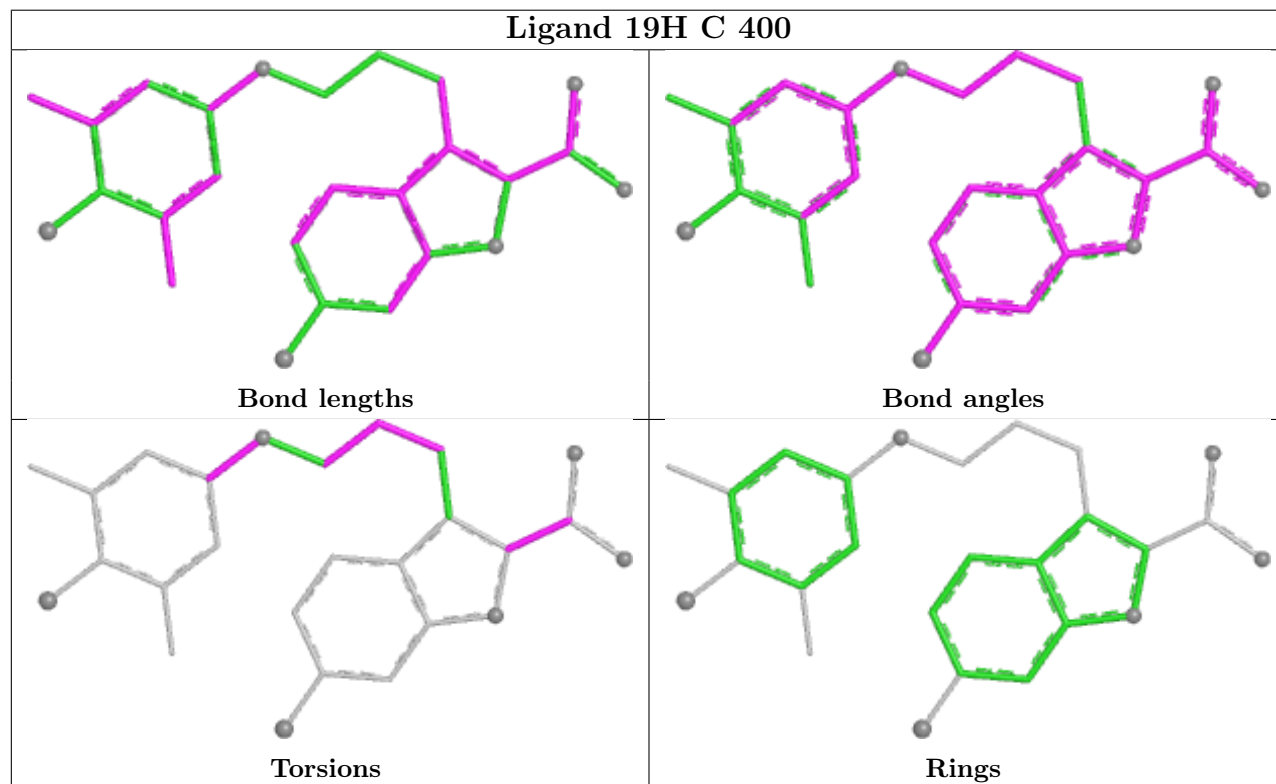
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PGE	4	0
3	B	403	PGE	2	0
2	F	400	19H	1	0
4	B	404	EDO	1	0
2	C	400	19H	5	0
2	A	401	19H	1	0
2	E	400	19H	1	0
2	D	400	19H	1	0

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.

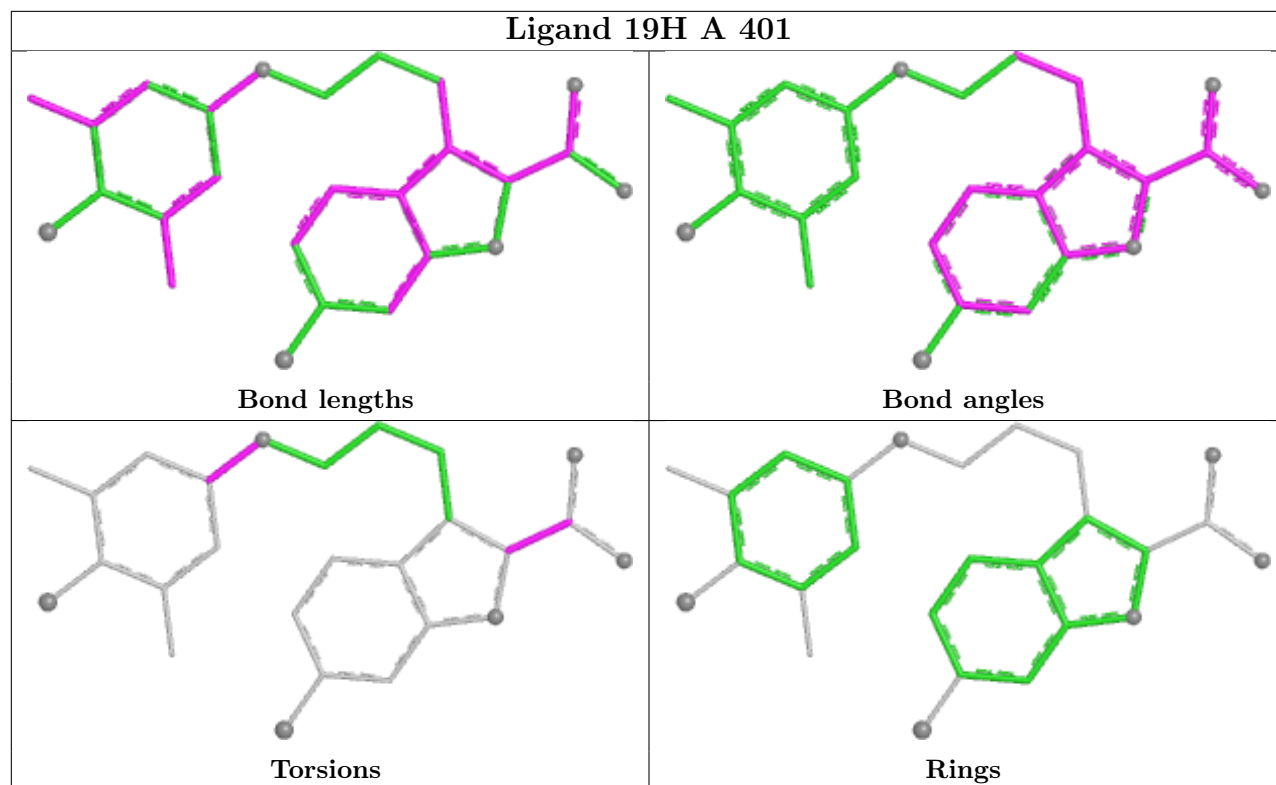
Ligand 19H F 400



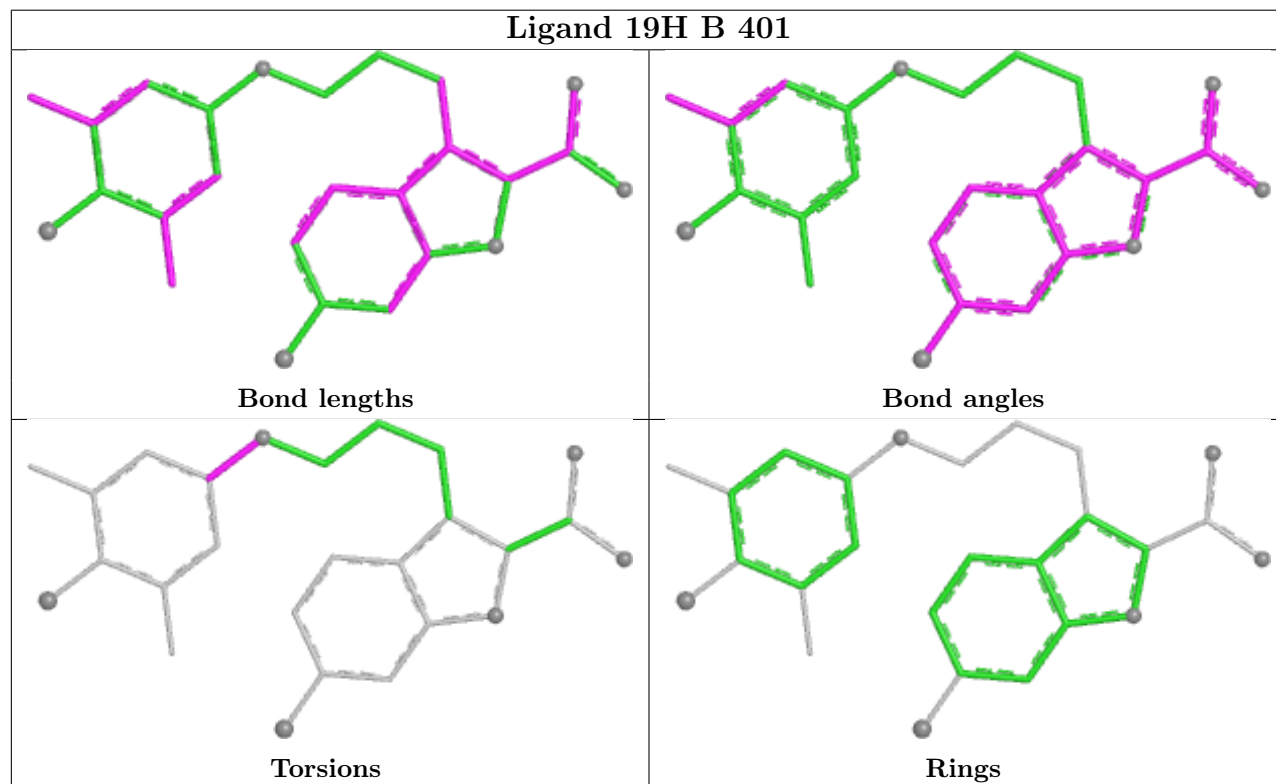
Ligand 19H C 400

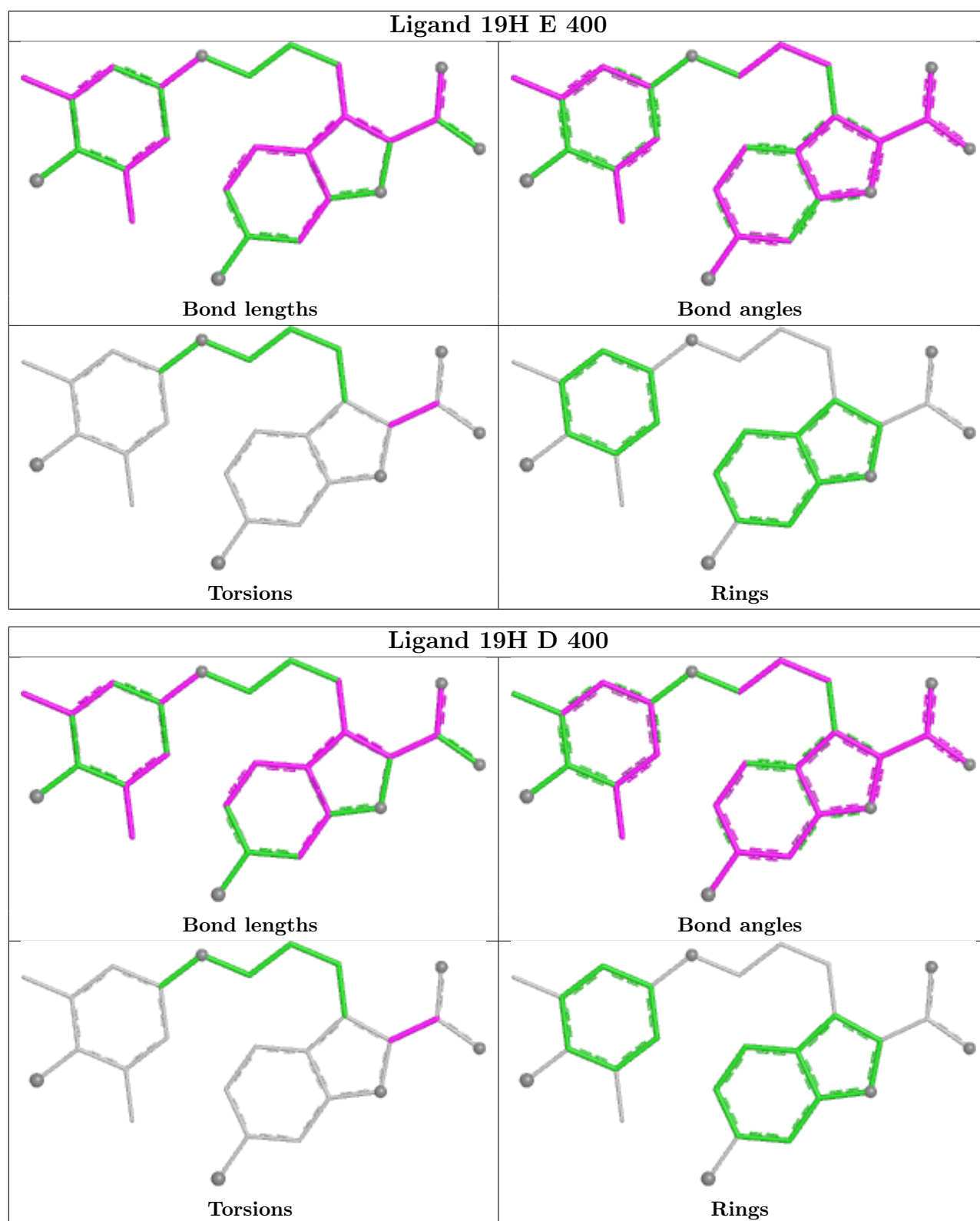


Ligand 19H A 401



Ligand 19H B 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	149/153 (97%)	-0.03	2 (1%) 75 66	26, 46, 70, 85	0
1	B	151/153 (98%)	-0.01	2 (1%) 75 66	7, 44, 65, 73	0
1	C	150/153 (98%)	-0.19	0 100 100	27, 50, 72, 78	0
1	D	151/153 (98%)	-0.11	3 (1%) 65 56	28, 48, 69, 81	0
1	E	151/153 (98%)	-0.02	2 (1%) 75 66	28, 49, 71, 87	0
1	F	150/153 (98%)	-0.04	3 (2%) 65 56	24, 49, 77, 87	0
All	All	902/918 (98%)	-0.07	12 (1%) 75 66	7, 48, 71, 87	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ALA	3.5
1	A	218	ASP	3.3
1	E	223	ASN	3.2
1	E	200	GLY	2.7
1	D	193	ALA	2.6
1	D	321	VAL	2.5
1	B	296	ASP	2.3
1	A	236	ASP	2.2
1	F	193	ALA	2.2
1	D	191	THR	2.1
1	F	196	THR	2.0
1	F	200	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](#)

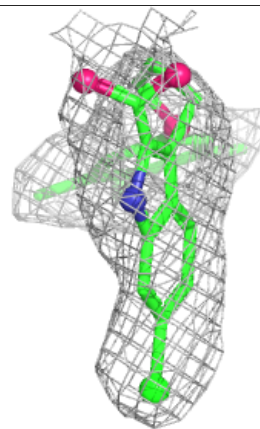
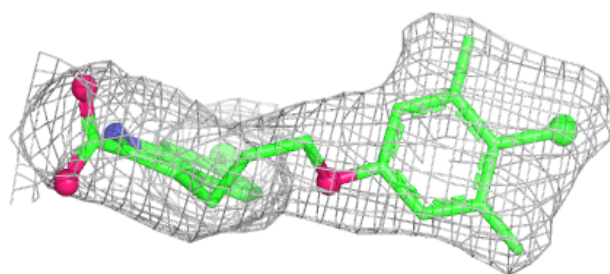
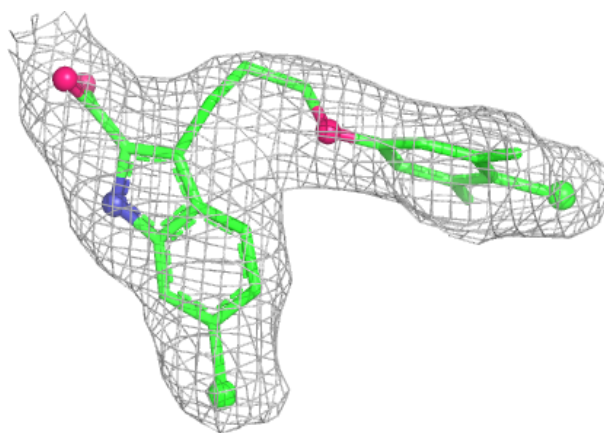
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PGE	A	402	10/10	0.82	0.13	36,56,76,79	0
3	PGE	B	402	10/10	0.87	0.13	26,60,74,80	0
3	PGE	B	403	10/10	0.87	0.15	32,48,61,65	0
4	EDO	B	404	4/4	0.87	0.12	33,41,62,77	0
2	19H	C	400	26/26	0.93	0.09	29,55,73,89	0
2	19H	B	401	26/26	0.94	0.08	1,23,37,47	0
2	19H	D	400	26/26	0.95	0.07	17,37,59,79	0
2	19H	F	400	26/26	0.95	0.07	10,42,61,87	0
2	19H	A	401	26/26	0.95	0.08	1,40,57,66	0
2	19H	E	400	26/26	0.96	0.07	1,43,62,70	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.

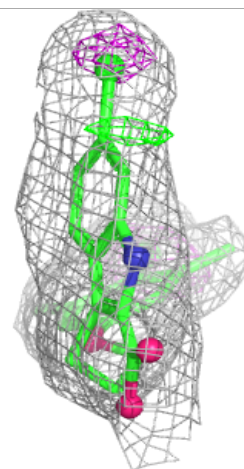
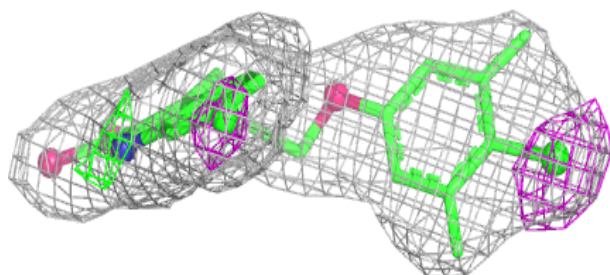
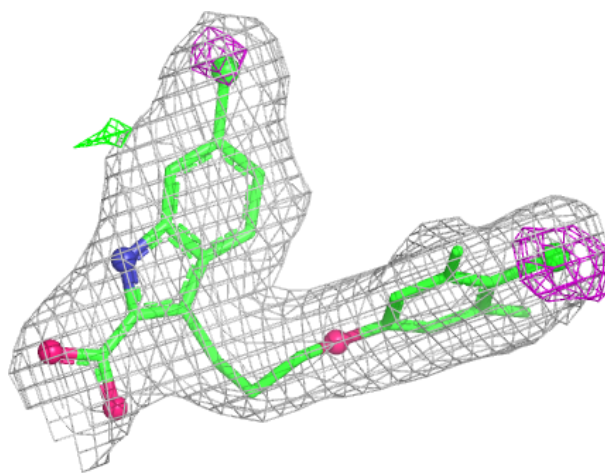
Electron density around 19H C 400:

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



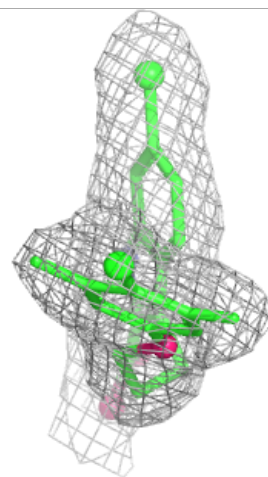
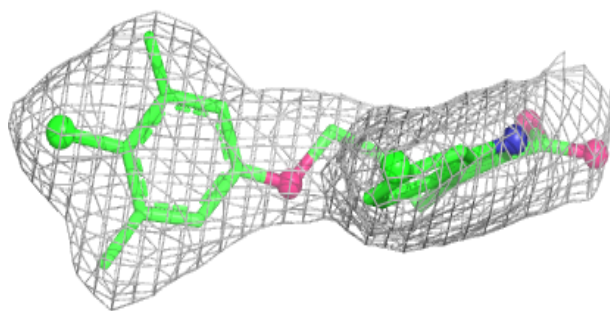
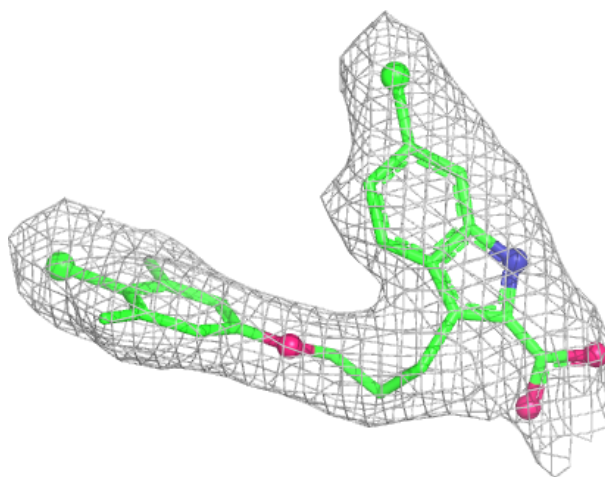
Electron density around 19H B 401:

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



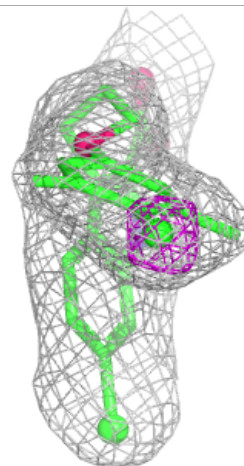
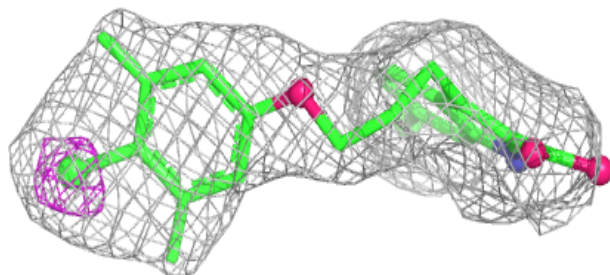
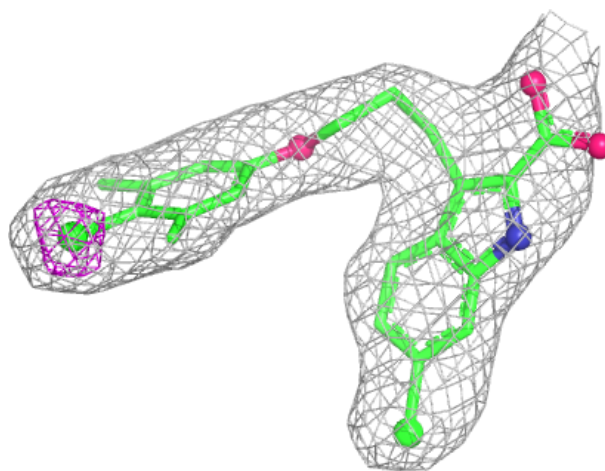
Electron density around 19H D 400:

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



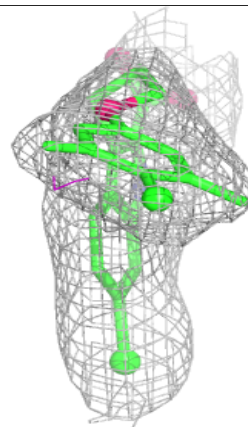
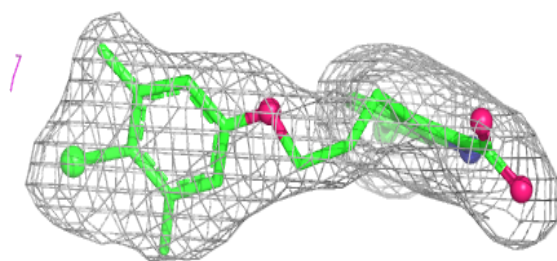
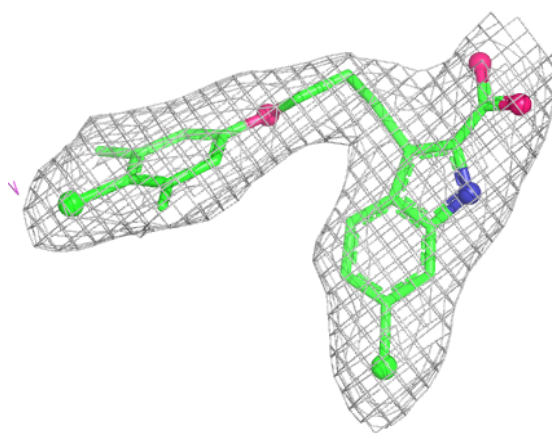
Electron density around 19H F 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



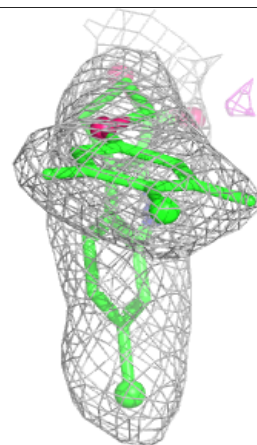
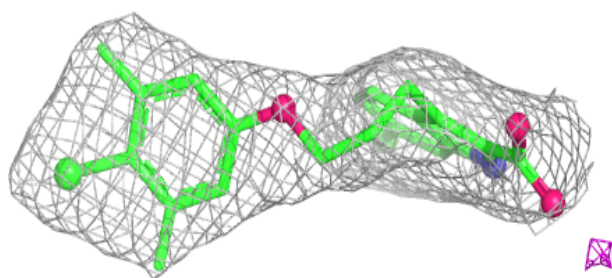
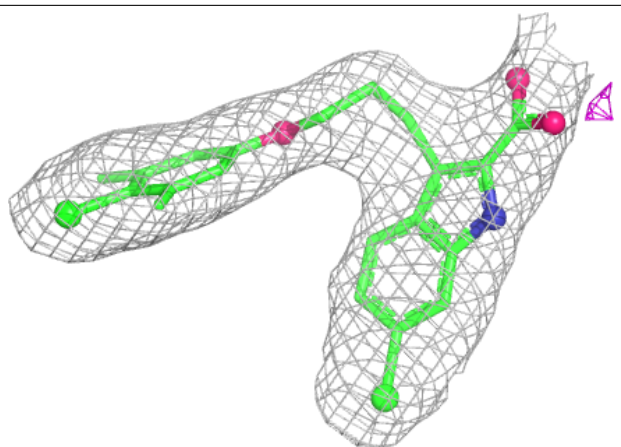
Electron density around 19H A 401:

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



Electron density around 19H E 400:

$2mF_o-DF_c$ (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.