



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:07 PM UTC

PDB ID : 4MZO / pdb_00004mzo
Title : Mouse cathepsin s with covalent ligand (3S,4S)-N-[(2E)-2-IMINOETHYL]-4-(MORPHOLIN-4-YLCARBONYL)-1-(PHENYLSULFONYL)PYRROLIDINE-3-CARBOXAMIDE
Authors : Kuglstatter, A.; Stihle, M.
Deposited on : 2013-09-30
Resolution : 1.47 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

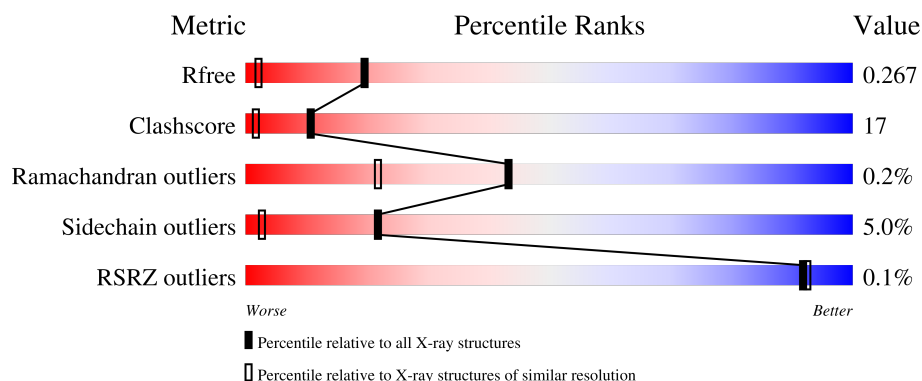
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	225	
1	B	225	
1	C	225	
1	D	225	

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Mol	Chain	Length	Quality of chain
1	E	225	50%40%7%
1	F	225	58%32%7%
1	G	225	62%30%5%
1	H	225	59%33%5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14421 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.

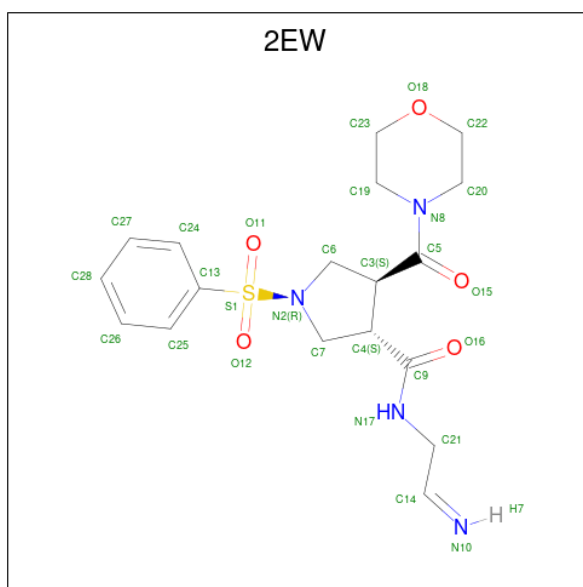
- Molecule 1 is a protein called Cathepsin S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	2	0
			1683	1059	281	330	13			
1	B	219	Total	C	N	O	S	0	1	0
			1682	1055	282	332	13			
1	C	218	Total	C	N	O	S	0	2	0
			1678	1054	280	331	13			
1	D	218	Total	C	N	O	S	0	2	0
			1683	1059	281	330	13			
1	E	218	Total	C	N	O	S	0	3	0
			1680	1058	280	328	14			
1	F	219	Total	C	N	O	S	0	1	0
			1679	1054	281	330	14			
1	G	218	Total	C	N	O	S	0	0	0
			1669	1048	280	328	13			
1	H	218	Total	C	N	O	S	0	0	0
			1669	1048	280	328	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	MET	THR	variant	UNP O70370
B	218	MET	THR	variant	UNP O70370
C	218	MET	THR	variant	UNP O70370
D	218	MET	THR	variant	UNP O70370
E	218	MET	THR	variant	UNP O70370
F	218	MET	THR	variant	UNP O70370
G	218	MET	THR	variant	UNP O70370
H	218	MET	THR	variant	UNP O70370

- Molecule 2 is (3S,4S)-N-[(2E)-2-iminoethyl]-4-(morpholin-4-ylcarbonyl)-1-(phenylsulfonyl)pyrrolidine-3-carboxamide (CCD ID: 2EW) (formula: C₁₈H₂₄N₄O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	B	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	C	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	D	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	E	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	F	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	G	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
2	H	1	Total	C	N	O	S	0	0
			28	18	4	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	101	Total	O	0	0
			101	101		
3	C	97	Total	O	0	0
			97	97		
3	D	86	Total	O	0	0
			86	86		

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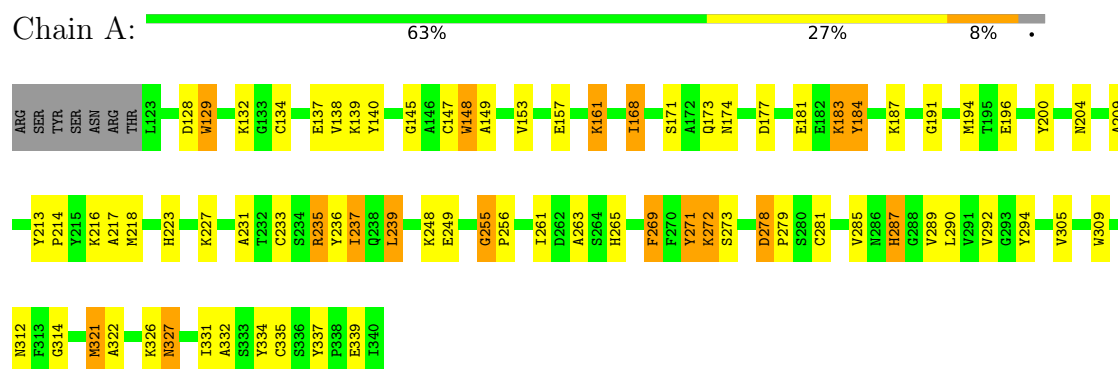
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	91	Total 91	O 91	0	0
3	F	97	Total 97	O 97	0	0
3	G	86	Total 86	O 86	0	0
3	H	97	Total 97	O 97	0	0

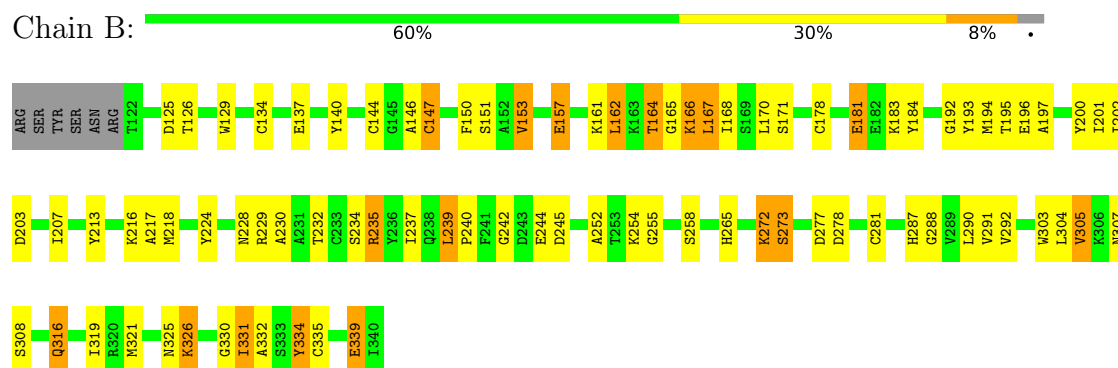
3 Residue-property plots

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.

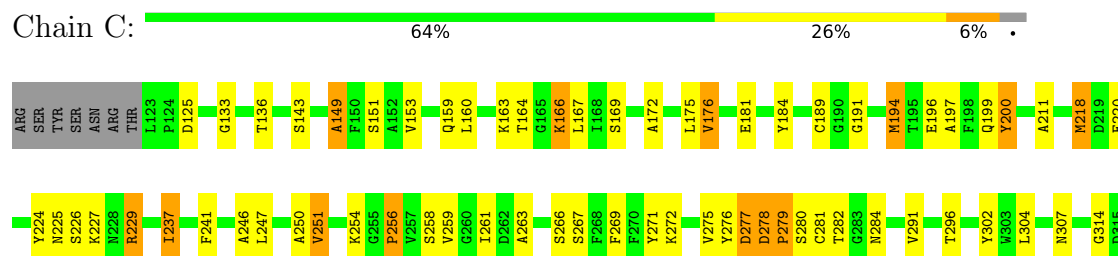
• Molecule 1: Cathepsin S

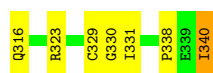


• Molecule 1: Cathepsin S



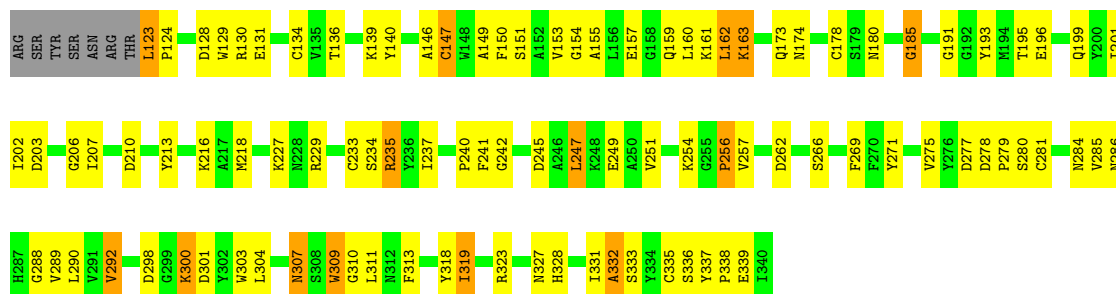
• Molecule 1: Cathepsin S





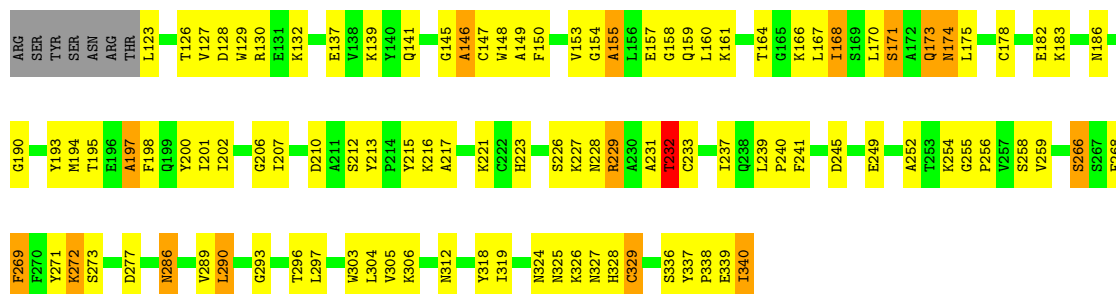
• Molecule 1: Cathepsin S

Chain D: 53% 38% 6%



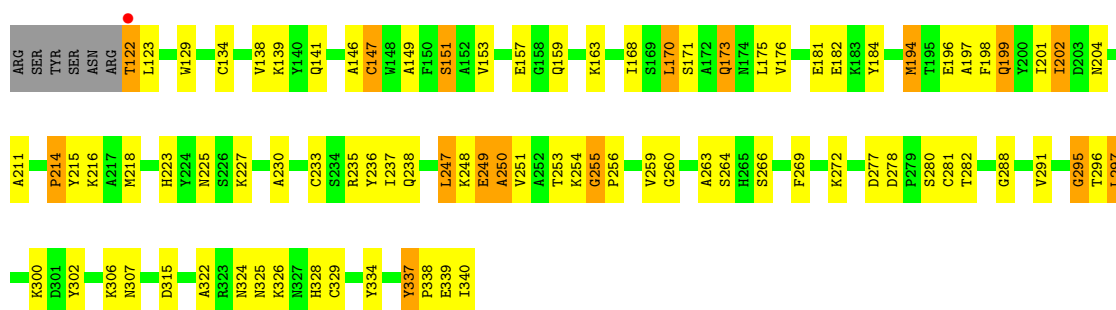
• Molecule 1: Cathepsin S

Chain E: 50% 40% 7%



• Molecule 1: Cathepsin S

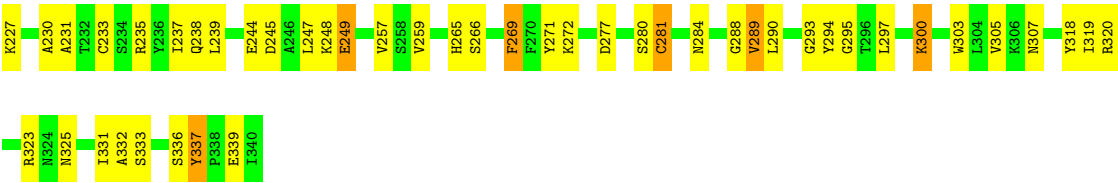
Chain F: 58% 32% 7%



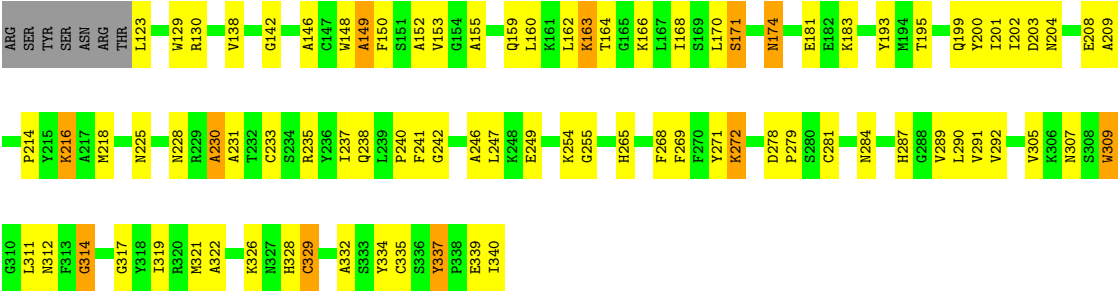
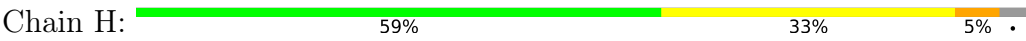
• Molecule 1: Cathepsin S

Chain G: 62% 30% 5%





• Molecule 1: Cathepsin S



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.20Å 86.06Å 119.32Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	49.03 – 1.47 49.03 – 1.47	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.03-1.47) 92.5 (49.03-1.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.231 , 0.275 0.223 , 0.267	Depositor DCC
R_{free} test set	11773 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 14.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.279 for h,-k,-l	Xtriage
Reported twinning fraction	0.703 for H, K, L 0.297 for -h,-k,l	Depositor
Outliers	0 of 234146 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14421	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 69.66 % 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 3.5618e-06.*

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: 2EW

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	24/1726 (1.4%)	1.67	21/2331 (0.9%)
1	B	1.62	20/1721 (1.2%)	1.71	26/2325 (1.1%)
1	C	1.71	20/1723 (1.2%)	1.74	20/2327 (0.9%)
1	D	1.61	20/1726 (1.2%)	1.76	35/2331 (1.5%)
1	E	1.59	20/1728 (1.2%)	1.64	19/2335 (0.8%)
1	F	1.72	24/1721 (1.4%)	1.75	25/2325 (1.1%)
1	G	1.71	20/1708 (1.2%)	1.80	27/2307 (1.2%)
1	H	1.60	15/1708 (0.9%)	1.64	24/2307 (1.0%)
All	All	1.66	163/13761 (1.2%)	1.72	197/18588 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	286	ASN	N-CA	10.93	1.56	1.46
1	H	291	VAL	N-CA	-10.16	1.34	1.46
1	D	290	LEU	C-O	9.59	1.34	1.23
1	F	260	GLY	CA-C	9.25	1.59	1.52
1	G	231	ALA	C-O	9.14	1.34	1.23
1	C	263	ALA	N-CA	8.31	1.55	1.46
1	C	338	PRO	CA-C	-8.06	1.43	1.52
1	A	271	TYR	C-O	-8.06	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	TYR	C-O	-8.01	1.15	1.24
1	G	191	GLY	N-CA	7.99	1.52	1.45
1	G	333	SER	C-O	7.98	1.33	1.24
1	E	168	ILE	C-O	7.84	1.32	1.24
1	H	292	VAL	N-CA	7.65	1.53	1.46
1	A	231	ALA	C-O	7.62	1.32	1.23
1	E	232	THR	C-O	-7.37	1.14	1.23
1	B	144	CYS	CA-C	-7.24	1.44	1.52
1	H	321	MET	CA-C	7.22	1.61	1.52
1	C	279	PRO	N-CA	-7.20	1.38	1.47
1	F	295	GLY	C-O	7.17	1.31	1.23
1	H	314	GLY	N-CA	-7.17	1.36	1.45
1	H	309	TRP	C-O	-7.14	1.14	1.23
1	D	333	SER	C-O	7.13	1.32	1.24
1	C	261	ILE	C-O	7.12	1.31	1.23
1	E	273	SER	C-O	7.11	1.32	1.23
1	H	265	HIS	CA-C	7.09	1.61	1.52
1	B	287	HIS	N-CA	6.98	1.54	1.46
1	F	173	GLN	CA-C	6.96	1.61	1.52
1	F	194	MET	C-O	-6.96	1.15	1.24
1	F	214	PRO	C-O	6.91	1.32	1.23
1	G	265	HIS	N-CA	6.91	1.55	1.46
1	F	306	LYS	CA-C	-6.88	1.44	1.52
1	B	305	VAL	CA-C	6.87	1.60	1.52
1	F	250	ALA	C-O	6.85	1.32	1.24
1	E	190	GLY	C-O	6.82	1.31	1.23
1	B	291	VAL	C-O	6.70	1.30	1.24
1	E	245	ASP	C-O	6.66	1.31	1.24
1	G	199	GLN	C-O	6.59	1.31	1.24
1	A	249	GLU	C-O	6.48	1.31	1.24
1	H	142	GLY	C-O	6.48	1.32	1.24
1	H	322	ALA	C-O	6.41	1.31	1.23
1	D	319	ILE	C-O	-6.41	1.17	1.24
1	F	329	CYS	CA-C	6.41	1.61	1.52
1	E	290	LEU	CA-C	6.30	1.59	1.52
1	C	256	PRO	CA-C	6.28	1.60	1.52
1	F	296	THR	C-O	6.26	1.31	1.24
1	G	192	GLY	C-O	6.26	1.30	1.23
1	E	266	SER	C-O	6.21	1.31	1.24
1	A	145	GLY	C-O	6.19	1.32	1.23
1	A	331	ILE	C-O	6.18	1.31	1.24
1	D	199	GLN	N-CA	6.18	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	ASN	CA-CB	6.14	1.61	1.52
1	B	230	ALA	CA-C	6.09	1.60	1.52
1	B	258	SER	CA-C	6.08	1.61	1.52
1	A	321	MET	N-CA	6.08	1.53	1.46
1	C	282	THR	C-O	6.04	1.31	1.23
1	E	303	TRP	C-O	6.01	1.31	1.23
1	H	149	ALA	C-O	6.01	1.31	1.24
1	A	261	ILE	N-CA	-6.00	1.39	1.46
1	B	196	GLU	C-O	5.99	1.31	1.24
1	E	186	ASN	CA-C	-5.98	1.45	1.52
1	G	318	TYR	C-O	5.96	1.31	1.23
1	H	334	TYR	CA-CB	-5.96	1.45	1.53
1	G	259	VAL	C-O	5.94	1.30	1.23
1	A	204	ASN	C-O	5.93	1.31	1.24
1	G	149	ALA	C-O	5.92	1.31	1.24
1	C	246	ALA	N-CA	-5.92	1.39	1.46
1	C	291	VAL	C-O	5.90	1.30	1.24
1	A	128	ASP	C-O	5.89	1.30	1.23
1	F	168	ILE	C-O	-5.86	1.18	1.24
1	E	329	CYS	C-O	5.83	1.33	1.24
1	A	289	VAL	C-O	5.82	1.30	1.23
1	F	138	VAL	N-CA	5.81	1.53	1.46
1	G	213	TYR	CZ-OH	-5.79	1.25	1.38
1	D	210	ASP	C-O	5.79	1.30	1.24
1	H	242	GLY	C-O	-5.76	1.15	1.24
1	G	245	ASP	N-CA	5.76	1.53	1.46
1	B	307	ASN	C-O	5.75	1.31	1.23
1	D	146	ALA	C-O	5.75	1.31	1.24
1	A	196	GLU	CA-C	5.71	1.60	1.52
1	E	210	ASP	C-O	-5.71	1.17	1.24
1	C	199	GLN	N-CA	5.68	1.53	1.46
1	E	206	GLY	C-O	5.67	1.31	1.23
1	B	339	GLU	CA-C	5.63	1.59	1.52
1	F	250	ALA	CA-C	5.63	1.60	1.52
1	F	264	SER	CA-C	5.63	1.60	1.52
1	D	147	CYS	C-O	-5.61	1.17	1.24
1	F	315	ASP	C-O	5.61	1.30	1.23
1	B	287	HIS	C-N	5.59	1.37	1.33
1	F	202	ILE	C-O	-5.59	1.17	1.24
1	C	330	GLY	N-CA	5.58	1.53	1.45
1	D	159	GLN	N-CA	5.57	1.53	1.46
1	D	180	ASN	CA-CB	5.57	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	ASP	C-O	-5.56	1.17	1.24
1	A	173	GLN	N-CA	5.53	1.53	1.46
1	E	141	GLN	N-CA	-5.53	1.39	1.46
1	B	334	TYR	C-O	5.52	1.31	1.23
1	E	213	TYR	C-N	5.52	1.40	1.33
1	E	223	HIS	C-O	5.51	1.29	1.23
1	F	170	LEU	N-CA	-5.51	1.39	1.45
1	C	277	ASP	N-CA	-5.51	1.41	1.46
1	G	210	ASP	C-O	5.51	1.30	1.24
1	B	207	ILE	C-O	5.50	1.30	1.23
1	F	147	CYS	C-O	5.50	1.30	1.24
1	D	154	GLY	C-O	5.49	1.30	1.23
1	A	139	LYS	CA-C	5.49	1.60	1.52
1	C	261	ILE	N-CA	-5.47	1.40	1.46
1	A	209	ALA	CA-C	-5.47	1.45	1.53
1	C	296	THR	N-CA	-5.45	1.39	1.46
1	A	149	ALA	N-CA	5.43	1.52	1.46
1	D	309	TRP	CB-CG	-5.42	1.33	1.50
1	E	318	TYR	CA-C	-5.42	1.46	1.52
1	E	139	LYS	CA-C	5.42	1.59	1.52
1	G	160	LEU	CA-C	-5.41	1.46	1.52
1	F	230	ALA	N-CA	5.39	1.52	1.45
1	G	295	GLY	N-CA	5.39	1.52	1.45
1	B	308	SER	N-CA	5.38	1.53	1.46
1	E	286	ASN	N-CA	-5.38	1.39	1.46
1	D	207	ILE	C-O	-5.37	1.18	1.24
1	C	316	GLN	CA-C	5.36	1.59	1.52
1	F	176	VAL	CA-C	5.35	1.59	1.52
1	D	149	ALA	CA-C	5.34	1.59	1.52
1	B	170	LEU	C-O	5.33	1.30	1.23
1	A	327	ASN	CA-C	5.31	1.60	1.53
1	B	192	GLY	C-O	5.31	1.30	1.23
1	B	157	GLU	C-O	5.29	1.30	1.24
1	F	171	SER	CA-C	5.26	1.59	1.53
1	D	233	CYS	CA-C	5.25	1.58	1.52
1	A	161	LYS	N-CA	5.23	1.52	1.46
1	B	194	MET	C-O	-5.22	1.17	1.24
1	A	337	TYR	CA-C	-5.22	1.46	1.52
1	D	235	ARG	CA-C	-5.22	1.46	1.52
1	C	254	LYS	CA-C	5.20	1.57	1.52
1	E	146	ALA	CA-C	5.18	1.60	1.52
1	G	257	VAL	CA-C	5.17	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	266	SER	C-O	5.17	1.30	1.24
1	G	233	CYS	CA-C	5.17	1.58	1.52
1	H	307	ASN	N-CA	-5.17	1.39	1.45
1	A	273	SER	N-CA	5.16	1.52	1.46
1	D	195	THR	N-CA	5.14	1.52	1.46
1	C	191	GLY	N-CA	5.14	1.49	1.45
1	B	254	LYS	N-CA	5.14	1.52	1.46
1	A	287	HIS	CA-C	5.14	1.58	1.52
1	G	162	LEU	N-CA	5.13	1.52	1.46
1	C	194	MET	C-O	-5.13	1.17	1.24
1	F	259	VAL	N-CA	5.13	1.51	1.46
1	G	247	LEU	C-O	-5.11	1.18	1.24
1	C	275	VAL	CA-CB	-5.11	1.48	1.54
1	H	287	HIS	N-CA	5.11	1.52	1.46
1	D	332	ALA	CA-CB	-5.09	1.45	1.53
1	F	255	GLY	C-O	5.08	1.30	1.24
1	C	267	SER	CA-C	5.07	1.59	1.52
1	A	171	SER	CA-C	5.06	1.59	1.52
1	C	159	GLN	N-CA	5.05	1.52	1.46
1	H	321	MET	C-O	5.05	1.30	1.23
1	B	193	TYR	C-O	5.04	1.30	1.23
1	G	266	SER	C-O	-5.04	1.17	1.24
1	D	327	ASN	CA-C	5.03	1.59	1.53
1	E	155	ALA	N-CA	5.03	1.52	1.46
1	A	255	GLY	C-O	-5.02	1.17	1.24
1	F	307	ASN	N-CA	-5.01	1.40	1.45
1	H	307	ASN	C-O	5.01	1.30	1.23
1	A	149	ALA	C-O	5.01	1.29	1.24
1	A	332	ALA	CA-C	-5.01	1.46	1.52

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	337	TYR	CA-C-N	12.16	132.23	120.31
1	F	337	TYR	C-N-CA	12.16	132.23	120.31
1	D	201	ILE	N-CA-C	-11.06	99.55	110.72
1	D	123	LEU	CA-C-N	-9.29	109.98	119.92
1	D	123	LEU	C-N-CA	-9.29	109.98	119.92
1	G	153	VAL	N-CA-CB	9.19	121.95	110.47
1	B	239	LEU	CA-C-N	-8.88	110.62	119.76
1	B	239	LEU	C-N-CA	-8.88	110.62	119.76
1	D	257	VAL	N-CA-C	8.73	121.20	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	ALA	N-CA-C	8.59	120.26	111.07
1	G	150	PHE	N-CA-C	8.19	120.29	111.36
1	H	204	ASN	N-CA-C	-7.89	103.65	113.28
1	A	239	LEU	CA-C-N	-7.87	111.80	120.14
1	A	239	LEU	C-N-CA	-7.87	111.80	120.14
1	E	197	ALA	N-CA-C	-7.71	102.96	111.36
1	A	184	TYR	N-CA-C	7.64	123.28	113.88
1	G	269	PHE	N-CA-C	-7.64	102.90	111.07
1	F	211	ALA	N-CA-C	7.61	119.57	111.28
1	F	247	LEU	N-CA-C	-7.56	103.12	111.36
1	C	307	ASN	N-CA-C	-7.54	99.10	109.95
1	C	200	TYR	N-CA-C	-7.49	102.47	111.69
1	G	289	VAL	N-CA-CB	-7.47	104.08	112.45
1	E	158	GLY	N-CA-C	-7.41	103.53	112.49
1	D	331	ILE	N-CA-C	7.30	120.18	111.05
1	B	195	THR	N-CA-C	-7.29	103.41	111.36
1	D	256	PRO	CB-CA-C	7.28	120.85	111.46
1	A	278	ASP	CA-C-N	7.20	127.83	119.47
1	A	278	ASP	C-N-CA	7.20	127.83	119.47
1	E	269	PHE	CB-CA-C	-7.07	99.05	110.79
1	A	168	ILE	CB-CA-C	-7.06	100.52	110.12
1	B	200	TYR	N-CA-C	-7.02	103.56	111.14
1	G	259	VAL	CA-C-O	-7.00	114.32	121.67
1	D	140	TYR	CA-C-O	-6.97	113.08	120.40
1	E	277	ASP	N-CA-C	-6.86	95.05	107.60
1	E	202	ILE	N-CA-C	-6.83	104.20	110.82
1	C	278	ASP	CA-C-N	6.80	127.36	119.47
1	C	278	ASP	C-N-CA	6.80	127.36	119.47
1	G	230	ALA	N-CA-C	6.73	121.77	113.50
1	F	201	ILE	N-CA-C	-6.70	103.96	110.72
1	G	259	VAL	N-CA-C	6.63	119.90	108.95
1	H	326	LYS	CB-CA-C	6.61	120.61	111.63
1	H	171	SER	N-CA-C	6.58	119.97	108.52
1	E	171	SER	N-CA-C	6.57	119.15	108.63
1	D	213	TYR	CA-C-N	6.53	126.45	119.85
1	D	213	TYR	C-N-CA	6.53	126.45	119.85
1	G	179	SER	N-CA-C	-6.52	103.75	112.94
1	A	177	ASP	N-CA-C	6.48	118.34	111.28
1	F	197	ALA	N-CA-C	-6.46	104.31	111.36
1	E	227	LYS	N-CA-C	-6.44	105.28	113.01
1	D	191	GLY	CA-C-O	-6.42	117.83	122.45
1	C	191	GLY	CA-C-O	-6.40	117.70	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	TYR	CA-C-O	-6.36	114.14	120.82
1	C	176	VAL	N-CA-C	6.35	117.03	110.36
1	H	130	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	B	147	CYS	CB-CA-C	-6.31	99.95	110.68
1	C	218	MET	N-CA-C	6.29	118.41	108.79
1	G	181	GLU	N-CA-C	6.27	118.67	108.76
1	D	151	SER	CA-C-N	-6.27	111.92	120.44
1	D	151	SER	C-N-CA	-6.27	111.92	120.44
1	C	237	ILE	CB-CA-C	-6.26	101.50	110.83
1	D	155	ALA	CA-C-N	-6.26	110.04	120.68
1	D	155	ALA	C-N-CA	-6.26	110.04	120.68
1	F	199	GLN	CB-CA-C	-6.26	100.80	110.81
1	H	255	GLY	CA-C-N	6.24	126.19	119.76
1	H	255	GLY	C-N-CA	6.24	126.19	119.76
1	H	329	CYS	N-CA-C	6.22	120.11	111.90
1	H	247	LEU	N-CA-C	-6.18	104.44	112.23
1	C	143	SER	N-CA-C	6.16	120.06	112.54
1	G	162	LEU	N-CA-C	6.14	118.78	111.71
1	B	277	ASP	N-CA-C	6.12	118.26	110.61
1	A	200	TYR	N-CA-C	-6.12	104.53	111.07
1	C	149	ALA	O-C-N	-6.12	115.48	122.09
1	B	290	LEU	N-CA-C	6.05	118.26	108.34
1	B	150	PHE	N-CA-C	6.04	118.35	111.11
1	H	152	ALA	N-CA-C	-6.03	104.79	111.36
1	B	153	VAL	CA-C-O	-6.02	114.69	120.95
1	B	167	LEU	N-CA-C	-6.01	99.44	109.24
1	A	148	TRP	O-C-N	6.01	128.34	122.09
1	B	252	ALA	N-CA-C	6.00	117.90	111.36
1	C	151	SER	N-CA-C	6.00	117.49	111.07
1	D	307	ASN	CA-C-O	-6.00	114.28	121.89
1	F	141	GLN	N-CA-C	5.99	119.77	112.23
1	F	175	LEU	N-CA-C	-5.97	104.69	111.14
1	H	314	GLY	N-CA-C	5.91	122.10	111.34
1	E	268	PHE	N-CA-C	-5.91	104.76	111.14
1	E	212	SER	N-CA-C	5.90	120.21	112.89
1	D	191	GLY	N-CA-C	-5.88	106.04	112.04
1	D	178	CYS	N-CA-C	5.88	120.73	113.50
1	H	214	PRO	N-CA-C	5.87	120.44	111.34
1	H	146	ALA	N-CA-C	5.84	119.47	112.93
1	G	280	SER	N-CA-C	5.79	119.95	113.01
1	G	337	TYR	CA-C-N	5.79	125.69	119.85
1	G	337	TYR	C-N-CA	5.79	125.69	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	159	GLN	N-CA-C	-5.78	105.06	111.36
1	B	242	GLY	N-CA-C	5.76	123.20	115.59
1	B	330	GLY	N-CA-C	-5.76	107.31	115.43
1	E	173	GLN	CA-C-N	5.75	128.31	120.54
1	E	173	GLN	C-N-CA	5.75	128.31	120.54
1	D	185	GLY	N-CA-C	-5.74	107.72	115.36
1	F	171	SER	N-CA-C	5.74	118.51	108.52
1	B	316	GLN	CA-CB-CG	-5.74	102.63	114.10
1	D	203	ASP	N-CA-CB	5.72	118.63	110.16
1	D	311	LEU	N-CA-C	5.70	118.26	111.71
1	G	281	CYS	N-CA-C	-5.68	103.03	110.53
1	C	304	LEU	CA-C-O	-5.68	114.07	120.43
1	A	273	SER	N-CA-C	5.66	116.86	108.60
1	B	265	HIS	CB-CA-C	5.65	118.98	109.48
1	C	276	TYR	CE1-CZ-CE2	-5.65	109.00	120.30
1	C	323	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	D	285	VAL	N-CA-C	5.64	121.07	109.34
1	B	164	THR	N-CA-C	-5.63	106.22	114.39
1	F	159	GLN	N-CA-CB	5.61	118.46	110.16
1	H	208	GLU	CA-C-N	5.57	129.69	120.94
1	H	208	GLU	C-N-CA	5.57	129.69	120.94
1	F	249	GLU	N-CA-C	-5.54	105.16	111.14
1	D	150	PHE	N-CA-CB	5.53	118.03	110.01
1	F	255	GLY	CA-C-N	5.50	125.44	119.78
1	F	255	GLY	C-N-CA	5.50	125.44	119.78
1	H	230	ALA	N-CA-C	5.50	120.14	113.38
1	G	175	LEU	CB-CG-CD1	5.49	127.16	110.70
1	F	151	SER	CA-C-O	5.48	126.57	120.82
1	G	239	LEU	CA-C-N	-5.48	114.15	119.90
1	G	239	LEU	C-N-CA	-5.48	114.15	119.90
1	B	273	SER	N-CA-C	5.47	116.59	108.60
1	A	149	ALA	O-C-N	5.47	127.70	122.07
1	A	305	VAL	N-CA-C	5.46	115.82	108.17
1	A	213	TYR	CA-C-N	-5.46	114.71	120.66
1	A	213	TYR	C-N-CA	-5.46	114.71	120.66
1	E	259	VAL	CB-CA-C	-5.46	102.75	110.82
1	E	164	THR	N-CA-C	-5.44	107.65	114.56
1	D	136	THR	N-CA-C	5.43	117.34	110.33
1	B	151	SER	CA-C-O	-5.41	114.81	120.55
1	B	162	LEU	N-CA-C	-5.41	106.52	113.01
1	H	269	PHE	N-CA-C	-5.41	104.78	111.33
1	B	125	ASP	N-CA-C	5.41	117.17	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	GLY	N-CA-C	5.39	125.97	113.18
1	H	174	ASN	N-CA-C	-5.36	105.33	111.07
1	D	151	SER	N-CA-C	-5.33	105.37	111.07
1	G	201	ILE	N-CA-CB	5.32	116.21	110.62
1	A	129	TRP	N-CA-C	5.30	118.84	112.38
1	D	160	LEU	N-CA-C	-5.30	105.59	111.36
1	D	149	ALA	CA-C-O	5.29	126.11	120.24
1	D	129	TRP	CA-C-N	-5.29	112.89	120.82
1	D	129	TRP	C-N-CA	-5.29	112.89	120.82
1	B	171	SER	N-CA-CB	5.28	117.96	110.46
1	A	331	ILE	N-CA-C	5.28	118.45	111.17
1	B	325	ASN	CB-CA-C	5.27	119.50	111.70
1	B	171	SER	CA-C-O	-5.26	115.50	121.66
1	H	246	ALA	N-CA-C	-5.25	105.67	111.71
1	F	151	SER	CA-CB-OG	-5.25	100.60	111.10
1	D	247	LEU	N-CA-C	-5.24	105.64	111.36
1	F	334	TYR	CA-CB-CG	-5.24	104.48	113.90
1	D	256	PRO	CA-C-N	-5.23	116.35	123.10
1	D	256	PRO	C-N-CA	-5.23	116.35	123.10
1	G	166	LYS	N-CA-C	5.23	117.28	108.96
1	A	233	CYS	CA-C-O	-5.22	114.66	120.66
1	G	307	ASN	CA-C-O	-5.22	114.69	121.73
1	F	202	ILE	N-CA-C	-5.21	104.89	110.36
1	E	324	ASN	N-CA-C	5.20	118.77	111.74
1	A	287	HIS	CB-CA-C	5.20	118.75	109.65
1	F	204	ASN	N-CA-C	5.20	119.10	112.87
1	H	155	ALA	N-CA-C	-5.19	105.71	111.36
1	H	337	TYR	CA-C-N	5.17	126.29	120.66
1	H	337	TYR	C-N-CA	5.17	126.29	120.66
1	E	175	LEU	N-CA-C	5.17	116.99	111.36
1	E	148	TRP	O-C-N	5.16	127.59	122.12
1	H	290	LEU	N-CA-C	5.16	116.82	108.41
1	G	293	GLY	N-CA-C	5.15	118.21	110.18
1	F	139	LYS	O-C-N	5.13	128.82	123.03
1	F	248	LYS	CG-CD-CE	-5.12	99.54	111.30
1	G	332	ALA	N-CA-C	5.11	119.21	112.92
1	G	204	ASN	N-CA-C	-5.11	106.90	113.23
1	G	305	VAL	N-CA-C	5.11	115.32	108.17
1	A	249	GLU	CA-C-O	5.10	126.18	120.82
1	G	305	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	C	259	VAL	CA-CB-CG2	-5.08	101.76	110.40
1	F	324	ASN	CA-C-N	-5.08	115.56	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	324	ASN	C-N-CA	-5.08	115.56	122.87
1	G	289	VAL	N-CA-C	5.07	115.00	108.82
1	E	171	SER	CB-CA-C	-5.07	102.77	110.88
1	B	184	TYR	OH-CZ-CE2	-5.07	104.71	119.90
1	C	331	ILE	N-CA-C	5.05	117.37	111.05
1	E	150	PHE	CA-CB-CG	-5.05	108.75	113.80
1	B	331	ILE	CB-CA-C	-5.05	104.33	112.16
1	H	317	GLY	N-CA-C	-5.05	108.15	115.27
1	B	278	ASP	CB-CA-C	5.05	118.15	109.82
1	H	203	ASP	CB-CA-C	-5.04	100.98	110.67
1	F	157	GLU	O-C-N	-5.04	116.78	122.12
1	D	292	VAL	N-CA-C	-5.03	108.07	112.90
1	C	251	VAL	CA-C-N	-5.03	113.15	120.29
1	C	251	VAL	C-N-CA	-5.03	113.15	120.29
1	E	174	ASN	N-CA-C	-5.03	105.08	111.11
1	C	125	ASP	N-CA-C	-5.02	106.66	112.89
1	D	331	ILE	O-C-N	5.02	126.94	121.87
1	A	223	HIS	N-CA-C	5.02	118.49	111.56
1	G	153	VAL	CA-C-O	-5.01	115.84	121.05
1	D	139	LYS	N-CA-C	5.01	117.87	110.46

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	154	GLY	Mainchain
1	G	337	TYR	Mainchain

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	1683	0	1583	50	0
1	B	1682	0	1581	68	0
1	C	1678	0	1581	40	0
1	D	1683	0	1583	55	0
1	E	1680	0	1593	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1679	0	1582	57	0
1	G	1669	0	1570	53	0
1	H	1669	0	1570	46	1
2	A	28	0	22	0	0
2	B	28	0	22	0	0
2	C	28	0	22	0	0
2	D	28	0	22	0	0
2	E	28	0	22	1	0
2	F	28	0	22	1	0
2	G	28	0	22	4	0
2	H	28	0	22	1	0
3	A	119	0	0	8	0
3	B	101	0	0	32	0
3	C	97	0	0	10	0
3	D	86	0	0	9	0
3	E	91	0	0	24	0
3	F	97	0	0	18	0
3	G	86	0	0	20	1
3	H	97	0	0	8	0
All	All	14421	0	12819	441	1

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 17.

All (441) 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:126:THR:HB	3:B:543:HOH:O	1.33	1.28
1:B:319:ILE:HG23	3:B:599:HOH:O	1.41	1.21
1:G:171:SER:HA	3:G:535:HOH:O	1.39	1.19
1:G:187:LYS:HE2	3:G:576:HOH:O	1.45	1.17
1:G:238:GLN:HB2	3:G:534:HOH:O	1.51	1.08
1:B:331:ILE:HG22	3:B:586:HOH:O	1.52	1.07
1:E:289[B]:VAL:CG2	1:E:306:LYS:O	2.02	1.07
1:G:272:LYS:HD2	1:H:240:PRO:HB3	1.36	1.04
3:E:532:HOH:O	2:H:401:2EW:H18	1.58	1.03
1:E:289[B]:VAL:HG22	1:E:290:LEU:H	1.18	1.02
1:B:218:MET:SD	3:B:526:HOH:O	2.20	1.00
1:E:153[B]:VAL:HG22	1:E:170:LEU:HB2	1.39	1.00
1:B:237:ILE:HD11	1:B:339:GLU:HG3	1.45	0.98
1:E:195:THR:HA	3:E:520:HOH:O	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289[B]:VAL:HG23	1:E:306:LYS:O	1.66	0.96
1:E:297:LEU:HG	3:E:586:HOH:O	1.66	0.95
1:F:272:LYS:HE3	3:F:589:HOH:O	1.67	0.93
1:H:170:LEU:HD22	3:H:560:HOH:O	1.68	0.93
1:H:199:GLN:HA	1:H:202:ILE:HD12	1.47	0.92
1:D:338:PRO:HD2	3:D:568:HOH:O	1.68	0.92
1:B:134:CYS:SG	1:B:162:LEU:HD21	2.10	0.91
1:E:166:LYS:HA	3:E:516:HOH:O	1.69	0.91
1:H:193:TYR:CD1	3:H:531:HOH:O	2.25	0.90
1:B:181:GLU:HG3	3:B:598:HOH:O	1.71	0.89
1:B:153:VAL:O	1:B:157:GLU:HG3	1.73	0.88
1:F:326:LYS:HB3	3:F:573:HOH:O	1.71	0.88
1:E:272:LYS:HD3	3:E:554:HOH:O	1.75	0.87
1:B:164:THR:HG22	3:B:569:HOH:O	1.75	0.86
1:B:137:GLU:HG3	1:D:284:ASN:HD21	1.40	0.85
1:B:316:GLN:HG3	3:D:564:HOH:O	1.77	0.85
1:B:213:TYR:HE2	3:B:582:HOH:O	1.60	0.84
1:D:134:CYS:SG	1:D:162:LEU:CD1	2.66	0.83
1:B:164:THR:OG1	1:B:166:LYS:HG2	1.80	0.82
1:C:340:ILE:HA	3:C:559:HOH:O	1.79	0.81
1:G:215:TYR:HB2	3:G:580:HOH:O	1.81	0.81
1:D:216:LYS:HB2	3:D:562:HOH:O	1.81	0.81
1:C:269:PHE:HB2	3:C:580:HOH:O	1.78	0.80
1:A:140:TYR:CE2	3:A:560:HOH:O	2.35	0.80
1:B:316:GLN:CG	3:B:534:HOH:O	2.29	0.80
1:B:237:ILE:CD1	1:B:339:GLU:HG3	2.12	0.79
1:B:213:TYR:CE2	3:B:582:HOH:O	2.34	0.79
1:D:235:ARG:CG	1:D:339:GLU:HB2	2.13	0.79
1:E:289[B]:VAL:HG22	1:E:290:LEU:N	1.98	0.78
1:D:235:ARG:HG2	1:D:339:GLU:HB2	1.66	0.78
1:C:225:ASN:OD1	1:C:227:LYS:HG3	1.85	0.77
1:E:237:ILE:HD11	1:E:339:GLU:HG3	1.67	0.77
1:A:327:ASN:O	3:A:579:HOH:O	2.04	0.76
1:H:168:ILE:HD11	1:H:209:ALA:HB2	1.65	0.76
1:F:272:LYS:CE	3:F:589:HOH:O	2.27	0.76
1:E:198:PHE:HD1	3:E:520:HOH:O	1.69	0.76
1:F:198:PHE:HB3	3:F:530:HOH:O	1.86	0.76
1:E:237:ILE:HD13	1:E:337:TYR:CE2	2.21	0.75
1:E:153[B]:VAL:CG2	1:E:170:LEU:HB2	2.15	0.75
1:C:266:SER:HB2	3:C:544:HOH:O	1.85	0.75
1:E:126:THR:HG22	3:E:507:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233[B]:CYS:SG	1:E:338:PRO:HB2	2.27	0.75
1:B:218:MET:HB2	3:B:526:HOH:O	1.86	0.74
1:B:232:THR:HB	3:B:575:HOH:O	1.86	0.74
1:B:134:CYS:SG	1:B:162:LEU:CD2	2.74	0.74
1:G:331:ILE:HG23	3:G:536:HOH:O	1.88	0.74
1:E:289[B]:VAL:HG22	1:E:306:LYS:O	1.86	0.73
1:A:237:ILE:N	1:A:237:ILE:HD12	2.04	0.73
1:B:232:THR:CB	3:B:575:HOH:O	2.35	0.73
1:F:325:ASN:HB3	3:F:516:HOH:O	1.89	0.73
1:D:134:CYS:SG	1:D:162:LEU:HD13	2.30	0.71
1:E:129:TRP:CE2	1:E:255:GLY:HA2	2.26	0.71
1:E:289[B]:VAL:HG21	1:E:305:VAL:CG1	2.19	0.71
1:A:134:CYS:SG	1:A:161:LYS:HG2	2.31	0.71
1:D:173:GLN:NE2	3:D:562:HOH:O	2.24	0.71
1:B:321:MET:SD	3:B:599:HOH:O	2.48	0.71
1:D:163:LYS:HD2	1:D:163:LYS:N	2.04	0.71
1:F:263:ALA:O	1:F:269:PHE:HE1	1.74	0.71
1:H:272:LYS:HD2	3:H:595:HOH:O	1.90	0.70
1:D:218:MET:HE2	3:D:561:HOH:O	1.90	0.70
1:D:271:TYR:CD1	1:D:319:ILE:HG13	2.27	0.70
1:F:338:PRO:HB3	3:F:546:HOH:O	1.91	0.70
1:B:316:GLN:HG3	3:B:534:HOH:O	1.90	0.70
1:B:202:ILE:HD12	3:B:583:HOH:O	1.90	0.69
1:E:161:LYS:HD3	1:E:167:LEU:HB2	1.73	0.69
1:B:237:ILE:HD11	1:B:339:GLU:CG	2.22	0.69
1:F:297:LEU:HA	3:F:541:HOH:O	1.93	0.69
1:F:325:ASN:ND2	3:F:557:HOH:O	2.24	0.69
1:B:305:VAL:HB	3:B:599:HOH:O	1.93	0.68
1:B:235:ARG:HG3	1:B:339:GLU:HB2	1.74	0.68
1:G:272:LYS:HD2	1:H:240:PRO:CB	2.19	0.68
1:A:137:GLU:HG3	1:C:284:ASN:HD21	1.57	0.68
1:A:236:TYR:C	1:A:237:ILE:HD12	2.19	0.67
1:E:166:LYS:HD2	1:E:168:ILE:HD11	1.75	0.67
1:E:266:SER:HA	1:E:269:PHE:CD1	2.30	0.67
1:E:296:THR:HB	3:E:535:HOH:O	1.93	0.67
1:A:263:ALA:O	1:A:269[A]:PHE:HE2	1.78	0.66
1:B:178:CYS:SG	3:B:582:HOH:O	2.53	0.66
1:B:232:THR:HA	3:B:575:HOH:O	1.96	0.66
1:H:193:TYR:HD1	3:H:531:HOH:O	1.69	0.66
3:B:601:HOH:O	1:D:185:GLY:HA2	1.95	0.65
1:E:195:THR:HG22	3:E:520:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:LYS:H	1:G:221:LYS:HD2	1.62	0.65
1:C:340:ILE:CA	3:C:559:HOH:O	2.39	0.65
1:C:218:MET:HE2	1:C:220:GLU:OE1	1.97	0.64
1:F:216:LYS:HD3	1:F:216:LYS:N	2.11	0.64
1:E:198:PHE:CD1	3:E:520:HOH:O	2.45	0.64
1:E:289[B]:VAL:HG21	1:E:305:VAL:HG12	1.80	0.64
1:B:321:MET:HG3	3:B:599:HOH:O	1.99	0.63
1:A:272:LYS:HE3	1:C:196:GLU:OE1	1.98	0.63
1:B:244:GLU:HB3	1:B:303:TRP:HZ2	1.63	0.63
1:E:166:LYS:CD	1:E:168:ILE:HD11	2.29	0.63
1:G:237:ILE:CD1	1:G:339:GLU:HG3	2.29	0.63
1:E:325:ASN:ND2	3:E:547:HOH:O	2.31	0.63
1:B:292:VAL:HG23	1:B:304:LEU:HD23	1.79	0.63
1:G:244:GLU:HG2	3:G:536:HOH:O	1.99	0.63
1:D:292:VAL:HG23	1:D:304:LEU:HD23	1.79	0.62
1:B:232:THR:CA	3:B:575:HOH:O	2.46	0.62
1:E:325:ASN:CG	3:E:552:HOH:O	2.43	0.62
1:H:163:LYS:HB3	3:H:573:HOH:O	1.98	0.62
1:E:297:LEU:CG	3:E:586:HOH:O	2.32	0.61
1:E:129:TRP:CZ2	1:E:255:GLY:HA2	2.36	0.61
1:C:227:LYS:HG2	1:F:182:GLU:O	2.01	0.61
1:E:297:LEU:CB	3:E:586:HOH:O	2.48	0.61
1:G:215:TYR:CB	3:G:580:HOH:O	2.42	0.61
1:H:168:ILE:HD13	1:H:230:ALA:HB1	1.82	0.61
1:E:269:PHE:HB3	1:G:269:PHE:HZ	1.66	0.61
1:D:235:ARG:HG3	1:D:339:GLU:HB2	1.82	0.61
1:G:237:ILE:HD11	1:G:339:GLU:HG3	1.83	0.60
1:F:129:TRP:CE2	1:F:255:GLY:HA2	2.36	0.60
1:G:210:ASP:CB	3:G:535:HOH:O	2.50	0.60
1:A:161:LYS:NZ	1:B:334:TYR:OH	2.31	0.60
1:E:197:ALA:O	1:E:201:ILE:HG13	2.01	0.60
1:B:216:LYS:O	1:B:217:ALA:HB3	2.01	0.59
1:A:137:GLU:HG3	1:C:284:ASN:ND2	2.18	0.59
1:E:127:VAL:HG13	3:E:515:HOH:O	2.03	0.59
1:G:179:SER:C	3:G:568:HOH:O	2.46	0.59
1:D:247:LEU:O	1:D:251:VAL:HG23	2.03	0.59
1:G:210:ASP:HB2	3:G:535:HOH:O	2.01	0.59
1:G:284:ASN:CB	3:G:538:HOH:O	2.50	0.59
1:G:284:ASN:HB3	3:G:538:HOH:O	2.01	0.59
1:F:338:PRO:HA	3:F:546:HOH:O	2.03	0.59
1:G:297:LEU:O	1:G:300:LYS:HG3	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:TYR:C	1:F:216:LYS:HD3	2.29	0.58
1:H:168:ILE:HD11	1:H:209:ALA:CB	2.33	0.58
1:F:236:TYR:C	1:F:237:ILE:HD12	2.28	0.58
1:A:235:ARG:CB	1:A:235:ARG:HH11	2.16	0.58
1:G:168:ILE:HD11	1:G:209:ALA:HB1	1.84	0.58
1:E:130:ARG:CZ	3:E:568:HOH:O	2.52	0.58
1:E:137:GLU:HG3	1:H:284:ASN:ND2	2.19	0.58
1:F:173:GLN:HG2	1:F:214:PRO:O	2.04	0.58
1:A:138:VAL:HG23	3:A:506:HOH:O	2.03	0.57
1:A:235:ARG:HG3	1:A:339:GLU:HG3	1.86	0.57
1:B:224:TYR:HB2	3:B:582:HOH:O	2.03	0.57
1:C:149:ALA:O	1:C:153:VAL:HG22	2.05	0.57
1:D:277:ASP:HA	1:D:328:HIS:CE1	2.39	0.57
1:G:210:ASP:CA	3:G:535:HOH:O	2.52	0.57
1:G:210:ASP:HA	3:G:535:HOH:O	2.04	0.57
1:A:140:TYR:CD2	3:A:560:HOH:O	2.54	0.57
1:C:271:TYR:HE2	3:C:575:HOH:O	1.87	0.57
1:F:223:HIS:HE1	3:F:560:HOH:O	1.86	0.57
1:H:254:LYS:HG3	1:H:337:TYR:CZ	2.40	0.57
1:C:184:TYR:O	1:C:196:GLU:OE1	2.23	0.57
1:F:202:ILE:HD11	3:F:530:HOH:O	2.04	0.57
1:C:284:ASN:HB3	3:C:546:HOH:O	2.04	0.57
1:B:316:GLN:HG2	3:B:534:HOH:O	2.00	0.56
1:D:256:PRO:HB3	1:D:292:VAL:HG12	1.87	0.56
1:E:237:ILE:HD11	1:E:339:GLU:CG	2.34	0.56
1:G:248:LYS:HE3	1:G:294:TYR:CE2	2.39	0.56
1:E:137:GLU:HG3	1:H:284:ASN:HD21	1.69	0.56
1:F:295:GLY:HA3	1:F:302:TYR:CZ	2.40	0.56
1:B:129:TRP:CE2	1:B:255:GLY:HA2	2.40	0.56
1:D:173:GLN:CD	3:D:562:HOH:O	2.48	0.56
1:E:256:PRO:HD2	3:E:529:HOH:O	2.06	0.56
1:B:272:LYS:HD2	3:B:548:HOH:O	2.06	0.55
1:D:128:ASP:HB3	1:D:131:GLU:HG3	1.88	0.55
1:F:338:PRO:CA	3:F:546:HOH:O	2.53	0.55
1:G:277:ASP:OD1	1:G:325:ASN:ND2	2.40	0.55
1:F:249:GLU:OE1	1:F:253:THR:CG2	2.53	0.55
1:G:221:LYS:HD2	1:G:221:LYS:N	2.22	0.55
1:B:126:THR:CB	3:B:543:HOH:O	2.15	0.55
1:C:163:LYS:NZ	1:F:238:GLN:O	2.39	0.55
1:A:187:LYS:HB3	3:A:564:HOH:O	2.06	0.55
1:C:340:ILE:C	3:C:559:HOH:O	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:HG2	1:D:339:GLU:CB	2.37	0.54
1:D:275:VAL:HB	1:D:300:LYS:HD2	1.89	0.54
1:E:289[B]:VAL:CG2	1:E:290:LEU:H	2.03	0.54
1:C:164:THR:O	1:C:166:LYS:HD2	2.07	0.54
1:H:271:TYR:O	1:H:272:LYS:HE3	2.08	0.54
1:E:149:ALA:O	1:E:153[A]:VAL:HG22	2.07	0.54
1:A:187:LYS:HB2	1:A:191:GLY:O	2.08	0.54
1:A:271:TYR:O	1:A:314:GLY:HA2	2.08	0.54
1:F:236:TYR:HB3	3:F:546:HOH:O	2.06	0.54
1:H:268:PHE:CE2	1:H:319:ILE:HD13	2.42	0.54
1:A:269[A]:PHE:H	1:A:269[A]:PHE:HD2	1.55	0.54
1:F:235:ARG:HG2	1:F:339:GLU:HB2	1.89	0.54
1:G:215:TYR:HD2	3:G:580:HOH:O	1.91	0.53
1:B:167:LEU:O	1:B:168:ILE:HG13	2.08	0.53
1:G:271:TYR:CE1	1:G:319:ILE:HG13	2.44	0.53
1:F:233:CYS:SG	3:F:530:HOH:O	2.37	0.53
1:A:214:PRO:HD2	3:A:519:HOH:O	2.07	0.53
1:C:172:ALA:O	1:C:176:VAL:HG23	2.09	0.53
1:G:168:ILE:HD11	1:G:209:ALA:CB	2.38	0.53
1:D:271:TYR:CG	1:D:319:ILE:HG13	2.43	0.52
1:A:269[B]:PHE:CG	1:A:269[B]:PHE:O	2.62	0.52
1:H:225:ASN:HB3	1:H:228:ASN:HD22	1.75	0.52
1:C:163:LYS:CE	1:F:238:GLN:O	2.57	0.52
1:E:226:SER:C	1:E:228:ASN:H	2.18	0.52
1:G:193:TYR:CZ	2:G:401:2EW:H12	2.44	0.52
1:E:161:LYS:HA	1:E:166:LYS:O	2.10	0.52
1:A:269[B]:PHE:HD2	1:A:309:TRP:CZ3	2.27	0.52
1:B:234:SER:C	1:B:235:ARG:HG2	2.33	0.52
1:B:319:ILE:CA	3:B:513:HOH:O	2.56	0.52
1:G:179:SER:CA	3:G:568:HOH:O	2.58	0.52
1:B:202:ILE:CD1	3:B:583:HOH:O	2.54	0.52
1:E:146:ALA:O	1:E:147:CYS:C	2.51	0.52
1:H:160:LEU:HD13	1:H:231:ALA:CB	2.40	0.52
1:D:245:ASP:HB3	3:D:543:HOH:O	2.10	0.51
1:D:301:ASP:HB2	1:D:323:ARG:O	2.10	0.51
1:F:338:PRO:CB	3:F:546:HOH:O	2.53	0.51
1:C:256:PRO:HD2	3:C:519:HOH:O	2.09	0.51
1:C:200:TYR:CD1	1:C:200:TYR:C	2.88	0.51
1:C:133:GLY:O	1:C:167:LEU:HD13	2.09	0.51
1:A:269[B]:PHE:CD2	1:A:309:TRP:CZ3	2.98	0.51
1:B:147:CYS:HB2	1:B:288:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:CYS:HB2	1:F:288:GLY:O	2.10	0.51
1:D:134:CYS:SG	1:D:162:LEU:HD11	2.48	0.51
1:B:237:ILE:HD12	1:B:237:ILE:N	2.26	0.51
1:A:263:ALA:O	1:A:269[A]:PHE:CE2	2.61	0.51
1:D:227:LYS:HD2	1:E:183:LYS:O	2.11	0.51
1:B:235:ARG:NH2	3:B:541:HOH:O	2.44	0.50
1:B:235:ARG:HB2	3:B:528:HOH:O	2.10	0.50
1:D:237:ILE:O	1:D:336[B]:SER:HA	2.12	0.50
1:F:256:PRO:HA	1:F:291:VAL:O	2.12	0.50
1:A:269[A]:PHE:N	1:A:269[A]:PHE:CD2	2.79	0.50
1:E:304:LEU:HD21	3:E:568:HOH:O	2.11	0.50
1:G:173:GLN:HB2	3:G:580:HOH:O	2.12	0.50
1:E:221:LYS:HE3	3:E:584:HOH:O	2.12	0.50
1:F:184:TYR:HE2	1:F:199:GLN:HG2	1.77	0.49
1:F:249:GLU:OE1	1:F:253:THR:HG23	2.11	0.49
1:H:166:LYS:O	1:H:166:LYS:HG3	2.11	0.49
1:D:123:LEU:HD13	1:D:249:GLU:HA	1.94	0.49
1:G:160:LEU:HD23	1:G:168:ILE:HG22	1.94	0.49
1:A:237:ILE:N	1:A:237:ILE:CD1	2.69	0.49
1:A:239:LEU:HD12	1:A:335:CYS:HB3	1.94	0.49
1:D:174:ASN:C	1:D:174:ASN:HD22	2.19	0.49
1:A:269[B]:PHE:HD2	1:A:309:TRP:HZ3	1.60	0.49
1:B:319:ILE:C	3:B:513:HOH:O	2.55	0.49
1:H:159:GLN:HB3	3:H:589:HOH:O	2.12	0.49
1:H:163:LYS:HD2	1:H:340:ILE:HB	1.94	0.49
1:B:326:LYS:HE2	1:B:326:LYS:O	2.13	0.49
1:G:179:SER:O	1:G:186:ASN:HB2	2.12	0.49
1:A:129:TRP:CE2	1:A:255:GLY:HA2	2.48	0.49
1:E:123:LEU:HD11	1:E:249:GLU:OE1	2.13	0.49
1:A:214:PRO:HG2	1:A:216:LYS:HE2	1.93	0.48
1:B:183:LYS:HE2	1:B:203:ASP:OD1	2.13	0.48
1:C:224:TYR:HE1	1:C:226[B]:SER:HG	1.60	0.48
1:G:123:LEU:HD21	1:G:249:GLU:OE1	2.12	0.48
1:G:179:SER:HA	3:G:568:HOH:O	2.13	0.48
1:E:241:PHE:CD1	1:E:241:PHE:C	2.90	0.48
1:F:254:LYS:HG3	1:F:337:TYR:CZ	2.49	0.48
1:F:250:ALA:O	1:F:254:LYS:HB2	2.14	0.48
1:H:254:LYS:HG3	1:H:337:TYR:CE2	2.49	0.48
1:A:269[A]:PHE:HD2	1:A:269[A]:PHE:N	2.10	0.48
1:D:206:GLY:HA3	1:D:229:ARG:HG3	1.94	0.48
1:D:153:VAL:O	1:D:157:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:237:ILE:HD13	1:H:337:TYR:CE2	2.49	0.47
1:B:316:GLN:NE2	1:D:193:TYR:OH	2.47	0.47
1:E:237:ILE:CD1	1:E:339:GLU:CG	2.92	0.47
1:E:312:ASN:HB2	3:E:510:HOH:O	2.14	0.47
1:H:235:ARG:NH1	3:H:550:HOH:O	2.45	0.47
1:A:153:VAL:O	1:A:157:GLU:HG3	2.14	0.47
1:A:239:LEU:HB2	1:A:335:CYS:HB2	1.96	0.47
2:G:401:2EW:H1	2:G:401:2EW:H13	1.61	0.47
1:H:160:LEU:HD13	1:H:231:ALA:HB2	1.96	0.47
1:E:128:ASP:OD2	1:E:130:ARG:HB2	2.14	0.47
1:A:237:ILE:HD11	1:A:339:GLU:HG3	1.96	0.47
1:G:331:ILE:CG2	3:G:536:HOH:O	2.55	0.47
1:A:216:LYS:O	1:A:217:ALA:HB3	2.14	0.46
1:E:207:ILE:HG22	1:E:231:ALA:HB3	1.97	0.46
1:F:237:ILE:HD12	1:F:237:ILE:N	2.29	0.46
1:G:154:GLY:HA3	1:G:290:LEU:HD22	1.97	0.46
1:C:175:LEU:HD13	1:C:197:ALA:HB1	1.96	0.46
1:E:328:HIS:O	1:E:329:CYS:HB2	2.16	0.46
1:F:278:ASP:OD2	1:F:280:SER:HB2	2.14	0.46
1:B:146:ALA:O	1:B:147:CYS:C	2.57	0.46
1:C:340:ILE:OXT	3:C:559:HOH:O	2.20	0.46
1:G:271:TYR:CD1	1:G:319:ILE:HG13	2.49	0.46
1:A:285:VAL:HG21	1:A:334:TYR:HD1	1.80	0.46
2:F:401:2EW:H13	2:F:401:2EW:H1	1.66	0.46
1:D:147:CYS:HB2	1:D:288:GLY:O	2.15	0.46
1:E:127:VAL:O	1:E:293:GLY:HA3	2.16	0.46
1:E:289[B]:VAL:CG2	1:E:305:VAL:CG1	2.90	0.46
1:F:196:GLU:O	1:F:199:GLN:HB3	2.16	0.46
1:G:272:LYS:HE2	1:G:272:LYS:HB2	1.57	0.46
1:E:239:LEU:HB3	1:E:240:PRO:HD2	1.97	0.46
1:G:303:TRP:CE2	1:G:323:ARG:HG3	2.50	0.46
1:B:316:GLN:CD	1:D:193:TYR:OH	2.59	0.46
1:C:237:ILE:N	1:C:237:ILE:HD12	2.31	0.46
1:D:278:ASP:HA	1:D:279:PRO:HD2	1.87	0.46
1:F:173:GLN:HB2	1:F:215:TYR:HA	1.96	0.46
1:F:216:LYS:O	1:F:218:MET:HG3	2.17	0.46
1:H:309:TRP:O	3:H:546:HOH:O	2.21	0.46
1:H:319:ILE:HD13	1:H:319:ILE:HG21	1.74	0.46
1:B:319:ILE:N	3:B:513:HOH:O	2.49	0.45
1:C:160:LEU:HD23	3:C:504:HOH:O	2.16	0.45
1:G:297:LEU:O	1:G:300:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LEU:O	1:B:240:PRO:C	2.58	0.45
1:H:328:HIS:CE1	1:H:329:CYS:SG	3.09	0.45
1:D:237:ILE:O	1:D:336[A]:SER:HA	2.16	0.45
1:H:202:ILE:HA	1:H:233:CYS:O	2.17	0.45
1:A:248:LYS:HE3	1:A:294:TYR:CE2	2.52	0.45
1:C:211:ALA:HB1	1:E:340:ILE:HG21	1.99	0.45
1:D:254:LYS:HA	1:D:254:LYS:HD3	1.84	0.45
1:A:235:ARG:NH1	1:A:235:ARG:HB2	2.32	0.45
1:A:265:HIS:O	1:A:269[A]:PHE:CD2	2.70	0.45
1:E:155:ALA:HB1	1:E:338:PRO:HD3	1.97	0.45
1:F:282:THR:CG2	3:F:579:HOH:O	2.64	0.45
1:A:290:LEU:HD22	3:A:618:HOH:O	2.16	0.45
1:D:196:GLU:HA	1:D:196:GLU:OE2	2.16	0.45
1:E:237:ILE:HD13	1:E:337:TYR:HE2	1.79	0.45
1:F:322:ALA:HB1	1:F:325:ASN:HD22	1.81	0.45
1:C:277:ASP:O	1:C:278:ASP:C	2.58	0.45
1:C:278:ASP:HA	1:C:279:PRO:HD2	1.56	0.45
1:D:237:ILE:HD13	1:D:337:TYR:CE2	2.52	0.45
1:B:237:ILE:CD1	1:B:339:GLU:CG	2.86	0.44
1:F:249:GLU:OE1	1:F:253:THR:HG21	2.17	0.44
1:E:160:LEU:O	1:E:161:LYS:C	2.57	0.44
1:A:285:VAL:HG21	1:A:334:TYR:CD1	2.52	0.44
1:C:136:THR:HG21	1:C:169:SER:HA	1.99	0.44
1:E:170:LEU:HD23	1:E:170:LEU:HA	1.81	0.44
1:C:229:ARG:NH2	1:F:199:GLN:OE1	2.50	0.44
1:E:289[B]:VAL:HG11	1:E:305:VAL:HG11	1.99	0.44
1:F:170:LEU:HA	1:F:170:LEU:HD23	1.60	0.44
1:G:193:TYR:OH	2:G:401:2EW:H12	2.17	0.44
1:H:332:ALA:HA	1:H:335:CYS:SG	2.57	0.44
1:B:235:ARG:HG3	1:B:235:ARG:NH1	2.33	0.44
1:C:272:LYS:CD	1:D:240:PRO:HB3	2.47	0.44
1:E:271:TYR:CD1	1:E:271:TYR:C	2.96	0.44
1:C:241:PHE:CD1	1:C:241:PHE:C	2.95	0.44
1:D:266:SER:HA	1:D:269[A]:PHE:CD1	2.52	0.44
1:E:167:LEU:N	3:E:516:HOH:O	2.45	0.44
1:E:171:SER:OG	1:E:174:ASN:HB2	2.17	0.44
1:G:235:ARG:HB2	3:G:533:HOH:O	2.18	0.44
1:F:297:LEU:HD13	3:F:541:HOH:O	2.17	0.44
1:G:200:TYR:CD1	1:G:200:TYR:C	2.95	0.44
1:B:316:GLN:CD	1:D:193:TYR:CZ	2.96	0.44
1:F:122:THR:HB	1:F:123:LEU:H	1.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:THR:CG2	3:E:520:HOH:O	2.62	0.44
1:A:148:TRP:O	1:A:194:MET:HG3	2.18	0.43
1:A:235:ARG:HD3	1:A:339:GLU:OE1	2.17	0.43
1:E:159:GLN:HG3	1:E:338:PRO:O	2.18	0.43
1:G:123:LEU:HA	1:G:124:PRO:HD2	1.76	0.43
1:H:195:THR:HG21	1:H:238:GLN:OE1	2.18	0.43
1:H:289:VAL:HG21	1:H:305:VAL:HG11	2.00	0.43
1:D:332:ALA:HA	1:D:335:CYS:SG	2.59	0.43
1:E:137:GLU:CD	1:E:137:GLU:H	2.26	0.43
1:H:148:TRP:H	1:H:148:TRP:CD1	2.34	0.43
1:A:235:ARG:CB	1:A:235:ARG:NH1	2.81	0.43
1:C:271:TYR:O	1:C:314:GLY:HA2	2.17	0.43
1:F:202:ILE:CD1	3:F:530:HOH:O	2.66	0.43
1:D:288:GLY:C	1:D:289:VAL:HG13	2.43	0.43
1:E:289[B]:VAL:CG2	1:E:290:LEU:N	2.71	0.43
1:G:148:TRP:CD1	1:G:148:TRP:H	2.36	0.43
1:H:278:ASP:HA	1:H:279:PRO:HD2	1.71	0.43
1:A:147:CYS:HB3	1:A:287:HIS:CE1	2.54	0.43
1:B:239:LEU:HB2	1:B:335:CYS:HB2	2.01	0.43
1:F:129:TRP:O	1:F:134[B]:CYS:HB2	2.18	0.43
1:G:320:ARG:HG3	1:G:320:ARG:HH11	1.83	0.43
1:H:216:LYS:HA	1:H:216:LYS:HD2	1.63	0.43
1:E:305:VAL:HB	1:E:319:ILE:HG23	2.01	0.43
1:H:129:TRP:CZ3	1:H:162:LEU:HD21	2.54	0.43
1:B:161:LYS:NZ	1:B:165:GLY:O	2.50	0.42
1:D:277:ASP:C	1:D:328:HIS:CE1	2.97	0.42
1:D:309:TRP:HE3	1:D:313:PHE:CD2	2.37	0.42
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.81	0.42
1:E:127:VAL:HG21	1:E:252:ALA:HA	2.01	0.42
1:E:178:CYS:HB3	1:E:200:TYR:OH	2.19	0.42
1:E:226:SER:C	1:E:228:ASN:N	2.76	0.42
1:A:183:LYS:HG2	1:A:184:TYR:CE1	2.54	0.42
1:E:127:VAL:HG12	1:E:128:ASP:N	2.33	0.42
1:E:312:ASN:ND2	3:E:565:HOH:O	2.35	0.42
1:F:269:PHE:N	1:F:269:PHE:CD1	2.88	0.42
1:A:235:ARG:HH11	1:A:235:ARG:HB3	1.85	0.42
1:B:332:ALA:HA	1:B:335:CYS:SG	2.60	0.42
1:H:195:THR:CG2	1:H:238:GLN:OE1	2.67	0.42
1:E:229:ARG:HD2	1:E:232:THR:HG23	2.02	0.42
1:E:269:PHE:CD1	1:G:269:PHE:HE2	2.37	0.42
1:E:326:LYS:O	1:E:327:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:TYR:CE2	2:G:401:2EW:H4	2.55	0.42
1:H:271:TYR:O	1:H:314:GLY:HA2	2.20	0.42
1:B:321:MET:CG	3:B:599:HOH:O	2.58	0.42
1:E:216:LYS:O	1:E:217:ALA:HB3	2.20	0.42
1:F:151:SER:HB3	1:F:194:MET:HG2	2.02	0.42
1:A:321:MET:O	1:A:322:ALA:C	2.62	0.42
1:F:149:ALA:O	1:F:153:VAL:HG22	2.20	0.42
1:A:265:HIS:HD2	3:A:527:HOH:O	2.02	0.42
1:A:239:LEU:HD12	1:A:335:CYS:CB	2.50	0.41
1:F:184:TYR:CE2	1:F:199:GLN:HG2	2.55	0.41
1:F:247:LEU:O	1:F:251:VAL:HG23	2.20	0.41
1:E:237:ILE:O	1:E:336:SER:HA	2.19	0.41
1:B:134:CYS:SG	1:B:162:LEU:HD23	2.58	0.41
1:C:189:CYS:SG	1:C:218:MET:HA	2.61	0.41
1:E:153[B]:VAL:CG2	1:E:170:LEU:CB	2.93	0.41
1:H:150:PHE:HA	1:H:153:VAL:HG22	2.02	0.41
1:H:241:PHE:CD1	1:H:241:PHE:C	2.98	0.41
1:C:247:LEU:O	1:C:251:VAL:HG23	2.20	0.41
1:H:168:ILE:HG23	1:H:168:ILE:O	2.21	0.41
1:C:302:TYR:CD2	1:C:302:TYR:C	2.98	0.41
1:D:123:LEU:O	1:D:124:PRO:C	2.62	0.41
1:D:130:ARG:HD3	1:D:318:TYR:CZ	2.56	0.41
1:D:241:PHE:C	1:D:241:PHE:CD1	2.97	0.41
1:H:200:TYR:O	1:H:201:ILE:C	2.63	0.41
1:B:197:ALA:O	1:B:201:ILE:HG13	2.20	0.41
1:H:160:LEU:O	1:H:164:THR:OG1	2.36	0.41
1:C:194:MET:HG2	1:C:258:SER:HB3	2.02	0.41
1:D:202:ILE:HG22	3:D:533:HOH:O	2.21	0.41
1:E:173:GLN:HB2	1:E:215:TYR:HA	2.03	0.41
1:F:129:TRP:CZ2	1:F:255:GLY:HA2	2.55	0.41
1:F:277:ASP:HA	1:F:328:HIS:CE1	2.54	0.41
1:B:228:ASN:O	1:B:229:ARG:C	2.62	0.41
1:D:307:ASN:ND2	1:D:309:TRP:CE3	2.89	0.41
1:E:193:TYR:CZ	2:E:401:2EW:H12	2.56	0.41
1:F:146:ALA:O	1:F:147:CYS:C	2.64	0.41
1:F:272:LYS:HA	1:F:272:LYS:HD2	1.93	0.41
1:H:171:SER:OG	1:H:174:ASN:HB2	2.21	0.41
1:B:134:CYS:HA	1:B:161:LYS:HG2	2.02	0.41
1:C:184:TYR:O	1:C:196:GLU:HG3	2.21	0.41
1:G:168:ILE:O	1:G:168:ILE:HG23	2.19	0.41
1:B:137:GLU:HG3	1:D:284:ASN:ND2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:LEU:HD23	1:D:303:TRP:CZ2	2.56	0.40
1:E:201:ILE:O	1:E:201:ILE:HG22	2.21	0.40
1:G:237:ILE:O	1:G:336:SER:HA	2.22	0.40
1:E:130:ARG:NH2	3:E:568:HOH:O	2.53	0.40
1:E:194:MET:HG2	1:E:258:SER:HB3	2.02	0.40
1:E:237:ILE:CD1	1:E:339:GLU:HG2	2.51	0.40
1:G:288:GLY:C	1:G:289:VAL:HG13	2.44	0.40
1:H:138:VAL:HB	1:H:311:LEU:HD23	2.04	0.40
1:H:149:ALA:O	1:H:153:VAL:HG22	2.21	0.40
1:B:129:TRP:CZ2	1:B:255:GLY:HA2	2.55	0.40
1:D:277:ASP:O	1:D:278:ASP:C	2.64	0.40
1:E:290:LEU:HD12	1:E:290:LEU:HA	2.00	0.40
1:D:310:GLY:HA2	3:D:571:HOH:O	2.21	0.40
1:F:194:MET:HE2	1:F:194:MET:HB2	2.00	0.40
1:G:177:ASP:HB3	1:G:222:CYS:HA	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:312:ASN:OD1	3:G:534:HOH:O[1_655]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/225 (97%)	207 (95%)	11 (5%)	0	100	100
1	B	218/225 (97%)	207 (95%)	11 (5%)	0	100	100
1	C	218/225 (97%)	203 (93%)	13 (6%)	2 (1%)	14	3
1	D	218/225 (97%)	206 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	219/225 (97%)	207 (94%)	10 (5%)	2 (1%)	14	3
1	F	218/225 (97%)	206 (94%)	12 (6%)	0	100	100
1	G	216/225 (96%)	207 (96%)	9 (4%)	0	100	100
1	H	216/225 (96%)	204 (94%)	12 (6%)	0	100	100
All	All	1741/1800 (97%)	1647 (95%)	90 (5%)	4 (0%)	43	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	GLU
1	E	286	ASN
1	C	329	CYS
1	E	145	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	177/182 (97%)	160 (90%)	17 (10%)	8	0
1	B	177/182 (97%)	169 (96%)	8 (4%)	24	3
1	C	177/182 (97%)	172 (97%)	5 (3%)	38	10
1	D	177/182 (97%)	169 (96%)	8 (4%)	24	3
1	E	178/182 (98%)	171 (96%)	7 (4%)	28	5
1	F	177/182 (97%)	168 (95%)	9 (5%)	21	2
1	G	175/182 (96%)	168 (96%)	7 (4%)	28	4
1	H	175/182 (96%)	165 (94%)	10 (6%)	18	2
All	All	1413/1456 (97%)	1342 (95%)	71 (5%)	22	3

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	168	ILE
1	A	174	ASN
1	A	181	GLU
1	A	183	LYS
1	A	218	MET
1	A	227	LYS
1	A	235	ARG
1	A	237	ILE
1	A	256	PRO
1	A	269[A]	PHE
1	A	269[B]	PHE
1	A	272	LYS
1	A	281	CYS
1	A	292	VAL
1	A	312	ASN
1	A	326	LYS
1	B	166	LYS
1	B	181	GLU
1	B	235	ARG
1	B	245	ASP
1	B	272	LYS
1	B	273	SER
1	B	281	CYS
1	B	326	LYS
1	C	166	LYS
1	C	229	ARG
1	C	280	SER
1	C	281	CYS
1	C	340	ILE
1	D	161	LYS
1	D	162	LEU
1	D	163	LYS
1	D	234	SER
1	D	280	SER
1	D	281	CYS
1	D	298	ASP
1	D	300	LYS
1	E	132	LYS
1	E	182	GLU
1	E	229	ARG
1	E	232	THR
1	E	254	LYS

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Mol	Chain	Res	Type
1	E	272	LYS
1	E	340	ILE
1	F	122	THR
1	F	163	LYS
1	F	181	GLU
1	F	225	ASN
1	F	227	LYS
1	F	281	CYS
1	F	297	LEU
1	F	300	LYS
1	F	340	ILE
1	G	168	ILE
1	G	181	GLU
1	G	221	LYS
1	G	227	LYS
1	G	249	GLU
1	G	281	CYS
1	G	300	LYS
1	H	123	LEU
1	H	163	LYS
1	H	181	GLU
1	H	183	LYS
1	H	216	LYS
1	H	218	MET
1	H	249	GLU
1	H	272	LYS
1	H	281	CYS
1	H	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	238	GLN
1	A	284	ASN
1	A	312	ASN
1	B	141	GLN
1	B	312	ASN
1	B	316	GLN
1	C	199	GLN
1	C	238	GLN
1	C	284	ASN

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Mol	Chain	Res	Type
1	D	238	GLN
1	D	284	ASN
1	E	159	GLN
1	E	325	ASN
1	F	223	HIS
1	F	225	ASN
1	F	265	HIS
1	F	312	ASN
1	F	325	ASN
1	F	328	HIS
1	G	180	ASN
1	G	316	GLN
1	H	223	HIS
1	H	228	ASN
1	H	284	ASN
1	H	316	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2EW	A	401	1	29,30,30	1.21	2 (6%)	35,42,42	2.41	16 (45%)
2	2EW	B	401	1	29,30,30	1.91	8 (27%)	35,42,42	2.74	17 (48%)
2	2EW	F	401	1	29,30,30	1.37	4 (13%)	35,42,42	3.55	11 (31%)
2	2EW	D	401	1	29,30,30	1.62	8 (27%)	35,42,42	2.79	19 (54%)
2	2EW	G	401	1	29,30,30	2.14	6 (20%)	35,42,42	2.03	12 (34%)
2	2EW	C	401	1	29,30,30	1.54	5 (17%)	35,42,42	3.71	15 (42%)
2	2EW	H	401	1	29,30,30	1.64	3 (10%)	35,42,42	3.38	14 (40%)
2	2EW	E	401	1	29,30,30	1.69	3 (10%)	35,42,42	2.72	20 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2EW	A	401	1	-	3/27/48/48	0/3/3/3
2	2EW	B	401	1	-	2/27/48/48	0/3/3/3
2	2EW	F	401	1	-	2/27/48/48	0/3/3/3
2	2EW	D	401	1	-	2/27/48/48	0/3/3/3
2	2EW	G	401	1	-	2/27/48/48	0/3/3/3
2	2EW	C	401	1	-	2/27/48/48	0/3/3/3
2	2EW	H	401	1	-	3/27/48/48	0/3/3/3
2	2EW	E	401	1	-	4/27/48/48	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	2EW	O11-S1	-7.94	1.35	1.43
2	H	401	2EW	O11-S1	-6.11	1.37	1.43
2	B	401	2EW	O12-S1	6.04	1.50	1.43
2	E	401	2EW	S1-N2	5.12	1.70	1.63
2	G	401	2EW	O12-S1	-4.80	1.38	1.43
2	E	401	2EW	O12-S1	-4.61	1.38	1.43
2	A	401	2EW	C19-N8	4.01	1.54	1.47
2	B	401	2EW	O11-S1	3.98	1.47	1.43
2	C	401	2EW	C25-C13	3.75	1.44	1.38
2	D	401	2EW	C9-N17	3.68	1.42	1.33
2	B	401	2EW	S1-N2	3.42	1.68	1.63
2	E	401	2EW	O11-S1	3.39	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	2EW	C5-N8	3.39	1.39	1.35
2	C	401	2EW	C9-N17	3.32	1.41	1.33
2	C	401	2EW	C6-N2	3.05	1.51	1.48
2	G	401	2EW	C7-N2	-3.01	1.45	1.48
2	G	401	2EW	C13-S1	2.98	1.80	1.76
2	F	401	2EW	O12-S1	-2.96	1.40	1.43
2	D	401	2EW	S1-N2	2.72	1.67	1.63
2	D	401	2EW	C6-C3	2.66	1.58	1.53
2	F	401	2EW	C13-S1	2.64	1.80	1.76
2	D	401	2EW	O11-S1	2.63	1.46	1.43
2	H	401	2EW	S1-N2	2.60	1.67	1.63
2	G	401	2EW	C19-N8	2.60	1.51	1.47
2	D	401	2EW	O12-S1	2.56	1.46	1.43
2	C	401	2EW	S1-N2	2.45	1.66	1.63
2	D	401	2EW	O16-C9	2.32	1.27	1.23
2	C	401	2EW	O12-S1	-2.32	1.41	1.43
2	A	401	2EW	C20-N8	2.31	1.51	1.47
2	B	401	2EW	C28-C27	2.18	1.43	1.38
2	D	401	2EW	C7-N2	2.16	1.50	1.48
2	B	401	2EW	C19-N8	2.15	1.50	1.47
2	D	401	2EW	C6-N2	-2.13	1.46	1.48
2	F	401	2EW	C9-N17	2.12	1.38	1.33
2	B	401	2EW	C13-S1	-2.12	1.73	1.76
2	B	401	2EW	C6-N2	2.09	1.50	1.48
2	G	401	2EW	C5-N8	2.07	1.38	1.35
2	F	401	2EW	C7-N2	-2.04	1.46	1.48
2	B	401	2EW	C20-N8	2.00	1.50	1.47

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	2EW	C13-S1-N2	-11.45	93.45	107.28
2	C	401	2EW	O12-S1-O11	10.59	136.11	119.59
2	C	401	2EW	O12-S1-N2	-10.42	96.87	106.69
2	F	401	2EW	O11-S1-N2	10.06	116.16	106.69
2	H	401	2EW	O12-S1-O11	9.89	135.02	119.59
2	C	401	2EW	O12-S1-C13	-9.84	95.87	108.10
2	H	401	2EW	O11-S1-C13	-9.09	96.80	108.10
2	H	401	2EW	O12-S1-N2	-8.87	98.33	106.69
2	F	401	2EW	C24-C13-S1	7.82	127.50	119.73
2	B	401	2EW	O11-S1-N2	-7.01	100.08	106.69
2	D	401	2EW	O12-S1-N2	-6.84	100.24	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	2EW	O12-S1-N2	-6.80	100.28	106.69
2	E	401	2EW	C13-S1-N2	-6.34	99.63	107.28
2	E	401	2EW	O12-S1-N2	-6.24	100.81	106.69
2	D	401	2EW	C28-C27-C24	-6.07	112.75	120.24
2	B	401	2EW	C13-S1-N2	-6.06	99.97	107.28
2	F	401	2EW	C25-C13-S1	-5.85	113.93	119.73
2	D	401	2EW	O12-S1-O11	5.26	127.80	119.59
2	F	401	2EW	O12-S1-C13	-5.26	101.56	108.10
2	C	401	2EW	O18-C22-C20	-5.21	100.54	111.77
2	A	401	2EW	O12-S1-O11	4.93	127.29	119.59
2	B	401	2EW	O12-S1-N2	4.92	111.31	106.69
2	C	401	2EW	C13-S1-N2	-4.79	101.50	107.28
2	C	401	2EW	O15-C5-N8	-4.75	115.94	121.61
2	H	401	2EW	C23-O18-C22	4.61	124.79	109.88
2	B	401	2EW	C7-N2-S1	-4.60	112.57	119.59
2	G	401	2EW	O11-S1-C13	-4.59	102.40	108.10
2	E	401	2EW	O11-S1-N2	4.44	110.87	106.69
2	B	401	2EW	C20-N8-C19	4.38	121.61	112.68
2	D	401	2EW	C27-C24-C13	4.15	123.19	118.95
2	H	401	2EW	C13-S1-N2	-4.10	102.33	107.28
2	B	401	2EW	O16-C9-C4	-4.02	116.86	121.67
2	E	401	2EW	O12-S1-C13	4.00	113.07	108.10
2	F	401	2EW	C20-N8-C19	3.91	120.65	112.68
2	D	401	2EW	C26-C25-C13	-3.90	114.96	118.95
2	E	401	2EW	C7-N2-S1	-3.90	113.64	119.59
2	F	401	2EW	C7-N2-S1	-3.79	113.81	119.59
2	A	401	2EW	C24-C13-S1	-3.75	116.01	119.73
2	D	401	2EW	C27-C28-C26	3.68	124.91	119.87
2	C	401	2EW	O11-S1-N2	3.67	110.14	106.69
2	D	401	2EW	C13-S1-N2	-3.63	102.89	107.28
2	G	401	2EW	O12-S1-O11	3.62	125.24	119.59
2	C	401	2EW	C27-C28-C26	3.61	124.81	119.87
2	E	401	2EW	C3-C6-N2	3.59	108.70	102.93
2	H	401	2EW	O15-C5-N8	-3.55	117.38	121.61
2	D	401	2EW	C7-N2-S1	-3.52	114.21	119.59
2	G	401	2EW	O12-S1-N2	3.52	110.00	106.69
2	A	401	2EW	O15-C5-C3	-3.44	115.77	121.85
2	A	401	2EW	C20-N8-C19	3.41	119.63	112.68
2	D	401	2EW	C3-C6-N2	3.40	108.40	102.93
2	E	401	2EW	C28-C26-C25	3.31	124.33	120.24
2	G	401	2EW	C20-N8-C19	3.30	119.41	112.68
2	E	401	2EW	C23-C19-N8	-3.29	102.88	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	2EW	C27-C28-C26	3.27	124.35	119.87
2	H	401	2EW	C28-C27-C24	-3.23	116.26	120.24
2	G	401	2EW	O12-S1-C13	-3.21	104.11	108.10
2	B	401	2EW	C23-C19-N8	-3.21	103.05	109.82
2	A	401	2EW	C3-C6-N2	3.17	108.03	102.93
2	G	401	2EW	O15-C5-N8	-3.13	117.88	121.61
2	D	401	2EW	C4-C7-N2	3.06	107.85	102.93
2	E	401	2EW	C20-N8-C19	3.05	118.90	112.68
2	H	401	2EW	O18-C22-C20	-3.05	105.21	111.77
2	H	401	2EW	C20-N8-C19	3.04	118.88	112.68
2	G	401	2EW	C27-C24-C13	3.02	122.03	118.95
2	F	401	2EW	C3-C6-N2	3.01	107.78	102.93
2	B	401	2EW	C27-C28-C26	-3.01	115.75	119.87
2	H	401	2EW	O11-S1-N2	3.01	109.52	106.69
2	G	401	2EW	C6-N2-S1	-2.99	115.03	119.59
2	D	401	2EW	C23-O18-C22	2.98	119.52	109.88
2	B	401	2EW	C7-C4-C3	-2.96	98.72	104.11
2	E	401	2EW	O16-C9-N17	2.93	129.18	122.98
2	H	401	2EW	O18-C23-C19	2.91	118.04	111.77
2	E	401	2EW	O16-C9-C4	-2.84	118.27	121.67
2	D	401	2EW	C7-C4-C3	-2.83	98.96	104.11
2	B	401	2EW	O12-S1-C13	2.83	111.62	108.10
2	B	401	2EW	C4-C7-N2	2.81	107.45	102.93
2	D	401	2EW	O15-C5-C3	-2.76	116.97	121.85
2	B	401	2EW	C6-N2-S1	-2.76	115.39	119.59
2	D	401	2EW	C25-C13-S1	-2.74	117.01	119.73
2	A	401	2EW	C23-O18-C22	2.74	118.72	109.88
2	E	401	2EW	C22-C20-N8	2.69	115.48	109.82
2	C	401	2EW	O18-C23-C19	-2.67	106.01	111.77
2	C	401	2EW	C25-C13-C24	2.64	123.90	120.47
2	A	401	2EW	C23-C19-N8	-2.62	104.30	109.82
2	A	401	2EW	C13-S1-N2	-2.62	104.11	107.28
2	F	401	2EW	O18-C22-C20	-2.60	106.16	111.77
2	B	401	2EW	C27-C24-C13	2.59	121.59	118.95
2	C	401	2EW	C28-C26-C25	-2.58	117.05	120.24
2	A	401	2EW	O12-S1-C13	2.57	111.30	108.10
2	F	401	2EW	O12-S1-O11	2.53	123.54	119.59
2	A	401	2EW	C25-C13-C24	2.53	123.77	120.47
2	E	401	2EW	C26-C25-C13	-2.53	116.36	118.95
2	E	401	2EW	C27-C24-C13	2.52	121.53	118.95
2	B	401	2EW	O15-C5-N8	2.52	124.62	121.61
2	H	401	2EW	O12-S1-C13	2.50	111.21	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	2EW	C13-S1-N2	-2.50	104.26	107.28
2	G	401	2EW	C28-C27-C24	-2.50	117.16	120.24
2	E	401	2EW	C4-C9-N17	-2.49	112.49	116.29
2	C	401	2EW	C25-C13-S1	-2.45	117.30	119.73
2	D	401	2EW	C20-N8-C19	2.45	117.67	112.68
2	C	401	2EW	C23-O18-C22	2.39	117.62	109.88
2	C	401	2EW	O11-S1-C13	2.38	111.07	108.10
2	A	401	2EW	O11-S1-N2	-2.37	104.45	106.69
2	H	401	2EW	C27-C24-C13	2.31	121.31	118.95
2	A	401	2EW	C7-C4-C3	-2.24	100.03	104.11
2	E	401	2EW	C23-O18-C22	2.23	117.10	109.88
2	E	401	2EW	C25-C13-S1	2.23	121.94	119.73
2	D	401	2EW	C25-C13-C24	2.22	123.36	120.47
2	E	401	2EW	C7-N2-C6	-2.20	105.42	109.62
2	F	401	2EW	C22-C20-N8	-2.19	105.21	109.82
2	B	401	2EW	C20-N8-C5	-2.17	115.17	123.30
2	C	401	2EW	C4-C7-N2	-2.14	99.49	102.93
2	D	401	2EW	O11-S1-N2	2.13	108.69	106.69
2	A	401	2EW	C28-C26-C25	-2.11	117.64	120.24
2	E	401	2EW	O18-C22-C20	-2.10	107.24	111.77
2	B	401	2EW	O15-C5-C3	-2.10	118.14	121.85
2	B	401	2EW	C28-C26-C25	2.10	122.82	120.24
2	H	401	2EW	C27-C28-C26	2.08	122.72	119.87
2	D	401	2EW	C7-N2-C6	-2.07	105.67	109.62
2	D	401	2EW	O16-C9-C4	-2.07	119.19	121.67
2	E	401	2EW	C28-C27-C24	-2.03	117.73	120.24
2	G	401	2EW	C7-N2-S1	-2.03	116.50	119.59
2	A	401	2EW	C28-C27-C24	-2.03	117.74	120.24
2	G	401	2EW	C4-C9-N17	-2.02	113.21	116.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	2EW	C7-N2-S1-C13
2	B	401	2EW	C7-N2-S1-O12
2	F	401	2EW	C7-N2-S1-O12
2	H	401	2EW	C7-N2-S1-O12
2	A	401	2EW	C7-N2-S1-O12
2	A	401	2EW	C7-N2-S1-C13
2	B	401	2EW	C7-N2-S1-C13
2	C	401	2EW	C7-N2-S1-O12

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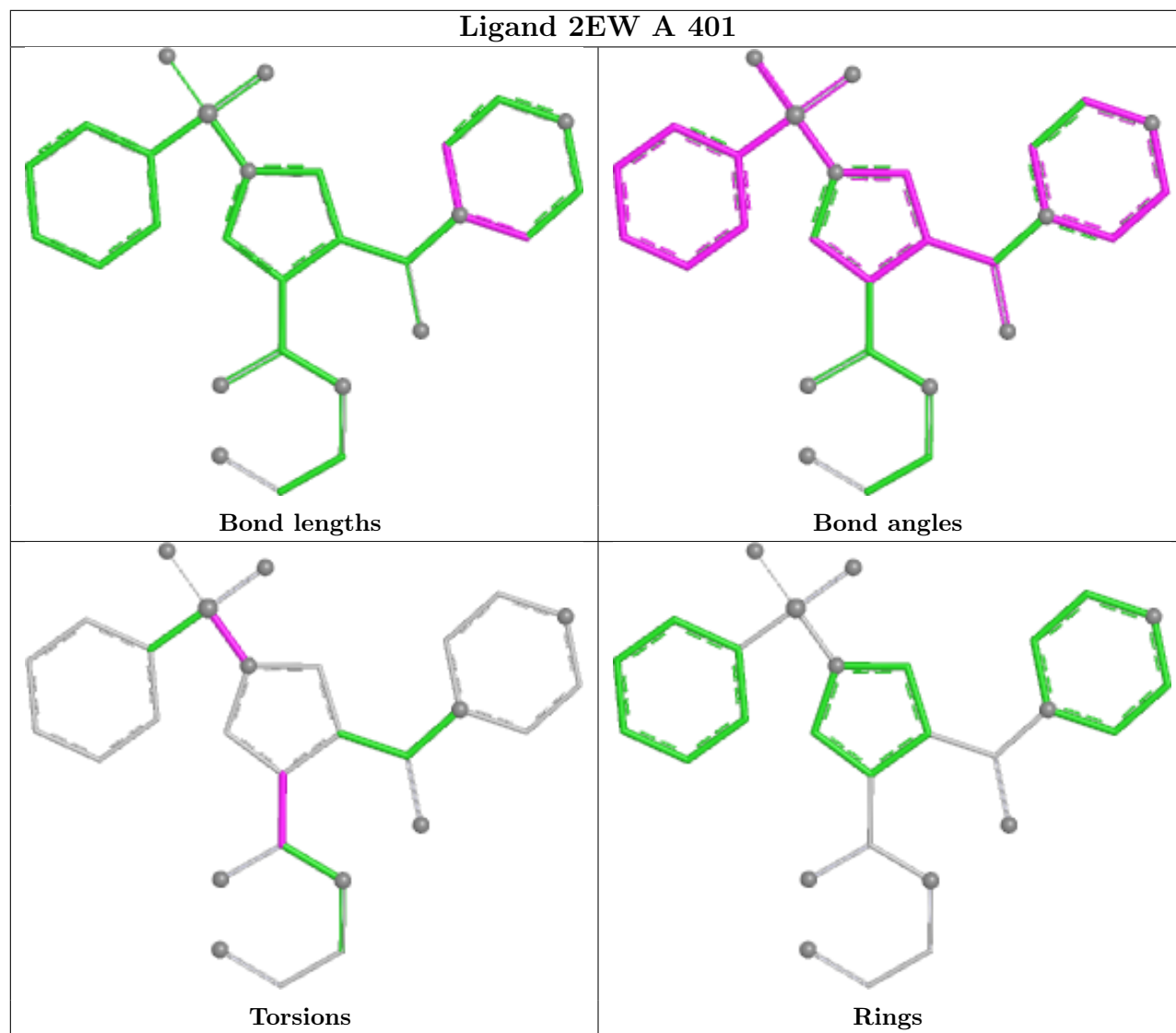
Mol	Chain	Res	Type	Atoms
2	D	401	2EW	C7-N2-S1-O12
2	G	401	2EW	C7-N2-S1-O12
2	G	401	2EW	C7-N2-S1-C13
2	H	401	2EW	C7-N2-S1-C13
2	C	401	2EW	C7-N2-S1-C13
2	D	401	2EW	C7-N2-S1-C13
2	F	401	2EW	C7-N2-S1-C13
2	E	401	2EW	C7-N2-S1-O12
2	E	401	2EW	C14-C21-N17-C9
2	E	401	2EW	C7-N2-S1-O11
2	A	401	2EW	C3-C4-C9-O16
2	H	401	2EW	C4-C3-C5-N8

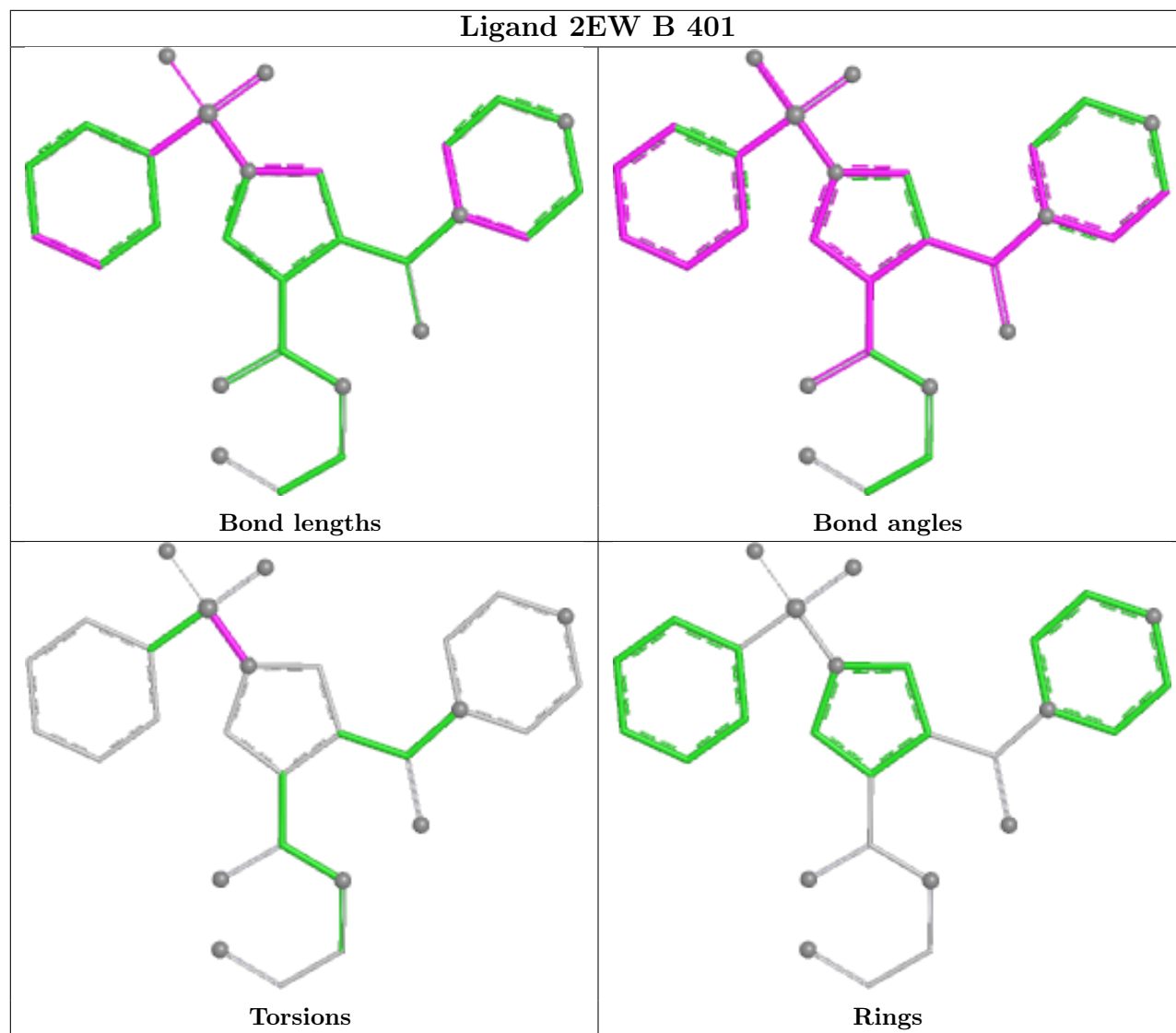
There are no ring outliers.

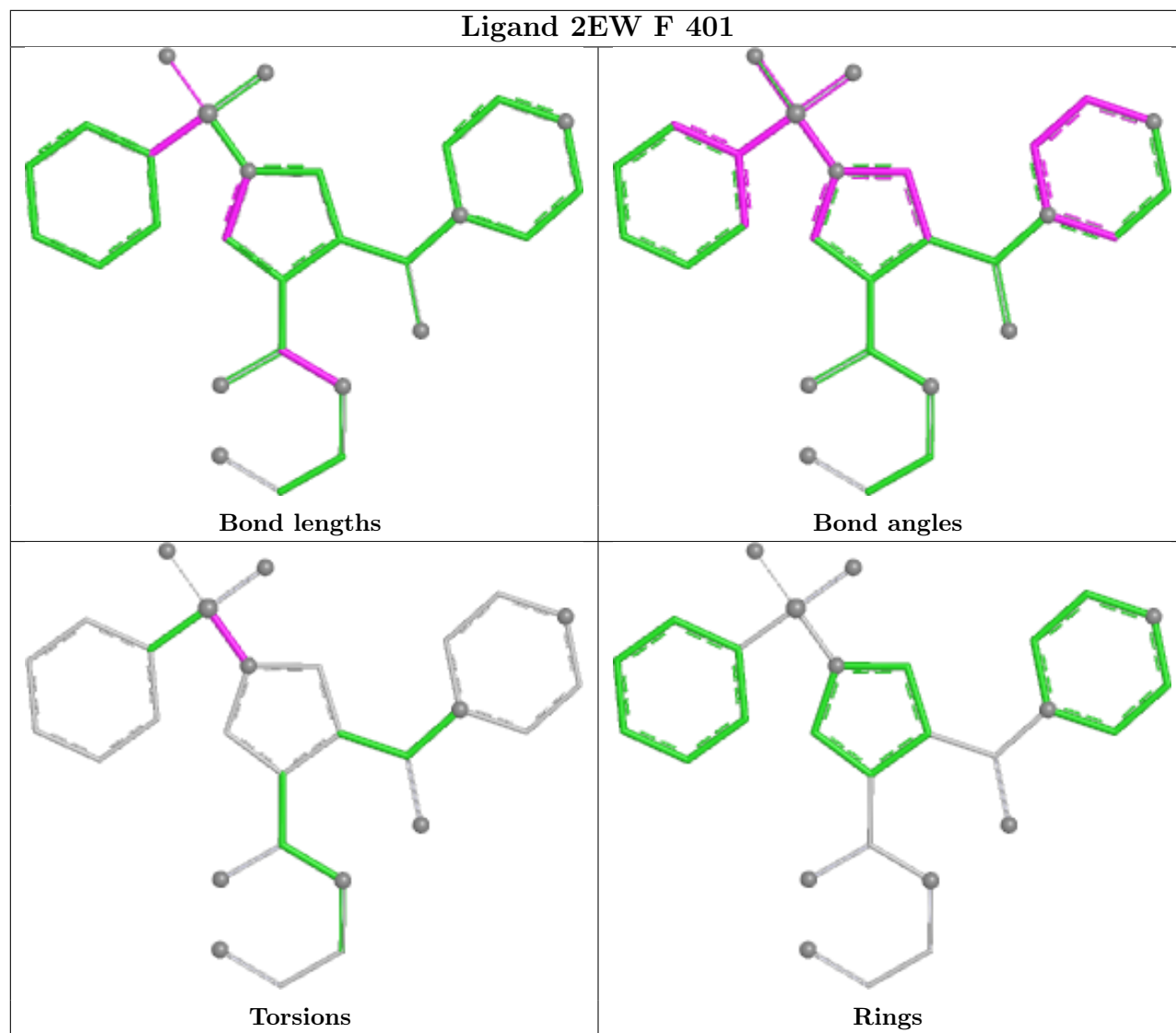
4 monomers are involved in 7 short contacts:

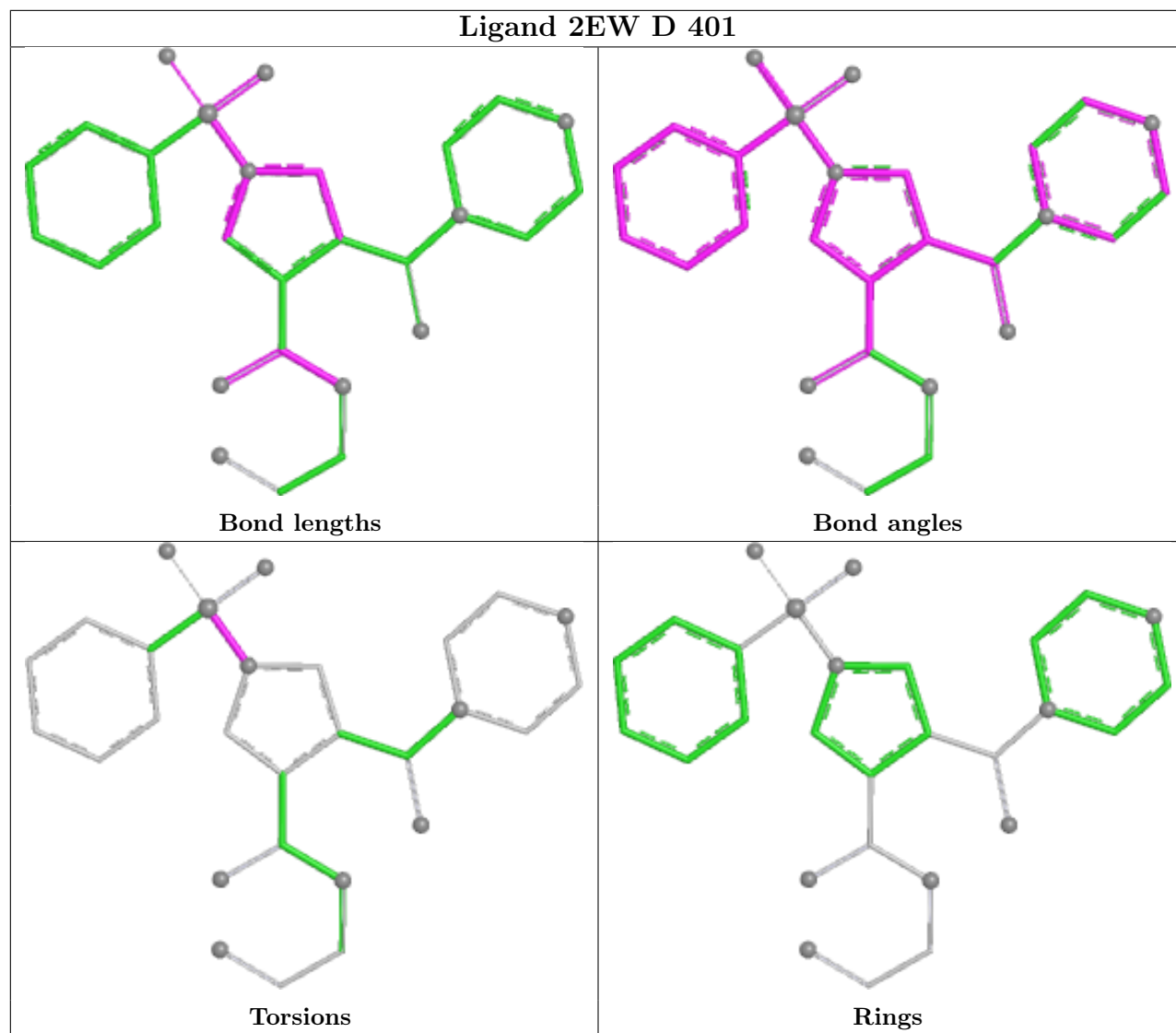
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	2EW	1	0
2	G	401	2EW	4	0
2	H	401	2EW	1	0
2	E	401	2EW	1	0

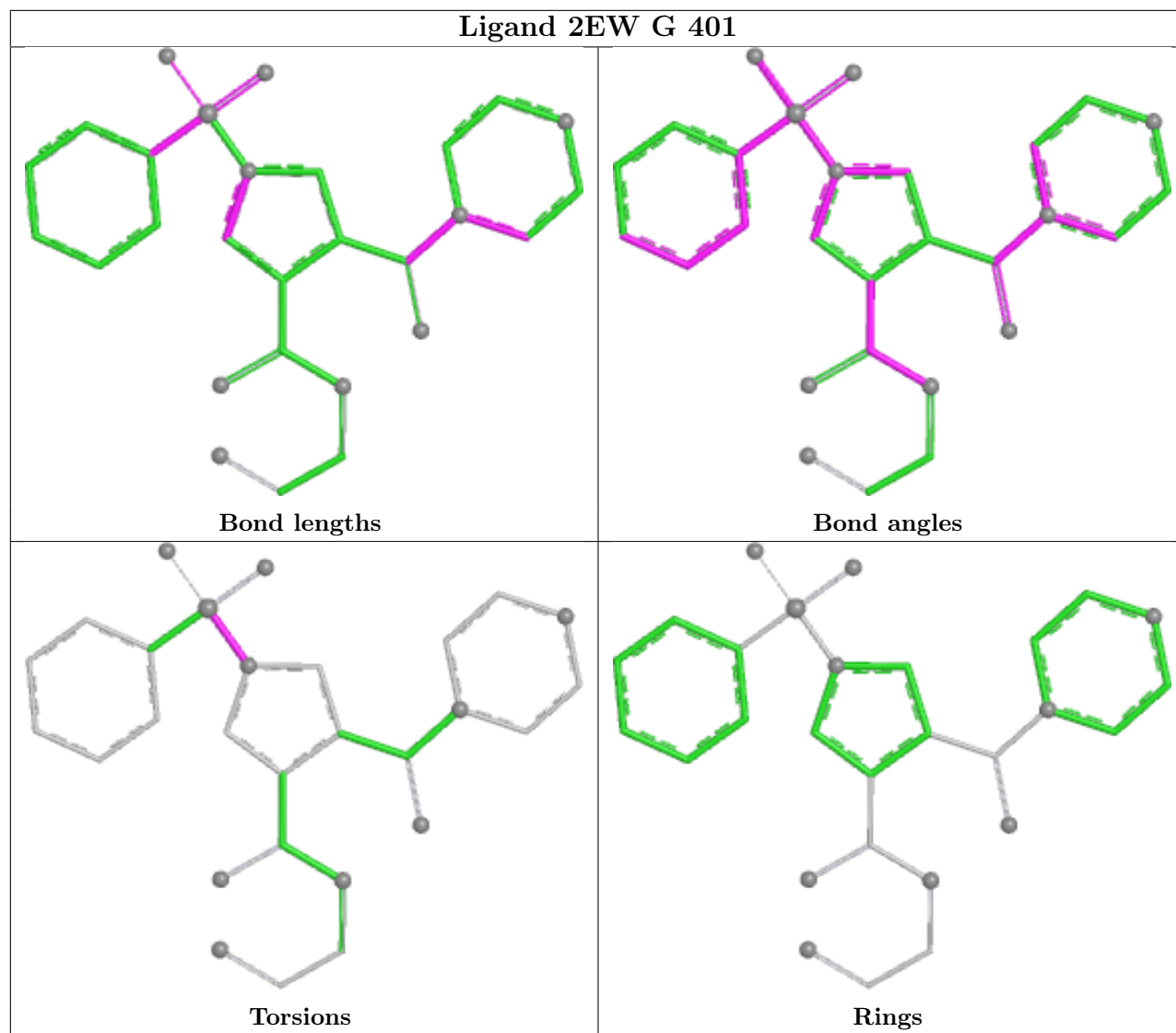
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

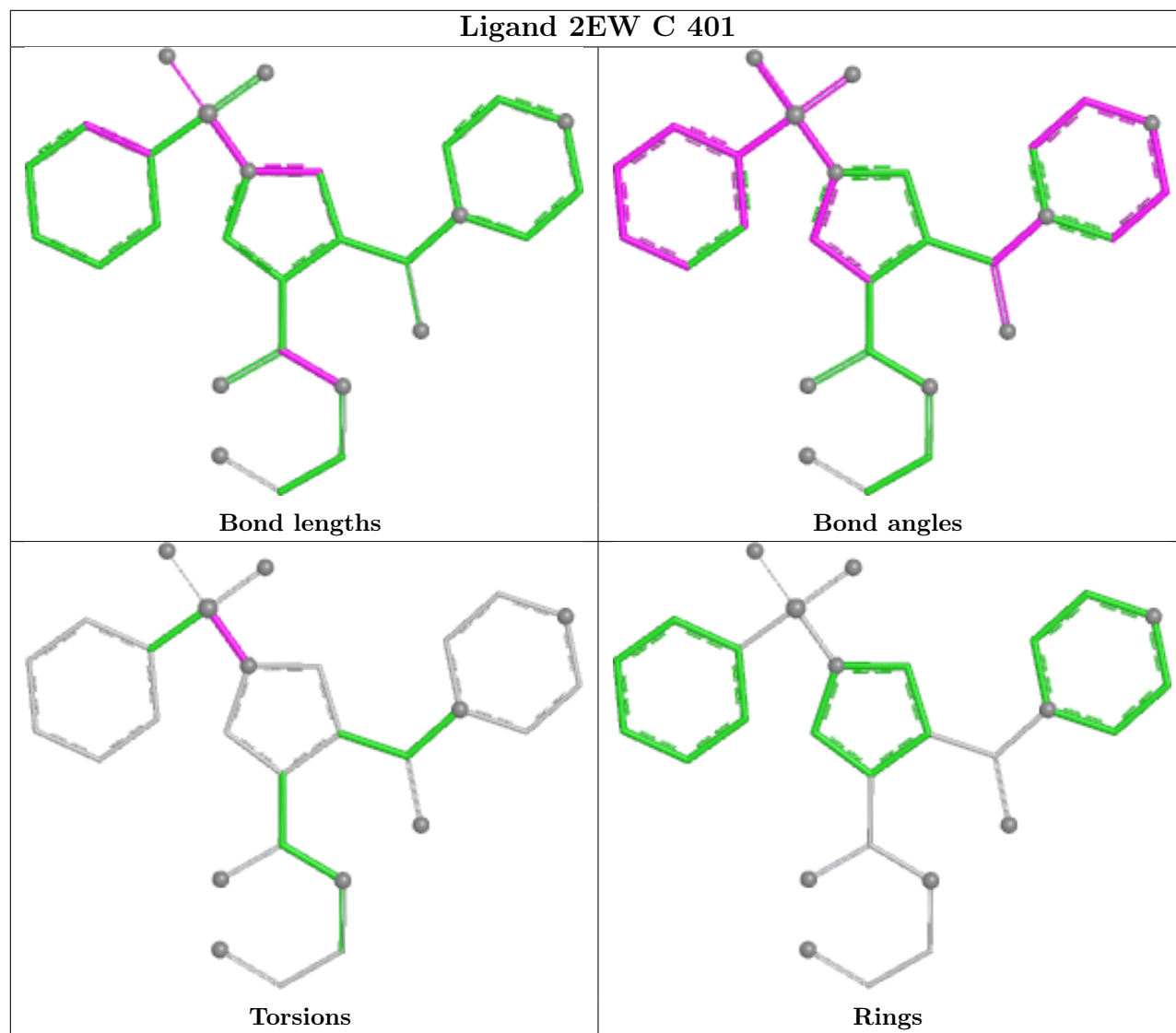


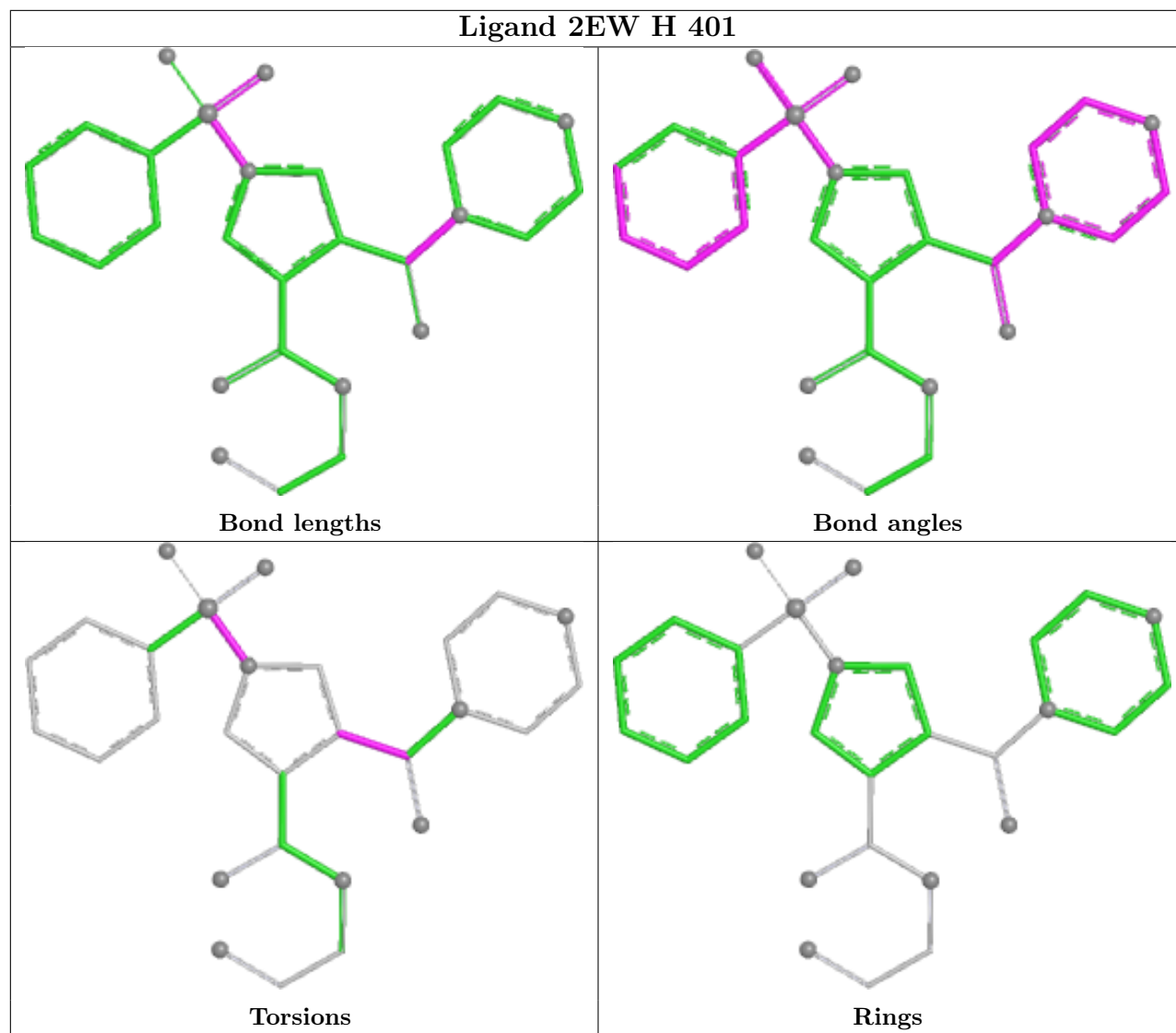


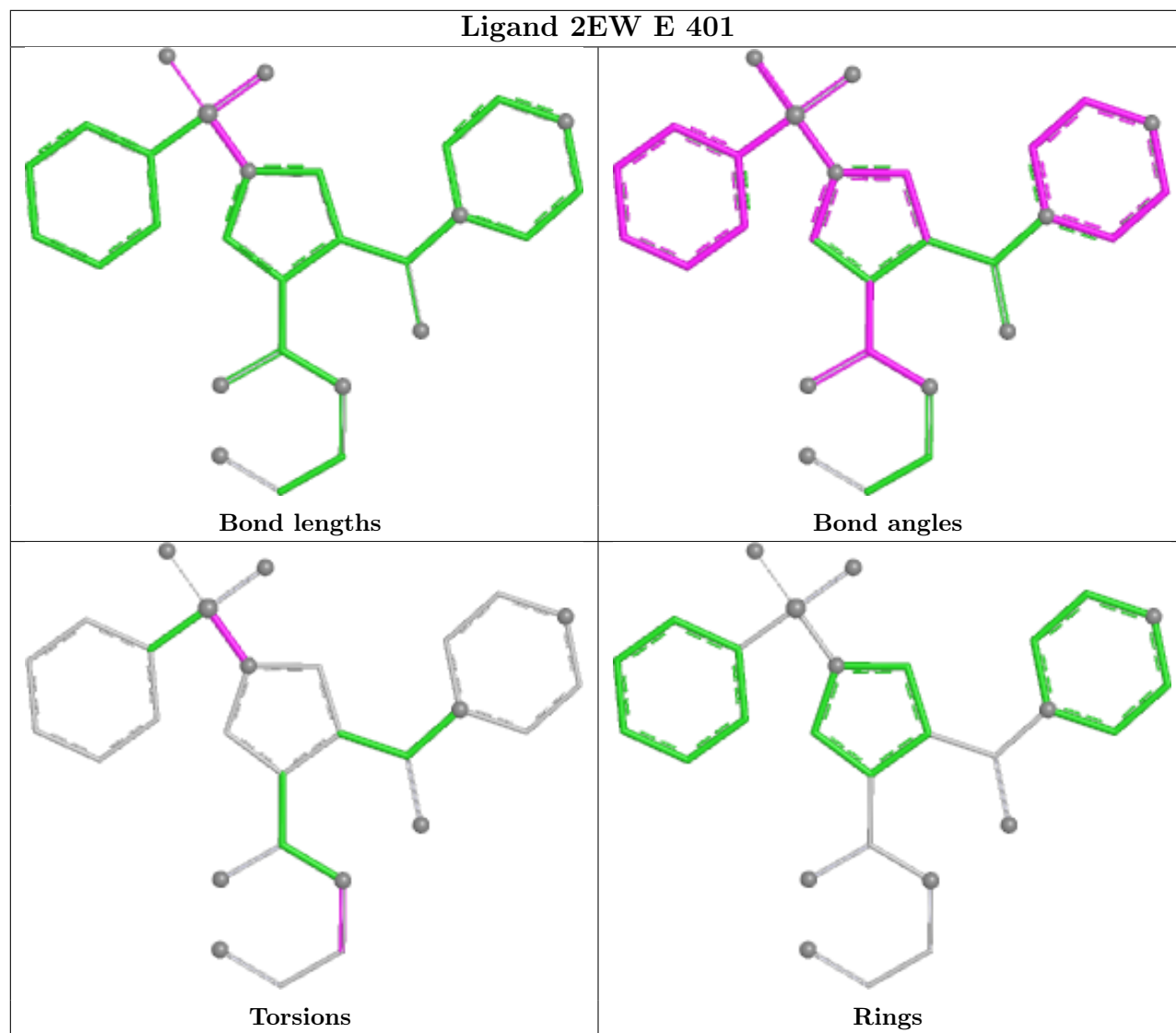












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	218/225 (96%)	-0.46	0 100 100	7, 15, 22, 31	17 (7%)
1	B	219/225 (97%)	-0.32	0 100 100	5, 16, 24, 38	17 (7%)
1	C	218/225 (96%)	-0.45	0 100 100	8, 15, 22, 35	17 (7%)
1	D	218/225 (96%)	-0.41	0 100 100	8, 16, 27, 38	17 (7%)
1	E	218/225 (96%)	-0.22	0 100 100	7, 17, 26, 32	18 (8%)
1	F	219/225 (97%)	-0.42	1 (0%) 87 90	9, 15, 22, 30	17 (7%)
1	G	218/225 (96%)	-0.54	0 100 100	8, 14, 21, 30	15 (6%)
1	H	218/225 (96%)	-0.36	0 100 100	10, 17, 27, 33	15 (6%)
All	All	1746/1800 (97%)	-0.40	1 (0%) 92 92	5, 16, 24, 38	133 (7%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	122	THR	2.2

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.

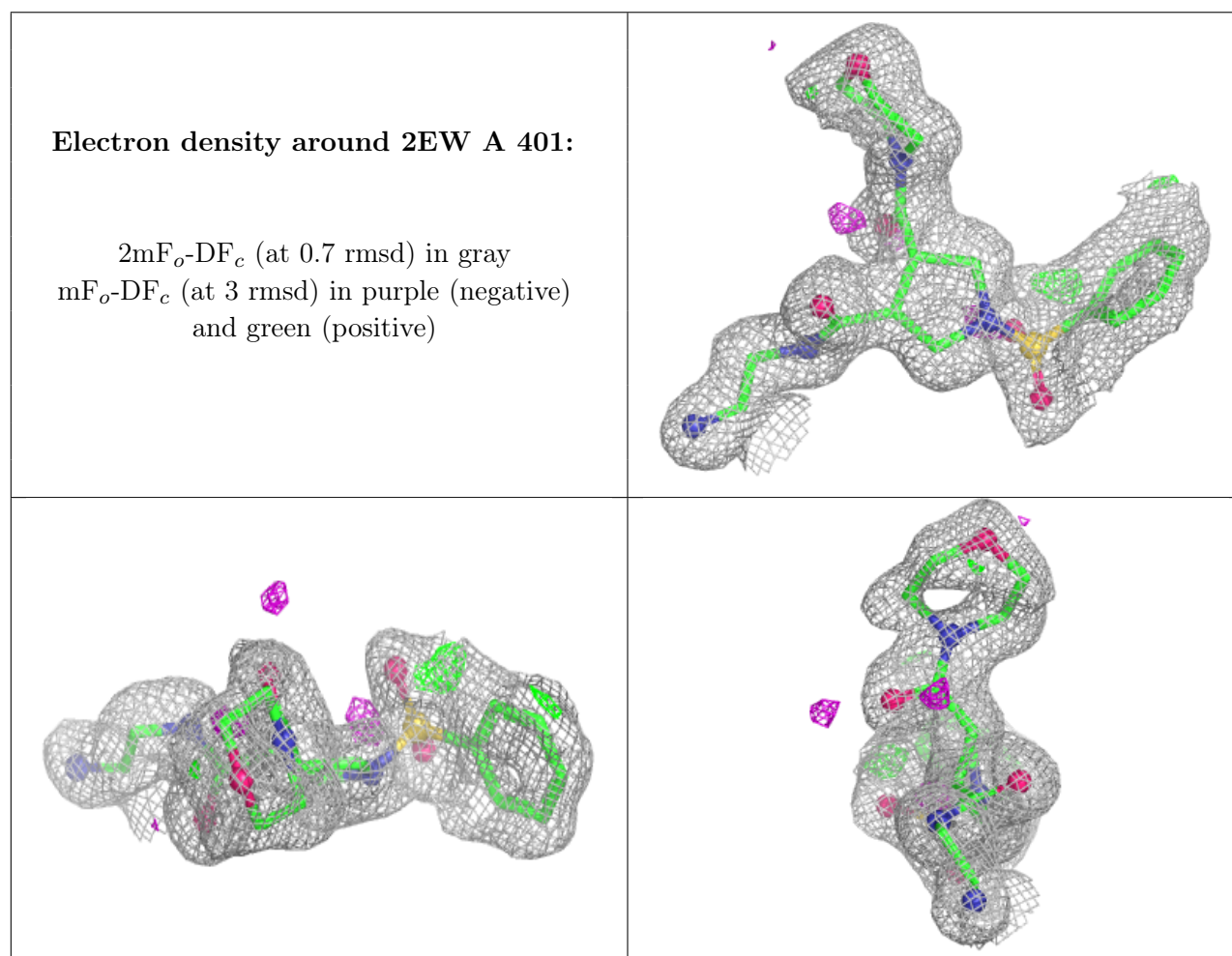
6.4 Ligands [i](#)

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.

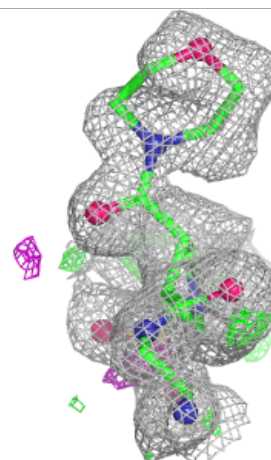
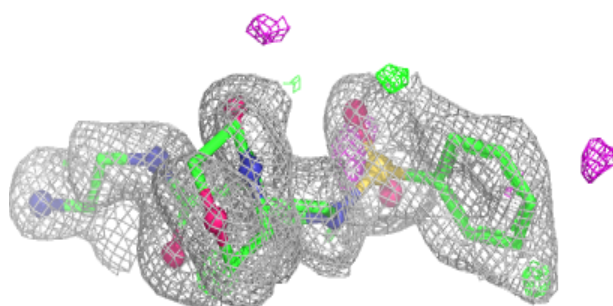
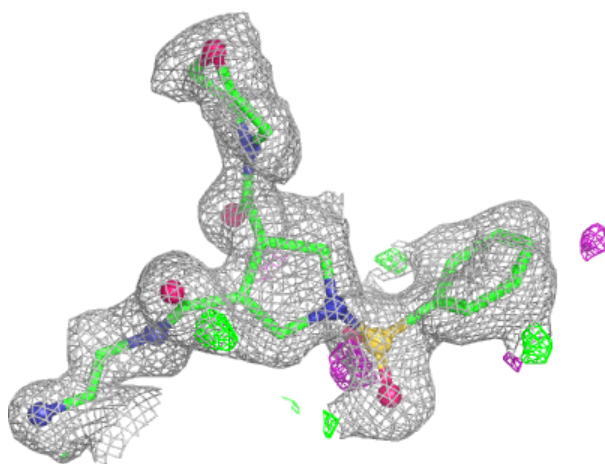
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	2EW	A	401	28/28	0.97	0.06	12,18,21,22	0
2	2EW	E	401	28/28	0.97	0.06	12,21,26,27	0
2	2EW	C	401	28/28	0.98	0.04	11,15,20,23	0
2	2EW	D	401	28/28	0.98	0.05	9,17,24,26	0
2	2EW	B	401	28/28	0.98	0.05	12,17,23,26	0
2	2EW	F	401	28/28	0.98	0.06	13,20,24,26	0
2	2EW	G	401	28/28	0.98	0.05	11,17,23,24	0
2	2EW	H	401	28/28	0.98	0.06	15,19,23,25	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.



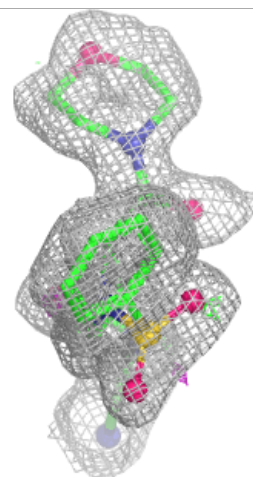
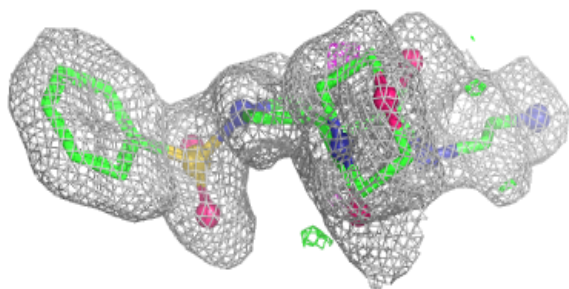
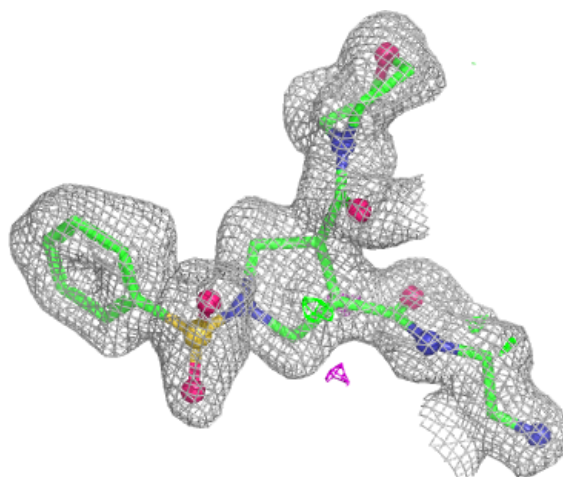
Electron density around 2EW E 401:

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



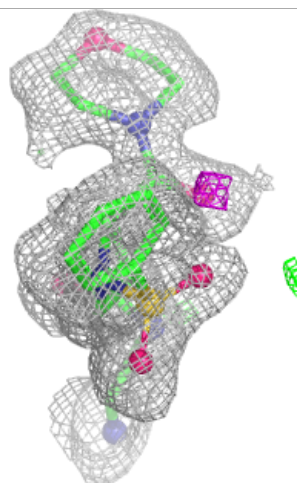
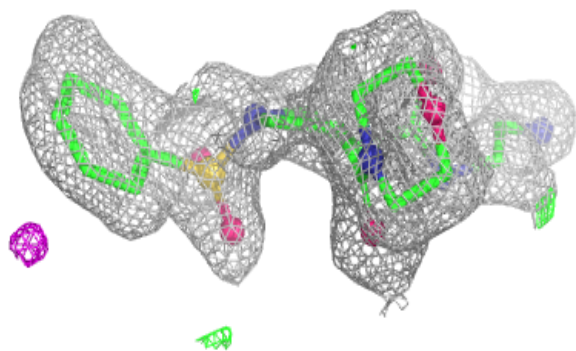
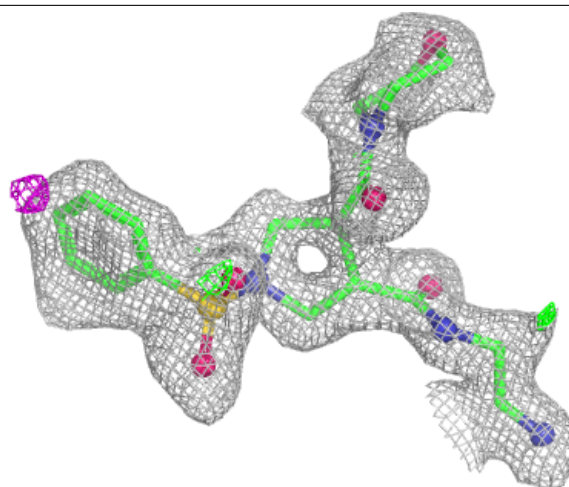
Electron density around 2EW C 401:

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



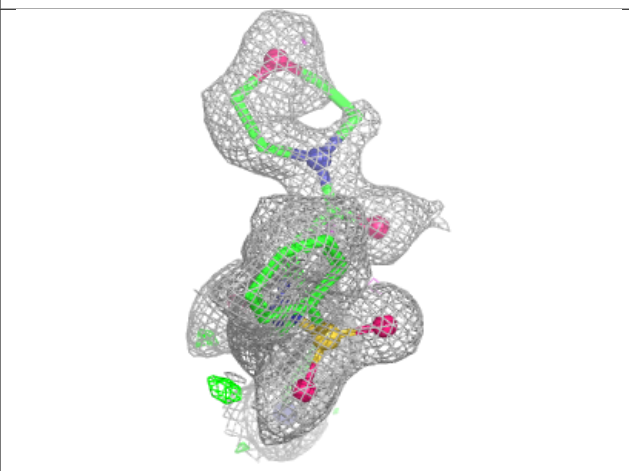
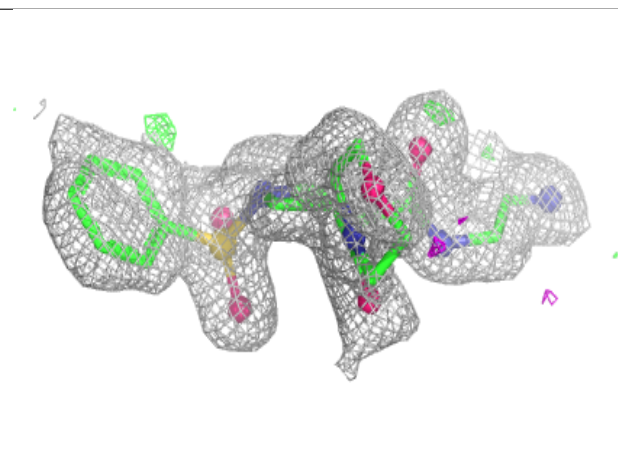
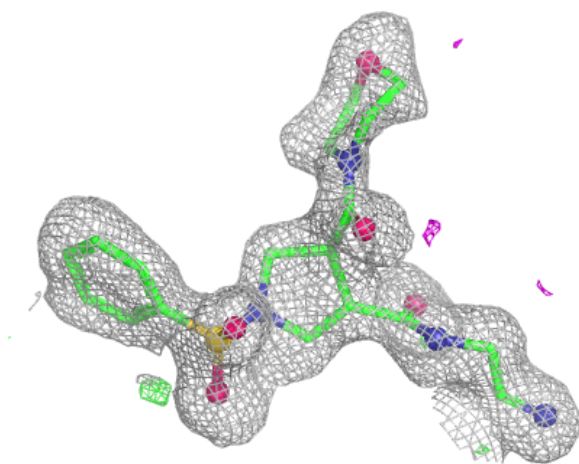
Electron density around 2EW D 401:

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



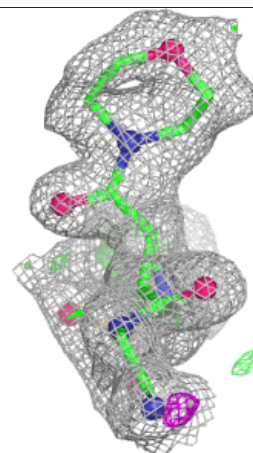
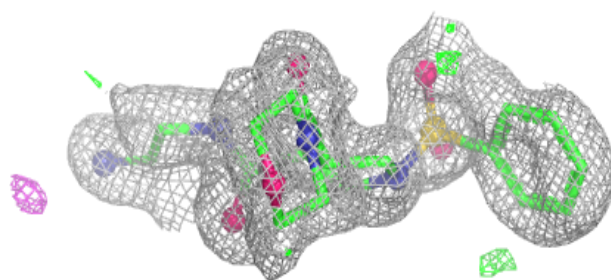
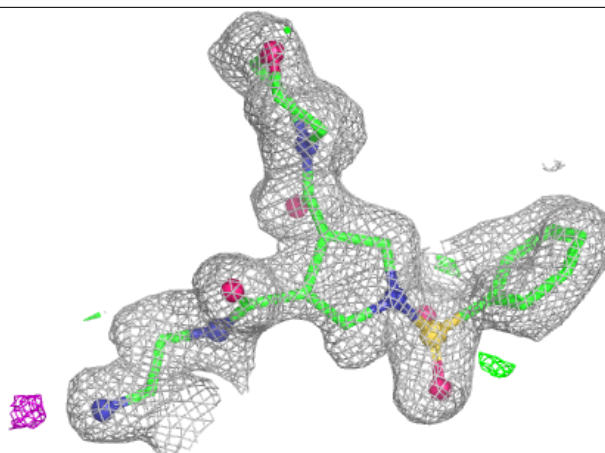
Electron density around 2EW B 401:

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



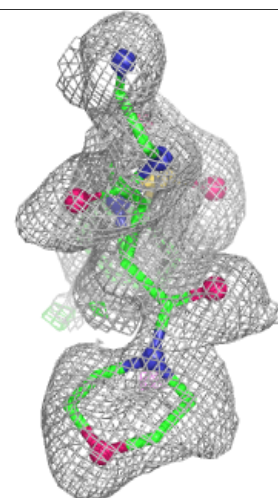
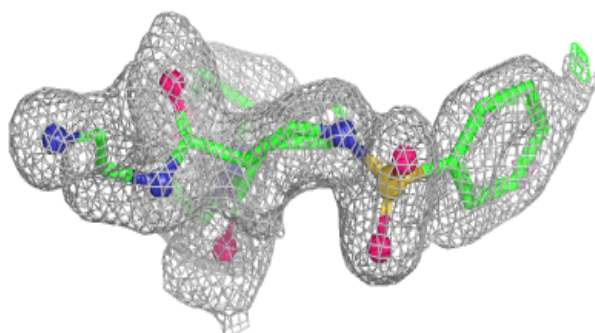
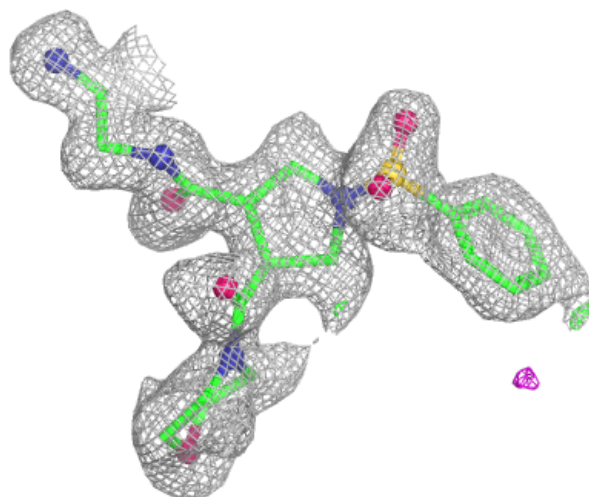
Electron density around 2EW F 401:

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



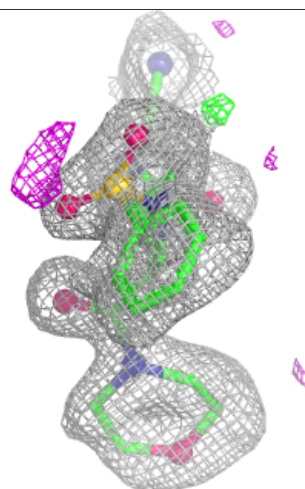
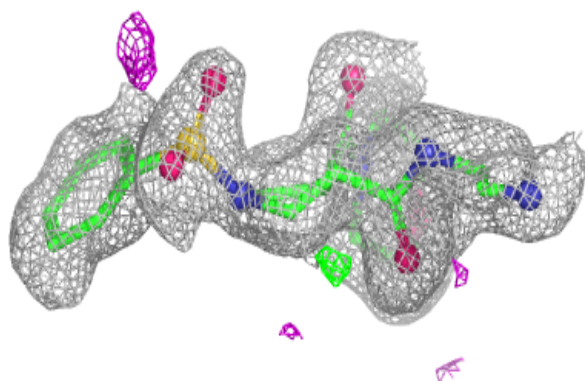
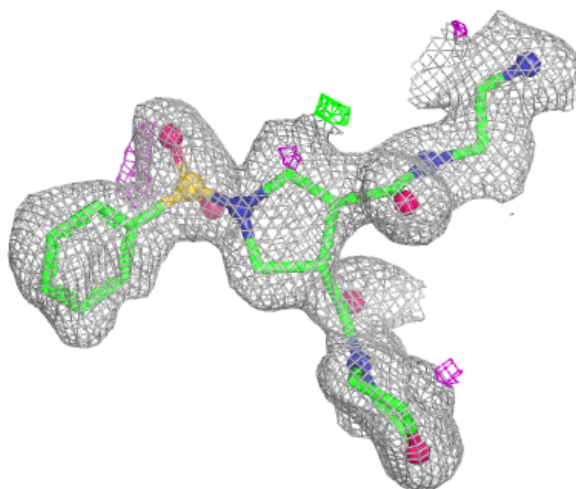
Electron density around 2EW G 401:

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



Electron density around 2EW H 401:

$2mF_o-DF_c$ (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.