



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:28 AM UTC

PDB ID : 3WCM / pdb_00003wcm
Title : The complex structure of HsSQS with ligand, ER119884
Authors : Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.;
Zhu, Z.; Chen, C.C.; Guo, R.T.
Deposited on : 2013-05-28
Resolution : 2.06 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

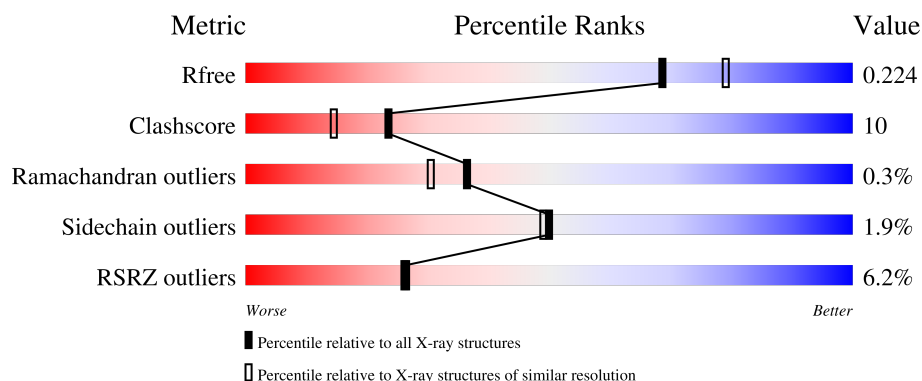
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	360	4% 76% 14% • 9%
1	B	360	7% 72% 19% • 8%
1	C	360	3% 73% 18% • 8%
1	D	360	6% 72% 17% • 10%
1	E	360	3% 73% 18% • 8%

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Mol	Chain	Length	Quality of chain
1	F	360	11% 60% 29% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17280 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 Squalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2659	1695	449	497	18			
1	B	332	Total	C	N	O	S	0	0	0
			2678	1705	452	503	18			
1	C	332	Total	C	N	O	S	0	0	0
			2683	1708	456	501	18			
1	D	325	Total	C	N	O	S	0	0	0
			2632	1674	446	494	18			
1	E	330	Total	C	N	O	S	0	0	0
			2664	1696	451	499	18			
1	F	328	Total	C	N	O	S	0	0	0
			2648	1686	448	496	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P37268
A	12	GLY	-	expression tag	UNP P37268
A	13	SER	-	expression tag	UNP P37268
A	14	SER	-	expression tag	UNP P37268
A	15	HIS	-	expression tag	UNP P37268
A	16	HIS	-	expression tag	UNP P37268
A	17	HIS	-	expression tag	UNP P37268
A	18	HIS	-	expression tag	UNP P37268
A	19	HIS	-	expression tag	UNP P37268
A	20	HIS	-	expression tag	UNP P37268
A	21	SER	-	expression tag	UNP P37268
A	22	SER	-	expression tag	UNP P37268
A	23	GLY	-	expression tag	UNP P37268
A	24	LEU	-	expression tag	UNP P37268
A	25	VAL	-	expression tag	UNP P37268
A	26	PRO	-	expression tag	UNP P37268
A	27	ARG	-	expression tag	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	expression tag	UNP P37268
A	29	SER	-	expression tag	UNP P37268
A	30	HIS	-	expression tag	UNP P37268
A	248	LEU	LYS	engineered mutation	UNP P37268
A	315	LEU	LYS	engineered mutation	UNP P37268
A	318	LEU	LYS	engineered mutation	UNP P37268
A	353	ASN	ASP	SEE REMARK 999	UNP P37268
B	11	MET	-	expression tag	UNP P37268
B	12	GLY	-	expression tag	UNP P37268
B	13	SER	-	expression tag	UNP P37268
B	14	SER	-	expression tag	UNP P37268
B	15	HIS	-	expression tag	UNP P37268
B	16	HIS	-	expression tag	UNP P37268
B	17	HIS	-	expression tag	UNP P37268
B	18	HIS	-	expression tag	UNP P37268
B	19	HIS	-	expression tag	UNP P37268
B	20	HIS	-	expression tag	UNP P37268
B	21	SER	-	expression tag	UNP P37268
B	22	SER	-	expression tag	UNP P37268
B	23	GLY	-	expression tag	UNP P37268
B	24	LEU	-	expression tag	UNP P37268
B	25	VAL	-	expression tag	UNP P37268
B	26	PRO	-	expression tag	UNP P37268
B	27	ARG	-	expression tag	UNP P37268
B	28	GLY	-	expression tag	UNP P37268
B	29	SER	-	expression tag	UNP P37268
B	30	HIS	-	expression tag	UNP P37268
B	248	LEU	LYS	engineered mutation	UNP P37268
B	315	LEU	LYS	engineered mutation	UNP P37268
B	318	LEU	LYS	engineered mutation	UNP P37268
B	353	ASN	ASP	SEE REMARK 999	UNP P37268
C	11	MET	-	expression tag	UNP P37268
C	12	GLY	-	expression tag	UNP P37268
C	13	SER	-	expression tag	UNP P37268
C	14	SER	-	expression tag	UNP P37268
C	15	HIS	-	expression tag	UNP P37268
C	16	HIS	-	expression tag	UNP P37268
C	17	HIS	-	expression tag	UNP P37268
C	18	HIS	-	expression tag	UNP P37268
C	19	HIS	-	expression tag	UNP P37268
C	20	HIS	-	expression tag	UNP P37268
C	21	SER	-	expression tag	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	SER	-	expression tag	UNP P37268
C	23	GLY	-	expression tag	UNP P37268
C	24	LEU	-	expression tag	UNP P37268
C	25	VAL	-	expression tag	UNP P37268
C	26	PRO	-	expression tag	UNP P37268
C	27	ARG	-	expression tag	UNP P37268
C	28	GLY	-	expression tag	UNP P37268
C	29	SER	-	expression tag	UNP P37268
C	30	HIS	-	expression tag	UNP P37268
C	248	LEU	LYS	engineered mutation	UNP P37268
C	315	LEU	LYS	engineered mutation	UNP P37268
C	318	LEU	LYS	engineered mutation	UNP P37268
C	353	ASN	ASP	SEE REMARK 999	UNP P37268
D	11	MET	-	expression tag	UNP P37268
D	12	GLY	-	expression tag	UNP P37268
D	13	SER	-	expression tag	UNP P37268
D	14	SER	-	expression tag	UNP P37268
D	15	HIS	-	expression tag	UNP P37268
D	16	HIS	-	expression tag	UNP P37268
D	17	HIS	-	expression tag	UNP P37268
D	18	HIS	-	expression tag	UNP P37268
D	19	HIS	-	expression tag	UNP P37268
D	20	HIS	-	expression tag	UNP P37268
D	21	SER	-	expression tag	UNP P37268
D	22	SER	-	expression tag	UNP P37268
D	23	GLY	-	expression tag	UNP P37268
D	24	LEU	-	expression tag	UNP P37268
D	25	VAL	-	expression tag	UNP P37268
D	26	PRO	-	expression tag	UNP P37268
D	27	ARG	-	expression tag	UNP P37268
D	28	GLY	-	expression tag	UNP P37268
D	29	SER	-	expression tag	UNP P37268
D	30	HIS	-	expression tag	UNP P37268
D	248	LEU	LYS	engineered mutation	UNP P37268
D	315	LEU	LYS	engineered mutation	UNP P37268
D	318	LEU	LYS	engineered mutation	UNP P37268
D	353	ASN	ASP	SEE REMARK 999	UNP P37268
E	11	MET	-	expression tag	UNP P37268
E	12	GLY	-	expression tag	UNP P37268
E	13	SER	-	expression tag	UNP P37268
E	14	SER	-	expression tag	UNP P37268
E	15	HIS	-	expression tag	UNP P37268

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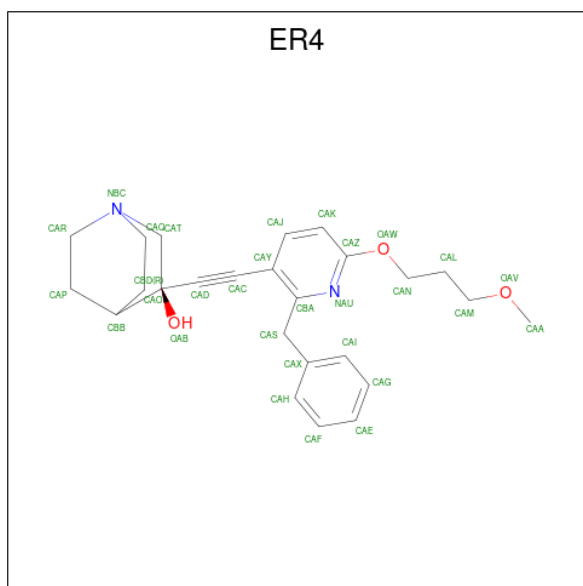
Chain	Residue	Modelled	Actual	Comment	Reference
E	16	HIS	-	expression tag	UNP P37268
E	17	HIS	-	expression tag	UNP P37268
E	18	HIS	-	expression tag	UNP P37268
E	19	HIS	-	expression tag	UNP P37268
E	20	HIS	-	expression tag	UNP P37268
E	21	SER	-	expression tag	UNP P37268
E	22	SER	-	expression tag	UNP P37268
E	23	GLY	-	expression tag	UNP P37268
E	24	LEU	-	expression tag	UNP P37268
E	25	VAL	-	expression tag	UNP P37268
E	26	PRO	-	expression tag	UNP P37268
E	27	ARG	-	expression tag	UNP P37268
E	28	GLY	-	expression tag	UNP P37268
E	29	SER	-	expression tag	UNP P37268
E	30	HIS	-	expression tag	UNP P37268
E	248	LEU	LYS	engineered mutation	UNP P37268
E	315	LEU	LYS	engineered mutation	UNP P37268
E	318	LEU	LYS	engineered mutation	UNP P37268
E	353	ASN	ASP	SEE REMARK 999	UNP P37268
F	11	MET	-	expression tag	UNP P37268
F	12	GLY	-	expression tag	UNP P37268
F	13	SER	-	expression tag	UNP P37268
F	14	SER	-	expression tag	UNP P37268
F	15	HIS	-	expression tag	UNP P37268
F	16	HIS	-	expression tag	UNP P37268
F	17	HIS	-	expression tag	UNP P37268
F	18	HIS	-	expression tag	UNP P37268
F	19	HIS	-	expression tag	UNP P37268
F	20	HIS	-	expression tag	UNP P37268
F	21	SER	-	expression tag	UNP P37268
F	22	SER	-	expression tag	UNP P37268
F	23	GLY	-	expression tag	UNP P37268
F	24	LEU	-	expression tag	UNP P37268
F	25	VAL	-	expression tag	UNP P37268
F	26	PRO	-	expression tag	UNP P37268
F	27	ARG	-	expression tag	UNP P37268
F	28	GLY	-	expression tag	UNP P37268
F	29	SER	-	expression tag	UNP P37268
F	30	HIS	-	expression tag	UNP P37268
F	248	LEU	LYS	engineered mutation	UNP P37268
F	315	LEU	LYS	engineered mutation	UNP P37268
F	318	LEU	LYS	engineered mutation	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
F	353	ASN	ASP	SEE REMARK 999	UNP P37268

- Molecule 2 is (3R)-3-[[2-benzyl-6-(3-methoxypropoxy)pyridin-3-yl]ethynyl]-1-azabicyclo[2.2.2]octan-3-ol (CCD ID: ER4) (formula: C₂₅H₃₀N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	25	2	3		
2	B	1	Total	C	N	O	0	0
			30	25	2	3		
2	C	1	Total	C	N	O	0	0
			30	25	2	3		
2	D	1	Total	C	N	O	0	0
			30	25	2	3		
2	E	1	Total	C	N	O	0	0
			30	25	2	3		
2	F	1	Total	C	N	O	0	0
			30	25	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	273	Total	O	0	0
			273	273		
3	B	234	Total	O	0	0
			234	234		

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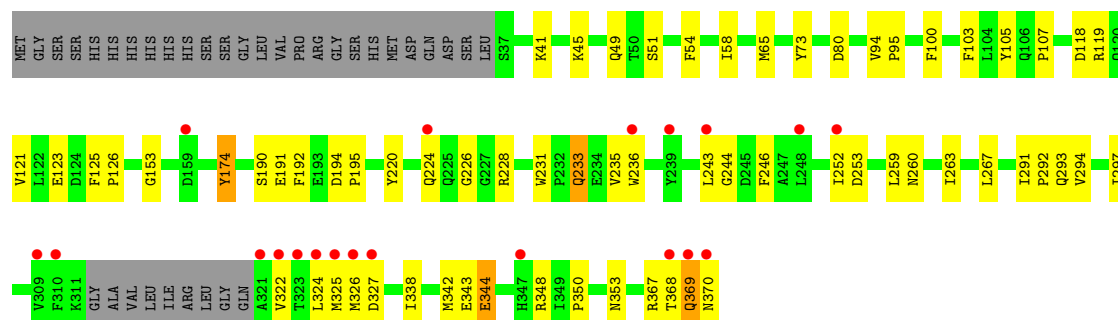
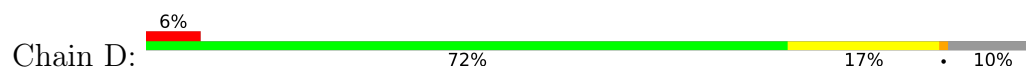
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	236	Total 236	O 236	0	0
3	D	168	Total 168	O 168	0	0
3	E	141	Total 141	O 141	0	0
3	F	84	Total 84	O 84	0	0

- Molecule 1: Squalene synthase

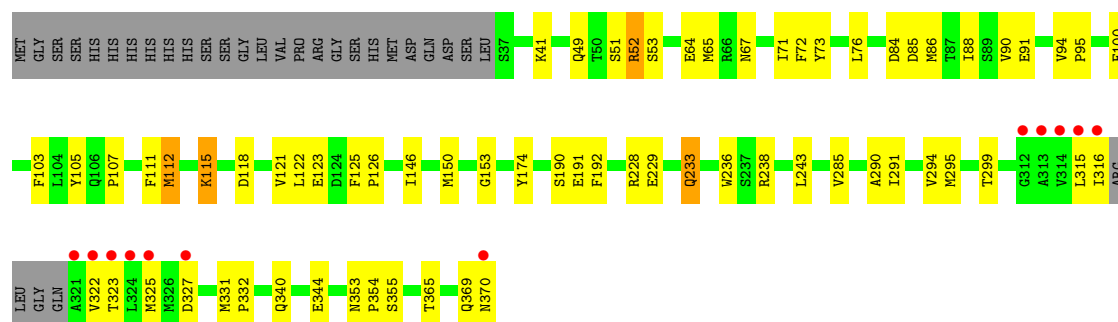
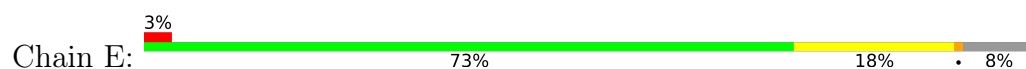




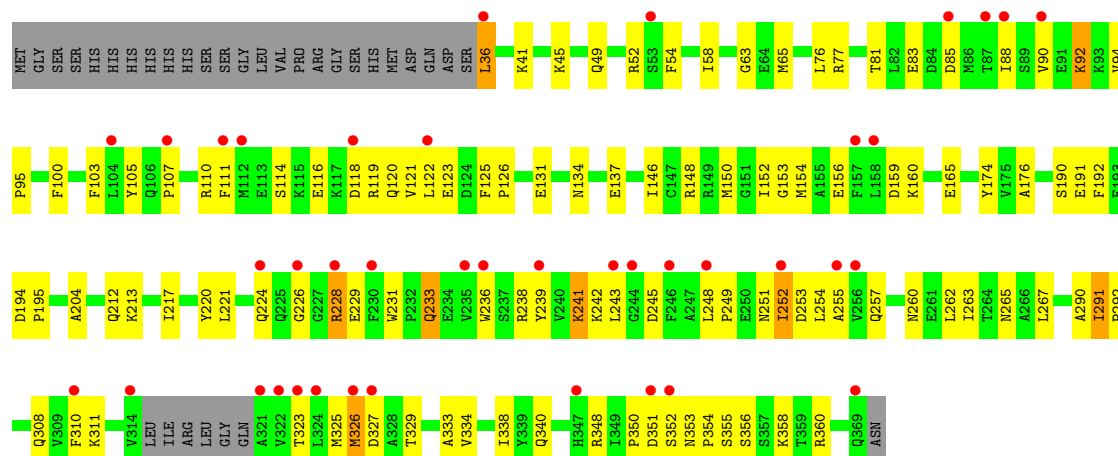
• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.62Å 153.45Å 92.12Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	25.00 – 2.06 25.00 – 2.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.06) 96.0 (25.00-2.06)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.06Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.186 , 0.222 0.190 , 0.224	Depositor DCC
R_{free} test set	7126 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17280	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: ER4

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	0.43	0/2713	0.84	6/3672 (0.2%)
1	B	0.39	0/2732	0.85	6/3698 (0.2%)
1	C	0.40	0/2737	0.83	3/3704 (0.1%)
1	D	0.36	0/2686	0.82	1/3635 (0.0%)
1	E	0.35	0/2718	0.81	2/3679 (0.1%)
1	F	0.33	0/2702	0.80	4/3657 (0.1%)
All	All	0.38	0/16288	0.83	22/22045 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	ASP	N-CA-C	-6.55	104.18	111.71
1	C	93	LYS	N-CA-C	6.08	117.99	111.36
1	A	204	ALA	N-CA-C	-6.07	104.75	111.36
1	F	290	ALA	N-CA-C	5.82	117.42	111.14
1	B	353	ASN	CA-C-N	5.62	125.72	119.87
1	B	353	ASN	C-N-CA	5.62	125.72	119.87
1	A	106	GLN	CA-C-N	5.57	125.67	119.32
1	A	106	GLN	C-N-CA	5.57	125.67	119.32
1	A	45	LYS	N-CA-C	-5.36	105.35	111.14
1	D	174	TYR	N-CA-C	5.36	117.12	111.28
1	A	368	THR	N-CA-C	5.35	117.19	111.36
1	F	204	ALA	N-CA-C	-5.29	105.52	111.28
1	F	165	GLU	N-CA-C	-5.21	105.78	111.82
1	F	291	ILE	CB-CA-C	-5.18	108.78	113.70
1	A	53	SER	N-CA-C	5.17	120.23	113.30
1	B	290	ALA	N-CA-C	5.17	116.72	111.14
1	E	344	GLU	N-CA-C	-5.11	105.80	111.36
1	E	290	ALA	N-CA-C	5.09	116.91	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	GLN	CA-C-N	5.06	126.16	119.84
1	C	106	GLN	C-N-CA	5.06	126.16	119.84
1	B	165	GLU	N-CA-C	-5.05	106.38	112.54
1	B	93	LYS	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2659	0	2635	45	0
1	B	2678	0	2649	57	0
1	C	2683	0	2659	63	0
1	D	2632	0	2596	54	0
1	E	2664	0	2635	57	0
1	F	2648	0	2618	87	0
2	A	30	0	30	1	0
2	B	30	0	30	1	0
2	C	30	0	30	0	0
2	D	30	0	30	1	0
2	E	30	0	30	0	0
2	F	30	0	30	1	0
3	A	273	0	0	3	0
3	B	234	0	0	1	0
3	C	236	0	0	5	0
3	D	168	0	0	1	0
3	E	141	0	0	3	0
3	F	84	0	0	3	0
All	All	17280	0	15972	328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:VAL:HG13	1:E:291:ILE:HG21	1.45	0.98
1:B:325:MET:HE2	1:C:295:MET:HG3	1.45	0.94
1:F:326:MET:HE2	1:F:333:ALA:HA	1.52	0.90
1:E:295:MET:HE2	1:E:295:MET:HA	1.53	0.90
1:B:326:MET:HE3	1:C:291:ILE:HD11	1.54	0.89
1:D:260:ASN:HD22	1:D:353:ASN:ND2	1.69	0.89
1:F:228:ARG:HH11	1:F:228:ARG:H	1.14	0.89
1:D:369:GLN:O	1:D:370:ASN:HB2	1.75	0.87
1:F:131:GLU:HA	1:F:134:ASN:HD22	1.41	0.85
1:F:260:ASN:HD22	1:F:353:ASN:ND2	1.74	0.84
1:C:95:PRO:HA	3:C:572:HOH:O	1.80	0.81
1:F:233:GLN:HA	1:F:236:TRP:NE1	1.96	0.81
1:D:368:THR:HG21	1:E:41:LYS:HA	1.66	0.78
1:E:150:MET:HG3	1:E:174:TYR:O	1.85	0.75
1:C:45:LYS:O	1:C:49:GLN:HG3	1.85	0.74
1:C:348:ARG:HB3	1:C:348:ARG:HH11	1.51	0.74
1:F:45:LYS:HG2	1:F:49:GLN:HE21	1.53	0.73
1:F:94:VAL:HB	1:F:95:PRO:HD3	1.70	0.73
1:A:325:MET:HE2	1:B:294:VAL:HG11	1.70	0.73
1:D:94:VAL:HB	1:D:95:PRO:HD3	1.70	0.72
1:B:233:GLN:HA	1:B:236:TRP:NE1	2.05	0.71
1:D:325:MET:HE2	1:E:294:VAL:HG11	1.72	0.70
1:A:291:ILE:HG21	1:C:322:VAL:HG22	1.71	0.70
1:B:325:MET:HE1	1:C:294:VAL:HG12	1.73	0.70
1:C:195:PRO:O	1:C:199:GLU:HG3	1.92	0.70
1:B:77:ARG:HD3	2:B:401:ER4:H7	1.74	0.69
1:F:228:ARG:HH11	1:F:228:ARG:N	1.88	0.69
1:A:357:SER:O	1:A:361:GLN:HG3	1.92	0.69
1:A:353:ASN:ND2	1:A:355:SER:H	1.91	0.69
1:F:228:ARG:HB2	1:F:228:ARG:NH1	2.08	0.68
1:C:322:VAL:HG12	1:C:340:GLN:CD	2.17	0.68
1:E:322:VAL:CG2	1:F:291:ILE:HG21	2.23	0.68
1:E:365:THR:O	1:E:369:GLN:HG3	1.94	0.67
1:F:118:ASP:O	1:F:121:VAL:HG22	1.96	0.66
1:D:224:GLN:HE21	1:D:244:GLY:HA2	1.61	0.66
1:E:322:VAL:HG12	1:E:340:GLN:NE2	2.11	0.66
1:B:322:VAL:HG13	1:C:291:ILE:HG21	1.77	0.66
1:C:348:ARG:HB3	1:C:348:ARG:NH1	2.12	0.65
1:D:233:GLN:HA	1:D:236:TRP:NE1	2.11	0.65
1:E:90:VAL:O	1:E:94:VAL:HG23	1.97	0.65
1:E:353:ASN:ND2	1:E:355:SER:H	1.94	0.65
1:B:260:ASN:HD22	1:B:353:ASN:ND2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:MET:HG3	1:F:174:TYR:O	1.97	0.63
1:C:100:PHE:HA	1:C:103:PHE:CD2	2.34	0.63
1:D:327:ASP:HB2	1:F:325:MET:O	1.98	0.63
1:C:315:LEU:O	1:C:315:LEU:HD12	1.99	0.63
1:A:326:MET:HA	1:B:327:ASP:HB2	1.81	0.62
1:D:260:ASN:HD22	1:D:353:ASN:HD22	1.46	0.62
1:F:242:LYS:HB2	1:F:245:ASP:OD2	1.98	0.62
1:E:52:ARG:HD2	1:E:53:SER:N	2.15	0.62
1:F:260:ASN:HD22	1:F:353:ASN:HD22	1.48	0.62
1:E:112:MET:HE1	1:E:123:GLU:HB3	1.81	0.62
1:A:245:ASP:HA	1:A:248:LEU:HD13	1.82	0.61
1:F:131:GLU:HA	1:F:134:ASN:ND2	2.14	0.61
1:D:45:LYS:O	1:D:49:GLN:HG3	2.00	0.61
1:F:228:ARG:H	1:F:228:ARG:NH1	1.94	0.61
1:E:233:GLN:HA	1:E:236:TRP:NE1	2.15	0.61
1:B:221:LEU:HD23	1:B:312:GLY:HA2	1.83	0.60
1:E:323:THR:HB	1:E:340:GLN:OE1	2.01	0.60
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.36	0.60
1:D:325:MET:HE2	1:E:294:VAL:CG1	2.32	0.59
1:E:322:VAL:HG23	1:F:291:ILE:HG21	1.83	0.59
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.17	0.59
3:A:1113:HOH:O	1:C:370:ASN:HB2	2.03	0.58
1:B:325:MET:HE1	1:C:294:VAL:CG1	2.32	0.58
1:B:253:ASP:O	1:B:257:GLN:HG3	2.03	0.58
1:A:65:MET:HE2	1:A:192:PHE:CD2	2.38	0.58
1:C:98:HIS:HB2	3:C:572:HOH:O	2.04	0.58
1:F:90:VAL:O	1:F:94:VAL:HG23	2.03	0.58
1:B:323:THR:CG2	1:B:340:GLN:HG3	2.34	0.58
1:A:343:GLU:OE1	1:A:367:ARG:NH2	2.37	0.57
1:E:52:ARG:CD	1:E:52:ARG:H	2.17	0.57
1:F:146:ILE:HG22	1:F:150:MET:HE3	1.87	0.57
1:A:325:MET:HE2	1:B:294:VAL:CG1	2.34	0.57
1:C:118:ASP:O	1:C:121:VAL:HG22	2.03	0.57
1:D:65:MET:HE2	1:D:192:PHE:CD2	2.39	0.57
1:D:326:MET:HE3	1:E:291:ILE:HG12	1.86	0.57
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.38	0.57
1:D:119:ARG:O	1:D:123:GLU:HG3	2.04	0.57
1:D:291:ILE:HB	1:D:292:PRO:HD3	1.86	0.57
1:E:115:LYS:HZ2	1:E:115:LYS:HB3	1.70	0.57
1:E:315:LEU:HD12	1:E:315:LEU:O	2.05	0.57
1:F:36:LEU:HB2	1:F:41:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASN:HB3	1:C:348:ARG:HH12	1.70	0.56
1:D:100:PHE:HA	1:D:103:PHE:CD2	2.41	0.56
1:C:150:MET:HG3	1:C:174:TYR:O	2.06	0.56
1:F:85:ASP:HB3	1:F:88:ILE:HD13	1.88	0.55
1:E:65:MET:HE2	1:E:192:PHE:CD2	2.42	0.55
1:F:253:ASP:O	1:F:257:GLN:HG3	2.07	0.55
1:C:348:ARG:O	1:C:350:PRO:HD3	2.07	0.55
1:E:52:ARG:HD2	1:E:53:SER:H	1.69	0.55
1:E:331:MET:HB3	1:E:332:PRO:HD3	1.89	0.55
1:A:322:VAL:O	1:A:326:MET:HG2	2.07	0.55
1:F:220:TYR:HB2	1:F:231:TRP:CZ2	2.42	0.55
1:F:36:LEU:N	1:F:36:LEU:HD22	2.21	0.55
1:C:94:VAL:HB	1:C:95:PRO:HD3	1.89	0.55
1:D:105:TYR:O	1:D:107:PRO:HD3	2.06	0.55
1:D:41:LYS:HE2	3:F:516:HOH:O	2.08	0.54
1:E:118:ASP:O	1:E:121:VAL:HG22	2.07	0.54
1:C:114:SER:C	1:C:115:LYS:HD2	2.33	0.54
1:F:323:THR:HB	1:F:340:GLN:OE1	2.06	0.54
1:E:323:THR:H	1:E:340:GLN:HE22	1.55	0.54
1:D:369:GLN:O	1:D:370:ASN:CB	2.52	0.54
1:E:105:TYR:O	1:E:107:PRO:HD3	2.07	0.54
1:D:125:PHE:N	1:D:126:PRO:CD	2.71	0.54
1:D:324:LEU:HD12	1:D:325:MET:HG2	1.90	0.54
1:E:125:PHE:N	1:E:126:PRO:CD	2.70	0.54
1:C:322:VAL:HG12	1:C:340:GLN:OE1	2.06	0.54
1:A:327:ASP:HB3	1:C:326:MET:HA	1.90	0.53
1:F:65:MET:HE2	1:F:192:PHE:CD2	2.43	0.53
1:E:67:ASN:O	1:E:71:ILE:HG12	2.09	0.53
1:C:314:VAL:CG1	1:C:315:LEU:N	2.72	0.53
1:E:370:ASN:HB3	3:F:522:HOH:O	2.08	0.53
1:F:88:ILE:N	1:F:88:ILE:HD12	2.24	0.52
1:F:88:ILE:HG23	1:F:92:LYS:HB3	1.91	0.52
1:A:325:MET:O	1:B:327:ASP:HB2	2.09	0.52
1:E:325:MET:O	1:F:327:ASP:HB3	2.10	0.52
1:F:116:GLU:O	1:F:119:ARG:HG2	2.10	0.52
1:A:36:LEU:HG	1:A:37:SER:N	2.24	0.52
1:C:348:ARG:HH11	1:C:348:ARG:CB	2.22	0.52
1:E:51:SER:HB2	1:E:73:TYR:CZ	2.44	0.52
1:D:325:MET:HG3	1:E:295:MET:HE3	1.91	0.52
1:C:37:SER:O	1:C:41:LYS:HG3	2.10	0.52
1:C:64:GLU:HG3	3:C:556:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:GLU:OE2	1:D:367:ARG:NE	2.43	0.52
1:D:348:ARG:O	1:D:350:PRO:HD3	2.10	0.52
1:D:51:SER:HB2	1:D:73:TYR:CZ	2.44	0.52
1:E:228:ARG:HG3	1:E:228:ARG:HH11	1.75	0.52
1:A:233:GLN:HA	1:A:236:TRP:NE1	2.25	0.51
1:C:314:VAL:HG12	1:C:315:LEU:N	2.25	0.51
1:F:263:ILE:O	1:F:267:LEU:HG	2.10	0.51
1:A:252:ILE:HG13	1:A:307:GLN:HG2	1.92	0.51
1:C:105:TYR:O	1:C:107:PRO:HD3	2.10	0.51
1:D:293:GLN:O	1:D:297:ILE:HG13	2.11	0.51
1:D:325:MET:CG	1:E:295:MET:HE3	2.40	0.51
1:D:220:TYR:HB2	1:D:231:TRP:CZ2	2.44	0.51
1:D:350:PRO:HG2	1:D:353:ASN:HB2	1.93	0.51
1:C:365:THR:O	1:C:369:GLN:HG3	2.09	0.51
1:E:295:MET:HA	1:E:295:MET:CE	2.32	0.51
1:F:291:ILE:HB	1:F:292:PRO:HD3	1.92	0.51
1:B:325:MET:O	1:C:327:ASP:HB2	2.10	0.50
1:C:248:LEU:HB2	1:C:251:ASN:HD22	1.75	0.50
1:F:118:ASP:HA	1:F:120:GLN:OE1	2.12	0.50
1:F:350:PRO:C	1:F:352:SER:H	2.19	0.50
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.47	0.50
1:A:291:ILE:CG2	1:C:322:VAL:HG22	2.41	0.50
1:E:84:ASP:O	1:E:86:MET:HE2	2.11	0.50
1:F:81:THR:HG23	1:F:116:GLU:HG3	1.92	0.50
1:A:325:MET:CE	1:B:294:VAL:HG11	2.39	0.50
1:B:150:MET:O	1:B:154:MET:HG3	2.10	0.50
1:A:36:LEU:HG	1:A:37:SER:H	1.76	0.50
1:D:233:GLN:HG3	1:D:236:TRP:CZ2	2.46	0.50
1:F:52:ARG:HG3	3:F:583:HOH:O	2.11	0.50
1:F:255:ALA:HB1	1:F:310:PHE:CE2	2.47	0.50
1:B:125:PHE:N	1:B:126:PRO:CD	2.75	0.49
1:F:308:GLN:OE1	1:F:311:LYS:HD2	2.11	0.49
1:F:92:LYS:O	1:F:95:PRO:HD2	2.12	0.49
1:F:233:GLN:HA	1:F:236:TRP:CD1	2.47	0.49
1:B:118:ASP:O	1:B:121:VAL:HG22	2.12	0.49
1:D:224:GLN:C	1:D:226:GLY:H	2.20	0.49
1:E:299:THR:HA	1:E:316:ILE:HD12	1.94	0.49
1:A:241:LYS:HD3	3:A:1188:HOH:O	2.12	0.49
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.95	0.49
1:C:291:ILE:HB	1:C:292:PRO:HD3	1.94	0.49
1:C:327:ASP:OD2	1:C:329:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:HB1	1:A:344:GLU:HG2	1.95	0.49
1:C:299:THR:HA	1:C:316:ILE:HD12	1.95	0.49
1:F:236:TRP:C	1:F:238:ARG:H	2.21	0.48
1:C:125:PHE:N	1:C:126:PRO:CD	2.76	0.48
1:F:239:TYR:O	1:F:254:LEU:HD13	2.13	0.48
1:E:64:GLU:HG3	3:E:506:HOH:O	2.13	0.48
1:F:252:ILE:HG23	1:F:253:ASP:N	2.28	0.48
1:B:326:MET:HE3	1:C:291:ILE:CD1	2.36	0.48
1:B:344:GLU:O	1:B:348:ARG:HD3	2.12	0.48
1:B:252:ILE:HG23	1:B:253:ASP:N	2.28	0.48
1:C:233:GLN:HA	1:C:236:TRP:CD1	2.49	0.48
1:F:153:GLY:O	1:F:156:GLU:HB3	2.14	0.48
1:F:262:LEU:O	1:F:265:ASN:HB3	2.13	0.48
1:F:190:SER:O	1:F:191:GLU:HB2	2.14	0.48
1:F:150:MET:O	1:F:154:MET:HG3	2.14	0.48
1:A:252:ILE:CG1	1:A:307:GLN:HG2	2.44	0.47
1:C:353:ASN:ND2	1:C:355:SER:H	2.12	0.47
1:D:344:GLU:CD	1:D:348:ARG:HH12	2.23	0.47
3:E:580:HOH:O	1:F:329:THR:HG21	2.13	0.47
1:A:326:MET:HE3	1:B:291:ILE:HG12	1.95	0.47
1:B:77:ARG:HD2	3:B:627:HOH:O	2.14	0.47
1:D:153:GLY:HA3	1:D:174:TYR:CG	2.48	0.47
1:A:45:LYS:O	1:A:49:GLN:HG3	2.14	0.47
1:D:220:TYR:OH	1:D:246:PHE:HB2	2.14	0.47
1:E:322:VAL:HG12	1:E:340:GLN:CD	2.39	0.47
1:A:119:ARG:O	1:A:123:GLU:HG3	2.15	0.47
1:E:233:GLN:HA	1:E:236:TRP:CD1	2.50	0.47
1:A:125:PHE:N	1:A:126:PRO:CD	2.78	0.47
1:E:190:SER:O	1:E:191:GLU:HB2	2.14	0.47
1:F:236:TRP:CG	1:F:243:LEU:HD13	2.50	0.47
1:A:252:ILE:O	1:A:256:VAL:HG23	2.15	0.46
1:A:326:MET:HA	1:B:327:ASP:CB	2.45	0.46
1:B:331:MET:HB3	1:B:332:PRO:HD3	1.96	0.46
1:F:334:VAL:O	1:F:338:ILE:HG13	2.15	0.46
1:A:85:ASP:HB3	1:A:88:ILE:HD12	1.97	0.46
1:C:110:ARG:HB3	1:C:126:PRO:HD3	1.98	0.46
1:C:315:LEU:O	1:C:317:ARG:N	2.48	0.46
1:F:228:ARG:HB2	1:F:228:ARG:CZ	2.44	0.46
1:A:190:SER:O	1:A:191:GLU:HB2	2.15	0.46
1:B:343:GLU:OE1	1:B:367:ARG:NH2	2.49	0.46
1:E:115:LYS:HB3	1:E:115:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:HA	1:A:248:LEU:CD1	2.46	0.46
1:A:369:GLN:HE22	1:B:36:LEU:CD2	2.29	0.46
1:B:220:TYR:HB2	1:B:231:TRP:CZ2	2.50	0.46
1:A:36:LEU:CG	1:A:37:SER:H	2.27	0.46
1:B:348:ARG:O	1:B:350:PRO:HD3	2.15	0.46
1:B:291:ILE:HB	1:B:292:PRO:HD3	1.97	0.46
1:C:331:MET:HB3	1:C:332:PRO:HD3	1.98	0.46
1:D:233:GLN:HA	1:D:236:TRP:CE2	2.50	0.46
1:B:163:THR:HA	1:B:233:GLN:HB3	1.98	0.46
1:B:326:MET:HA	1:C:327:ASP:OD2	2.15	0.46
1:F:255:ALA:HB1	1:F:310:PHE:CZ	2.50	0.46
1:C:190:SER:O	1:C:191:GLU:HB2	2.16	0.46
1:D:118:ASP:O	1:D:121:VAL:HG22	2.16	0.46
1:F:213:LYS:O	1:F:217:ILE:HG13	2.16	0.46
1:A:153:GLY:HA3	1:A:174:TYR:CG	2.51	0.46
1:A:295:MET:SD	1:C:322:VAL:HG23	2.56	0.46
1:B:190:SER:O	1:B:191:GLU:HB2	2.15	0.46
1:E:94:VAL:HB	1:E:95:PRO:HD3	1.97	0.46
1:E:354:PRO:HG2	3:E:515:HOH:O	2.14	0.46
1:F:355:SER:O	1:F:356:SER:C	2.59	0.46
1:B:120:GLN:HA	1:B:120:GLN:NE2	2.30	0.45
1:B:221:LEU:O	1:B:225:GLN:HG3	2.16	0.45
1:F:125:PHE:N	1:F:126:PRO:CD	2.78	0.45
1:B:157:PHE:CE2	1:B:160:LYS:HE3	2.51	0.45
1:C:94:VAL:HG11	3:C:704:HOH:O	2.16	0.45
1:B:255:ALA:HB1	1:B:310:PHE:CZ	2.52	0.45
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.98	0.45
1:D:190:SER:O	1:D:191:GLU:HB2	2.15	0.45
1:E:85:ASP:HB3	1:E:88:ILE:HD12	1.99	0.45
1:B:334:VAL:O	1:B:338:ILE:HG13	2.17	0.45
1:F:252:ILE:O	1:F:255:ALA:HB3	2.17	0.45
1:B:51:SER:HB2	1:B:73:TYR:CZ	2.52	0.45
1:B:117:LYS:HG3	1:B:118:ASP:N	2.31	0.45
1:F:83:GLU:CD	1:F:154:MET:HE2	2.42	0.45
1:B:314:VAL:HG12	1:B:315:LEU:N	2.31	0.44
1:B:315:LEU:O	1:B:316:ILE:C	2.60	0.44
1:D:224:GLN:OE1	1:D:224:GLN:HA	2.17	0.44
1:F:156:GLU:HG2	1:F:160:LYS:HE2	1.98	0.44
1:E:72:PHE:O	1:E:76:LEU:HG	2.17	0.44
1:D:228:ARG:HG2	3:D:668:HOH:O	2.18	0.44
1:A:77:ARG:NH1	2:A:901:ER4:H9	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:GLY:HA3	1:E:174:TYR:CG	2.52	0.44
1:F:351:ASP:HB3	1:F:360:ARG:HH22	1.83	0.44
1:C:297:ILE:CD1	1:C:338:ILE:HG12	2.48	0.44
1:C:299:THR:HA	1:C:316:ILE:CD1	2.47	0.44
1:D:338:ILE:O	1:D:342:MET:HG2	2.17	0.44
1:D:343:GLU:OE1	1:D:367:ARG:NH2	2.51	0.44
1:E:353:ASN:HD22	1:E:355:SER:H	1.61	0.44
1:F:111:PHE:HB3	1:F:122:LEU:HB3	1.98	0.44
1:F:148:ARG:O	1:F:152:ILE:HG13	2.18	0.44
1:B:228:ARG:HD2	1:B:230:PHE:CE2	2.52	0.44
1:C:255:ALA:HB1	1:C:310:PHE:CZ	2.52	0.44
1:A:120:GLN:HG2	1:A:121:VAL:N	2.33	0.43
1:F:114:SER:O	1:F:119:ARG:HD3	2.18	0.43
1:E:233:GLN:HA	1:E:236:TRP:CE2	2.53	0.43
1:B:350:PRO:C	1:B:352:SER:N	2.73	0.43
1:C:305:ASN:HB3	1:C:348:ARG:NH1	2.32	0.43
1:F:229:GLU:HB3	1:F:243:LEU:HD23	2.00	0.43
1:E:146:ILE:HG22	1:E:150:MET:HE3	2.00	0.43
1:E:315:LEU:HD12	1:E:315:LEU:C	2.44	0.43
1:F:236:TRP:CE2	1:F:243:LEU:HB2	2.53	0.43
1:C:94:VAL:CG1	3:C:704:HOH:O	2.67	0.43
1:D:263:ILE:O	1:D:267:LEU:HG	2.19	0.43
1:F:241:LYS:HB2	1:F:241:LYS:NZ	2.33	0.43
1:C:119:ARG:O	1:C:123:GLU:HG3	2.18	0.43
1:D:233:GLN:C	1:D:235:VAL:H	2.24	0.43
1:E:65:MET:HE1	1:E:285:VAL:HG23	2.01	0.43
1:F:76:LEU:HD12	2:F:401:ER4:H28	2.00	0.43
1:D:343:GLU:CD	1:D:367:ARG:HH21	2.27	0.43
1:F:224:GLN:C	1:F:226:GLY:H	2.25	0.43
1:F:248:LEU:HA	1:F:249:PRO:HD3	1.92	0.43
1:B:343:GLU:OE1	1:C:48:ASN:HB3	2.19	0.43
1:D:260:ASN:HB2	1:D:353:ASN:HD21	1.83	0.43
1:B:367:ARG:C	1:B:369:GLN:H	2.26	0.43
1:E:322:VAL:HG22	1:F:291:ILE:HG21	2.00	0.42
1:C:51:SER:HB2	1:C:73:TYR:CZ	2.54	0.42
1:F:221:LEU:HD23	1:F:311:LYS:O	2.19	0.42
1:F:233:GLN:HE21	1:F:233:GLN:HB3	1.60	0.42
1:A:120:GLN:HB2	3:A:1125:HOH:O	2.19	0.42
1:B:350:PRO:HB2	1:B:353:ASN:H	1.84	0.42
1:D:260:ASN:HD22	1:D:353:ASN:HD21	1.62	0.42
1:F:54:PHE:O	1:F:58:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:ARG:O	1:F:350:PRO:HD3	2.19	0.42
1:F:355:SER:O	1:F:358:LYS:N	2.52	0.42
1:C:65:MET:HE1	1:C:285:VAL:HG23	2.02	0.42
1:D:259:LEU:O	1:D:263:ILE:HG13	2.20	0.42
1:F:105:TYR:O	1:F:107:PRO:HD3	2.20	0.42
1:B:67:ASN:O	1:B:71:ILE:HG12	2.20	0.42
1:C:350:PRO:HG2	1:C:353:ASN:HB2	2.01	0.42
1:F:353:ASN:HA	1:F:354:PRO:HD3	1.85	0.42
1:A:297:ILE:CD1	1:A:338:ILE:HG12	2.50	0.41
1:B:120:GLN:HA	1:B:120:GLN:HE21	1.85	0.41
1:C:316:ILE:HD13	1:C:316:ILE:HA	1.93	0.41
1:F:260:ASN:ND2	1:F:353:ASN:ND2	2.55	0.41
1:B:262:LEU:O	1:B:265:ASN:HB3	2.21	0.41
1:D:236:TRP:CD1	1:D:243:LEU:HD13	2.55	0.41
1:E:111:PHE:HB3	1:E:122:LEU:HB3	2.02	0.41
1:F:119:ARG:HD2	1:F:123:GLU:OE2	2.21	0.41
1:F:159:ASP:OD2	1:F:160:LYS:N	2.54	0.41
1:F:228:ARG:HH11	1:F:228:ARG:HB2	1.85	0.41
1:F:251:ASN:O	1:F:252:ILE:C	2.63	0.41
1:A:341:TYR:O	1:A:344:GLU:HB3	2.21	0.41
1:B:248:LEU:HB3	1:B:250:GLU:OE1	2.21	0.41
1:E:229:GLU:HB3	1:E:243:LEU:HD23	2.02	0.41
1:D:294:VAL:HG11	1:F:325:MET:HE1	2.02	0.41
1:B:233:GLN:HB3	1:B:233:GLN:HE21	1.60	0.41
1:B:343:GLU:HA	1:B:367:ARG:NH2	2.36	0.41
1:D:54:PHE:O	1:D:58:ILE:HG13	2.20	0.41
1:D:80:ASP:OD1	2:D:401:ER4:H8	2.21	0.41
1:E:91:GLU:CD	1:E:91:GLU:H	2.28	0.41
1:A:233:GLN:HE21	1:A:233:GLN:HB3	1.65	0.40
1:A:259:LEU:HD21	1:A:303:CYS:O	2.21	0.40
1:C:100:PHE:HA	1:C:103:PHE:CE2	2.55	0.40
1:D:194:ASP:CG	1:D:195:PRO:HD2	2.45	0.40
1:C:162:VAL:HG11	1:C:168:TRP:HA	2.02	0.40
1:F:176:ALA:CB	1:F:212:GLN:HB2	2.51	0.40
1:B:153:GLY:HA3	1:B:174:TYR:CG	2.56	0.40
1:F:120:GLN:HG2	1:F:121:VAL:N	2.37	0.40
1:A:41:LYS:NZ	1:C:365:THR:HA	2.37	0.40
1:A:233:GLN:HA	1:A:236:TRP:CD1	2.56	0.40
1:D:252:ILE:HG23	1:D:253:ASP:N	2.36	0.40
1:F:194:ASP:OD1	1:F:195:PRO:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/360 (90%)	317 (98%)	8 (2%)	0	100	100
1	B	328/360 (91%)	315 (96%)	12 (4%)	1 (0%)	36	30
1	C	328/360 (91%)	318 (97%)	9 (3%)	1 (0%)	36	30
1	D	321/360 (89%)	304 (95%)	16 (5%)	1 (0%)	36	30
1	E	326/360 (91%)	315 (97%)	11 (3%)	0	100	100
1	F	324/360 (90%)	306 (94%)	16 (5%)	2 (1%)	21	13
All	All	1952/2160 (90%)	1875 (96%)	72 (4%)	5 (0%)	36	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	LEU
1	D	369	GLN
1	C	316	ILE
1	F	252	ILE
1	F	63	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	294/320 (92%)	289 (98%)	5 (2%)	53	53
1	B	296/320 (92%)	291 (98%)	5 (2%)	53	53
1	C	296/320 (92%)	290 (98%)	6 (2%)	48	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	291/320 (91%)	289 (99%)	2 (1%)	76	79
1	E	294/320 (92%)	287 (98%)	7 (2%)	43	40
1	F	292/320 (91%)	283 (97%)	9 (3%)	35	30
All	All	1763/1920 (92%)	1729 (98%)	34 (2%)	50	49

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

Mol	Chain	Res	Type
1	A	167	GLU
1	A	233	GLN
1	A	241	LYS
1	A	344	GLU
1	A	369	GLN
1	B	84	ASP
1	B	117	LYS
1	B	233	GLN
1	B	308	GLN
1	B	369	GLN
1	C	84	ASP
1	C	110	ARG
1	C	203	ARG
1	C	233	GLN
1	C	315	LEU
1	C	322	VAL
1	D	233	GLN
1	D	344	GLU
1	E	49	GLN
1	E	52	ARG
1	E	112	MET
1	E	115	LYS
1	E	233	GLN
1	E	238	ARG
1	E	327	ASP
1	F	36	LEU
1	F	77	ARG
1	F	92	LYS
1	F	110	ARG
1	F	137	GLU
1	F	228	ARG
1	F	233	GLN
1	F	241	LYS

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Mol	Chain	Res	Type
1	F	326	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	59	GLN
1	A	106	GLN
1	A	140	GLN
1	A	225	GLN
1	A	233	GLN
1	A	260	ASN
1	A	293	GLN
1	A	305	ASN
1	A	308	GLN
1	A	353	ASN
1	A	361	GLN
1	A	369	GLN
1	B	120	GLN
1	B	224	GLN
1	B	225	GLN
1	B	233	GLN
1	B	308	GLN
1	C	48	ASN
1	C	59	GLN
1	C	140	GLN
1	C	161	HIS
1	C	224	GLN
1	C	225	GLN
1	C	233	GLN
1	C	251	ASN
1	C	257	GLN
1	C	293	GLN
1	C	347	HIS
1	D	233	GLN
1	D	283	GLN
1	D	353	ASN
1	D	370	ASN
1	E	48	ASN
1	E	49	GLN
1	E	59	GLN
1	E	224	GLN

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Mol	Chain	Res	Type
1	E	225	GLN
1	E	233	GLN
1	E	283	GLN
1	E	293	GLN
1	E	353	ASN
1	F	48	ASN
1	F	59	GLN
1	F	98	HIS
1	F	134	ASN
1	F	224	GLN
1	F	225	GLN
1	F	233	GLN
1	F	257	GLN
1	F	283	GLN
1	F	293	GLN
1	F	347	HIS
1	F	353	ASN

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ER4	B	401	-	30,33,33	2.46	6 (20%)	36,45,45	1.09	2 (5%)
2	ER4	E	401	-	30,33,33	2.63	6 (20%)	36,45,45	1.08	2 (5%)
2	ER4	D	401	-	30,33,33	2.53	6 (20%)	36,45,45	1.10	2 (5%)
2	ER4	A	901	-	30,33,33	2.47	6 (20%)	36,45,45	1.10	2 (5%)
2	ER4	C	401	-	30,33,33	2.57	6 (20%)	36,45,45	1.10	2 (5%)
2	ER4	F	401	-	30,33,33	2.63	5 (16%)	36,45,45	1.08	2 (5%)

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	ER4	B	401	-	-	5/14/37/37	0/5/4/4
2	ER4	E	401	-	-	5/14/37/37	0/5/4/4
2	ER4	D	401	-	-	4/14/37/37	0/5/4/4
2	ER4	A	901	-	-	4/14/37/37	0/5/4/4
2	ER4	C	401	-	-	4/14/37/37	0/5/4/4
2	ER4	F	401	-	-	5/14/37/37	0/5/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	ER4	CAS-CBA	-11.83	1.42	1.51
2	F	401	ER4	CAS-CBA	-11.69	1.42	1.51
2	C	401	ER4	CAS-CBA	-11.40	1.43	1.51
2	D	401	ER4	CAS-CBA	-11.25	1.43	1.51
2	A	901	ER4	CAS-CBA	-11.06	1.43	1.51
2	B	401	ER4	CAS-CBA	-10.97	1.43	1.51
2	F	401	ER4	CAS-CAX	-3.26	1.41	1.52
2	E	401	ER4	CAS-CAX	-3.18	1.42	1.52
2	D	401	ER4	CAZ-NAU	3.17	1.38	1.33
2	A	901	ER4	CAS-CAX	-3.12	1.42	1.52
2	F	401	ER4	CAZ-NAU	3.03	1.38	1.33
2	C	401	ER4	CAS-CAX	-3.03	1.42	1.52
2	C	401	ER4	CAZ-NAU	3.01	1.38	1.33
2	D	401	ER4	CAS-CAX	-3.00	1.42	1.52
2	A	901	ER4	CAZ-NAU	2.95	1.38	1.33
2	B	401	ER4	CAS-CAX	-2.84	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ER4	CAZ-NAU	2.73	1.37	1.33
2	E	401	ER4	CAZ-NAU	2.69	1.37	1.33
2	F	401	ER4	CAH-CAX	2.42	1.43	1.38
2	D	401	ER4	CAH-CAX	2.38	1.43	1.38
2	C	401	ER4	CAH-CAX	2.38	1.43	1.38
2	E	401	ER4	CAH-CAX	2.32	1.43	1.38
2	A	901	ER4	CAH-CAX	2.29	1.43	1.38
2	A	901	ER4	CAF-CAH	2.21	1.42	1.38
2	C	401	ER4	CAG-CAI	2.13	1.42	1.38
2	B	401	ER4	CAH-CAX	2.12	1.43	1.38
2	F	401	ER4	CAG-CAI	2.12	1.42	1.38
2	E	401	ER4	CAI-CAX	2.09	1.43	1.38
2	B	401	ER4	CAF-CAH	2.09	1.42	1.38
2	B	401	ER4	CAG-CAI	2.08	1.42	1.38
2	A	901	ER4	CAG-CAI	2.06	1.42	1.38
2	D	401	ER4	CAG-CAI	2.06	1.42	1.38
2	C	401	ER4	CAF-CAH	2.04	1.42	1.38
2	E	401	ER4	CAG-CAI	2.02	1.42	1.38
2	D	401	ER4	CAG-CAE	2.00	1.42	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ER4	CAZ-NAU-CBA	3.79	122.97	117.63
2	E	401	ER4	CAZ-NAU-CBA	3.76	122.94	117.63
2	C	401	ER4	CAZ-NAU-CBA	3.71	122.87	117.63
2	D	401	ER4	CAZ-NAU-CBA	3.69	122.84	117.63
2	A	901	ER4	CAZ-NAU-CBA	3.68	122.82	117.63
2	F	401	ER4	CAZ-NAU-CBA	3.54	122.63	117.63
2	B	401	ER4	CAJ-CAY-CAC	-2.87	114.48	120.05
2	C	401	ER4	CAJ-CAY-CAC	-2.86	114.49	120.05
2	A	901	ER4	CAJ-CAY-CAC	-2.85	114.51	120.05
2	D	401	ER4	CAJ-CAY-CAC	-2.78	114.64	120.05
2	E	401	ER4	CAJ-CAY-CAC	-2.60	115.00	120.05
2	F	401	ER4	CAJ-CAY-CAC	-2.58	115.05	120.05

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	ER4	CAY-CAC-CAD-CBD
2	F	401	ER4	CAC-CAD-CBD-CAT

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Mol	Chain	Res	Type	Atoms
2	B	401	ER4	CAD-CAC-CAY-CBA
2	A	901	ER4	CAD-CAC-CAY-CBA
2	E	401	ER4	CAD-CAC-CAY-CBA
2	F	401	ER4	CAD-CAC-CAY-CBA
2	D	401	ER4	CAD-CAC-CAY-CBA
2	A	901	ER4	CAD-CAC-CAY-CAJ
2	F	401	ER4	CAM-CAL-CAN-OAW
2	B	401	ER4	CAD-CAC-CAY-CAJ
2	E	401	ER4	CAD-CAC-CAY-CAJ
2	F	401	ER4	CAD-CAC-CAY-CAJ
2	B	401	ER4	CAY-CAC-CAD-CBD
2	D	401	ER4	CAY-CAC-CAD-CBD
2	D	401	ER4	CAD-CAC-CAY-CAJ
2	C	401	ER4	CAD-CAC-CAY-CAJ
2	E	401	ER4	CAN-CAL-CAM-OAV
2	A	901	ER4	CAM-CAL-CAN-OAW
2	C	401	ER4	CAD-CAC-CAY-CBA
2	D	401	ER4	CAM-CAL-CAN-OAW
2	A	901	ER4	CAC-CAD-CBD-CAT
2	E	401	ER4	CAC-CAD-CBD-CAT
2	B	401	ER4	CAN-CAL-CAM-OAV
2	C	401	ER4	CAM-CAL-CAN-OAW
2	B	401	ER4	CAM-CAL-CAN-OAW
2	E	401	ER4	CAM-CAL-CAN-OAW
2	F	401	ER4	CAL-CAM-OAV-CAA

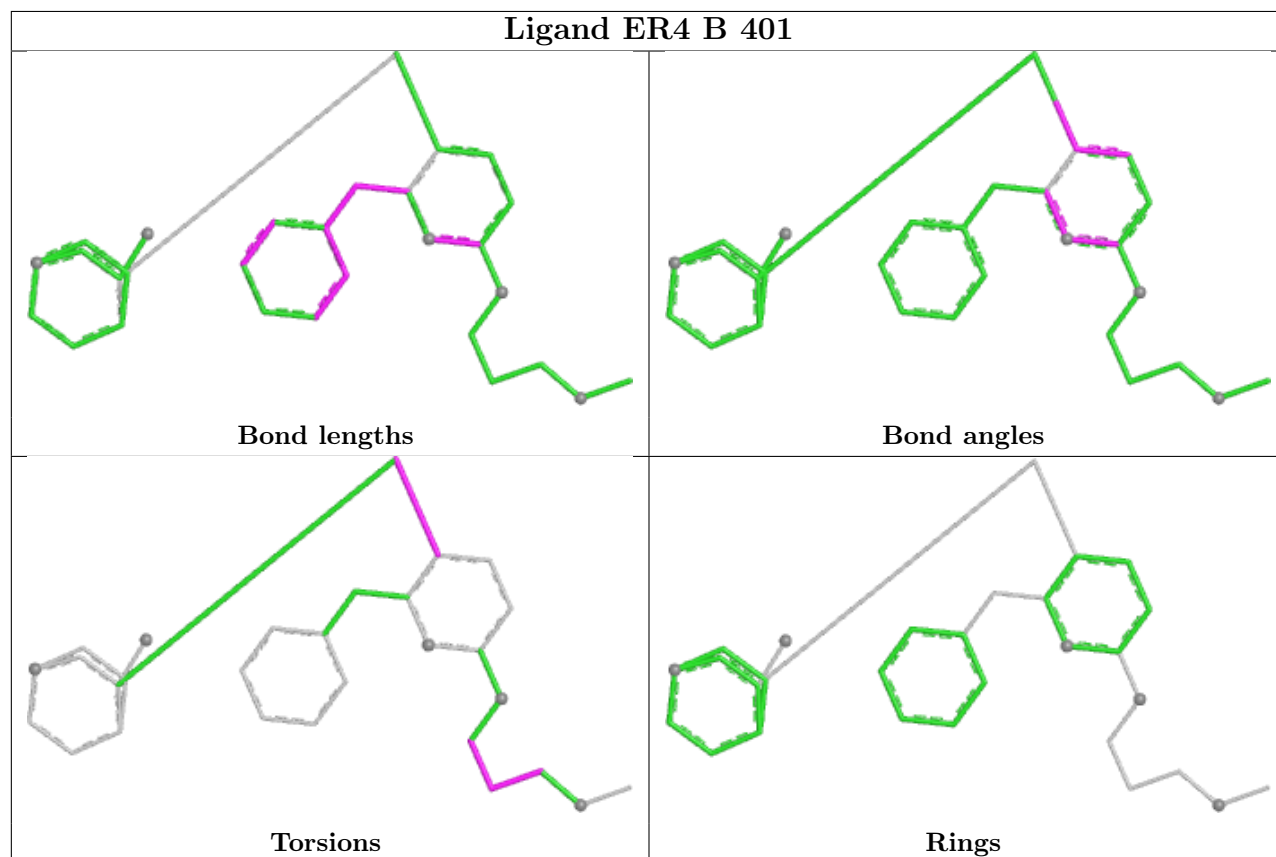
There are no ring outliers.

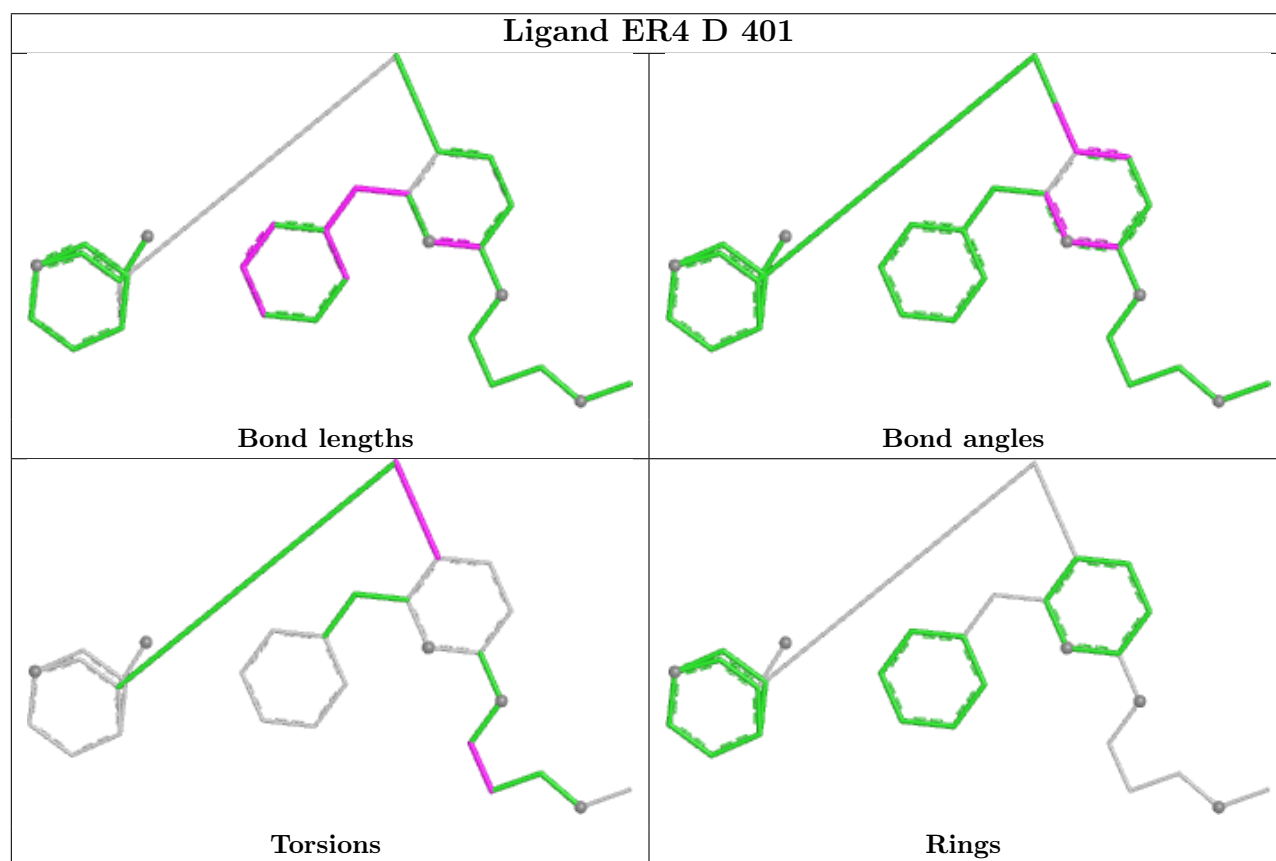
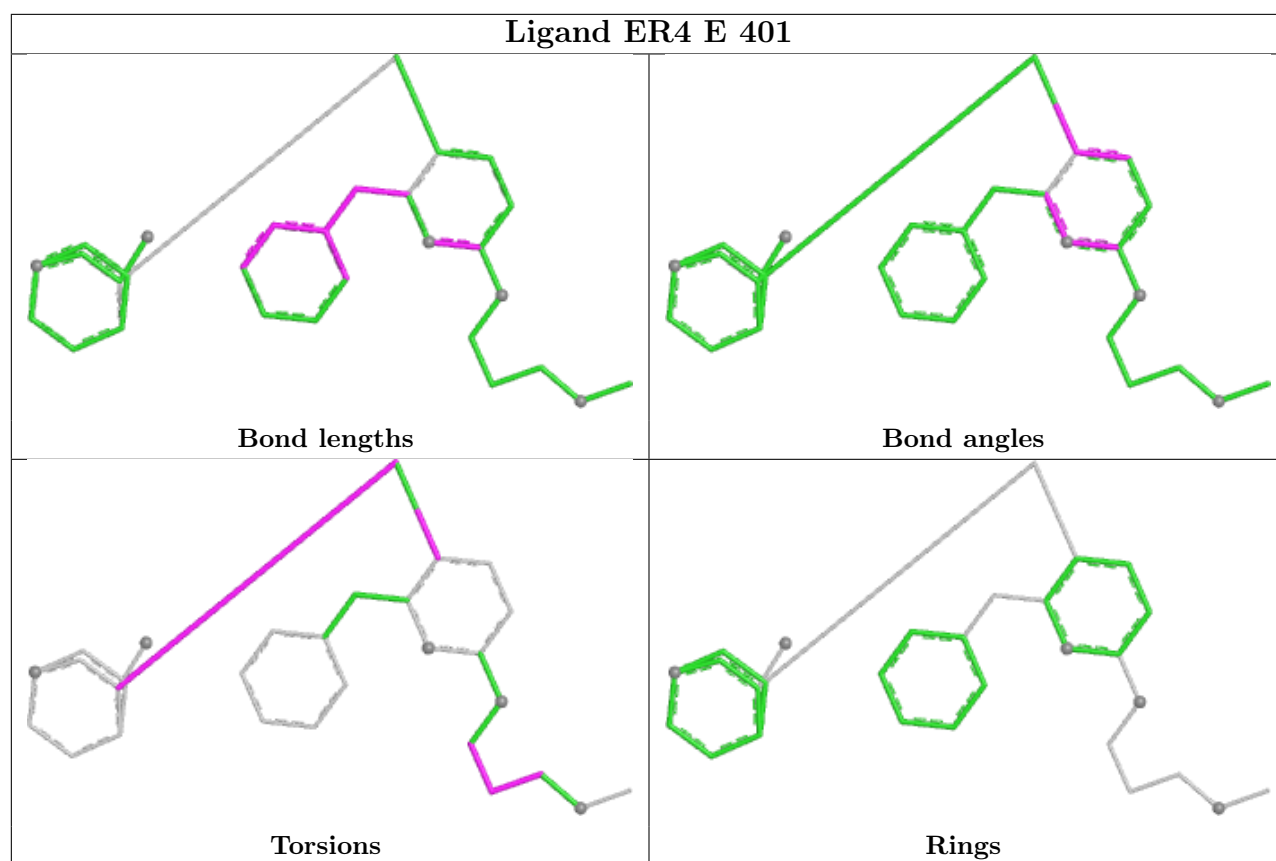
4 monomers are involved in 4 short contacts:

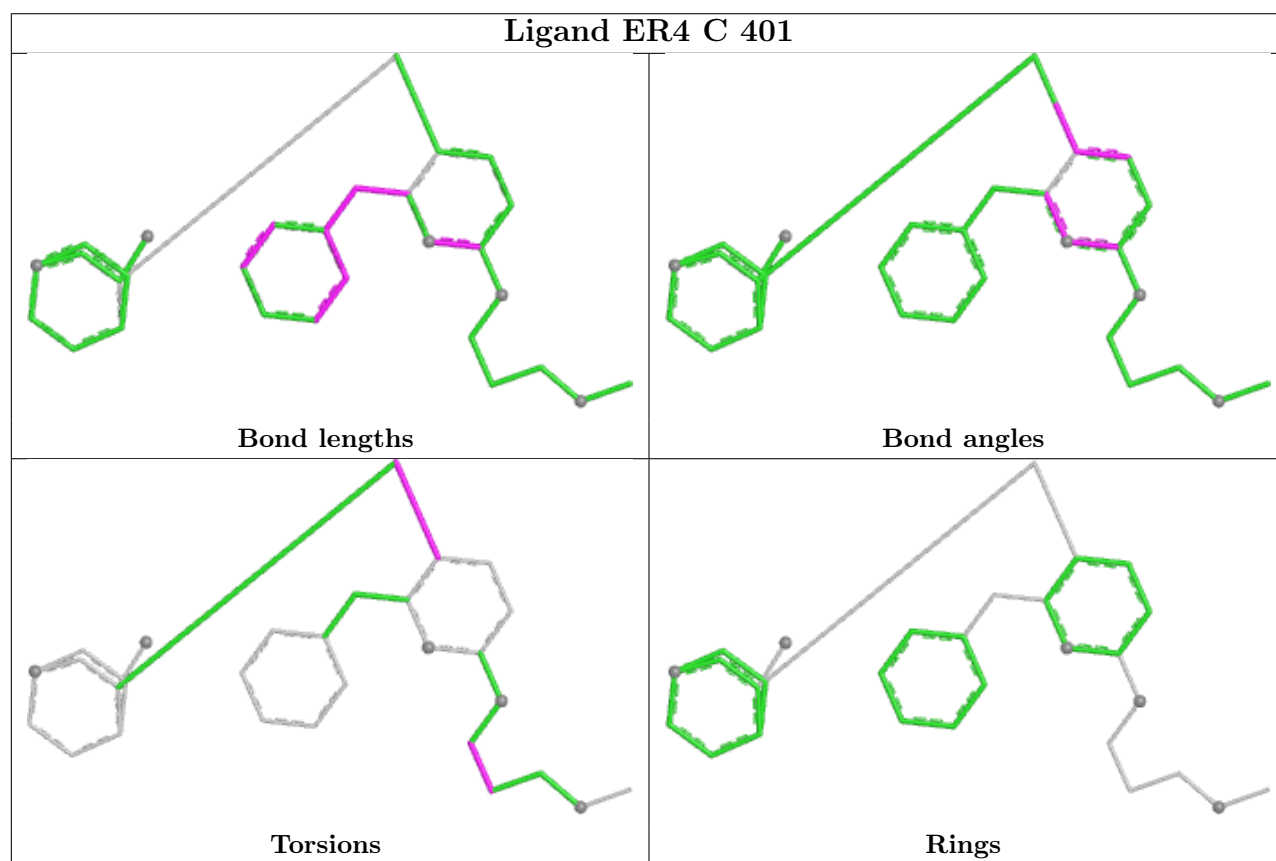
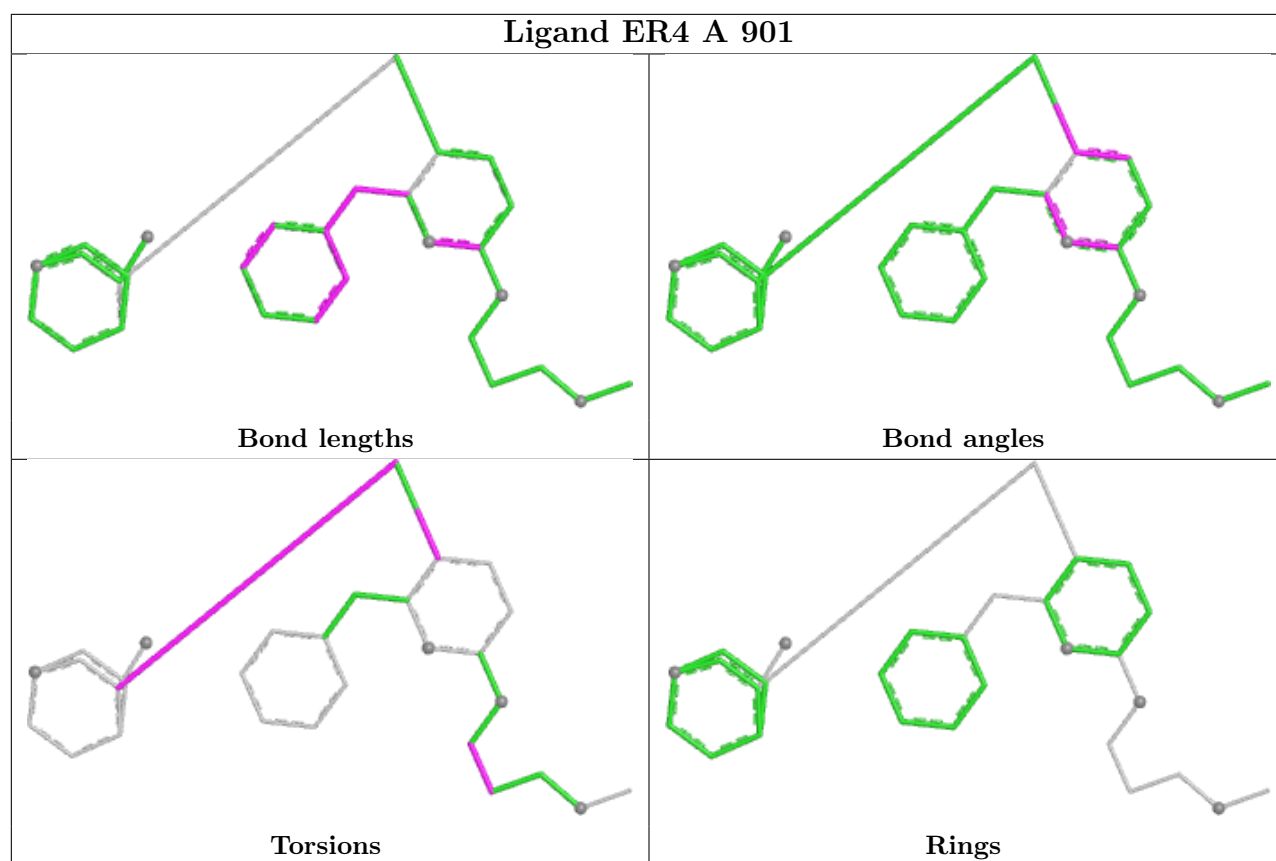
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ER4	1	0
2	D	401	ER4	1	0
2	A	901	ER4	1	0
2	F	401	ER4	1	0

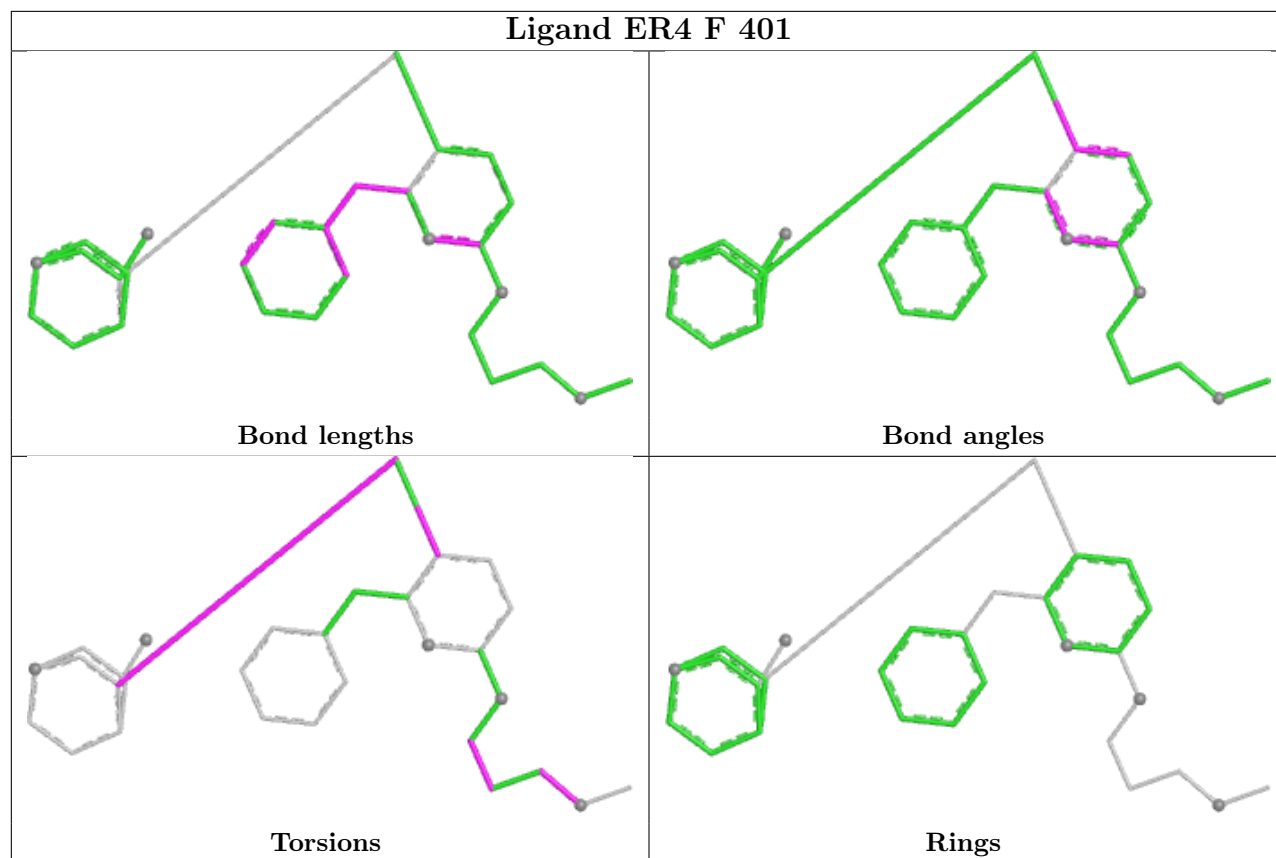
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	329/360 (91%)	-0.31	13 (3%)	42	43	13, 24, 50, 78	0
1	B	332/360 (92%)	0.07	26 (7%)	19	19	17, 28, 64, 79	0
1	C	332/360 (92%)	-0.07	11 (3%)	49	49	18, 29, 57, 76	0
1	D	325/360 (90%)	0.19	20 (6%)	26	26	19, 33, 67, 80	0
1	E	330/360 (91%)	0.29	12 (3%)	46	47	23, 38, 65, 80	0
1	F	328/360 (91%)	0.78	40 (12%)	8	8	22, 49, 78, 90	0
All	All	1976/2160 (91%)	0.16	122 (6%)	26	26	13, 33, 70, 90	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	315	LEU	4.6
1	F	322	VAL	4.2
1	D	321	ALA	4.2
1	F	235	VAL	4.0
1	A	315	LEU	4.0
1	D	322	VAL	3.9
1	C	321	ALA	3.9
1	F	321	ALA	3.8
1	B	35	SER	3.7
1	E	323	THR	3.7
1	A	316	ILE	3.6
1	F	323	THR	3.5
1	F	369	GLN	3.5
1	C	313	ALA	3.4
1	E	321	ALA	3.4
1	C	323	THR	3.4
1	A	323	THR	3.4
1	F	327	ASP	3.3
1	B	315	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	248	LEU	3.3
1	A	313	ALA	3.3
1	A	327	ASP	3.3
1	D	309	VAL	3.2
1	F	324	LEU	3.2
1	D	368	THR	3.2
1	E	370	ASN	3.2
1	A	322	VAL	3.1
1	B	34	ASP	3.1
1	A	324	LEU	3.1
1	B	368	THR	3.1
1	B	355	SER	3.1
1	F	248	LEU	3.1
1	F	252	ILE	3.1
1	D	370	ASN	3.0
1	B	313	ALA	3.0
1	A	314	VAL	3.0
1	C	324	LEU	3.0
1	D	323	THR	3.0
1	F	230	PHE	3.0
1	E	313	ALA	2.9
1	F	310	PHE	2.9
1	A	36	LEU	2.9
1	C	312	GLY	2.9
1	F	87	THR	2.9
1	F	236	TRP	2.9
1	A	325	MET	2.8
1	C	36	LEU	2.8
1	D	224	GLN	2.8
1	E	322	VAL	2.8
1	D	327	ASP	2.8
1	B	36	LEU	2.8
1	D	324	LEU	2.8
1	E	324	LEU	2.8
1	C	316	ILE	2.8
1	F	246	PHE	2.8
1	B	316	ILE	2.8
1	D	369	GLN	2.8
1	A	159	ASP	2.8
1	D	310	PHE	2.8
1	F	244	GLY	2.7
1	D	325	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	2.7
1	B	240	VAL	2.7
1	F	36	LEU	2.6
1	F	158	LEU	2.6
1	F	243	LEU	2.6
1	B	322	VAL	2.6
1	F	112	MET	2.6
1	B	236	TRP	2.6
1	B	312	GLY	2.5
1	F	326	MET	2.5
1	B	358	LYS	2.5
1	E	327	ASP	2.5
1	F	314	VAL	2.5
1	F	239	TYR	2.5
1	F	111	PHE	2.5
1	F	351	ASP	2.5
1	B	323	THR	2.5
1	D	243	LEU	2.5
1	F	88	ILE	2.5
1	B	354	PRO	2.4
1	B	310	PHE	2.4
1	E	314	VAL	2.4
1	F	226	GLY	2.4
1	F	352	SER	2.4
1	B	369	GLN	2.3
1	E	315	LEU	2.3
1	B	321	ALA	2.3
1	C	314	VAL	2.3
1	C	322	VAL	2.3
1	F	107	PRO	2.3
1	F	122	LEU	2.3
1	E	325	MET	2.3
1	B	256	VAL	2.3
1	B	254	LEU	2.3
1	F	53	SER	2.2
1	F	118	ASP	2.2
1	B	347	HIS	2.2
1	D	239	TYR	2.2
1	B	352	SER	2.2
1	C	159	ASP	2.2
1	D	326	MET	2.2
1	F	255	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	347	HIS	2.2
1	D	347	HIS	2.1
1	D	252	ILE	2.1
1	A	53	SER	2.1
1	B	243	LEU	2.1
1	B	252	ILE	2.1
1	F	228	ARG	2.1
1	D	159	ASP	2.1
1	F	157	PHE	2.1
1	F	104	LEU	2.0
1	F	224	GLN	2.0
1	A	52	ARG	2.0
1	E	316	ILE	2.0
1	F	90	VAL	2.0
1	F	256	VAL	2.0
1	D	236	TRP	2.0
1	F	85	ASP	2.0
1	B	228	ARG	2.0
1	E	312	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
2	ER4	F	401	30/30	0.90	0.11	39,48,61,61	0
2	ER4	E	401	30/30	0.92	0.10	33,38,58,59	0
2	ER4	D	401	30/30	0.94	0.08	24,30,44,44	0
2	ER4	B	401	30/30	0.94	0.08	19,29,50,51	0

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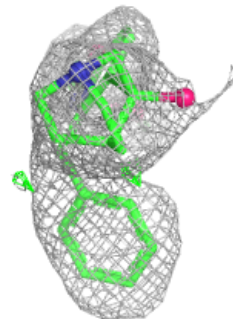
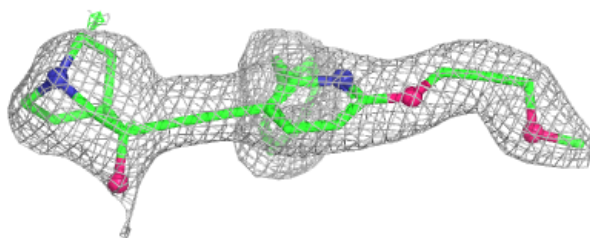
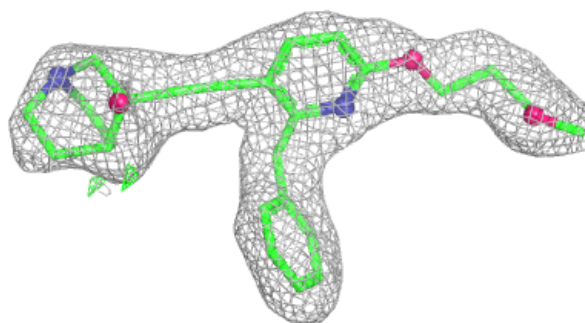
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ER4	C	401	30/30	0.94	0.08	23,29,48,48	0
2	ER4	A	901	30/30	0.95	0.07	20,25,44,45	0

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.

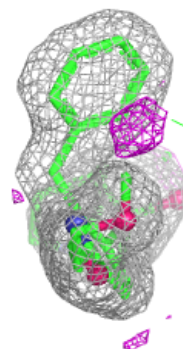
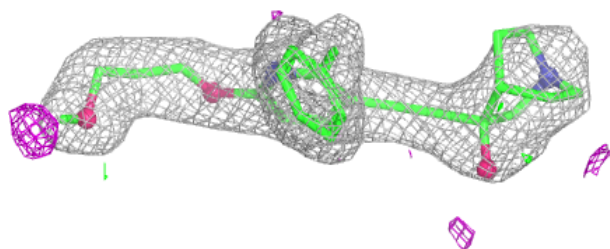
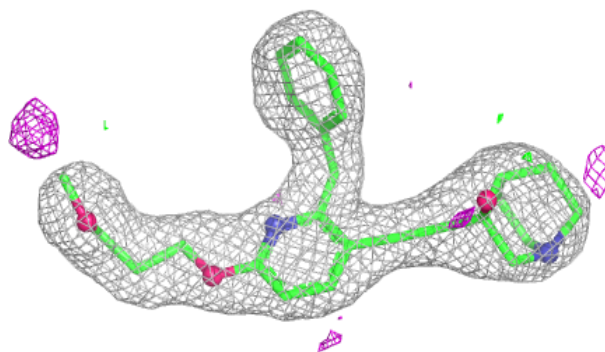
Electron density around ER4 F 401:

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

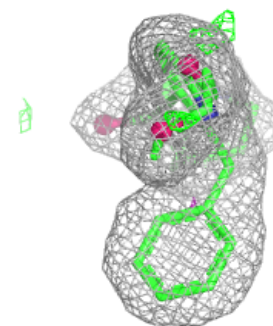
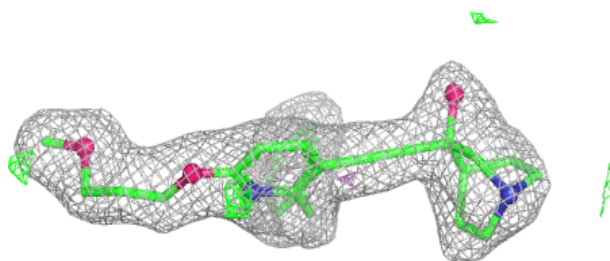
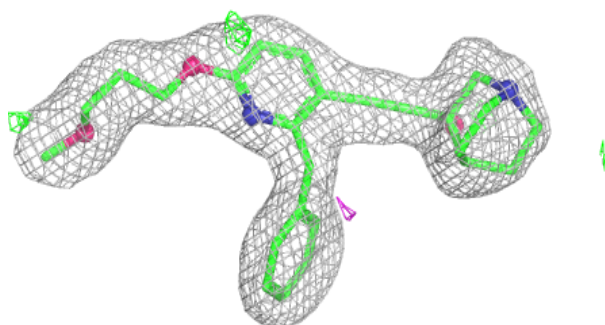


Electron density around ER4 E 401:

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

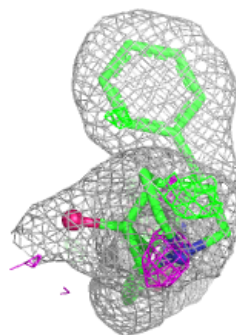
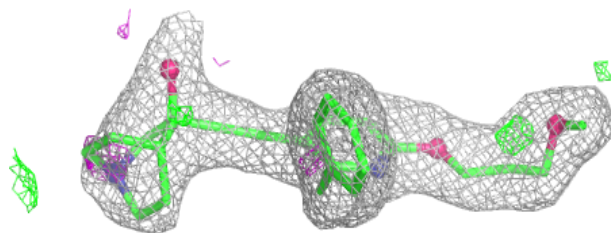
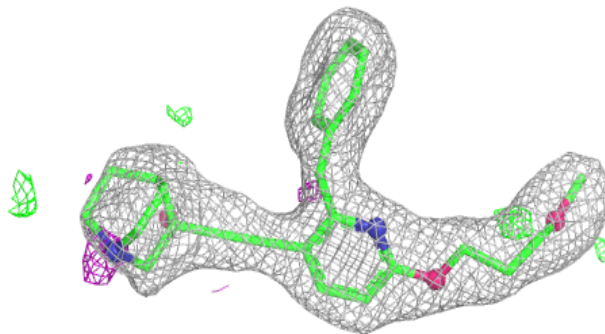
**Electron density around ER4 D 401:**

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

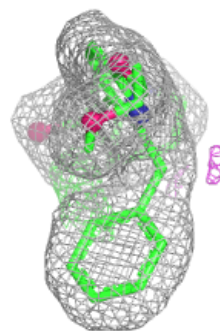
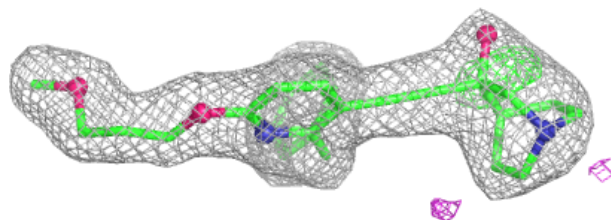
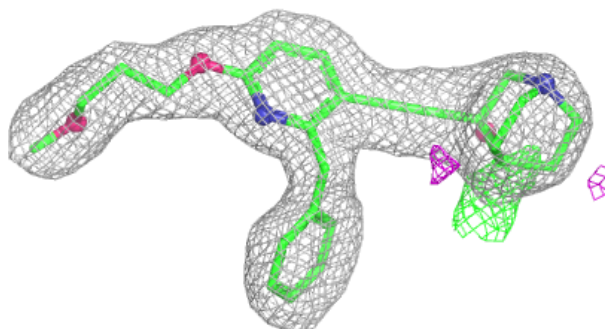


Electron density around ER4 B 401:

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

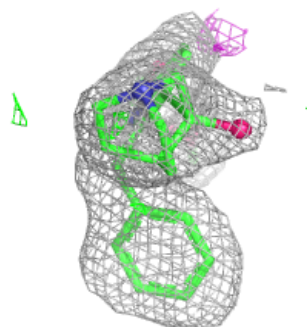
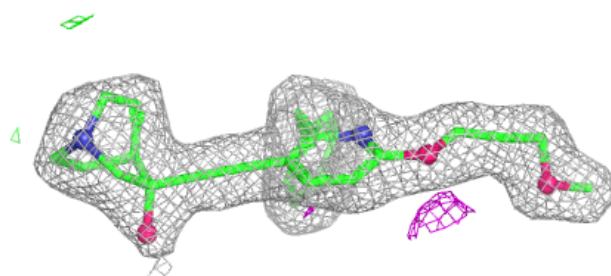
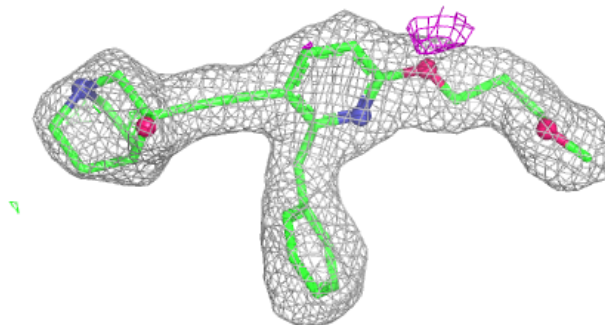
**Electron density around ER4 C 401:**

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



Electron density around ER4 A 901:

$2mF_o-DF_c$ (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.