



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:15 am BST

PDB ID : 3WCJ
Title : The complex structure of HsSQS wtih ligand,E5700
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 : 2013-05-27
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

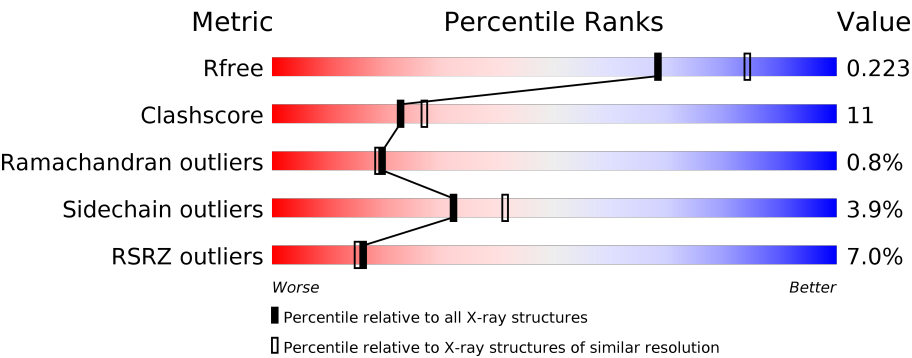
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>76%14%• 7%</div></div>
1	B	360	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>75%15%• 8%</div></div>
1	C	360	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>72%19%• 7%</div></div>
1	D	360	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>67%24%• 7%</div></div>
1	E	360	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>70%21%• 7%</div></div>
1	F	360	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>63%27%• 7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17199 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	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	B	332	Total	C	N	O	S	0	0	0
			2678	1705	453	502	18			
1	C	335	Total	C	N	O	S	0	0	0
			2704	1721	460	505	18			
1	D	335	Total	C	N	O	S	0	0	0
			2704	1721	460	505	18			
1	E	335	Total	C	N	O	S	0	0	0
			2704	1721	460	505	18			
1	F	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	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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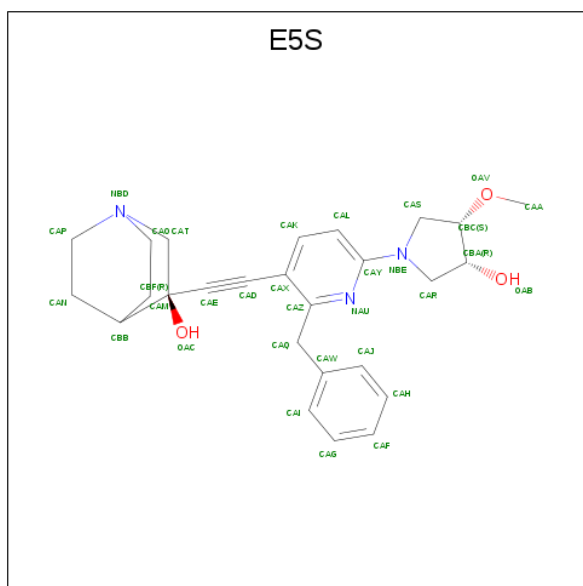
Chain	Residue	Modelled	Actual	Comment	Reference
E	16	HIS	-	EXPRESSION TAG	UNP P37268
E	17	HIS	-	EXPRESSION TAG	UNP P37268
E	18	HIS	-	EXPRESSION TAG	UNP P37268
E	19	HIS	-	EXPRESSION TAG	UNP P37268
E	20	HIS	-	EXPRESSION TAG	UNP P37268
E	21	SER	-	EXPRESSION TAG	UNP P37268
E	22	SER	-	EXPRESSION TAG	UNP P37268
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-($\{2\text{-benzyl-6-}[(3R,4S)\text{-3-hydroxy-4-methoxypyrrolidin-1-yl}]pyridin\text{-3-yl}\}$ ethynyl)-1-azabicyclo[2.2.2]octan-3-ol (three-letter code: E5S) (formula: $C_{26}H_{31}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 32	C 26	N 3	O 3	0	0
2	B	1	Total 32	C 26	N 3	O 3	0	0
2	C	1	Total 32	C 26	N 3	O 3	0	0
2	D	1	Total 32	C 26	N 3	O 3	0	0
2	E	1	Total 32	C 26	N 3	O 3	0	0
2	F	1	Total 32	C 26	N 3	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	178	Total O 178 178	0	0
3	B	204	Total O 204 204	0	0

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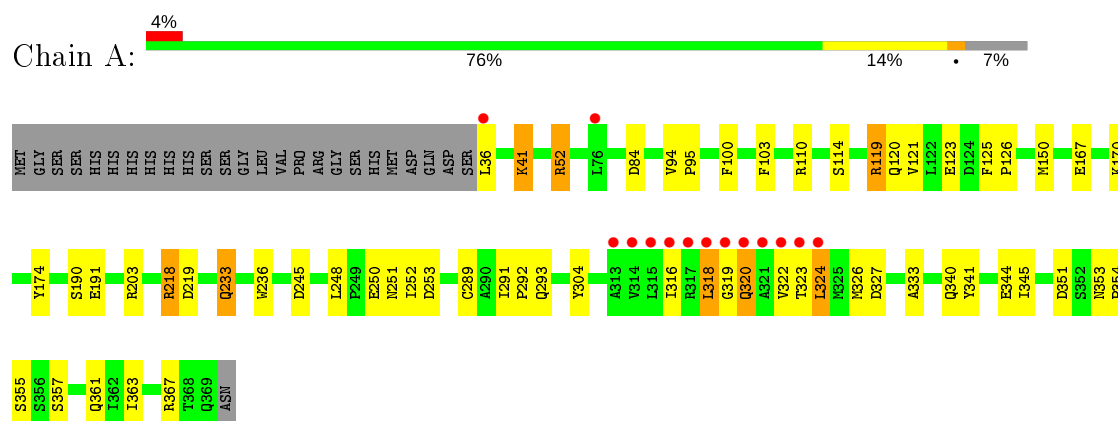
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	160	Total 160	O 160	0	0
3	D	131	Total 131	O 131	0	0
3	E	86	Total 86	O 86	0	0
3	F	66	Total 66	O 66	0	0

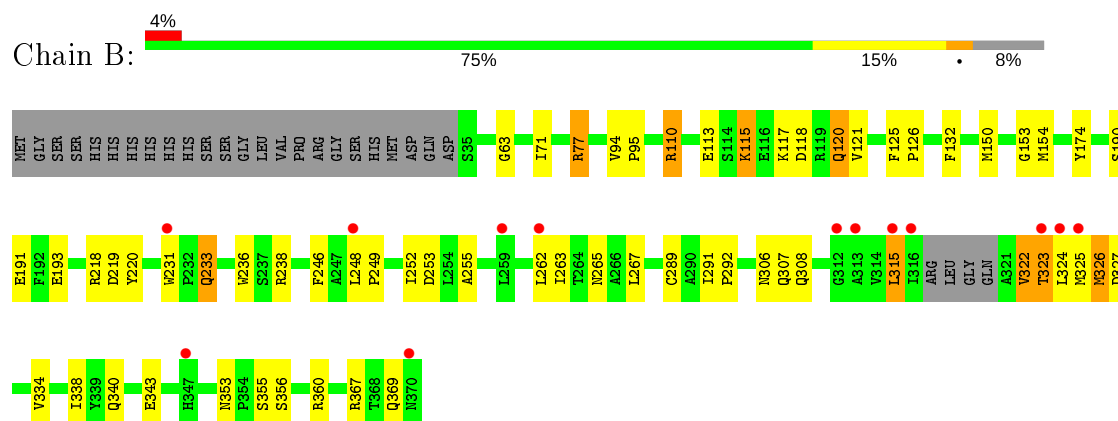
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

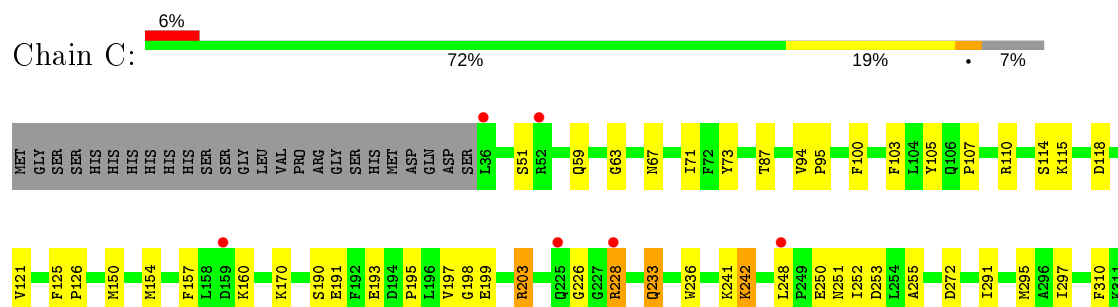
• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase

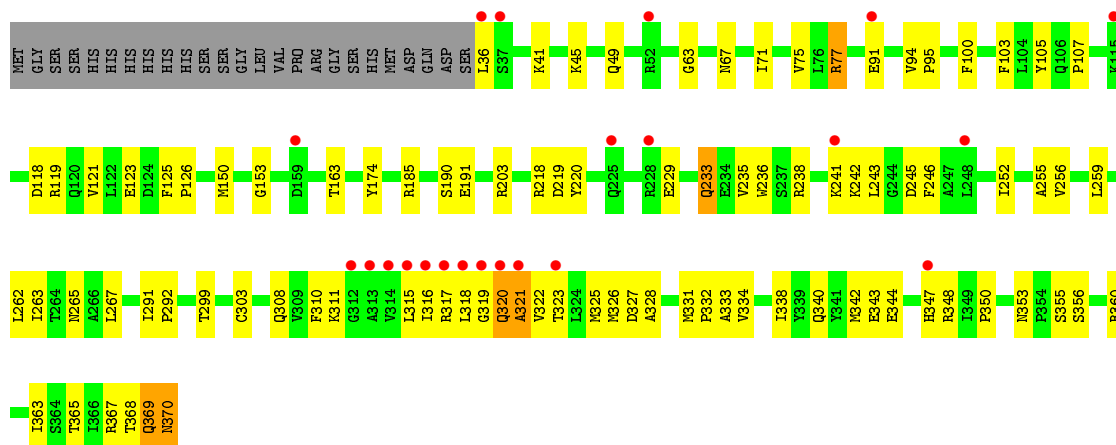


• Molecule 1: Squalene synthase

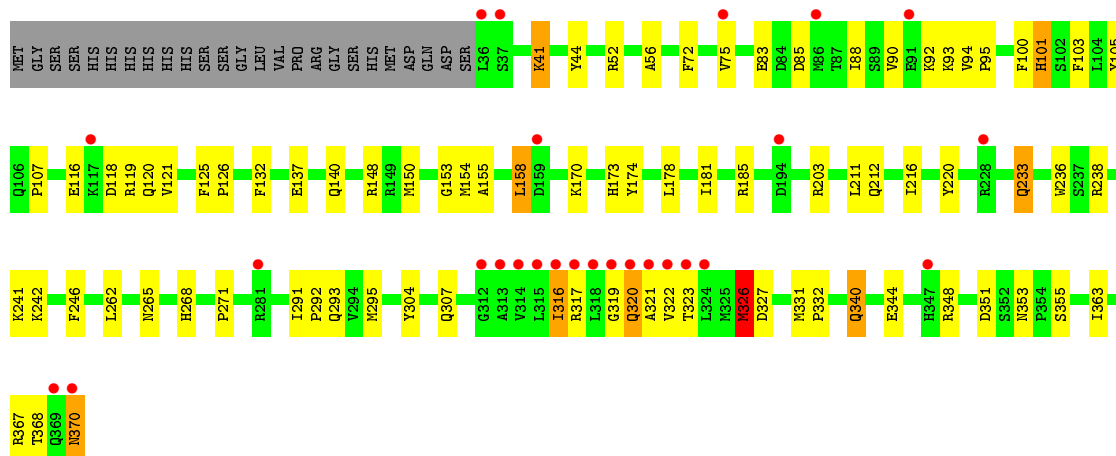




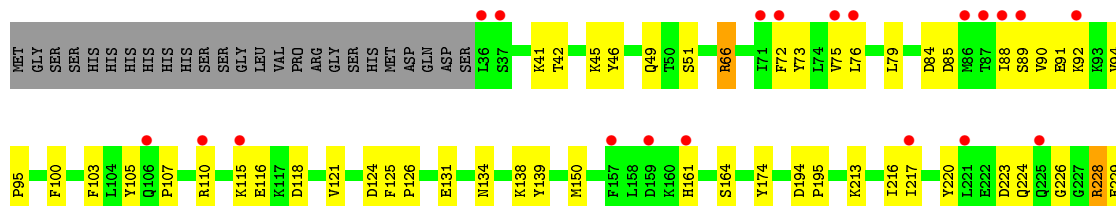
• Molecule 1: Squalene synthase

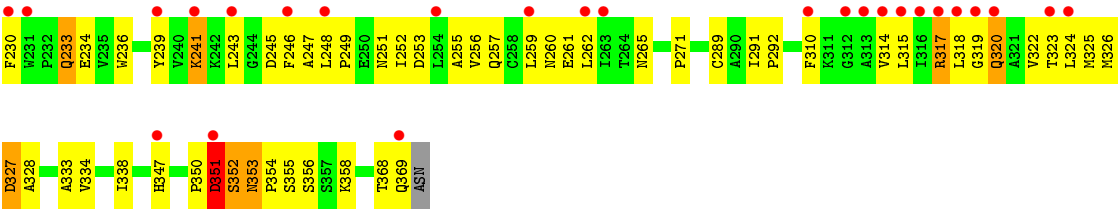


• Molecule 1: Squalene synthase



• 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	85.33Å 153.62Å 92.11Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.86 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.20) 93.8 (24.86-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.198 , 0.225 0.194 , 0.223	Depositor DCC
R_{free} test set	5697 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17199	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: E5S

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	0.39	0/2751	0.59	0/3724
1	B	0.37	0/2732	0.57	1/3698 (0.0%)
1	C	0.36	0/2759	0.57	0/3735
1	D	0.34	0/2759	0.54	0/3735
1	E	0.33	0/2759	0.53	0/3735
1	F	0.32	0/2751	0.52	0/3724
All	All	0.35	0/16511	0.55	1/22351 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	LEU	CA-CB-CG	6.63	130.56	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2696	0	2676	51	0
1	B	2678	0	2651	56	0
1	C	2704	0	2682	72	0
1	D	2704	0	2682	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2704	0	2682	72	0
1	F	2696	0	2676	87	0
2	A	32	0	31	1	0
2	B	32	0	31	1	0
2	C	32	0	31	0	0
2	D	32	0	31	0	0
2	E	32	0	31	0	0
2	F	32	0	31	1	0
3	A	178	0	0	0	0
3	B	204	0	0	2	0
3	C	160	0	0	3	0
3	D	131	0	0	1	0
3	E	86	0	0	3	0
3	F	66	0	0	0	0
All	All	17199	0	16235	374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (374) 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:C:315:LEU:HG	1:C:316:ILE:H	1.20	1.04
1:E:319:GLY:HA3	1:E:323:THR:HG21	1.40	1.01
1:B:323:THR:O	1:B:325:MET:N	1.98	0.96
1:F:260:ASN:HD22	1:F:353:ASN:ND2	1.65	0.94
1:C:317:ARG:HG3	1:C:317:ARG:HH21	1.32	0.92
1:C:317:ARG:HB2	3:C:578:HOH:O	1.69	0.92
1:C:315:LEU:HG	1:C:316:ILE:N	1.86	0.91
1:F:233:GLN:HA	1:F:236:TRP:NE1	1.86	0.90
1:E:319:GLY:CA	1:E:323:THR:HG21	2.03	0.89
1:E:326:MET:HA	1:F:327:ASP:OD2	1.75	0.86
1:C:226:GLY:HA3	1:C:228:ARG:HH11	1.40	0.86
1:C:317:ARG:CG	1:C:317:ARG:HH21	1.89	0.85
1:A:320:GLN:HG3	1:A:340:GLN:HB3	1.58	0.83
1:F:228:ARG:HB2	1:F:228:ARG:NH1	1.94	0.82
1:F:318:LEU:HD12	1:F:318:LEU:H	1.44	0.82
1:E:320:GLN:HG2	1:E:321:ALA:H	1.46	0.80
1:A:320:GLN:O	1:A:323:THR:HG22	1.81	0.79
1:D:368:THR:HG21	1:E:41:LYS:HA	1.64	0.78
1:A:326:MET:HA	1:B:327:ASP:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ASN:HD22	1:F:353:ASN:HD21	1.31	0.77
1:B:233:GLN:HA	1:B:236:TRP:NE1	1.99	0.77
1:A:319:GLY:CA	1:A:323:THR:HG21	2.15	0.76
1:B:120:GLN:NE2	1:B:120:GLN:H	1.82	0.76
1:A:323:THR:HG23	1:A:324:LEU:N	2.00	0.75
1:E:326:MET:HA	1:F:327:ASP:CG	2.07	0.75
1:A:319:GLY:HA2	1:A:323:THR:HG21	1.69	0.74
1:A:320:GLN:NE2	1:A:344:GLU:HG3	2.02	0.74
1:F:233:GLN:HA	1:F:236:TRP:CD1	2.23	0.74
1:B:322:VAL:HG12	1:B:340:GLN:NE2	2.03	0.73
1:C:226:GLY:HA3	1:C:228:ARG:NH1	2.03	0.72
1:E:150:MET:HG3	1:E:174:TYR:O	1.90	0.72
1:D:233:GLN:HA	1:D:236:TRP:NE1	2.05	0.71
1:D:235:VAL:HA	1:D:238:ARG:HH21	1.53	0.71
1:E:105:TYR:O	1:E:107:PRO:HD3	1.91	0.70
1:E:90:VAL:O	1:E:94:VAL:HG23	1.91	0.70
1:D:327:ASP:CG	1:F:326:MET:HA	2.12	0.69
1:C:320:GLN:HG2	1:C:321:ALA:H	1.57	0.69
1:D:327:ASP:OD1	1:F:326:MET:HA	1.92	0.69
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.27	0.69
1:F:319:GLY:HA3	1:F:323:THR:HG21	1.74	0.69
1:A:357:SER:O	1:A:361:GLN:HG3	1.93	0.68
1:F:229:GLU:HB2	1:F:243:LEU:HD13	1.76	0.68
1:B:326:MET:HE3	1:C:291:ILE:HD11	1.76	0.67
1:C:314:VAL:HG12	1:C:315:LEU:H	1.60	0.67
1:D:94:VAL:HB	1:D:95:PRO:HD3	1.77	0.66
1:D:365:THR:O	1:D:369:GLN:HB3	1.95	0.66
1:B:118:ASP:C	1:B:120:GLN:HE21	1.99	0.66
1:A:323:THR:HG23	1:A:324:LEU:H	1.61	0.66
1:E:93:LYS:HD2	1:E:158:LEU:HD11	1.76	0.65
1:A:322:VAL:HG12	1:A:326:MET:SD	2.36	0.65
1:E:155:ALA:O	1:E:158:LEU:HB2	1.96	0.65
1:A:327:ASP:OD1	1:C:327:ASP:HB3	1.97	0.65
1:F:105:TYR:O	1:F:107:PRO:HD3	1.96	0.65
1:F:320:GLN:O	1:F:324:LEU:HG	1.98	0.64
1:A:218:ARG:NH1	1:A:219:ASP:OD1	2.31	0.64
1:A:320:GLN:HB2	1:A:340:GLN:OE1	1.98	0.64
1:A:248:LEU:HD23	1:A:250:GLU:OE1	1.98	0.63
1:C:315:LEU:HG	1:C:316:ILE:HG12	1.81	0.63
1:C:315:LEU:CG	1:C:316:ILE:N	2.58	0.63
1:D:368:THR:HG22	1:E:44:TYR:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:ASP:O	1:E:121:VAL:HG22	1.99	0.63
1:A:326:MET:HE2	1:A:333:ALA:HA	1.80	0.63
1:C:365:THR:O	1:C:369:GLN:HG3	1.98	0.63
1:C:320:GLN:HG2	1:C:321:ALA:N	2.14	0.62
1:A:245:ASP:HA	1:A:248:LEU:HD13	1.81	0.62
1:C:317:ARG:NH2	1:C:317:ARG:HG3	2.05	0.62
1:E:132:PHE:CZ	1:E:140:GLN:HB2	2.34	0.62
1:E:353:ASN:ND2	1:E:355:SER:H	1.98	0.62
1:F:89:SER:HB2	1:F:91:GLU:OE1	2.00	0.62
1:C:118:ASP:O	1:C:121:VAL:HG22	2.00	0.61
1:C:203:ARG:HD2	1:C:272:ASP:OD1	2.00	0.61
1:D:322:VAL:HG13	1:E:291:ILE:HG21	1.81	0.61
1:A:318:LEU:HB3	1:A:341:TYR:HE1	1.65	0.61
1:C:314:VAL:HG12	1:C:315:LEU:N	2.16	0.60
1:E:317:ARG:NH1	1:E:348:ARG:NH1	2.49	0.60
1:C:320:GLN:CG	1:C:321:ALA:H	2.13	0.60
1:D:100:PHE:HA	1:D:103:PHE:CD2	2.37	0.60
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.17	0.60
1:E:331:MET:HB3	1:E:332:PRO:HD3	1.84	0.60
1:F:236:TRP:CE2	1:F:243:LEU:HG	2.37	0.60
1:F:94:VAL:HB	1:F:95:PRO:HD3	1.83	0.60
1:B:353:ASN:ND2	1:B:355:SER:H	1.98	0.60
1:D:368:THR:HG21	1:E:41:LYS:HG3	1.84	0.60
1:B:323:THR:C	1:B:325:MET:H	1.99	0.59
1:F:322:VAL:O	1:F:325:MET:HB2	2.01	0.59
1:C:315:LEU:O	1:C:317:ARG:HD3	2.03	0.59
1:E:233:GLN:HA	1:E:236:TRP:NE1	2.17	0.59
1:A:323:THR:CG2	1:A:324:LEU:N	2.65	0.59
1:B:117:LYS:O	1:B:120:GLN:NE2	2.35	0.59
1:D:308:GLN:NE2	1:D:311:LYS:HD2	2.18	0.59
1:D:299:THR:HA	1:D:316:ILE:HD11	1.84	0.59
1:C:94:VAL:HB	1:C:95:PRO:HD3	1.85	0.58
1:B:322:VAL:HA	1:C:295:MET:CE	2.33	0.58
1:F:228:ARG:HB2	1:F:228:ARG:CZ	2.32	0.58
1:C:348:ARG:O	1:C:350:PRO:HD3	2.03	0.58
1:B:110:ARG:NH2	3:B:534:HOH:O	2.37	0.58
1:B:252:ILE:HG23	1:B:253:ASP:N	2.18	0.58
1:F:118:ASP:O	1:F:121:VAL:HG22	2.04	0.57
1:D:370:ASN:H	1:D:370:ASN:ND2	2.02	0.57
1:D:363:ILE:O	1:D:367:ARG:HG2	2.02	0.57
1:A:323:THR:CG2	1:A:324:LEU:H	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLN:O	1:C:324:LEU:HG	2.03	0.57
1:B:190:SER:O	1:B:191:GLU:HB2	2.03	0.57
1:F:90:VAL:O	1:F:94:VAL:HG23	2.05	0.57
1:D:308:GLN:NE2	1:D:308:GLN:HA	2.20	0.57
1:B:323:THR:O	1:B:326:MET:N	2.37	0.56
1:A:233:GLN:HA	1:A:236:TRP:NE1	2.20	0.56
1:C:248:LEU:HB2	1:C:251:ASN:HD22	1.70	0.56
1:A:363:ILE:O	1:A:367:ARG:HG2	2.05	0.56
1:D:308:GLN:HE21	1:D:308:GLN:HA	1.69	0.56
1:F:260:ASN:ND2	1:F:353:ASN:HD21	2.03	0.56
1:C:353:ASN:ND2	1:C:355:SER:H	2.02	0.56
1:D:150:MET:HG3	1:D:174:TYR:O	2.03	0.56
1:B:150:MET:HG3	1:B:174:TYR:O	2.06	0.56
1:D:353:ASN:ND2	1:D:355:SER:H	2.04	0.56
1:D:71:ILE:O	1:D:75:VAL:HG13	2.06	0.56
1:E:212:GLN:HE21	1:E:216:ILE:HG13	1.70	0.56
1:C:318:LEU:O	1:C:318:LEU:HD23	2.06	0.56
1:B:252:ILE:HD11	1:B:307:GLN:HB3	1.88	0.55
1:D:370:ASN:HD22	1:D:370:ASN:H	1.52	0.55
1:D:319:GLY:HA3	1:D:323:THR:HG21	1.88	0.55
1:E:125:PHE:N	1:E:126:PRO:CD	2.69	0.55
1:C:100:PHE:HA	1:C:103:PHE:CD2	2.42	0.55
1:A:36:LEU:N	1:A:36:LEU:HD12	2.22	0.55
1:F:220:TYR:OH	1:F:246:PHE:HB2	2.06	0.55
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.89	0.55
1:C:195:PRO:O	1:C:199:GLU:HG3	2.07	0.55
1:B:325:MET:O	1:C:327:ASP:HB2	2.07	0.54
1:A:150:MET:HG3	1:A:174:TYR:O	2.07	0.54
1:A:326:MET:CE	1:A:333:ALA:HA	2.38	0.54
1:A:245:ASP:O	1:A:248:LEU:HB2	2.08	0.54
1:A:326:MET:HA	1:B:327:ASP:CB	2.33	0.54
1:D:348:ARG:O	1:D:350:PRO:HD3	2.08	0.54
1:C:105:TYR:O	1:C:107:PRO:HD3	2.07	0.54
1:A:41:LYS:HA	1:C:368:THR:HG21	1.89	0.54
1:D:327:ASP:OD2	1:D:328:ALA:N	2.40	0.54
1:F:325:MET:CE	1:F:325:MET:HA	2.38	0.54
1:A:353:ASN:ND2	1:A:355:SER:H	2.06	0.53
1:B:120:GLN:CD	1:B:120:GLN:H	2.09	0.53
1:E:320:GLN:CG	1:E:321:ALA:H	2.16	0.53
1:F:262:LEU:O	1:F:265:ASN:HB3	2.08	0.53
1:D:220:TYR:OH	1:D:246:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LYS:HG2	1:F:49:GLN:HE21	1.74	0.53
1:D:163:THR:HA	1:D:233:GLN:HB3	1.91	0.53
1:D:299:THR:HA	1:D:316:ILE:CD1	2.38	0.53
1:F:150:MET:HG3	1:F:174:TYR:O	2.09	0.53
1:F:85:ASP:OD2	1:F:88:ILE:HG13	2.09	0.53
1:C:248:LEU:HB3	1:C:250:GLU:OE1	2.10	0.52
1:F:255:ALA:HB1	1:F:310:PHE:CE2	2.44	0.52
1:F:239:TYR:HE2	1:F:261:GLU:OE1	1.93	0.52
1:F:350:PRO:C	1:F:352:SER:H	2.13	0.52
1:F:247:ALA:O	1:F:249:PRO:HD3	2.10	0.52
1:C:318:LEU:HD23	1:C:324:LEU:HD21	1.91	0.52
1:D:326:MET:HE2	1:D:333:ALA:HA	1.92	0.52
1:B:322:VAL:HA	1:C:295:MET:HE3	1.91	0.52
1:D:327:ASP:OD2	1:F:325:MET:O	2.28	0.52
1:B:289:CYS:HA	2:B:401:E5S:H20	1.92	0.51
1:D:153:GLY:HA3	1:D:174:TYR:CG	2.45	0.51
1:E:56:ALA:HB3	3:E:520:HOH:O	2.10	0.51
1:F:326:MET:HE2	1:F:333:ALA:HA	1.91	0.51
1:E:344:GLU:O	1:E:348:ARG:HD3	2.10	0.51
1:D:218:ARG:HD2	1:D:219:ASP:OD1	2.11	0.51
1:F:115:LYS:NZ	1:F:115:LYS:HB3	2.24	0.51
1:D:370:ASN:HD22	1:D:370:ASN:N	2.08	0.51
1:D:45:LYS:O	1:D:49:GLN:HG3	2.11	0.51
1:E:153:GLY:HA3	1:E:174:TYR:CG	2.45	0.51
1:F:260:ASN:ND2	1:F:353:ASN:ND2	2.48	0.51
1:B:218:ARG:HD2	1:B:219:ASP:OD1	2.11	0.51
1:B:369:GLN:HB2	3:B:679:HOH:O	2.10	0.51
1:C:51:SER:HB2	1:C:73:TYR:CZ	2.46	0.51
1:C:316:ILE:C	1:C:318:LEU:H	2.14	0.51
1:D:125:PHE:N	1:D:126:PRO:CD	2.73	0.50
1:F:320:GLN:O	1:F:323:THR:HG22	2.12	0.50
1:B:343:GLU:OE1	1:B:367:ARG:NH2	2.43	0.50
1:E:236:TRP:CZ3	1:E:242:LYS:HA	2.46	0.50
1:F:138:LYS:HE3	1:F:139:TYR:CZ	2.47	0.50
1:E:323:THR:HB	1:E:340:GLN:NE2	2.26	0.50
1:F:89:SER:OG	1:F:92:LYS:HB2	2.12	0.50
1:C:326:MET:HE2	1:C:333:ALA:HA	1.94	0.50
1:E:295:MET:CE	1:E:295:MET:HA	2.42	0.50
1:F:228:ARG:HB2	1:F:228:ARG:HH11	1.71	0.50
1:E:323:THR:HA	1:E:326:MET:CG	2.42	0.50
1:F:79:LEU:HB2	1:F:100:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:ILE:HB	1:F:292:PRO:HD3	1.94	0.50
1:E:322:VAL:HB	1:E:340:GLN:OE1	2.12	0.49
1:F:236:TRP:HZ3	1:F:241:LYS:C	2.16	0.49
1:A:170:LYS:HE2	1:A:174:TYR:OH	2.12	0.49
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.47	0.49
1:F:75:VAL:HG23	1:F:76:LEU:N	2.27	0.49
1:E:320:GLN:HG2	1:E:321:ALA:N	2.21	0.49
1:D:242:LYS:HB2	1:D:245:ASP:OD2	2.13	0.49
1:E:92:LYS:O	1:E:95:PRO:HD2	2.11	0.49
1:A:248:LEU:HB2	1:A:251:ASN:HD22	1.78	0.49
1:A:291:ILE:HG21	1:C:322:VAL:HG13	1.94	0.49
1:C:317:ARG:O	1:C:319:GLY:N	2.45	0.49
1:D:252:ILE:O	1:D:256:VAL:HG23	2.12	0.49
1:E:233:GLN:HA	1:E:236:TRP:CD1	2.48	0.49
1:F:115:LYS:HB3	1:F:115:LYS:HZ2	1.77	0.49
1:C:170:LYS:HA	3:C:585:HOH:O	2.11	0.49
1:D:259:LEU:HB2	1:D:310:PHE:HZ	1.76	0.49
1:C:190:SER:O	1:C:191:GLU:HB2	2.13	0.49
1:E:233:GLN:HA	1:E:236:TRP:CE2	2.48	0.49
1:D:319:GLY:C	1:D:323:THR:HB	2.33	0.49
1:E:170:LYS:O	1:E:173:HIS:HB3	2.13	0.48
1:B:353:ASN:HD21	1:B:355:SER:HB2	1.77	0.48
1:C:250:GLU:CD	1:C:250:GLU:H	2.17	0.48
1:E:320:GLN:HB3	1:E:340:GLN:OE1	2.14	0.48
1:B:322:VAL:HA	1:C:295:MET:HE1	1.96	0.48
1:E:307:GLN:HG3	3:E:513:HOH:O	2.13	0.48
1:B:233:GLN:HA	1:B:236:TRP:CD1	2.49	0.48
1:D:291:ILE:HB	1:D:292:PRO:HD3	1.95	0.48
1:A:326:MET:CA	1:B:327:ASP:HB2	2.40	0.47
1:A:289:CYS:HA	2:A:901:E5S:H20	1.95	0.47
1:C:364:SER:O	1:C:368:THR:HG23	2.14	0.47
1:A:114:SER:O	1:A:119:ARG:HD3	2.14	0.47
1:F:125:PHE:N	1:F:126:PRO:CD	2.77	0.47
1:B:125:PHE:N	1:B:126:PRO:CD	2.77	0.47
1:D:233:GLN:HA	1:D:236:TRP:CE2	2.50	0.47
1:C:150:MET:O	1:C:154:MET:HG3	2.14	0.47
1:D:67:ASN:O	1:D:71:ILE:HG12	2.15	0.47
1:C:320:GLN:CG	1:C:321:ALA:N	2.77	0.47
1:B:323:THR:HG22	1:B:340:GLN:OE1	2.14	0.47
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.96	0.47
1:E:326:MET:HE3	1:F:291:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:TYR:O	1:E:348:ARG:NH2	2.47	0.47
1:E:72:PHE:O	1:E:75:VAL:HG22	2.15	0.47
1:D:316:ILE:O	1:D:316:ILE:HG22	2.16	0.46
1:F:325:MET:HA	1:F:325:MET:HE2	1.97	0.46
1:E:319:GLY:CA	1:E:323:THR:CG2	2.87	0.46
1:C:193:GLU:HB3	1:C:197:VAL:HG21	1.98	0.46
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.29	0.46
1:A:119:ARG:O	1:A:123:GLU:HG3	2.15	0.46
1:C:228:ARG:H	1:C:228:ARG:HD3	1.80	0.46
1:E:291:ILE:HB	1:E:292:PRO:HD3	1.98	0.46
1:E:92:LYS:C	1:E:95:PRO:HD2	2.35	0.46
1:D:185:ARG:HD2	3:D:512:HOH:O	2.16	0.46
1:D:338:ILE:O	1:D:342:MET:HG2	2.16	0.46
1:E:116:GLU:O	1:E:119:ARG:HG3	2.15	0.46
1:E:85:ASP:HB3	1:E:88:ILE:HD12	1.98	0.46
1:A:125:PHE:N	1:A:126:PRO:CD	2.79	0.45
1:C:250:GLU:N	1:C:250:GLU:OE2	2.49	0.45
1:D:119:ARG:O	1:D:123:GLU:HG3	2.15	0.45
1:D:246:PHE:CD1	1:D:255:ALA:HA	2.51	0.45
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.52	0.45
1:E:368:THR:OG1	1:F:41:LYS:HA	2.16	0.45
1:F:72:PHE:CZ	1:F:76:LEU:HD11	2.52	0.45
1:E:94:VAL:N	1:E:95:PRO:CD	2.80	0.45
1:F:51:SER:HB2	1:F:73:TYR:CZ	2.51	0.45
1:D:325:MET:O	1:E:327:ASP:HB2	2.17	0.45
1:B:306:ASN:OD1	1:B:308:GLN:HB2	2.17	0.44
1:C:87:THR:OG1	1:C:115:LYS:HG2	2.17	0.44
1:F:245:ASP:O	1:F:248:LEU:HB2	2.17	0.44
1:F:246:PHE:CD1	1:F:255:ALA:HA	2.52	0.44
1:C:157:PHE:CE2	1:C:160:LYS:HE3	2.52	0.44
1:E:370:ASN:HB3	1:F:66:ARG:CD	2.47	0.44
1:F:334:VAL:O	1:F:338:ILE:HG13	2.18	0.44
1:B:153:GLY:HA3	1:B:174:TYR:CG	2.52	0.44
1:D:105:TYR:O	1:D:107:PRO:HD3	2.18	0.44
1:D:308:GLN:HE22	1:D:311:LYS:HD2	1.83	0.44
1:E:268:HIS:O	1:E:271:PRO:HD2	2.17	0.44
1:B:262:LEU:O	1:B:265:ASN:HB3	2.18	0.44
1:D:153:GLY:HA3	1:D:174:TYR:CD1	2.53	0.44
1:F:131:GLU:HA	1:F:134:ASN:HD22	1.83	0.44
1:F:248:LEU:HB2	1:F:251:ASN:HD22	1.82	0.44
1:F:318:LEU:H	1:F:318:LEU:CD1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:CG	1:A:52:ARG:HH11	2.29	0.43
1:E:93:LYS:CD	1:E:158:LEU:HD11	2.47	0.43
1:C:233:GLN:HA	1:C:236:TRP:CD1	2.53	0.43
1:F:194:ASP:OD1	1:F:195:PRO:HD2	2.18	0.43
1:D:41:LYS:HA	1:F:368:THR:HG21	1.99	0.43
1:A:289:CYS:O	1:A:293:GLN:HG2	2.18	0.43
1:D:320:GLN:O	1:D:321:ALA:C	2.56	0.43
1:B:291:ILE:HB	1:B:292:PRO:HD3	1.99	0.43
1:C:317:ARG:HD2	1:C:317:ARG:HA	1.89	0.43
1:A:327:ASP:HB3	1:C:326:MET:HA	2.00	0.43
1:D:190:SER:O	1:D:191:GLU:HB2	2.18	0.43
1:D:77:ARG:CG	1:D:77:ARG:HH11	2.32	0.43
1:F:124:ASP:O	1:F:124:ASP:CG	2.57	0.43
1:F:85:ASP:HA	1:F:116:GLU:OE2	2.17	0.43
1:B:246:PHE:CD1	1:B:255:ALA:HA	2.53	0.43
1:B:248:LEU:HA	1:B:249:PRO:HD3	1.87	0.43
1:B:353:ASN:ND2	1:B:355:SER:HB2	2.34	0.43
1:C:67:ASN:O	1:C:71:ILE:HG12	2.18	0.43
1:F:353:ASN:HA	1:F:354:PRO:HD3	1.79	0.43
1:F:92:LYS:C	1:F:95:PRO:HD2	2.39	0.43
1:A:316:ILE:N	1:A:316:ILE:HD12	2.33	0.43
1:E:181:ILE:O	1:E:185:ARG:HG3	2.19	0.43
1:F:239:TYR:HE1	1:F:257:GLN:HE21	1.67	0.43
1:C:297:ILE:CD1	1:C:338:ILE:HG12	2.49	0.43
1:E:137:GLU:HA	1:E:140:GLN:HG2	2.00	0.43
1:E:211:LEU:HG	1:E:293:GLN:HE22	1.83	0.43
1:E:83:GLU:HB2	1:E:154:MET:HE2	2.00	0.43
1:A:252:ILE:HG23	1:A:253:ASP:N	2.33	0.42
1:B:263:ILE:O	1:B:267:LEU:HG	2.18	0.42
1:F:213:LYS:O	1:F:217:ILE:HG13	2.19	0.42
1:A:233:GLN:HA	1:A:236:TRP:CD1	2.54	0.42
1:C:114:SER:C	1:C:115:LYS:HD2	2.39	0.42
1:D:229:GLU:HG2	1:D:243:LEU:HD23	2.02	0.42
1:E:320:GLN:O	1:E:323:THR:HG22	2.19	0.42
1:F:317:ARG:HG3	1:F:318:LEU:O	2.20	0.42
1:B:326:MET:HA	1:C:327:ASP:HB2	2.02	0.42
1:E:101:HIS:ND1	1:E:148:ARG:HB2	2.34	0.42
1:D:343:GLU:OE1	1:D:367:ARG:NH2	2.52	0.42
1:F:355:SER:O	1:F:358:LYS:N	2.52	0.42
1:B:326:MET:HE3	1:C:291:ILE:CD1	2.44	0.42
1:F:271:PRO:HA	1:F:369:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:O	1:B:326:MET:HG3	2.19	0.42
1:B:71:ILE:HG21	1:B:132:PHE:HA	2.02	0.42
1:C:331:MET:HB3	1:C:332:PRO:HD3	2.02	0.42
1:E:320:GLN:CG	1:E:321:ALA:N	2.81	0.42
1:F:256:VAL:O	1:F:259:LEU:HB3	2.19	0.42
1:A:233:GLN:HE21	1:A:233:GLN:HB3	1.62	0.42
1:B:113:GLU:O	1:B:115:LYS:HD2	2.20	0.42
1:B:193:GLU:OE1	1:B:193:GLU:HA	2.19	0.42
1:E:295:MET:HE2	1:E:295:MET:HA	2.02	0.42
1:F:42:THR:HG22	1:F:46:TYR:CE2	2.55	0.42
1:B:220:TYR:HB2	1:B:231:TRP:CZ2	2.54	0.42
1:C:241:LYS:HE3	1:C:241:LYS:HB3	1.85	0.42
1:D:344:GLU:HG2	1:D:348:ARG:HH12	1.85	0.42
1:D:356:SER:O	1:D:360:ARG:HG3	2.18	0.42
1:E:317:ARG:HB2	3:E:507:HOH:O	2.19	0.42
1:F:92:LYS:O	1:F:95:PRO:HD2	2.20	0.42
1:D:331:MET:HB3	1:D:332:PRO:HD3	2.02	0.42
1:D:320:GLN:HB3	1:D:340:GLN:OE1	2.19	0.42
1:E:353:ASN:HD21	1:E:355:SER:HB2	1.85	0.42
1:F:223:ASP:O	1:F:228:ARG:O	2.37	0.42
1:F:220:TYR:CZ	1:F:246:PHE:HB2	2.54	0.42
1:F:355:SER:O	1:F:356:SER:C	2.58	0.42
1:F:216:ILE:HG23	1:F:230:PHE:HB2	2.02	0.41
1:F:241:LYS:NZ	1:F:241:LYS:HB2	2.35	0.41
1:C:252:ILE:HG23	1:C:253:ASP:N	2.34	0.41
1:D:262:LEU:O	1:D:265:ASN:HB3	2.21	0.41
1:F:224:GLN:C	1:F:226:GLY:H	2.23	0.41
1:F:252:ILE:HG23	1:F:253:ASP:N	2.36	0.41
1:F:318:LEU:N	1:F:318:LEU:HD12	2.22	0.41
1:E:363:ILE:O	1:E:367:ARG:HG3	2.20	0.41
1:F:289:CYS:HA	2:F:401:E5S:H20	2.02	0.41
1:F:164:SER:HB3	1:F:234:GLU:OE1	2.20	0.41
1:A:353:ASN:HA	1:A:354:PRO:HD3	1.83	0.41
1:B:118:ASP:O	1:B:121:VAL:HG22	2.21	0.41
1:B:233:GLN:HE21	1:B:233:GLN:HB3	1.57	0.41
1:B:252:ILE:CG2	1:B:253:ASP:N	2.84	0.41
1:E:326:MET:N	1:F:327:ASP:HB2	2.35	0.41
1:B:150:MET:O	1:B:154:MET:HG3	2.19	0.41
1:B:334:VAL:O	1:B:338:ILE:HG13	2.21	0.41
1:B:356:SER:O	1:B:360:ARG:HG3	2.20	0.41
1:E:370:ASN:HB3	1:F:66:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HG2	1:A:121:VAL:N	2.36	0.41
1:A:291:ILE:HB	1:A:292:PRO:HD3	2.02	0.41
1:A:304:TYR:CD2	1:A:345:ILE:HG23	2.56	0.41
1:B:77:ARG:HD3	1:B:77:ARG:HA	1.90	0.41
1:E:150:MET:HG2	1:E:154:MET:SD	2.61	0.41
1:E:233:GLN:HB3	1:E:233:GLN:HE21	1.71	0.41
1:E:94:VAL:HB	1:E:95:PRO:HD3	2.02	0.41
1:A:322:VAL:CG1	1:A:326:MET:SD	3.07	0.41
1:D:263:ILE:O	1:D:267:LEU:HG	2.21	0.41
1:D:334:VAL:O	1:D:338:ILE:HG13	2.20	0.41
1:C:59:GLN:HE21	1:C:59:GLN:HB2	1.75	0.41
1:D:259:LEU:HD21	1:D:303:CYS:O	2.20	0.40
1:B:233:GLN:HA	1:B:236:TRP:CE2	2.55	0.40
1:F:351:ASP:OD1	1:F:351:ASP:N	2.45	0.40
1:A:190:SER:O	1:A:191:GLU:HB2	2.20	0.40
1:C:198:GLY:HA3	3:C:592:HOH:O	2.21	0.40
1:C:236:TRP:CZ3	1:C:242:LYS:HA	2.57	0.40
1:C:255:ALA:HB1	1:C:310:PHE:CZ	2.56	0.40
1:C:356:SER:O	1:C:360:ARG:HG3	2.20	0.40
1:B:353:ASN:HD22	1:B:355:SER:H	1.66	0.40
1:C:125:PHE:N	1:C:126:PRO:CD	2.85	0.40
1:C:248:LEU:HB2	1:C:251:ASN:ND2	2.34	0.40
1:D:118:ASP:O	1:D:121:VAL:HG22	2.22	0.40
1:E:220:TYR:CZ	1:E:246:PHE:HB2	2.56	0.40
1:E:262:LEU:O	1:E:265:ASN:HB3	2.21	0.40
1:F:72:PHE:CE1	1:F:76:LEU:HD11	2.56	0.40
1:E:178:LEU:HD23	1:E:181:ILE:HD12	2.02	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	332/360 (92%)	318 (96%)	13 (4%)	1 (0%)	41	46
1	B	328/360 (91%)	314 (96%)	12 (4%)	2 (1%)	25	26
1	C	333/360 (92%)	320 (96%)	10 (3%)	3 (1%)	17	16
1	D	333/360 (92%)	315 (95%)	14 (4%)	4 (1%)	13	10
1	E	333/360 (92%)	315 (95%)	15 (4%)	3 (1%)	17	16
1	F	332/360 (92%)	305 (92%)	24 (7%)	3 (1%)	17	16
All	All	1991/2160 (92%)	1887 (95%)	88 (4%)	16 (1%)	19	19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	LEU
1	B	324	LEU
1	C	316	ILE
1	C	318	LEU
1	D	320	GLN
1	E	316	ILE
1	F	328	ALA
1	D	318	LEU
1	E	320	GLN
1	D	321	ALA
1	C	63	GLY
1	D	63	GLY
1	E	326	MET
1	F	66	ARG
1	F	351	ASP
1	B	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	297/320 (93%)	285 (96%)	12 (4%)	31	40
1	B	296/320 (92%)	286 (97%)	10 (3%)	37	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	298/320 (93%)	290 (97%)	8 (3%)	44	57
1	D	298/320 (93%)	287 (96%)	11 (4%)	34	43
1	E	298/320 (93%)	284 (95%)	14 (5%)	26	33
1	F	297/320 (93%)	282 (95%)	15 (5%)	24	29
All	All	1784/1920 (93%)	1714 (96%)	70 (4%)	32	41

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	52	ARG
1	A	84	ASP
1	A	110	ARG
1	A	119	ARG
1	A	167	GLU
1	A	203	ARG
1	A	218	ARG
1	A	233	GLN
1	A	320	GLN
1	A	324	LEU
1	A	351	ASP
1	B	77	ARG
1	B	110	ARG
1	B	115	LYS
1	B	120	GLN
1	B	233	GLN
1	B	238	ARG
1	B	315	LEU
1	B	322	VAL
1	B	323	THR
1	B	326	MET
1	C	110	ARG
1	C	203	ARG
1	C	228	ARG
1	C	233	GLN
1	C	242	LYS
1	C	315	LEU
1	C	317	ARG
1	C	368	THR
1	D	36	LEU
1	D	77	ARG

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Mol	Chain	Res	Type
1	D	91	GLU
1	D	203	ARG
1	D	233	GLN
1	D	241	LYS
1	D	315	LEU
1	D	317	ARG
1	D	347	HIS
1	D	369	GLN
1	D	370	ASN
1	E	41	LYS
1	E	52	ARG
1	E	101	HIS
1	E	120	GLN
1	E	158	LEU
1	E	203	ARG
1	E	233	GLN
1	E	238	ARG
1	E	241	LYS
1	E	316	ILE
1	E	326	MET
1	E	340	GLN
1	E	351	ASP
1	E	370	ASN
1	F	84	ASP
1	F	110	ARG
1	F	161	HIS
1	F	228	ARG
1	F	233	GLN
1	F	241	LYS
1	F	314	VAL
1	F	315	LEU
1	F	317	ARG
1	F	320	GLN
1	F	327	ASP
1	F	347	HIS
1	F	351	ASP
1	F	352	SER
1	F	353	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	233	GLN
1	A	251	ASN
1	A	257	GLN
1	A	308	GLN
1	A	320	GLN
1	A	361	GLN
1	B	120	GLN
1	B	225	GLN
1	B	233	GLN
1	B	251	ASN
1	B	257	GLN
1	B	308	GLN
1	B	340	GLN
1	C	49	GLN
1	C	225	GLN
1	C	251	ASN
1	C	257	GLN
1	D	225	GLN
1	D	233	GLN
1	D	257	GLN
1	D	308	GLN
1	D	353	ASN
1	D	370	ASN
1	E	49	GLN
1	E	212	GLN
1	E	225	GLN
1	E	233	GLN
1	E	257	GLN
1	E	293	GLN
1	E	353	ASN
1	F	134	ASN
1	F	161	HIS
1	F	225	GLN
1	F	233	GLN
1	F	251	ASN
1	F	257	GLN
1	F	308	GLN
1	F	353	ASN
1	F	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	E5S	A	901	-	34,36,36	2.89	4 (11%)	39,52,52	1.41	3 (7%)
2	E5S	B	401	-	34,36,36	2.86	3 (8%)	39,52,52	1.36	3 (7%)
2	E5S	D	401	-	34,36,36	2.91	3 (8%)	39,52,52	1.48	4 (10%)
2	E5S	C	401	-	34,36,36	2.88	4 (11%)	39,52,52	1.41	4 (10%)
2	E5S	F	401	-	34,36,36	2.92	4 (11%)	39,52,52	1.38	4 (10%)
2	E5S	E	401	-	34,36,36	2.91	4 (11%)	39,52,52	1.38	3 (7%)

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	E5S	A	901	-	-	5/14/49/49	0/6/5/5
2	E5S	B	401	-	-	3/14/49/49	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E5S	D	401	-	-	4/14/49/49	0/6/5/5
2	E5S	C	401	-	-	2/14/49/49	0/6/5/5
2	E5S	F	401	-	-	3/14/49/49	0/6/5/5
2	E5S	E	401	-	-	1/14/49/49	0/6/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	E5S	CAQ-CAZ	-15.83	1.39	1.51
2	E	401	E5S	CAQ-CAZ	-15.82	1.39	1.51
2	D	401	E5S	CAQ-CAZ	-15.81	1.39	1.51
2	A	901	E5S	CAQ-CAZ	-15.72	1.39	1.51
2	C	401	E5S	CAQ-CAZ	-15.58	1.39	1.51
2	B	401	E5S	CAQ-CAZ	-15.53	1.39	1.51
2	A	901	E5S	CAQ-CAW	-3.95	1.39	1.52
2	E	401	E5S	CAQ-CAW	-3.94	1.39	1.52
2	D	401	E5S	CAQ-CAW	-3.94	1.39	1.52
2	F	401	E5S	CAQ-CAW	-3.94	1.39	1.52
2	C	401	E5S	CAQ-CAW	-3.92	1.39	1.52
2	B	401	E5S	CAQ-CAW	-3.87	1.39	1.52
2	C	401	E5S	CAD-CAE	2.72	1.23	1.19
2	F	401	E5S	CAD-CAE	2.46	1.22	1.19
2	E	401	E5S	CAD-CAE	2.45	1.22	1.19
2	D	401	E5S	CAD-CAE	2.33	1.22	1.19
2	B	401	E5S	CAD-CAE	2.32	1.22	1.19
2	A	901	E5S	CAD-CAE	2.28	1.22	1.19
2	E	401	E5S	CAY-NBE	-2.13	1.33	1.37
2	F	401	E5S	CAY-NBE	-2.08	1.33	1.37
2	C	401	E5S	CAY-NBE	-2.08	1.33	1.37
2	A	901	E5S	CAY-NBE	-2.06	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	E5S	CAR-CBA-CBC	-5.90	98.52	104.18
2	C	401	E5S	CAR-CBA-CBC	-5.44	98.96	104.18
2	B	401	E5S	CAR-CBA-CBC	-5.43	98.97	104.18
2	F	401	E5S	CAR-CBA-CBC	-5.43	98.97	104.18
2	E	401	E5S	CAR-CBA-CBC	-5.36	99.03	104.18
2	A	901	E5S	CAR-CBA-CBC	-5.13	99.25	104.18
2	C	401	E5S	CAS-NBE-CAY	3.48	127.85	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	E5S	CAS-NBE-CAY	3.28	127.61	123.60
2	D	401	E5S	CAS-NBE-CAY	3.20	127.51	123.60
2	A	901	E5S	NAU-CAY-NBE	3.00	119.91	116.55
2	C	401	E5S	CAR-NBE-CAS	-2.54	108.32	111.67
2	F	401	E5S	CAN-CBB-CBF	-2.50	108.04	109.46
2	D	401	E5S	CAR-NBE-CAS	-2.41	108.50	111.67
2	F	401	E5S	CAS-NBE-CAY	2.40	126.54	123.60
2	A	901	E5S	CAR-NBE-CAS	-2.38	108.53	111.67
2	B	401	E5S	CAR-NBE-CAS	-2.31	108.62	111.67
2	B	401	E5S	CAS-NBE-CAY	2.31	126.43	123.60
2	F	401	E5S	CAR-NBE-CAS	-2.30	108.64	111.67
2	E	401	E5S	CAR-NBE-CAS	-2.27	108.67	111.67
2	D	401	E5S	CAN-CBB-CBF	-2.24	108.19	109.46
2	C	401	E5S	CAL-CAY-NAU	-2.19	119.96	123.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

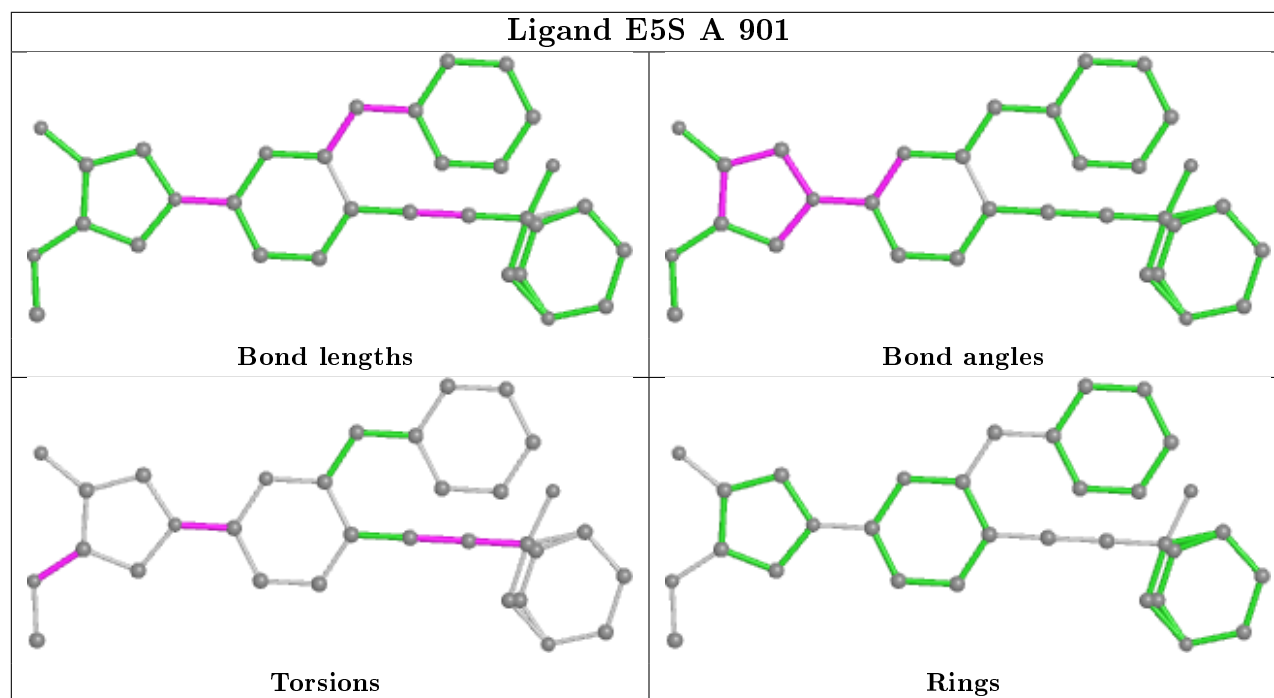
Mol	Chain	Res	Type	Atoms
2	D	401	E5S	CAD-CAE-CBF-CAT
2	D	401	E5S	CAX-CAD-CAE-CBF
2	A	901	E5S	CAX-CAD-CAE-CBF
2	C	401	E5S	CAX-CAD-CAE-CBF
2	F	401	E5S	CAS-CBC-OAV-CAA
2	A	901	E5S	CBA-CBC-OAV-CAA
2	B	401	E5S	NAU-CAY-NBE-CAS
2	C	401	E5S	NAU-CAY-NBE-CAS
2	B	401	E5S	CAX-CAD-CAE-CBF
2	F	401	E5S	CAX-CAD-CAE-CBF
2	A	901	E5S	CAS-CBC-OAV-CAA
2	F	401	E5S	CBA-CBC-OAV-CAA
2	D	401	E5S	CAE-CAD-CAX-CAZ
2	A	901	E5S	CAD-CAE-CBF-CAT
2	A	901	E5S	NAU-CAY-NBE-CAS
2	D	401	E5S	NAU-CAY-NBE-CAS
2	B	401	E5S	CAL-CAY-NBE-CAS
2	E	401	E5S	CAX-CAD-CAE-CBF

There are no ring outliers.

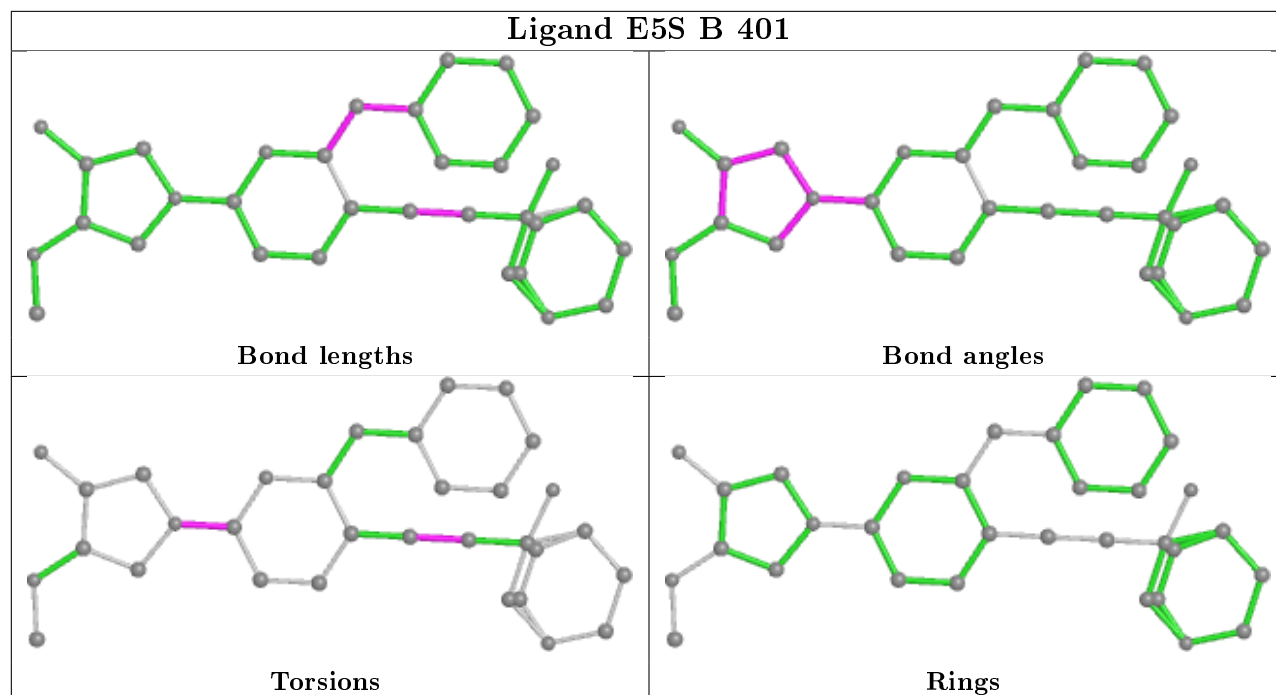
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	E5S	1	0
2	B	401	E5S	1	0
2	F	401	E5S	1	0

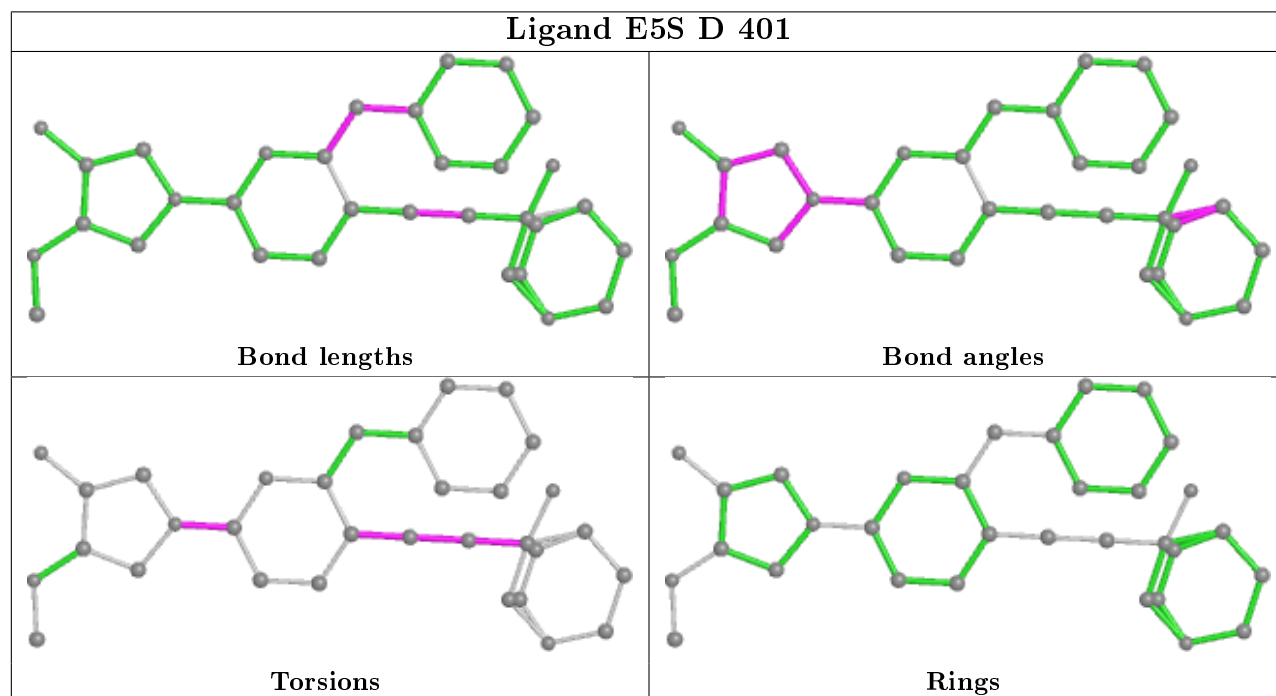
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



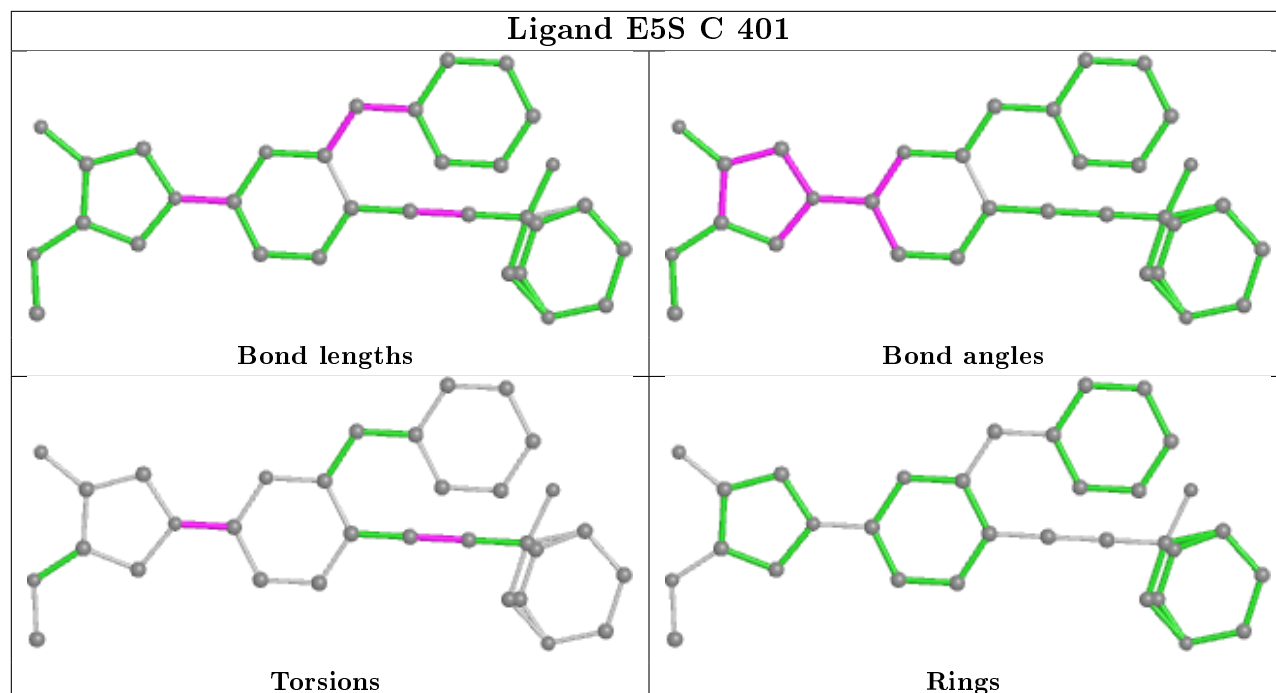
Ligand E5S B 401



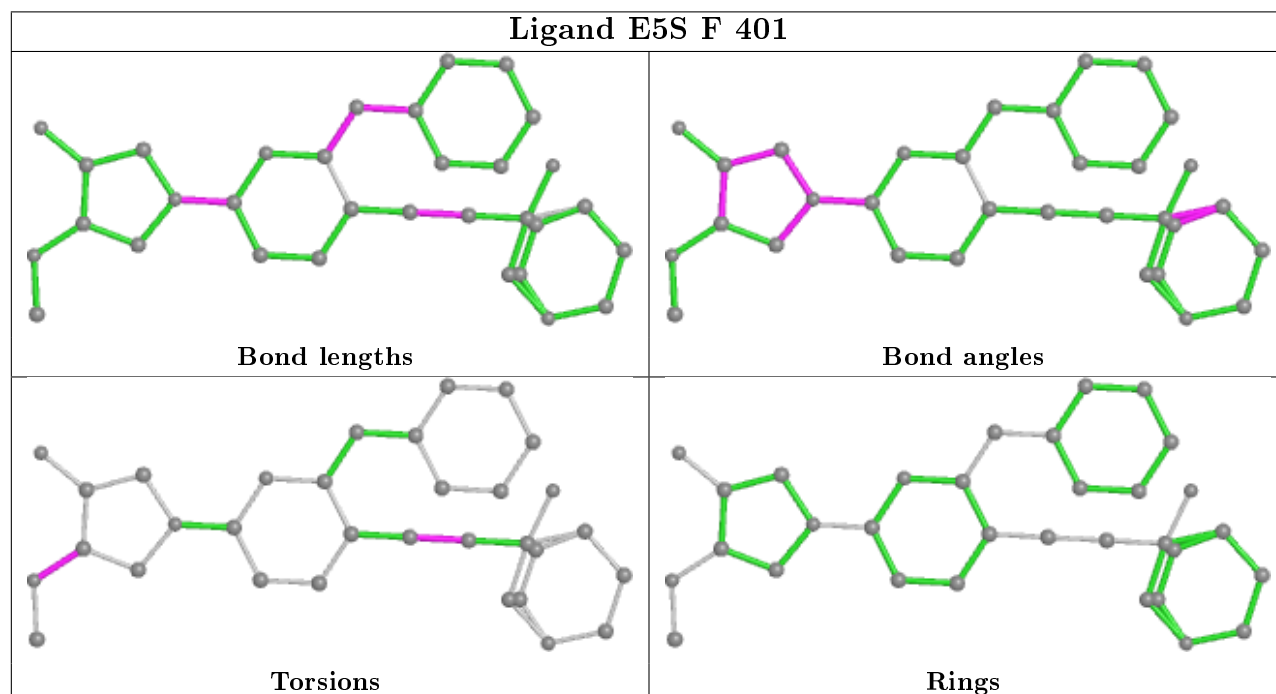
Ligand E5S D 401

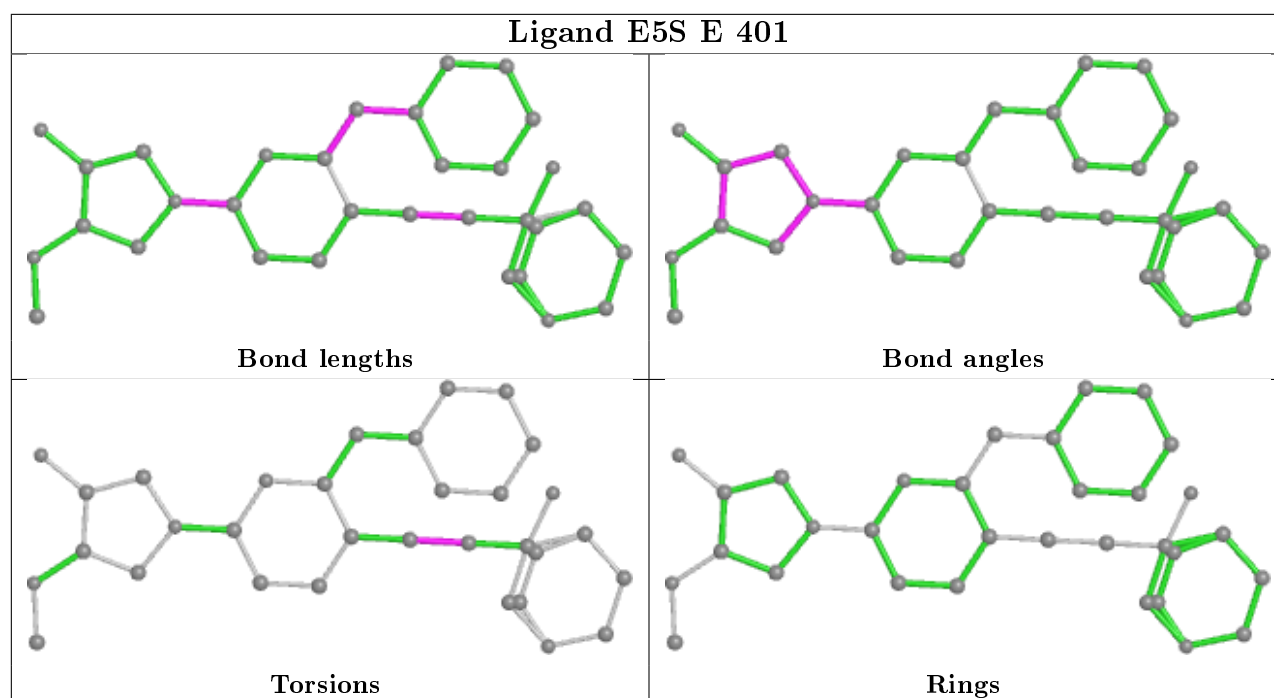


Ligand E5S C 401



Ligand E5S F 401





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	334/360 (92%)	-0.25	14 (4%)	36 34	16, 27, 57, 101	0
1	B	332/360 (92%)	-0.12	13 (3%)	39 37	16, 30, 68, 95	0
1	C	335/360 (93%)	0.03	20 (5%)	21 20	20, 32, 64, 107	0
1	D	335/360 (93%)	0.14	22 (6%)	18 17	22, 38, 79, 112	0
1	E	335/360 (93%)	0.33	26 (7%)	13 11	29, 48, 82, 113	0
1	F	334/360 (92%)	0.69	46 (13%)	2 2	25, 59, 91, 112	0
All	All	2005/2160 (92%)	0.14	141 (7%)	16 15	16, 39, 84, 113	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	LEU	9.0
1	A	318	LEU	8.3
1	C	318	LEU	8.2
1	F	318	LEU	8.1
1	D	36	LEU	7.9
1	C	313	ALA	7.0
1	F	320	GLN	6.9
1	F	315	LEU	6.9
1	F	324	LEU	6.5
1	C	319	GLY	6.5
1	D	317	ARG	6.4
1	F	319	GLY	6.2
1	F	323	THR	6.1
1	A	315	LEU	6.1
1	D	319	GLY	5.9
1	C	321	ALA	5.8
1	D	313	ALA	5.6
1	C	315	LEU	5.6
1	E	317	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	320	GLN	5.5
1	D	323	THR	5.4
1	A	319	GLY	5.3
1	C	316	ILE	5.3
1	D	316	ILE	5.2
1	C	320	GLN	5.2
1	F	316	ILE	5.1
1	E	318	LEU	5.0
1	D	315	LEU	5.0
1	E	319	GLY	5.0
1	F	317	ARG	5.0
1	C	36	LEU	4.8
1	F	36	LEU	4.8
1	D	312	GLY	4.8
1	B	313	ALA	4.8
1	B	315	LEU	4.8
1	E	36	LEU	4.8
1	A	320	GLN	4.7
1	A	324	LEU	4.7
1	F	313	ALA	4.5
1	B	312	GLY	4.5
1	E	313	ALA	4.5
1	D	320	GLN	4.4
1	F	159	ASP	4.3
1	D	321	ALA	4.2
1	E	321	ALA	4.2
1	E	323	THR	4.2
1	D	37	SER	4.0
1	B	370	ASN	3.9
1	F	312	GLY	3.9
1	A	36	LEU	3.9
1	E	370	ASN	3.8
1	E	91	GLU	3.7
1	F	241	LYS	3.7
1	B	316	ILE	3.5
1	F	248	LEU	3.4
1	C	312	GLY	3.4
1	F	351	ASP	3.4
1	A	321	ALA	3.4
1	A	323	THR	3.4
1	F	225	GLN	3.3
1	F	92	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	317	ARG	3.3
1	F	87	THR	3.3
1	E	37	SER	3.2
1	C	248	LEU	3.2
1	F	89	SER	3.2
1	D	347	HIS	3.2
1	E	86	MET	3.2
1	F	231	TRP	3.1
1	E	315	LEU	3.1
1	A	313	ALA	3.1
1	F	217	ILE	3.1
1	B	323	THR	3.1
1	D	159	ASP	3.0
1	F	37	SER	3.0
1	C	314	VAL	3.0
1	D	115	LYS	3.0
1	F	115	LYS	2.9
1	D	314	VAL	2.9
1	F	230	PHE	2.8
1	C	317	ARG	2.8
1	E	159	ASP	2.8
1	F	75	VAL	2.7
1	F	314	VAL	2.7
1	A	322	VAL	2.7
1	E	75	VAL	2.6
1	F	239	TYR	2.6
1	E	281	ARG	2.6
1	D	248	LEU	2.6
1	D	228	ARG	2.5
1	F	106	GLN	2.5
1	C	323	THR	2.5
1	F	221	LEU	2.5
1	F	254	LEU	2.5
1	E	117	LYS	2.4
1	E	312	GLY	2.4
1	F	71	ILE	2.4
1	E	322	VAL	2.4
1	F	161	HIS	2.4
1	E	194	ASP	2.4
1	A	316	ILE	2.4
1	D	225	GLN	2.4
1	F	243	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	2.4
1	C	228	ARG	2.4
1	D	91	GLU	2.4
1	B	231	TRP	2.4
1	B	324	LEU	2.3
1	F	369	GLN	2.3
1	F	86	MET	2.3
1	E	347	HIS	2.3
1	C	52	ARG	2.3
1	F	72	PHE	2.3
1	C	159	ASP	2.3
1	F	76	LEU	2.2
1	E	316	ILE	2.2
1	C	324	LEU	2.2
1	E	369	GLN	2.2
1	B	325	MET	2.2
1	D	241	LYS	2.2
1	E	314	VAL	2.2
1	D	52	ARG	2.2
1	E	228	ARG	2.2
1	F	246	PHE	2.2
1	F	88	ILE	2.2
1	F	259	LEU	2.1
1	C	370	ASN	2.1
1	B	347	HIS	2.1
1	B	248	LEU	2.1
1	F	157	PHE	2.1
1	F	310	PHE	2.1
1	A	76	LEU	2.1
1	C	322	VAL	2.1
1	F	110	ARG	2.1
1	F	347	HIS	2.1
1	A	314	VAL	2.1
1	C	225	GLN	2.0
1	E	324	LEU	2.0
1	F	262	LEU	2.0
1	B	262	LEU	2.0
1	F	263	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

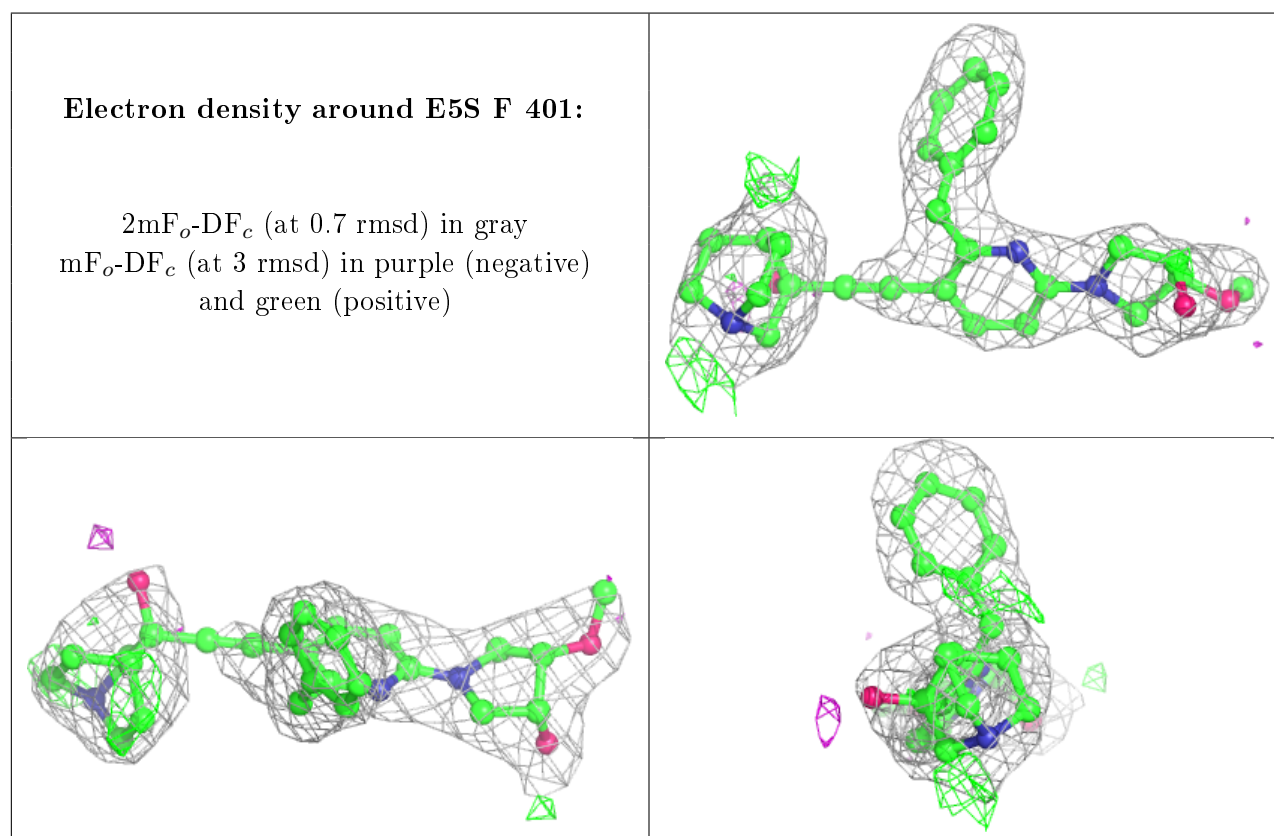
There are no carbohydrates in this entry.

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.

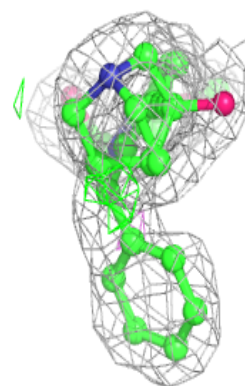
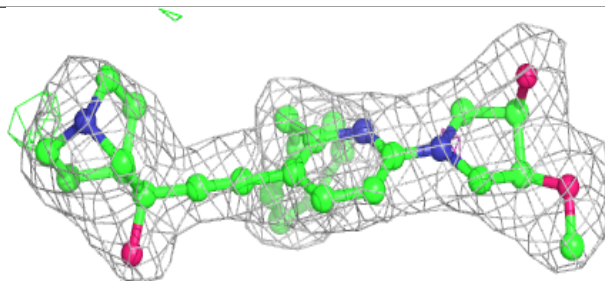
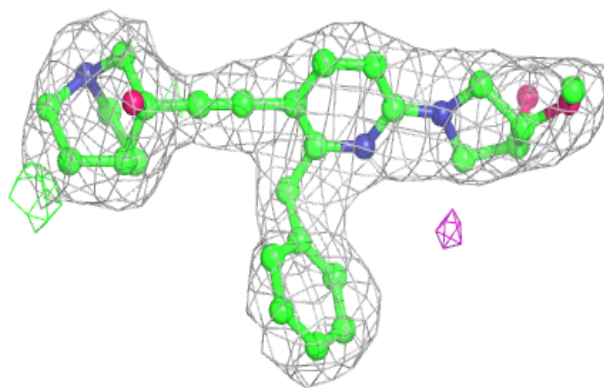
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	E5S	F	401	32/32	0.85	0.20	44,53,63,63	0
2	E5S	E	401	32/32	0.92	0.17	38,42,51,51	0
2	E5S	D	401	32/32	0.93	0.13	25,37,50,51	0
2	E5S	C	401	32/32	0.93	0.17	25,37,48,48	0
2	E5S	A	901	32/32	0.94	0.14	18,36,44,45	0
2	E5S	B	401	32/32	0.95	0.13	22,27,36,38	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.

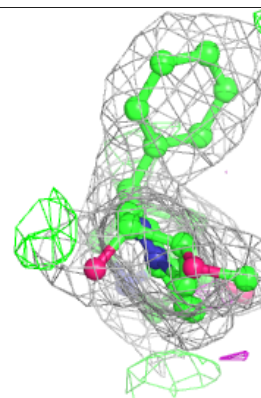
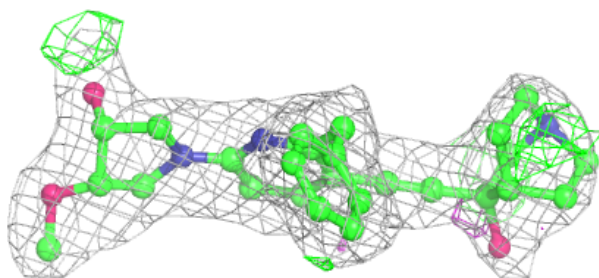
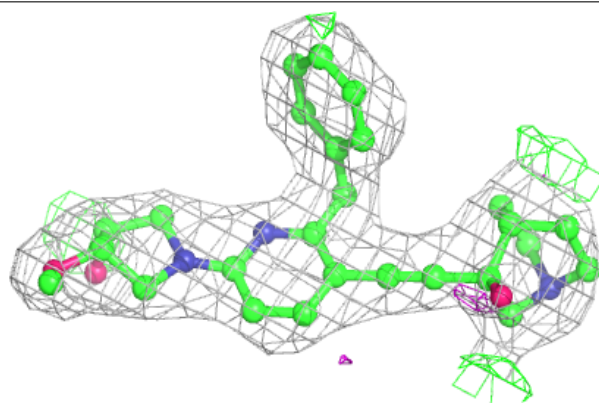


Electron density around E5S E 401:

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

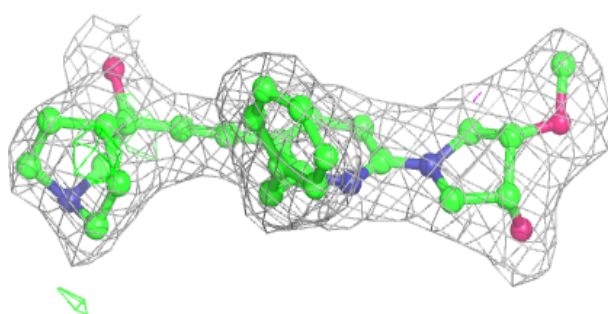
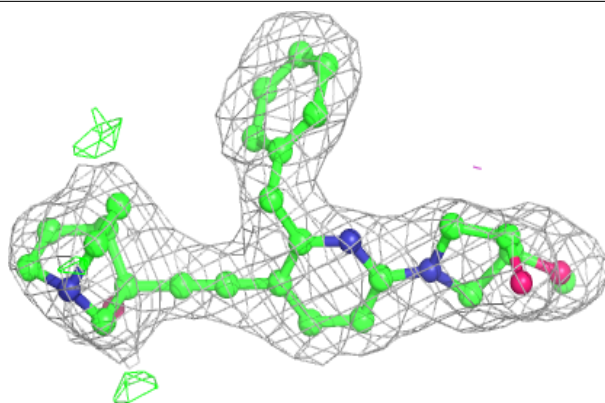
**Electron density around E5S D 401:**

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

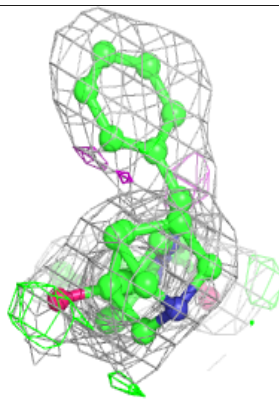
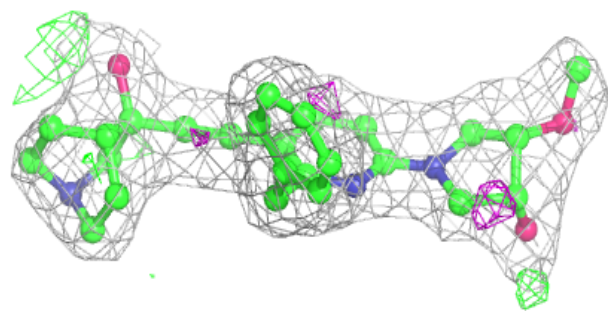
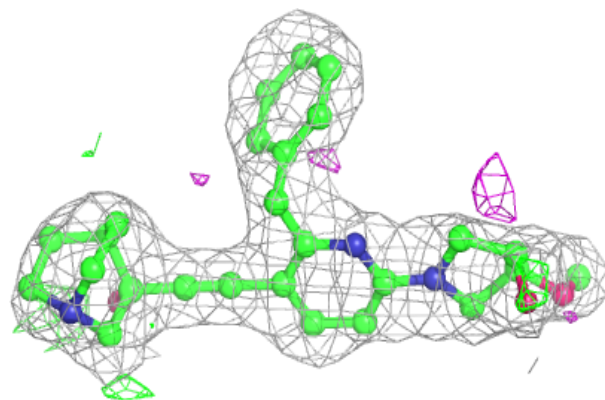


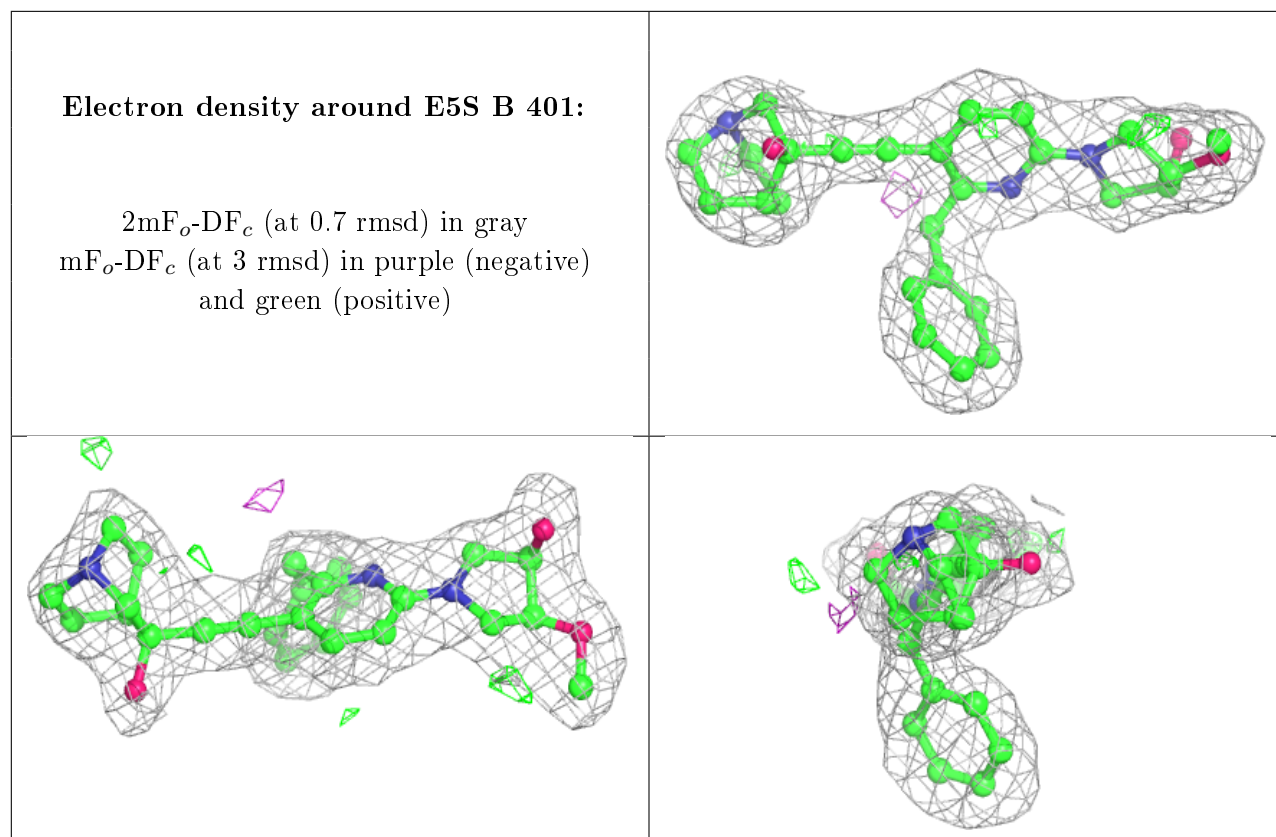
Electron density around E5S C 401:

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

**Electron density around E5S 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.