Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:53 PM EDT

PDB ID	:	3WCC
Title	:	The complex structure of TcSQS with 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	:	2.32 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 (i) 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 (i)) were used in the production of this report:

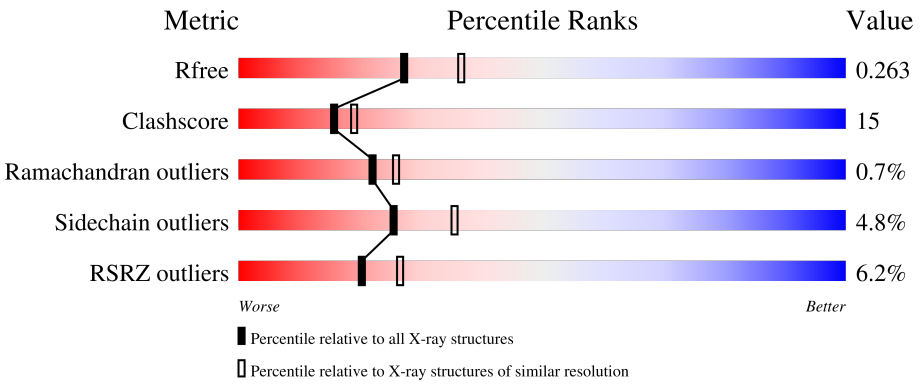
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	365	3% 74% 18% • 7%
1	B	365	3% 66% 26% • 7%
1	C	365	4% 68% 24% • 6%
1	D	365	13% 51% 38% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11641 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 Farnesyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2751	1745	473	511	22	0	0	0
1	B	341	2751	1745	473	511	22	0	0	0
1	C	342	2759	1749	475	513	22	0	0	0
1	D	341	2752	1745	473	512	22	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q4CWB4
A	5	GLY	-	expression tag	UNP Q4CWB4
A	6	SER	-	expression tag	UNP Q4CWB4
A	7	SER	-	expression tag	UNP Q4CWB4
A	8	HIS	-	expression tag	UNP Q4CWB4
A	9	HIS	-	expression tag	UNP Q4CWB4
A	10	HIS	-	expression tag	UNP Q4CWB4
A	11	HIS	-	expression tag	UNP Q4CWB4
A	12	HIS	-	expression tag	UNP Q4CWB4
A	13	HIS	-	expression tag	UNP Q4CWB4
A	14	SER	-	expression tag	UNP Q4CWB4
A	15	SER	-	expression tag	UNP Q4CWB4
A	16	GLY	-	expression tag	UNP Q4CWB4
A	17	LEU	-	expression tag	UNP Q4CWB4
A	18	VAL	-	expression tag	UNP Q4CWB4
A	19	PRO	-	expression tag	UNP Q4CWB4
A	20	ARG	-	expression tag	UNP Q4CWB4
A	21	GLY	-	expression tag	UNP Q4CWB4
A	22	SER	-	expression tag	UNP Q4CWB4
A	23	HIS	-	expression tag	UNP Q4CWB4
A	24	MET	-	expression tag	UNP Q4CWB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	engineered mutation	UNP Q4CWB4
B	4	MET	-	expression tag	UNP Q4CWB4
B	5	GLY	-	expression tag	UNP Q4CWB4
B	6	SER	-	expression tag	UNP Q4CWB4
B	7	SER	-	expression tag	UNP Q4CWB4
B	8	HIS	-	expression tag	UNP Q4CWB4
B	9	HIS	-	expression tag	UNP Q4CWB4
B	10	HIS	-	expression tag	UNP Q4CWB4
B	11	HIS	-	expression tag	UNP Q4CWB4
B	12	HIS	-	expression tag	UNP Q4CWB4
B	13	HIS	-	expression tag	UNP Q4CWB4
B	14	SER	-	expression tag	UNP Q4CWB4
B	15	SER	-	expression tag	UNP Q4CWB4
B	16	GLY	-	expression tag	UNP Q4CWB4
B	17	LEU	-	expression tag	UNP Q4CWB4
B	18	VAL	-	expression tag	UNP Q4CWB4
B	19	PRO	-	expression tag	UNP Q4CWB4
B	20	ARG	-	expression tag	UNP Q4CWB4
B	21	GLY	-	expression tag	UNP Q4CWB4
B	22	SER	-	expression tag	UNP Q4CWB4
B	23	HIS	-	expression tag	UNP Q4CWB4
B	24	MET	-	expression tag	UNP Q4CWB4
B	82	GLU	ASP	engineered mutation	UNP Q4CWB4
C	4	MET	-	expression tag	UNP Q4CWB4
C	5	GLY	-	expression tag	UNP Q4CWB4
C	6	SER	-	expression tag	UNP Q4CWB4
C	7	SER	-	expression tag	UNP Q4CWB4
C	8	HIS	-	expression tag	UNP Q4CWB4
C	9	HIS	-	expression tag	UNP Q4CWB4
C	10	HIS	-	expression tag	UNP Q4CWB4
C	11	HIS	-	expression tag	UNP Q4CWB4
C	12	HIS	-	expression tag	UNP Q4CWB4
C	13	HIS	-	expression tag	UNP Q4CWB4
C	14	SER	-	expression tag	UNP Q4CWB4
C	15	SER	-	expression tag	UNP Q4CWB4
C	16	GLY	-	expression tag	UNP Q4CWB4
C	17	LEU	-	expression tag	UNP Q4CWB4
C	18	VAL	-	expression tag	UNP Q4CWB4
C	19	PRO	-	expression tag	UNP Q4CWB4
C	20	ARG	-	expression tag	UNP Q4CWB4
C	21	GLY	-	expression tag	UNP Q4CWB4
C	22	SER	-	expression tag	UNP Q4CWB4

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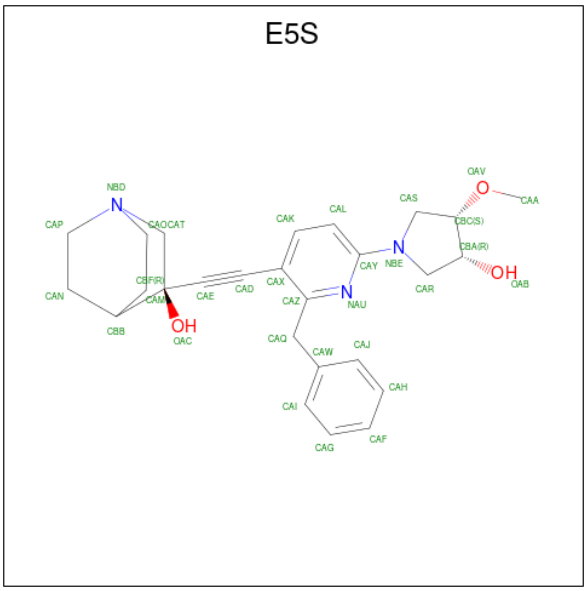
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	expression tag	UNP Q4CWB4
C	24	MET	-	expression tag	UNP Q4CWB4
C	82	GLU	ASP	engineered mutation	UNP Q4CWB4
D	4	MET	-	expression tag	UNP Q4CWB4
D	5	GLY	-	expression tag	UNP Q4CWB4
D	6	SER	-	expression tag	UNP Q4CWB4
D	7	SER	-	expression tag	UNP Q4CWB4
D	8	HIS	-	expression tag	UNP Q4CWB4
D	9	HIS	-	expression tag	UNP Q4CWB4
D	10	HIS	-	expression tag	UNP Q4CWB4
D	11	HIS	-	expression tag	UNP Q4CWB4
D	12	HIS	-	expression tag	UNP Q4CWB4
D	13	HIS	-	expression tag	UNP Q4CWB4
D	14	SER	-	expression tag	UNP Q4CWB4
D	15	SER	-	expression tag	UNP Q4CWB4
D	16	GLY	-	expression tag	UNP Q4CWB4
D	17	LEU	-	expression tag	UNP Q4CWB4
D	18	VAL	-	expression tag	UNP Q4CWB4
D	19	PRO	-	expression tag	UNP Q4CWB4
D	20	ARG	-	expression tag	UNP Q4CWB4
D	21	GLY	-	expression tag	UNP Q4CWB4
D	22	SER	-	expression tag	UNP Q4CWB4
D	23	HIS	-	expression tag	UNP Q4CWB4
D	24	MET	-	expression tag	UNP Q4CWB4
D	82	GLU	ASP	engineered mutation	UNP Q4CWB4

- Molecule 2 is (3R)-3-({2-benzyl-6-[(3R,4S)-3-hydroxy-4-methoxypyrrolidin-1-yl]pyridin-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
			Total	C	N	O		
2	A	1	32	26	3	3	0	0
			Total	C	N	O		
2	B	1	32	26	3	3	0	0
			Total	C	N	O		
2	C	1	32	26	3	3	0	0
			Total	C	N	O		
2	D	1	32	26	3	3	0	0

- Molecule 3 is water.

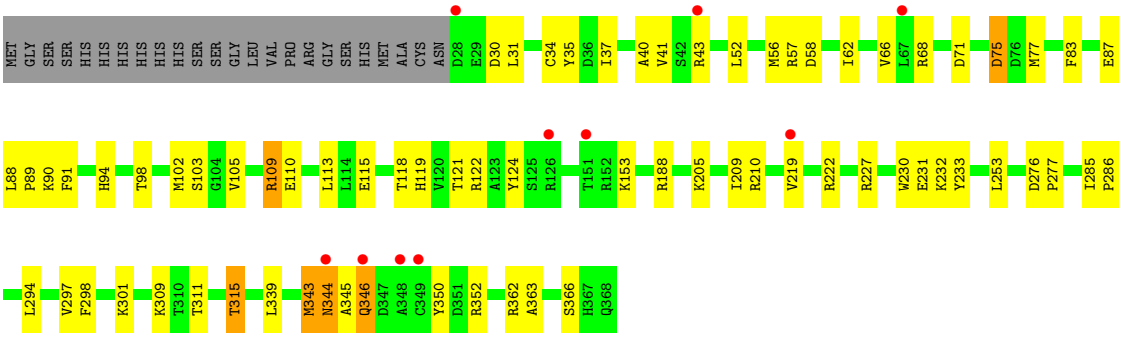
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	153	153	153	0	0
			Total	O		
3	B	154	154	154	0	0
			Total	O		
3	C	128	128	128	0	0
			Total	O		
3	D	65	65	65	0	0

3 Residue-property plots (i)

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

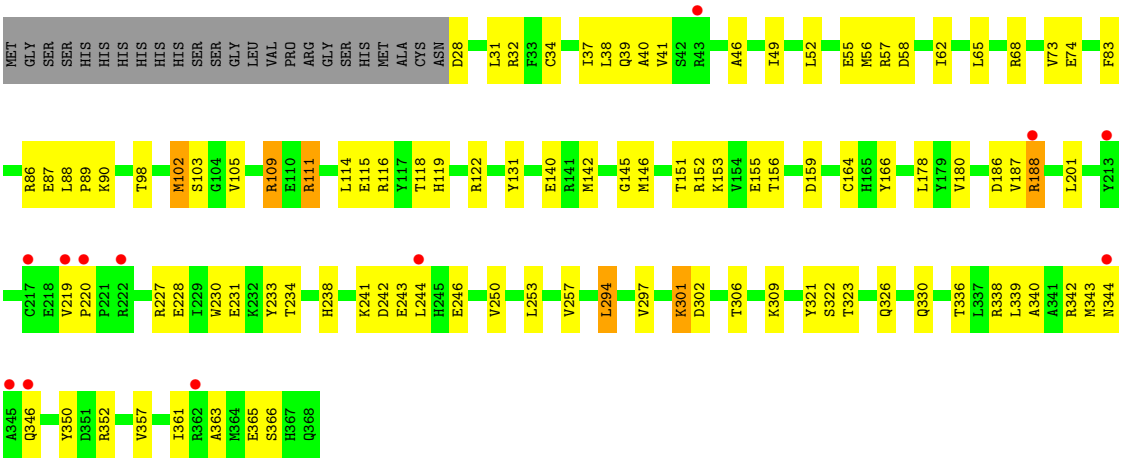
- Molecule 1: Farnesyltransferase, putative

Chain A:



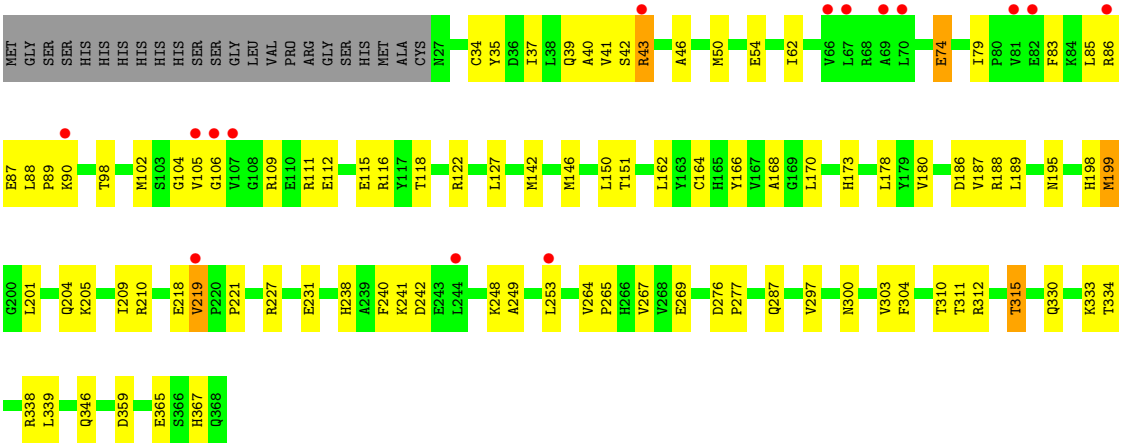
- Molecule 1: Farnesyltransferase, putative

Chain B:



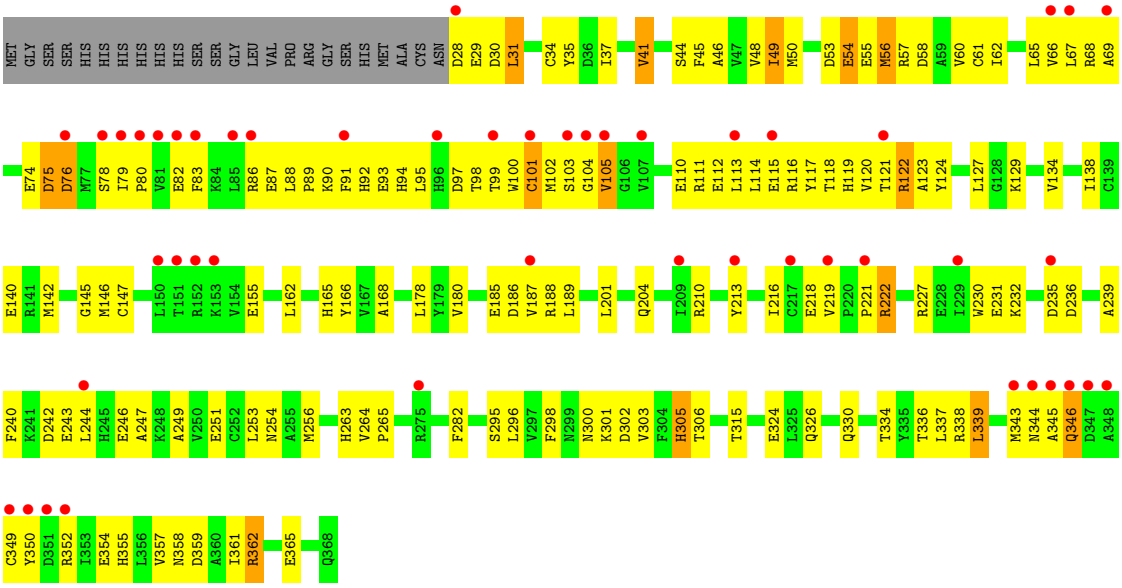
- Molecule 1: Farnesyltransferase, putative

Chain C:



- Molecule 1: Farnesyltransferase, putative

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.07Å 131.60Å 143.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.32 24.91 – 2.32	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.32) 96.5 (24.91-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.13 (at 2.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.262 0.211 , 0.263	Depositor DCC
R_{free} test set	3186 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/2809	0.57	0/3806
1	B	0.36	0/2809	0.58	1/3806 (0.0%)
1	C	0.35	0/2817	0.56	0/3817
1	D	0.32	0/2810	0.56	0/3806
All	All	0.35	0/11245	0.57	1/15235 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	SER	N-CA-C	5.24	125.15	111.00

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	2751	0	2698	53	0
1	B	2751	0	2698	78	0
1	C	2759	0	2704	76	0
1	D	2752	0	2698	122	0
2	A	32	0	31	1	0
2	B	32	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	32	0	31	0	0
2	D	32	0	31	0	0
3	A	153	0	0	2	0
3	B	154	0	0	5	0
3	C	128	0	0	1	0
3	D	65	0	0	0	0
All	All	11641	0	10922	325	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 15.

All (325) 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:199:MET:HE1	1:C:267:VAL:HG13	1.24	1.11
1:B:102:MET:HE3	1:B:105:VAL:HG21	1.39	1.00
1:D:31:LEU:H	1:D:31:LEU:HD22	1.32	0.92
1:D:242:ASP:OD2	1:D:244:LEU:HB2	1.71	0.91
1:C:104:GLY:HA2	1:C:111:ARG:HH12	1.34	0.90
1:C:104:GLY:HA2	1:C:111:ARG:NH1	1.90	0.85
1:D:62:ILE:HD12	1:D:127:LEU:HD11	1.58	0.84
1:B:186:ASP:OD2	1:B:188:ARG:HB2	1.76	0.83
1:D:155:GLU:HA	1:D:227:ARG:HB3	1.61	0.83
1:D:103:SER:HA	1:D:115:GLU:HG2	1.61	0.83
1:B:242:ASP:OD2	1:B:244:LEU:HB3	1.81	0.80
1:B:41:VAL:HG22	1:B:68:ARG:CZ	2.12	0.79
1:A:121:THR:O	1:A:124:TYR:HB3	1.85	0.77
1:C:46:ALA:O	1:C:50:MET:HG2	1.85	0.77
1:C:86:ARG:O	1:C:90:LYS:HE3	1.86	0.76
1:D:45:PHE:O	1:D:49:ILE:HB	1.86	0.76
1:C:104:GLY:CA	1:C:111:ARG:HH12	1.99	0.76
1:C:186:ASP:OD2	1:C:188:ARG:HB2	1.86	0.75
1:A:362:ARG:NH1	1:D:111:ARG:HH12	1.83	0.75
1:D:79:ILE:HG23	1:D:83:PHE:HD2	1.51	0.75
1:D:344:ASN:HB2	1:D:346:GLN:HB2	1.69	0.74
1:C:43:ARG:CZ	1:C:43:ARG:HB2	2.17	0.74
1:D:30:ASP:CG	1:D:122:ARG:HD2	2.08	0.74
1:B:73:VAL:HG22	1:B:102:MET:HE1	1.71	0.73
1:A:40:ALA:HB1	1:A:109:ARG:HG2	1.73	0.71
1:D:41:VAL:HG13	1:D:68:ARG:NH1	2.06	0.71
1:B:55:GLU:HG2	1:B:131:TYR:HE2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:O	1:B:49:ILE:HG22	1.90	0.70
1:C:199:MET:HE1	1:C:267:VAL:CG1	2.14	0.70
1:C:106:GLY:O	1:C:111:ARG:HB2	1.92	0.70
1:C:35:TYR:O	1:C:39:GLN:HG3	1.92	0.69
1:B:309:LYS:HD3	3:B:568:HOH:O	1.93	0.69
1:D:142:MET:O	1:D:146:MET:HG3	1.92	0.69
1:B:55:GLU:HG2	1:B:131:TYR:CE2	2.29	0.68
1:B:363:ALA:O	1:B:366:SER:HB3	1.95	0.67
1:C:199:MET:HE3	1:C:267:VAL:HG22	1.76	0.67
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.77	0.67
1:B:83:PHE:CZ	1:B:87:GLU:HG3	2.32	0.64
1:B:73:VAL:HG22	1:B:102:MET:CE	2.27	0.64
1:C:238:HIS:O	1:C:241:LYS:HB2	1.97	0.64
1:D:105:VAL:HG21	1:D:114:LEU:HD13	1.79	0.63
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.79	0.63
1:A:98:THR:O	1:A:118:THR:HG23	1.99	0.63
1:B:111:ARG:O	1:B:115:GLU:HG3	1.98	0.63
1:C:199:MET:CE	1:C:267:VAL:HG22	2.30	0.62
1:C:199:MET:HE2	1:C:199:MET:HA	1.81	0.62
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.14	0.62
1:D:46:ALA:O	1:D:49:ILE:HG22	2.00	0.62
1:A:298:PHE:HZ	1:A:343:MET:HE3	1.64	0.61
1:D:31:LEU:HD22	1:D:31:LEU:N	2.12	0.61
1:D:358:ASN:O	1:D:362:ARG:HG2	2.01	0.61
1:C:221:PRO:HG3	1:D:235:ASP:OD1	2.00	0.61
1:D:344:ASN:C	1:D:346:GLN:H	2.05	0.60
1:B:153:LYS:HB2	1:B:155:GLU:OE2	2.02	0.60
1:D:295:SER:HA	1:D:339:LEU:HD22	1.84	0.60
1:C:118:THR:HB	1:C:122:ARG:NH1	2.16	0.60
1:A:30:ASP:OD1	1:A:122:ARG:HD2	2.02	0.59
1:B:343:MET:CE	1:B:350:TYR:HA	2.33	0.58
1:A:34:CYS:O	1:A:37:ILE:HG22	2.03	0.58
1:D:142:MET:HG3	1:D:166:TYR:O	2.03	0.58
1:C:199:MET:CE	1:C:199:MET:HA	2.34	0.58
1:D:90:LYS:HE2	1:D:94:HIS:HE1	1.69	0.58
1:C:199:MET:CE	1:C:267:VAL:HG13	2.16	0.58
1:D:31:LEU:H	1:D:31:LEU:CD2	2.10	0.58
1:B:227:ARG:HA	1:B:230:TRP:CE2	2.38	0.57
1:A:35:TYR:OH	1:A:57:ARG:HG2	2.04	0.57
1:C:85:LEU:HD11	1:C:151:THR:CG2	2.34	0.57
1:B:257:VAL:HG13	1:B:294:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:HG2	1:D:188:ARG:HH11	1.69	0.57
1:B:102:MET:HE3	1:B:105:VAL:CG2	2.26	0.56
1:D:34:CYS:O	1:D:37:ILE:HG22	2.05	0.56
1:A:344:ASN:N	1:A:344:ASN:HD22	2.02	0.56
1:B:88:LEU:HB2	1:B:89:PRO:HD3	1.87	0.56
1:C:43:ARG:HB2	1:C:43:ARG:NH1	2.20	0.56
1:A:77:MET:HG2	1:A:222:ARG:HH22	1.70	0.56
1:B:145:GLY:HA3	1:B:166:TYR:CD1	2.40	0.56
1:D:87:GLU:O	1:D:90:LYS:N	2.31	0.56
1:C:330:GLN:O	1:C:334:THR:HG23	2.05	0.56
1:D:67:LEU:HD22	1:D:142:MET:SD	2.45	0.56
1:C:37:ILE:O	1:C:41:VAL:HG22	2.05	0.56
1:C:219:VAL:HG22	1:C:219:VAL:O	2.05	0.56
1:B:257:VAL:HG13	1:B:294:LEU:HD13	1.88	0.56
1:C:338:ARG:HG3	1:C:338:ARG:HH11	1.72	0.55
1:D:30:ASP:OD2	1:D:122:ARG:HD2	2.06	0.55
1:D:112:GLU:O	1:D:116:ARG:HD3	2.06	0.55
1:A:71:ASP:O	1:A:75:ASP:HB2	2.07	0.55
1:B:142:MET:O	1:B:146:MET:HG3	2.07	0.55
1:D:254:ASN:HB3	1:D:349:CYS:SG	2.46	0.55
1:D:344:ASN:C	1:D:346:GLN:N	2.60	0.55
1:C:86:ARG:O	1:C:90:LYS:CE	2.54	0.54
1:A:309:LYS:HE3	3:A:644:HOH:O	2.07	0.54
1:B:40:ALA:HB1	1:B:109:ARG:HG2	1.90	0.54
1:B:302:ASP:O	1:B:306:THR:HG22	2.08	0.54
1:A:285:ILE:HB	1:A:286:PRO:HD3	1.90	0.54
1:A:311:THR:O	1:A:315:THR:HG23	2.08	0.54
1:A:343:MET:CE	1:A:350:TYR:HA	2.37	0.54
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.73	0.53
1:D:79:ILE:CG2	1:D:83:PHE:HD2	2.18	0.53
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.90	0.53
1:A:344:ASN:HD22	1:A:344:ASN:H	1.56	0.53
1:C:85:LEU:HD11	1:C:151:THR:HG21	1.89	0.53
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.90	0.53
1:D:253:LEU:O	1:D:256:MET:HB2	2.09	0.53
1:A:227:ARG:HA	1:A:230:TRP:NE1	2.24	0.53
1:C:339:LEU:C	1:C:339:LEU:HD23	2.29	0.53
1:D:90:LYS:HE2	1:D:94:HIS:CE1	2.43	0.53
1:B:344:ASN:HB3	1:B:346:GLN:H	1.73	0.53
1:D:117:TYR:O	1:D:120:VAL:HB	2.09	0.53
1:D:100:TRP:O	1:D:101:CYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:THR:HG22	1:D:357:VAL:HG13	1.90	0.52
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.24	0.52
1:D:302:ASP:O	1:D:306:THR:HG22	2.09	0.52
1:D:58:ASP:O	1:D:62:ILE:HG13	2.08	0.52
1:D:326:GLN:O	1:D:330:GLN:HG3	2.09	0.52
1:D:145:GLY:HA3	1:D:166:TYR:CD1	2.45	0.52
1:D:79:ILE:HD13	1:D:83:PHE:HE2	1.74	0.52
1:C:98:THR:O	1:C:98:THR:HG22	2.09	0.52
1:C:338:ARG:HG3	1:C:338:ARG:NH1	2.24	0.52
1:D:185:GLU:HB3	1:D:189:LEU:HD22	1.90	0.52
1:A:62:ILE:O	1:A:66:VAL:HG23	2.10	0.52
1:B:142:MET:HG3	1:B:166:TYR:O	2.10	0.52
1:D:186:ASP:OD2	1:D:188:ARG:HB2	2.10	0.52
1:B:140:GLU:HA	3:B:554:HOH:O	2.08	0.52
1:B:31:LEU:O	1:B:34:CYS:HB2	2.10	0.52
1:B:34:CYS:O	1:B:37:ILE:HG22	2.10	0.52
1:B:326:GLN:O	1:B:330:GLN:HG3	2.10	0.51
1:D:102:MET:SD	1:D:105:VAL:HG11	2.50	0.51
1:D:361:ILE:O	1:D:365:GLU:HG3	2.10	0.51
1:A:309:LYS:HE2	3:A:564:HOH:O	2.11	0.51
1:C:164:CYS:HB3	1:C:201:LEU:HD22	1.93	0.51
1:D:86:ARG:NH1	1:D:90:LYS:HD2	2.25	0.51
1:B:344:ASN:HB3	1:B:346:GLN:HB2	1.92	0.51
1:D:121:THR:O	1:D:124:TYR:HB3	2.09	0.51
1:D:90:LYS:O	1:D:93:GLU:HG3	2.10	0.51
1:C:180:VAL:HG13	1:C:187:VAL:HA	1.92	0.51
1:D:227:ARG:O	1:D:231:GLU:HB3	2.10	0.51
1:A:210:ARG:HD2	1:A:210:ARG:O	2.11	0.51
1:C:227:ARG:HG3	1:C:231:GLU:HB3	1.93	0.51
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.93	0.50
1:D:112:GLU:HG2	1:D:116:ARG:HD3	1.93	0.50
1:C:111:ARG:O	1:C:115:GLU:HG3	2.11	0.50
1:D:227:ARG:HA	1:D:230:TRP:CE2	2.46	0.50
1:D:240:PHE:CE1	1:D:249:ALA:HA	2.47	0.50
1:A:40:ALA:CB	1:A:109:ARG:HG2	2.41	0.50
1:B:40:ALA:CB	1:B:109:ARG:HG2	2.42	0.50
1:B:41:VAL:CG2	1:B:68:ARG:CZ	2.86	0.50
1:D:105:VAL:CG2	1:D:114:LEU:HD13	2.41	0.49
1:D:110:GLU:O	1:D:113:LEU:HB3	2.11	0.49
1:D:243:GLU:O	1:D:246:GLU:HG3	2.12	0.49
1:A:110:GLU:O	1:A:113:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ILE:HG21	1:C:83:PHE:HD2	1.77	0.49
1:A:362:ARG:NH1	1:D:111:ARG:NH1	2.58	0.49
1:B:116:ARG:HH21	1:B:119:HIS:HE1	1.61	0.49
1:A:363:ALA:O	1:A:366:SER:HB3	2.12	0.49
1:C:199:MET:HE2	1:C:287:GLN:CD	2.33	0.49
1:A:91:PHE:HA	1:A:94:HIS:CD2	2.48	0.48
1:C:86:ARG:C	1:C:90:LYS:HZ1	2.17	0.48
1:C:54:GLU:CD	1:C:54:GLU:H	2.17	0.48
1:C:109:ARG:NH2	1:C:112:GLU:OE1	2.47	0.48
1:D:295:SER:HA	1:D:339:LEU:CD2	2.43	0.48
1:B:58:ASP:O	1:B:62:ILE:HG12	2.13	0.48
1:C:210:ARG:HD2	1:C:210:ARG:O	2.14	0.48
1:D:213:TYR:HA	1:D:216:ILE:HG22	1.96	0.48
1:B:102:MET:HB3	1:B:114:LEU:HB3	1.96	0.47
1:D:90:LYS:O	1:D:93:GLU:N	2.42	0.47
1:B:227:ARG:HG2	1:B:231:GLU:HB3	1.96	0.47
1:D:155:GLU:CA	1:D:227:ARG:HB3	2.40	0.47
1:A:31:LEU:HD21	1:A:58:ASP:OD1	2.13	0.47
1:A:83:PHE:C	1:A:83:PHE:CD2	2.87	0.47
1:A:227:ARG:HA	1:A:230:TRP:CD1	2.49	0.47
1:C:40:ALA:HB1	1:C:109:ARG:HG3	1.95	0.47
1:C:300:ASN:O	1:C:303:VAL:HG23	2.13	0.47
1:A:253:LEU:HD21	1:A:297:VAL:O	2.15	0.47
1:D:87:GLU:HA	1:D:90:LYS:HD3	1.96	0.47
1:A:232:LYS:HG3	1:A:233:TYR:CE2	2.49	0.47
1:B:164:CYS:HB3	1:B:201:LEU:HD22	1.96	0.47
1:B:180:VAL:HG13	1:B:187:VAL:HA	1.96	0.47
1:B:83:PHE:CE2	1:B:87:GLU:HG3	2.49	0.47
1:C:118:THR:O	1:C:122:ARG:HB2	2.15	0.47
1:D:69:ALA:HB1	1:D:114:LEU:HD21	1.97	0.47
1:D:87:GLU:O	1:D:88:LEU:C	2.52	0.47
1:B:41:VAL:HG22	1:B:68:ARG:NH1	2.28	0.47
1:C:87:GLU:HA	1:C:90:LYS:CE	2.44	0.47
1:D:162:LEU:HG	1:D:166:TYR:CE2	2.50	0.47
1:D:222:ARG:HG3	1:D:222:ARG:HH11	1.79	0.47
1:A:41:VAL:HG11	1:A:68:ARG:HG2	1.96	0.46
1:A:52:LEU:O	1:A:57:ARG:NH1	2.46	0.46
1:D:222:ARG:HG3	1:D:222:ARG:NH1	2.30	0.46
1:A:118:THR:O	1:A:122:ARG:HG2	2.15	0.46
1:B:156:THR:HA	1:B:228:GLU:HB2	1.97	0.46
1:B:233:TYR:O	1:B:234:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:HG2	1:B:243:GLU:O	2.15	0.46
1:B:344:ASN:C	1:B:346:GLN:N	2.69	0.46
1:C:205:LYS:O	1:C:209:ILE:HG13	2.16	0.46
1:C:312:ARG:HG2	3:C:514:HOH:O	2.14	0.46
1:A:41:VAL:HG13	1:A:68:ARG:CZ	2.45	0.46
1:A:219:VAL:HG23	1:A:219:VAL:O	2.15	0.46
1:C:249:ALA:HB1	1:C:304:PHE:CE2	2.51	0.46
1:D:56:MET:O	1:D:60:VAL:HG23	2.15	0.46
1:C:311:THR:O	1:C:315:THR:HG23	2.16	0.46
1:D:62:ILE:O	1:D:66:VAL:HG23	2.16	0.46
1:C:334:THR:O	1:C:338:ARG:HG2	2.16	0.46
1:D:76:ASP:OD1	1:D:78:SER:HB2	2.16	0.46
1:D:298:PHE:CD2	1:D:339:LEU:HD13	2.51	0.46
1:B:131:TYR:CD1	1:B:178:LEU:HD22	2.51	0.46
1:D:188:ARG:HG2	1:D:188:ARG:NH1	2.31	0.46
1:B:102:MET:O	1:B:115:GLU:HA	2.16	0.45
1:D:345:ALA:HA	1:D:350:TYR:CD2	2.51	0.45
1:D:357:VAL:O	1:D:361:ILE:HG13	2.17	0.45
1:B:219:VAL:HA	1:B:220:PRO:HA	1.85	0.45
1:B:338:ARG:NH2	3:B:599:HOH:O	2.49	0.45
1:B:338:ARG:O	1:B:342:ARG:HG3	2.16	0.45
1:C:142:MET:HG3	1:C:166:TYR:O	2.16	0.45
1:A:298:PHE:CZ	1:A:343:MET:HE3	2.48	0.45
1:A:344:ASN:ND2	1:A:346:GLN:HG3	2.31	0.45
1:C:98:THR:HG23	1:C:122:ARG:HD3	1.99	0.45
1:D:74:GLU:HG3	1:D:146:MET:HB3	1.98	0.45
1:C:34:CYS:O	1:C:37:ILE:HG22	2.17	0.45
1:D:61:CYS:O	1:D:65:LEU:HG	2.17	0.45
1:D:88:LEU:HD12	1:D:147:CYS:SG	2.56	0.45
1:D:162:LEU:O	1:D:165:HIS:HB3	2.17	0.45
1:A:205:LYS:O	1:A:209:ILE:HG13	2.17	0.44
1:B:242:ASP:CG	1:B:244:LEU:H	2.21	0.44
1:D:134:VAL:O	1:D:138:ILE:HG12	2.17	0.44
1:D:355:HIS:O	1:D:358:ASN:HB2	2.17	0.44
1:C:168:ALA:CB	1:C:204:GLN:HB2	2.47	0.44
1:C:248:LYS:HA	1:C:248:LYS:HD3	1.77	0.44
1:B:37:ILE:O	1:B:41:VAL:HG12	2.16	0.44
1:A:30:ASP:CG	1:A:122:ARG:HD2	2.37	0.44
2:A:401:E5S:H3	2:A:401:E5S:H32	1.99	0.44
1:D:79:ILE:CG2	1:D:83:PHE:CD2	2.99	0.44
1:D:201:LEU:HD12	1:D:263:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ASP:OD1	1:D:122:ARG:NE	2.49	0.44
1:D:232:LYS:HG2	1:D:232:LYS:O	2.17	0.44
1:A:30:ASP:OD1	1:A:119:HIS:HD2	2.01	0.44
1:B:38:LEU:HD21	1:B:49:ILE:HG21	2.00	0.44
1:D:86:ARG:HD3	1:D:86:ARG:C	2.38	0.44
1:B:122:ARG:HG3	1:B:122:ARG:HH11	1.82	0.44
1:C:62:ILE:HD12	1:C:127:LEU:HD21	2.00	0.44
1:D:79:ILE:HG23	1:D:83:PHE:CD2	2.42	0.44
1:D:213:TYR:O	1:D:216:ILE:HG22	2.18	0.44
1:B:336:THR:HG22	1:B:357:VAL:HG13	2.00	0.43
1:B:339:LEU:HD23	1:B:339:LEU:C	2.38	0.43
1:D:46:ALA:O	1:D:50:MET:HG2	2.18	0.43
1:C:102:MET:CE	1:C:105:VAL:HG21	2.48	0.43
1:C:264:VAL:HB	1:C:265:PRO:HD3	2.01	0.43
1:A:344:ASN:N	1:A:344:ASN:ND2	2.67	0.43
1:C:240:PHE:CE1	1:C:249:ALA:HA	2.53	0.43
1:D:35:TYR:OH	1:D:57:ARG:HG2	2.17	0.43
1:D:54:GLU:HG2	1:D:55:GLU:H	1.83	0.43
1:B:87:GLU:O	1:B:90:LYS:HG2	2.18	0.43
1:C:74:GLU:HG3	1:C:146:MET:HB3	1.99	0.43
1:C:210:ARG:HD2	1:C:210:ARG:C	2.38	0.43
1:B:238:HIS:CD2	1:B:241:LYS:CD	3.02	0.43
1:C:310:THR:OG1	1:C:315:THR:HG22	2.18	0.43
1:D:142:MET:HE2	1:D:166:TYR:O	2.17	0.43
1:A:41:VAL:CG1	1:A:68:ARG:CZ	2.97	0.43
1:A:301:LYS:HE3	1:B:32:ARG:CZ	2.49	0.43
1:D:48:VAL:HG12	1:D:282:PHE:CD2	2.54	0.43
1:D:83:PHE:CE1	1:D:87:GLU:HG3	2.54	0.43
1:D:168:ALA:HB2	1:D:204:GLN:HB2	2.01	0.43
1:D:92:HIS:O	1:D:95:LEU:HB2	2.19	0.43
1:B:340:ALA:O	1:B:343:MET:HG2	2.19	0.43
1:D:343:MET:CE	1:D:350:TYR:HA	2.49	0.42
1:C:162:LEU:HG	1:C:166:TYR:CE2	2.54	0.42
1:C:218:GLU:OE1	1:C:218:GLU:HA	2.19	0.42
1:D:54:GLU:HG2	1:D:55:GLU:N	2.34	0.42
1:A:294:LEU:HA	1:A:297:VAL:HG22	2.00	0.42
1:B:86:ARG:O	1:B:90:LYS:HD2	2.18	0.42
1:D:86:ARG:HD3	1:D:86:ARG:O	2.19	0.42
1:D:218:GLU:O	1:D:221:PRO:HA	2.19	0.42
1:D:302:ASP:HA	1:D:305:HIS:NE2	2.35	0.42
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:O	1:B:152:ARG:HB3	2.18	0.42
1:B:156:THR:O	1:B:159:ASP:HB2	2.19	0.42
1:C:253:LEU:HD21	1:C:297:VAL:O	2.20	0.42
1:D:44:SER:OG	1:D:45:PHE:N	2.53	0.42
1:B:243:GLU:HG2	3:B:639:HOH:O	2.19	0.42
1:B:246:GLU:O	1:B:250:VAL:HG23	2.19	0.42
1:B:246:GLU:CD	1:B:301:LYS:HG3	2.40	0.42
1:B:321:TYR:O	1:B:323:THR:N	2.48	0.42
1:B:361:ILE:O	1:B:365:GLU:HG3	2.20	0.42
1:D:56:MET:HE1	1:D:178:LEU:C	2.40	0.42
1:A:339:LEU:C	1:A:339:LEU:HD23	2.40	0.42
1:C:42:SER:O	1:C:46:ALA:HB2	2.20	0.42
1:D:92:HIS:ND1	1:D:140:GLU:HG3	2.35	0.42
1:B:52:LEU:O	1:B:57:ARG:HD3	2.19	0.42
1:C:170:LEU:O	1:C:173:HIS:HB2	2.19	0.42
1:D:56:MET:HE1	1:D:178:LEU:O	2.20	0.42
1:D:219:VAL:HG13	1:D:219:VAL:O	2.20	0.42
1:D:122:ARG:HG3	1:D:123:ALA:N	2.35	0.42
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.87	0.41
1:B:219:VAL:HG13	1:B:219:VAL:O	2.20	0.41
1:B:49:ILE:HG12	1:B:57:ARG:HG3	2.01	0.41
1:C:276:ASP:HA	1:C:277:PRO:HD3	1.92	0.41
1:B:28:ASP:N	3:B:646:HOH:O	2.53	0.41
1:D:116:ARG:C	1:D:118:THR:H	2.24	0.41
1:A:102:MET:SD	1:A:105:VAL:HG21	2.60	0.41
1:C:87:GLU:C	1:C:90:LYS:HZ3	2.24	0.41
1:C:269:GLU:OE2	1:C:367:HIS:NE2	2.43	0.41
1:A:87:GLU:OE1	1:A:90:LYS:HE3	2.20	0.41
1:B:253:LEU:HD21	1:B:297:VAL:O	2.20	0.41
1:B:257:VAL:HG13	1:B:294:LEU:HD11	2.02	0.41
1:C:195:ASN:O	1:C:198:HIS:HB2	2.20	0.41
1:D:28:ASP:N	1:D:31:LEU:CD2	2.83	0.41
1:C:238:HIS:HE1	1:D:235:ASP:OD2	2.03	0.41
1:B:37:ILE:HG23	1:B:65:LEU:HD21	2.02	0.41
1:C:249:ALA:HB1	1:C:304:PHE:CZ	2.56	0.41
1:D:79:ILE:HA	1:D:80:PRO:HD3	1.82	0.41
1:D:300:ASN:O	1:D:303:VAL:HG23	2.20	0.41
1:B:321:TYR:C	1:B:323:THR:H	2.23	0.41
1:D:75:ASP:OD1	1:D:222:ARG:NH2	2.54	0.41
1:D:97:ASP:O	1:D:99:THR:N	2.41	0.41
1:A:227:ARG:O	1:A:231:GLU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ALA:O	1:D:251:GLU:HG3	2.21	0.40
1:A:103:SER:HA	1:A:115:GLU:HG2	2.04	0.40
1:A:276:ASP:HA	1:A:277:PRO:HD3	1.81	0.40
1:D:210:ARG:C	1:D:210:ARG:HD2	2.41	0.40
1:C:90:LYS:HB2	1:C:90:LYS:HE2	1.70	0.40
1:C:116:ARG:C	1:C:118:THR:N	2.74	0.40
1:D:236:ASP:O	1:D:239:ALA:HB3	2.21	0.40
1:B:122:ARG:HG3	1:B:122:ARG:NH1	2.36	0.40
1:D:119:HIS:HD1	1:D:119:HIS:H	1.69	0.40
1:D:232:LYS:O	1:D:232:LYS:CG	2.69	0.40
1:D:334:THR:O	1:D:338:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/365 (93%)	324 (96%)	14 (4%)	1 (0%)	41	50
1	B	339/365 (93%)	320 (94%)	17 (5%)	2 (1%)	25	30
1	C	340/365 (93%)	322 (95%)	18 (5%)	0	100	100
1	D	339/365 (93%)	312 (92%)	20 (6%)	7 (2%)	7	5
All	All	1357/1460 (93%)	1278 (94%)	69 (5%)	10 (1%)	22	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	54	GLU
1	B	98	THR
1	D	98	THR
1	D	305	HIS

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Mol	Chain	Res	Type
1	A	345	ALA
1	D	76	ASP
1	D	91	PHE
1	D	101	CYS
1	B	322	SER
1	D	104	GLY

5.3.2 Protein sidechains (i)

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	298/318 (94%)	287 (96%)	11 (4%)	34	47
1	B	298/318 (94%)	287 (96%)	11 (4%)	34	47
1	C	299/318 (94%)	287 (96%)	12 (4%)	31	44
1	D	298/318 (94%)	275 (92%)	23 (8%)	13	16
All	All	1193/1272 (94%)	1136 (95%)	57 (5%)	25	35

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	56	MET
1	A	75	ASP
1	A	109	ARG
1	A	153	LYS
1	A	188	ARG
1	A	315	THR
1	A	343	MET
1	A	344	ASN
1	A	346	GLN
1	A	352	ARG
1	B	39	GLN
1	B	56	MET
1	B	74	GLU
1	B	102	MET

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Mol	Chain	Res	Type
1	B	109	ARG
1	B	111	ARG
1	B	118	THR
1	B	188	ARG
1	B	294	LEU
1	B	301	LYS
1	B	352	ARG
1	C	43	ARG
1	C	74	GLU
1	C	150	LEU
1	C	189	LEU
1	C	199	MET
1	C	219	VAL
1	C	242	ASP
1	C	315	THR
1	C	333	LYS
1	C	346	GLN
1	C	359	ASP
1	C	365	GLU
1	D	29	GLU
1	D	31	LEU
1	D	41	VAL
1	D	49	ILE
1	D	53	ASP
1	D	56	MET
1	D	75	ASP
1	D	82	GLU
1	D	105	VAL
1	D	122	ARG
1	D	129	LYS
1	D	222	ARG
1	D	296	LEU
1	D	301	LYS
1	D	315	THR
1	D	324	GLU
1	D	337	LEU
1	D	339	LEU
1	D	346	GLN
1	D	352	ARG
1	D	354	GLU
1	D	359	ASP
1	D	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	119	HIS
1	A	144	ASN
1	A	238	HIS
1	A	320	HIS
1	A	344	ASN
1	B	119	HIS
1	B	144	ASN
1	B	238	HIS
1	B	320	HIS
1	B	330	GLN
1	B	346	GLN
1	B	358	ASN
1	C	27	ASN
1	C	144	ASN
1	C	238	HIS
1	C	245	HIS
1	C	346	GLN
1	D	94	HIS
1	D	144	ASN
1	D	238	HIS
1	D	245	HIS
1	D	330	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	D	401	-	33,36,36	2.71	8 (24%)	42,52,52	2.81	8 (19%)
2	E5S	B	401	-	33,36,36	2.72	9 (27%)	42,52,52	2.93	8 (19%)
2	E5S	A	401	-	33,36,36	2.79	8 (24%)	42,52,52	2.84	7 (16%)
2	E5S	C	401	-	33,36,36	2.64	8 (24%)	42,52,52	2.72	8 (19%)

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	D	401	-	-	5/14/49/49	0/6/5/5
2	E5S	B	401	-	-	5/14/49/49	0/6/5/5
2	E5S	A	401	-	-	2/14/49/49	0/6/5/5
2	E5S	C	401	-	-	4/14/49/49	0/6/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	E5S	CAQ-CAZ	-12.87	1.41	1.51
2	D	401	E5S	CAQ-CAZ	-12.44	1.42	1.51
2	C	401	E5S	CAQ-CAZ	-12.15	1.42	1.51
2	B	401	E5S	CAQ-CAZ	-12.05	1.42	1.51
2	B	401	E5S	CAD-CAE	3.56	1.24	1.19
2	A	401	E5S	CAD-CAE	3.53	1.24	1.19
2	D	401	E5S	CAQ-CAW	-3.26	1.41	1.52
2	B	401	E5S	CAQ-CAW	-3.26	1.41	1.52
2	B	401	E5S	CAR-NBE	3.08	1.51	1.46
2	A	401	E5S	CAQ-CAW	-3.00	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	E5S	CAQ-CAW	-2.93	1.42	1.52
2	C	401	E5S	CAR-NBE	2.83	1.51	1.46
2	D	401	E5S	CAR-NBE	2.81	1.51	1.46
2	B	401	E5S	CAS-NBE	2.73	1.50	1.46
2	A	401	E5S	CAR-NBE	2.60	1.50	1.46
2	D	401	E5S	CAS-NBE	2.59	1.50	1.46
2	C	401	E5S	CAS-NBE	2.39	1.50	1.46
2	A	401	E5S	CAL-CAK	2.32	1.42	1.38
2	B	401	E5S	CAH-CAJ	2.29	1.42	1.38
2	A	401	E5S	CAS-NBE	2.17	1.50	1.46
2	D	401	E5S	CAI-CAW	2.17	1.43	1.38
2	C	401	E5S	CAH-CAJ	2.16	1.42	1.38
2	C	401	E5S	CAF-CAG	2.16	1.43	1.38
2	A	401	E5S	CAJ-CAW	2.16	1.43	1.38
2	B	401	E5S	CAJ-CAW	2.15	1.43	1.38
2	D	401	E5S	CAD-CAE	2.14	1.22	1.19
2	D	401	E5S	CAJ-CAW	2.14	1.43	1.38
2	B	401	E5S	CAF-CAG	2.13	1.42	1.38
2	B	401	E5S	CAL-CAK	2.13	1.42	1.38
2	C	401	E5S	CAJ-CAW	2.07	1.43	1.38
2	A	401	E5S	CAG-CAI	2.06	1.42	1.38
2	C	401	E5S	CAO-NBD	2.05	1.52	1.46
2	D	401	E5S	CAH-CAJ	2.02	1.42	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	E5S	CAY-NAU-CAZ	15.43	124.74	118.85
2	A	401	E5S	CAY-NAU-CAZ	15.16	124.64	118.85
2	D	401	E5S	CAY-NAU-CAZ	14.29	124.31	118.85
2	C	401	E5S	CAY-NAU-CAZ	14.08	124.23	118.85
2	D	401	E5S	CAR-CBA-CBC	-6.39	97.89	104.12
2	B	401	E5S	CAR-CBA-CBC	-6.27	98.01	104.12
2	C	401	E5S	CAR-CBA-CBC	-6.22	98.05	104.12
2	A	401	E5S	CAR-CBA-CBC	-5.81	98.46	104.12
2	D	401	E5S	CBC-CAS-NBE	-5.41	97.23	103.26
2	B	401	E5S	CBC-CAS-NBE	-5.07	97.61	103.26
2	C	401	E5S	CBC-CAS-NBE	-4.92	97.78	103.26
2	A	401	E5S	CBC-CAS-NBE	-4.65	98.07	103.26
2	B	401	E5S	CAS-NBE-CAY	4.21	128.69	123.58
2	D	401	E5S	CAS-NBE-CAY	4.12	128.57	123.58
2	A	401	E5S	CAS-NBE-CAY	4.01	128.44	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	E5S	CAS-NBE-CAY	3.09	127.33	123.58
2	A	401	E5S	CAS-CBC-CBA	-2.63	100.09	103.58
2	C	401	E5S	CAS-CBC-CBA	-2.56	100.19	103.58
2	D	401	E5S	CAS-CBC-CBA	-2.54	100.22	103.58
2	B	401	E5S	CAL-CAY-NAU	-2.49	119.55	123.62
2	D	401	E5S	CAR-NBE-CAS	-2.41	108.14	111.64
2	A	401	E5S	CAL-CAY-NAU	-2.40	119.70	123.62
2	A	401	E5S	CAR-NBE-CAS	-2.37	108.20	111.64
2	B	401	E5S	CAR-NBE-CAS	-2.32	108.27	111.64
2	C	401	E5S	CAL-CAY-NAU	-2.27	119.91	123.62
2	D	401	E5S	CAL-CAY-NAU	-2.25	119.93	123.62
2	B	401	E5S	CAS-CBC-CBA	-2.21	100.66	103.58
2	C	401	E5S	CAR-NBE-CAS	-2.08	108.62	111.64
2	B	401	E5S	CAT-CBF-CAE	-2.07	108.01	112.22
2	C	401	E5S	CAT-CBF-CAE	-2.07	108.01	112.22
2	D	401	E5S	CAT-CBF-CAE	-2.03	108.08	112.22

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	E5S	CAX-CAD-CAE-CBF
2	D	401	E5S	CAD-CAE-CBF-CAT
2	A	401	E5S	CAE-CAD-CAX-CAZ
2	D	401	E5S	CBA-CBC-OAV-CAA
2	B	401	E5S	CAE-CAD-CAX-CAZ
2	C	401	E5S	CAE-CAD-CAX-CAZ
2	D	401	E5S	CAE-CAD-CAX-CAZ
2	A	401	E5S	CAE-CAD-CAX-CAK
2	B	401	E5S	CAE-CAD-CAX-CAK
2	C	401	E5S	CAE-CAD-CAX-CAK
2	D	401	E5S	CAS-CBC-OAV-CAA
2	C	401	E5S	CBA-CBC-OAV-CAA
2	D	401	E5S	CAE-CAD-CAX-CAK
2	C	401	E5S	CAS-CBC-OAV-CAA
2	B	401	E5S	CBA-CBC-OAV-CAA
2	B	401	E5S	CAS-CBC-OAV-CAA

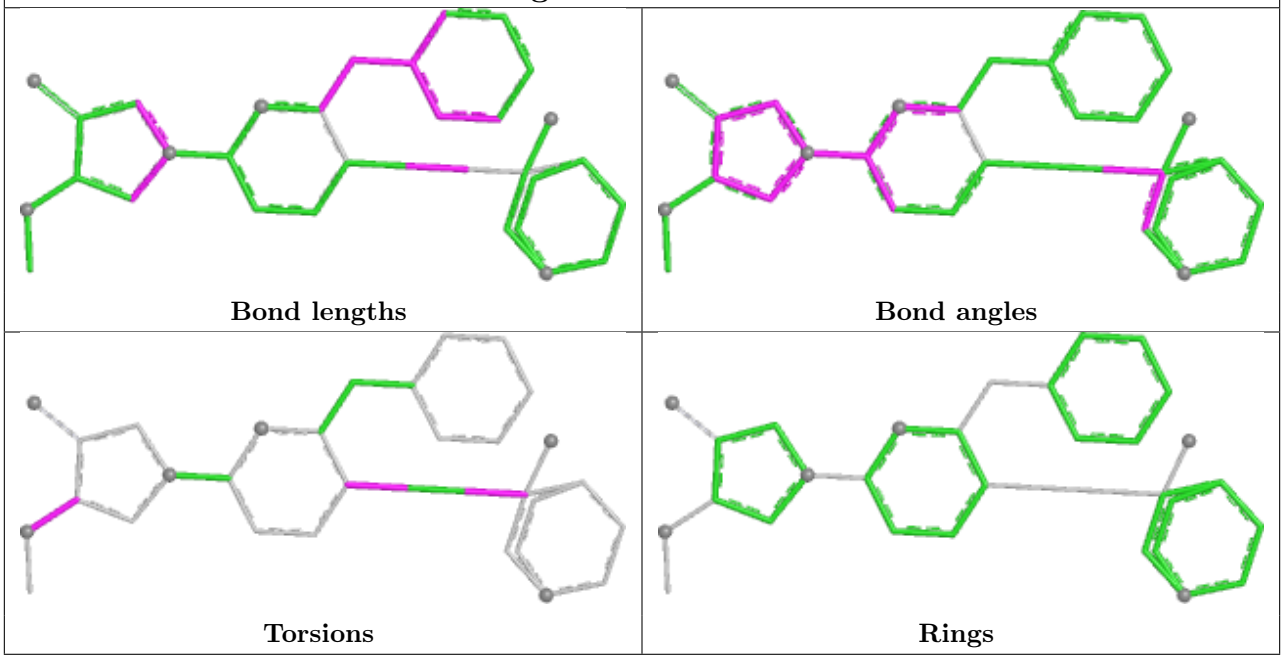
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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 then 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 D 401



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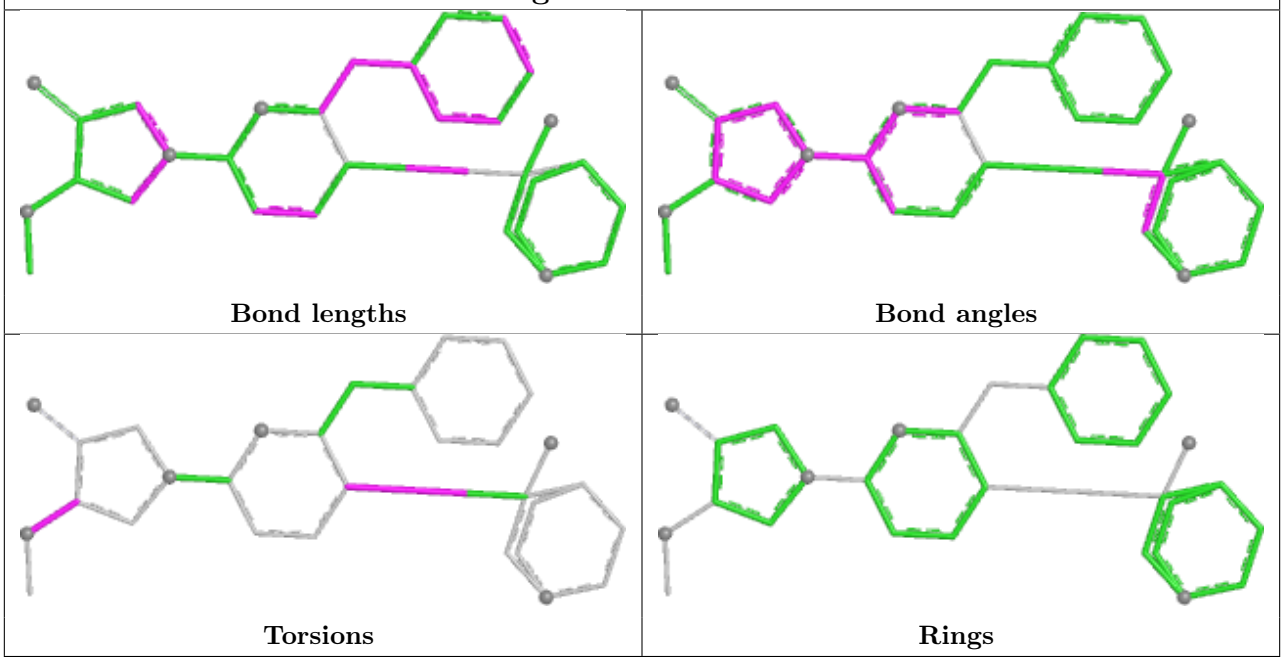

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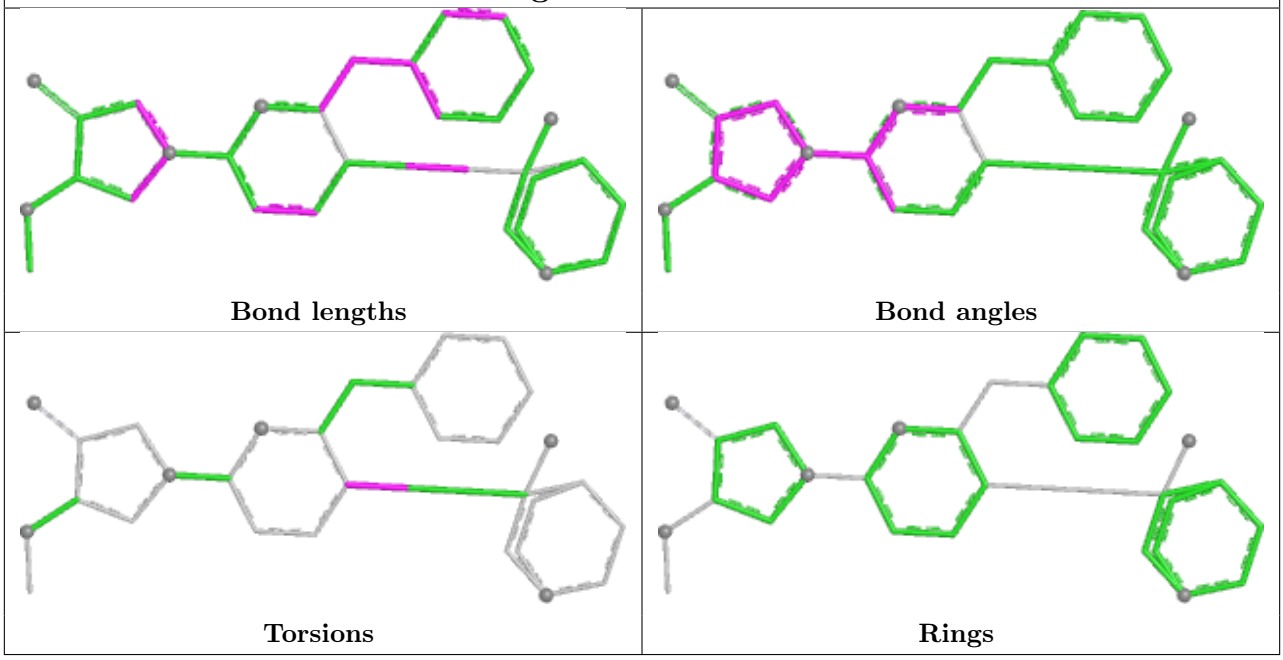

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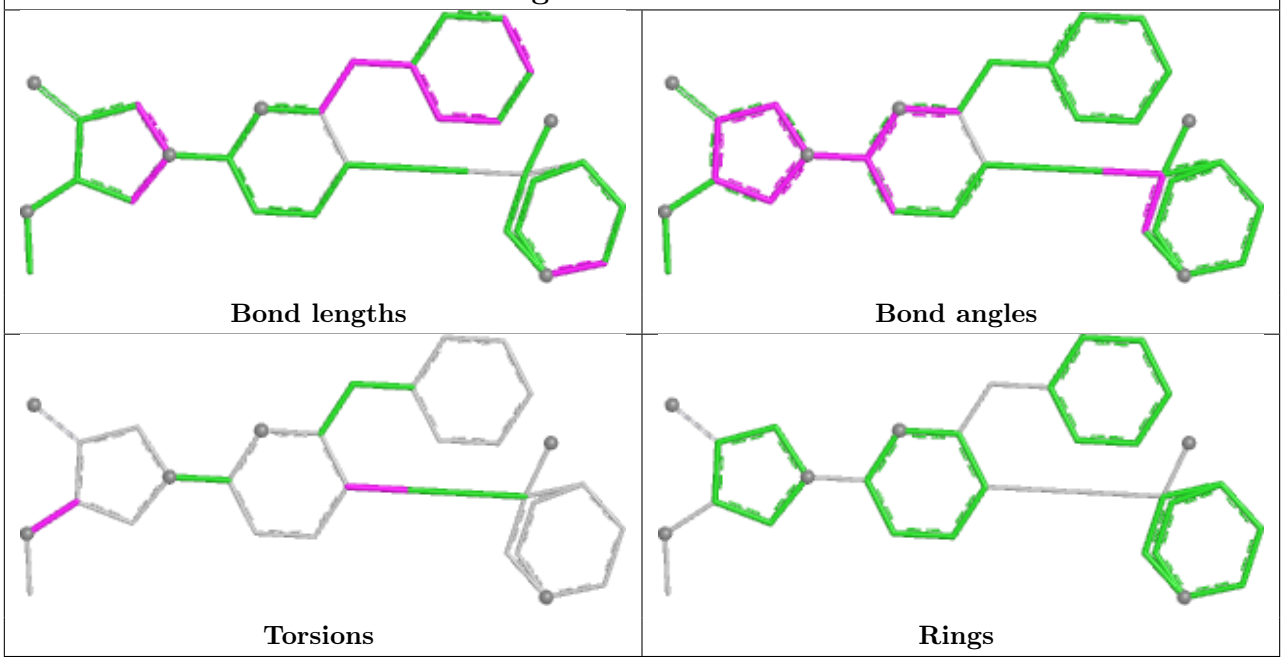

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	341/365 (93%)	0.07	10 (2%)	51	59	23, 40, 62, 91	0
1	B	341/365 (93%)	0.17	12 (3%)	44	51	22, 44, 77, 86	0
1	C	342/365 (93%)	0.31	15 (4%)	34	41	20, 46, 82, 89	0
1	D	341/365 (93%)	0.83	48 (14%)	2	4	27, 65, 110, 117	0
All	All	1365/1460 (93%)	0.34	85 (6%)	20	26	20, 47, 91, 117	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	345	ALA	6.3
1	D	80	PRO	5.8
1	D	346	GLN	5.6
1	D	78	SER	5.4
1	D	103	SER	5.3
1	A	346	GLN	4.6
1	D	86	ARG	4.5
1	B	345	ALA	4.5
1	D	82	GLU	4.5
1	B	219	VAL	4.4
1	D	348	ALA	4.2
1	D	69	ALA	4.1
1	A	349	CYS	4.1
1	C	43	ARG	4.0
1	C	66	VAL	4.0
1	D	217	CYS	3.9
1	D	151	THR	3.8
1	B	346	GLN	3.8
1	C	107	VAL	3.7
1	D	107	VAL	3.7
1	B	217	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	244	LEU	3.5
1	D	85	LEU	3.4
1	C	69	ALA	3.4
1	B	43	ARG	3.4
1	D	350	TYR	3.4
1	C	105	VAL	3.3
1	D	104	GLY	3.3
1	D	105	VAL	3.3
1	D	343	MET	3.3
1	D	79	ILE	3.3
1	A	344	ASN	3.2
1	D	347	ASP	3.2
1	A	67	LEU	3.2
1	D	121	THR	3.0
1	D	344	ASN	3.0
1	B	362	ARG	3.0
1	D	99	THR	3.0
1	D	153	LYS	3.0
1	B	213	TYR	2.9
1	D	28	ASP	2.9
1	A	348	ALA	2.9
1	C	90	LYS	2.9
1	D	209	ILE	2.9
1	C	219	VAL	2.8
1	C	81	VAL	2.8
1	C	86	ARG	2.8
1	D	66	VAL	2.8
1	C	244	LEU	2.8
1	D	96	HIS	2.8
1	D	213	TYR	2.8
1	D	67	LEU	2.7
1	D	349	CYS	2.7
1	C	253	LEU	2.7
1	D	113	LEU	2.6
1	D	81	VAL	2.4
1	C	82	GLU	2.4
1	D	244	LEU	2.4
1	D	152	ARG	2.4
1	C	67	LEU	2.4
1	D	235	ASP	2.3
1	C	70	LEU	2.3
1	A	219	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	188	ARG	2.3
1	D	150	LEU	2.3
1	B	344	ASN	2.3
1	D	115	GLU	2.2
1	D	91	PHE	2.2
1	A	28	ASP	2.2
1	D	219	VAL	2.1
1	D	275	ARG	2.1
1	D	83	PHE	2.1
1	C	106	GLY	2.1
1	D	351	ASP	2.1
1	A	151	THR	2.1
1	D	187	VAL	2.1
1	B	220	PRO	2.1
1	D	101	CYS	2.1
1	D	229	ILE	2.0
1	D	76	ASP	2.0
1	A	43	ARG	2.0
1	B	222	ARG	2.0
1	D	352	ARG	2.0
1	D	221	PRO	2.0
1	A	126	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	E5S	D	401	32/32	0.91	0.21	51,57,59,60	0

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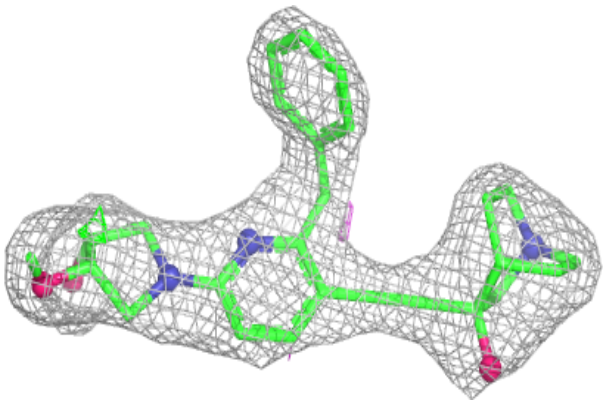
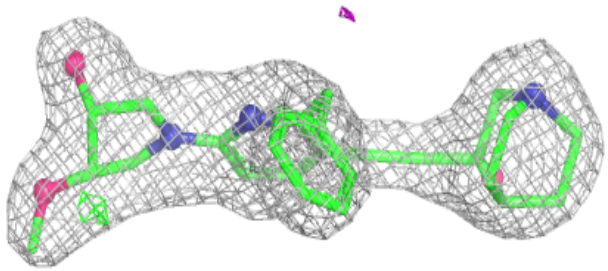
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	E5S	C	401	32/32	0.94	0.15	25,35,42,43	0
2	E5S	A	401	32/32	0.95	0.20	29,37,49,50	0
2	E5S	B	401	32/32	0.95	0.14	31,39,43,45	0

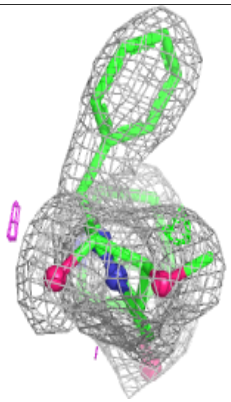
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

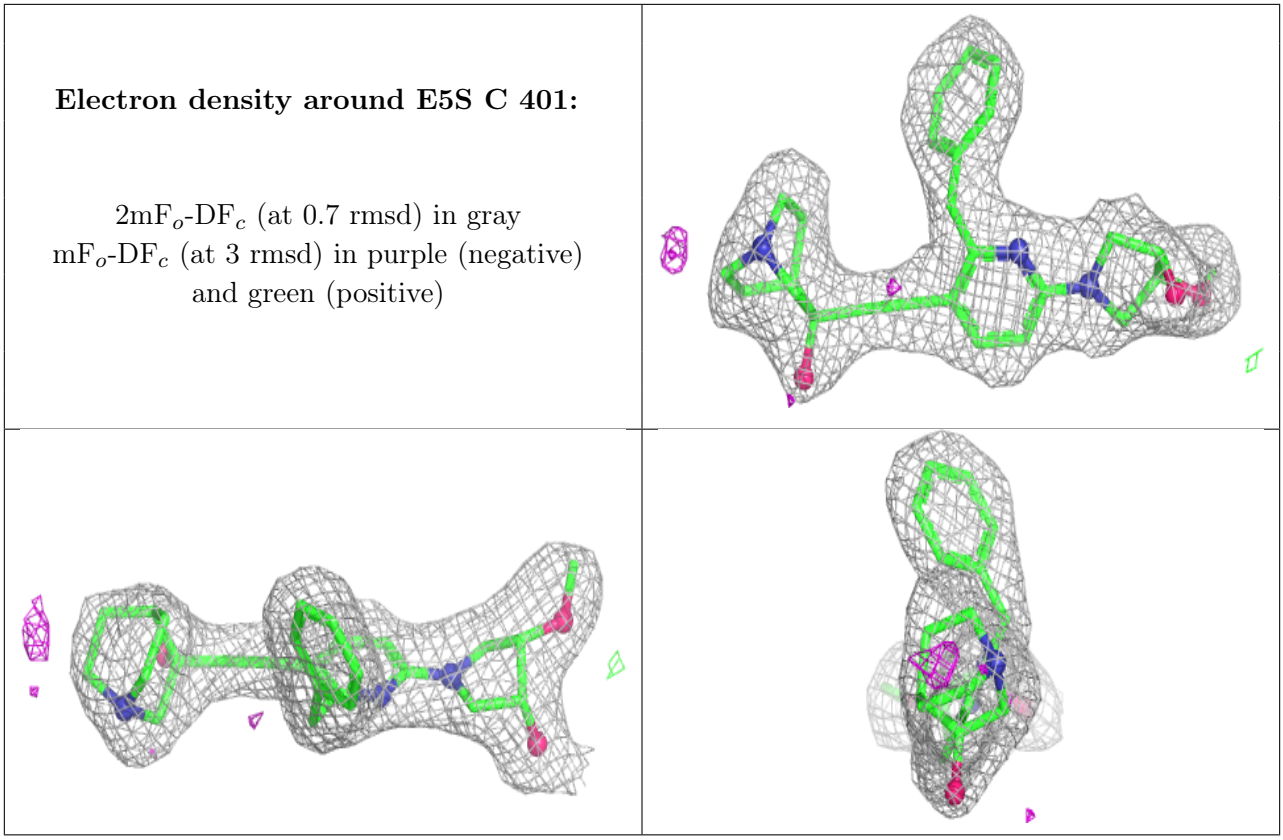






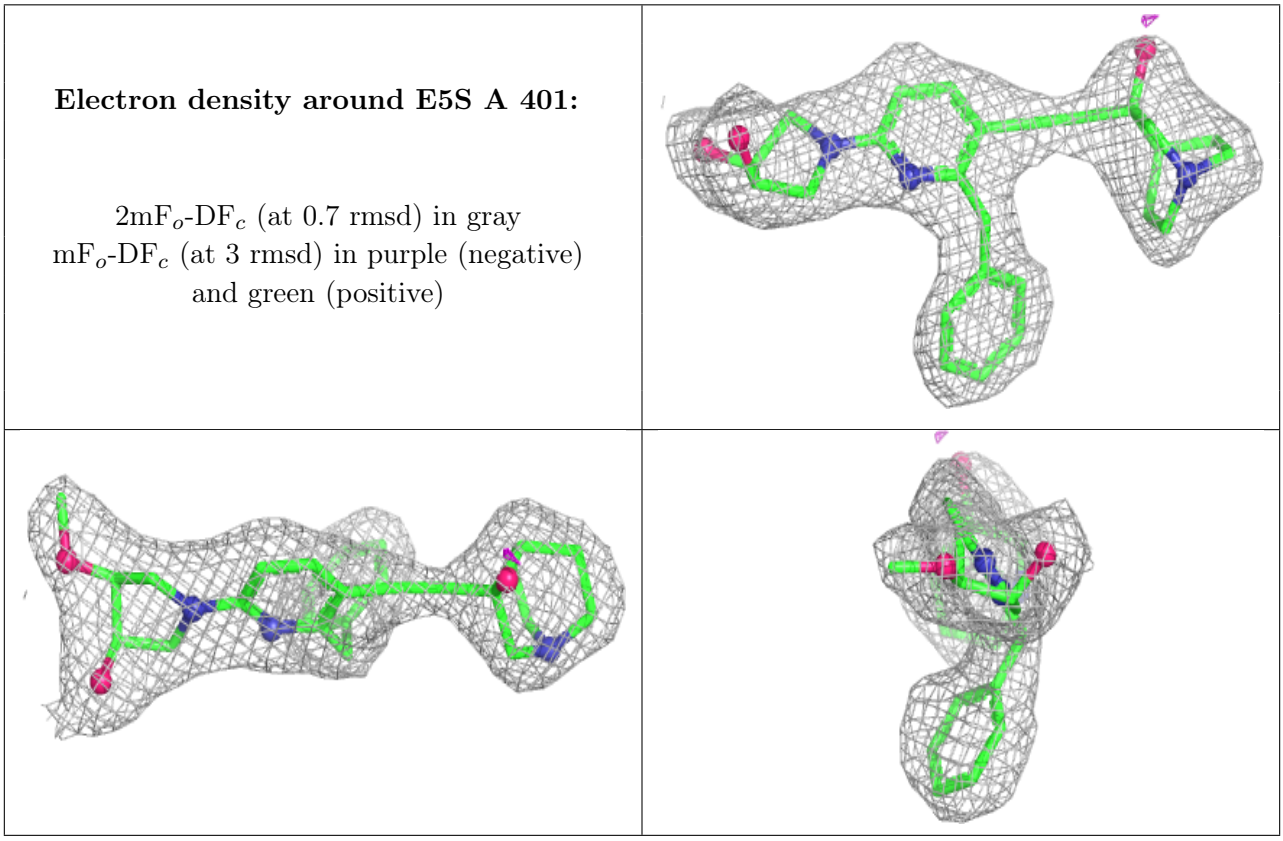
Electron density around E5S C 401:

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



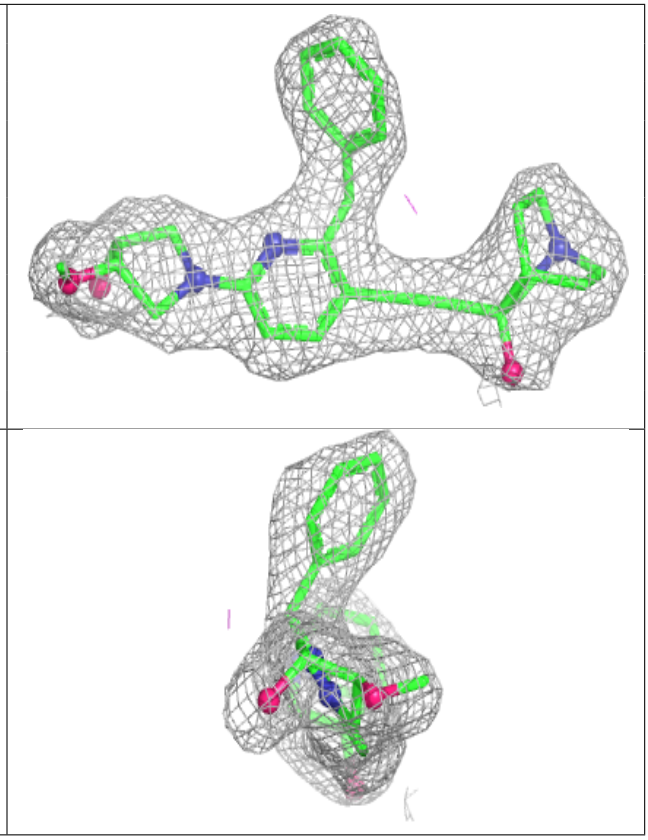
Electron density around E5S A 401:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.