



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:56 pm BST

PDB ID : 3WCE  
Title : The complex structure of TcSQS with ligand, ER119884  
Authors : Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.;  
Zhu, Z.; Chen, C.C.; Guo, R.T.  
Deposited on : 2013-05-27  
Resolution : 2.75 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](mailto: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.

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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

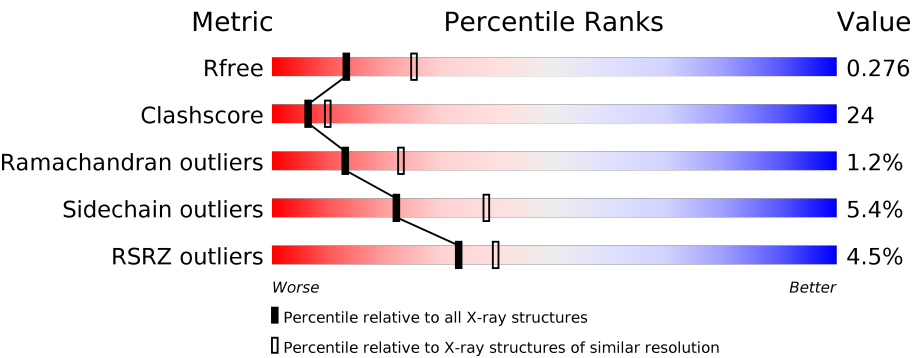
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	365	<div><div>2%</div><div><div></div><div>57%</div><div>35%</div><div>7%</div></div></div>
1	B	365	<div><div>3%</div><div><div></div><div>58%</div><div>34%</div><div>7%</div></div></div>
1	C	365	<div><div>2%</div><div><div></div><div>52%</div><div>39%</div><div>7%</div></div></div>
1	D	365	<div><div>10%</div><div><div></div><div>41%</div><div>45%</div><div>7%</div><div>7%</div></div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ER4	C	401	-	-	-	X
2	ER4	D	401	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11468 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
1	A	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	B	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	C	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	D	341	Total	C	N	O	S	0	0	0
			2748	1743	473	510	22			

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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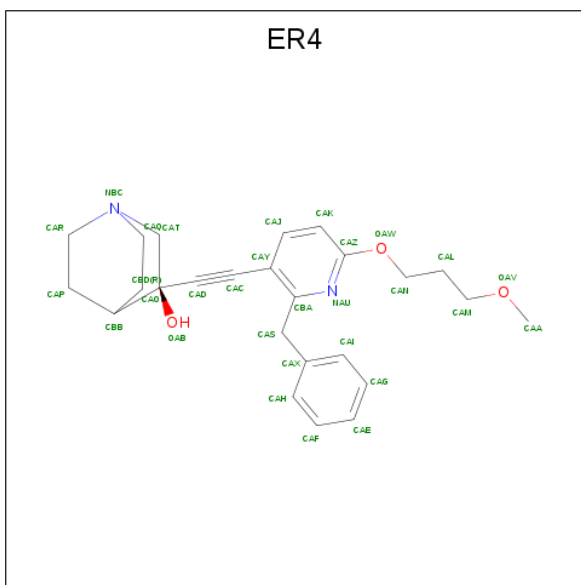
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
B	4	MET	-	EXPRESSION TAG	UNP Q4CWB4
B	5	GLY	-	EXPRESSION TAG	UNP Q4CWB4
B	6	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	7	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	8	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	9	HIS	-	EXPRESSION TAG	UNP 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-(3-methoxypropoxy)pyridin-3-yl}ethynyl}-1-azabicyclo[2.2.2]octan-3-ol (three-letter code: ER4) (formula: C<sub>25</sub>H<sub>30</sub>N<sub>2</sub>O<sub>3</sub>).



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

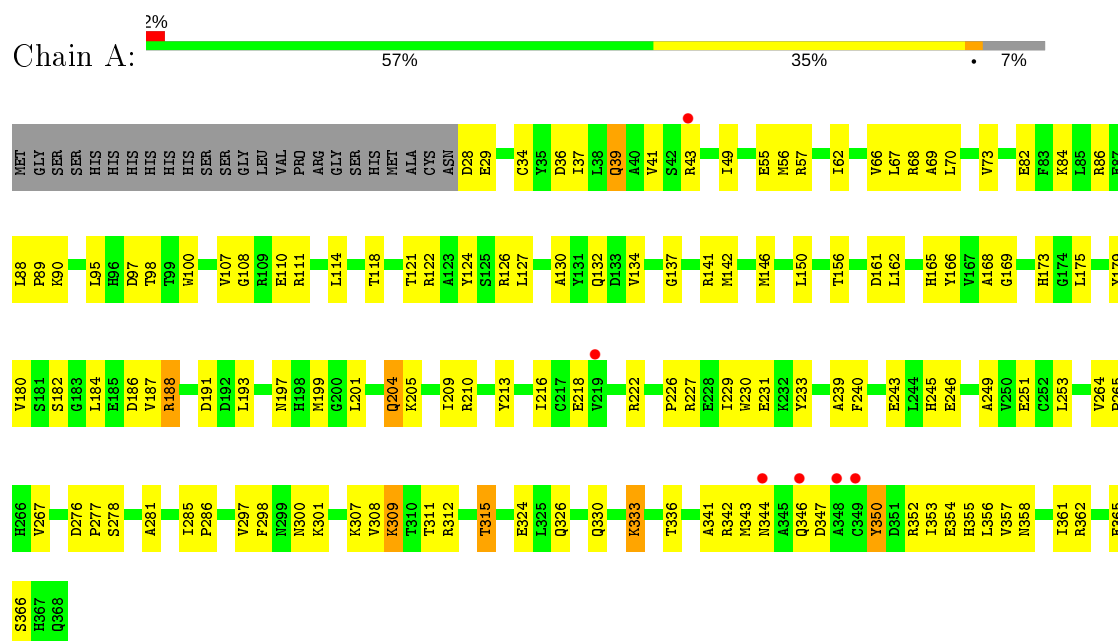
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	100	Total O 100 100	0	0
3	C	78	Total O 78 78	0	0
3	D	70	Total O 70 70	0	0

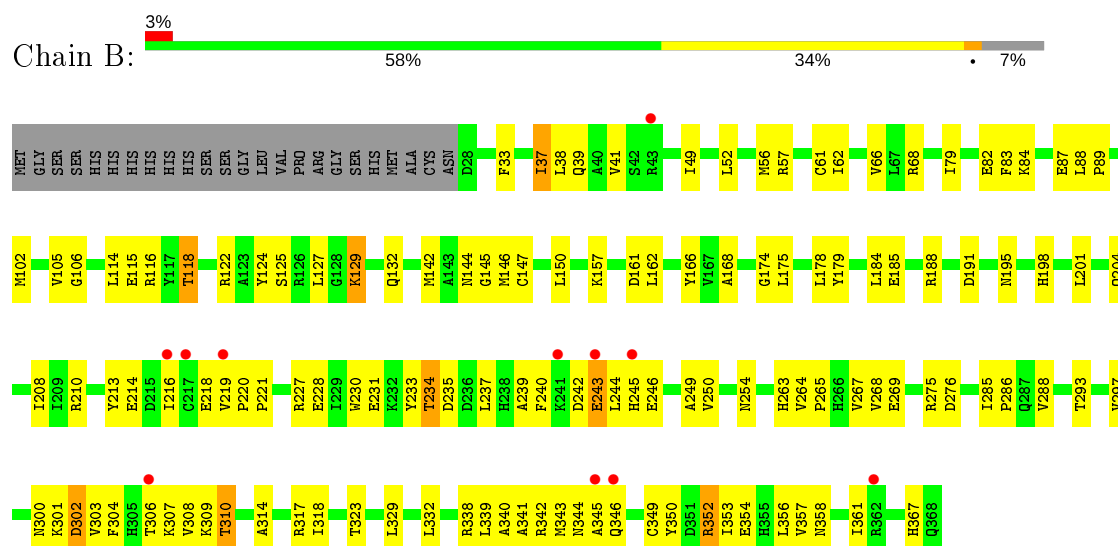
### 3 Residue-property plots

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: Farnesyltransferase, putative

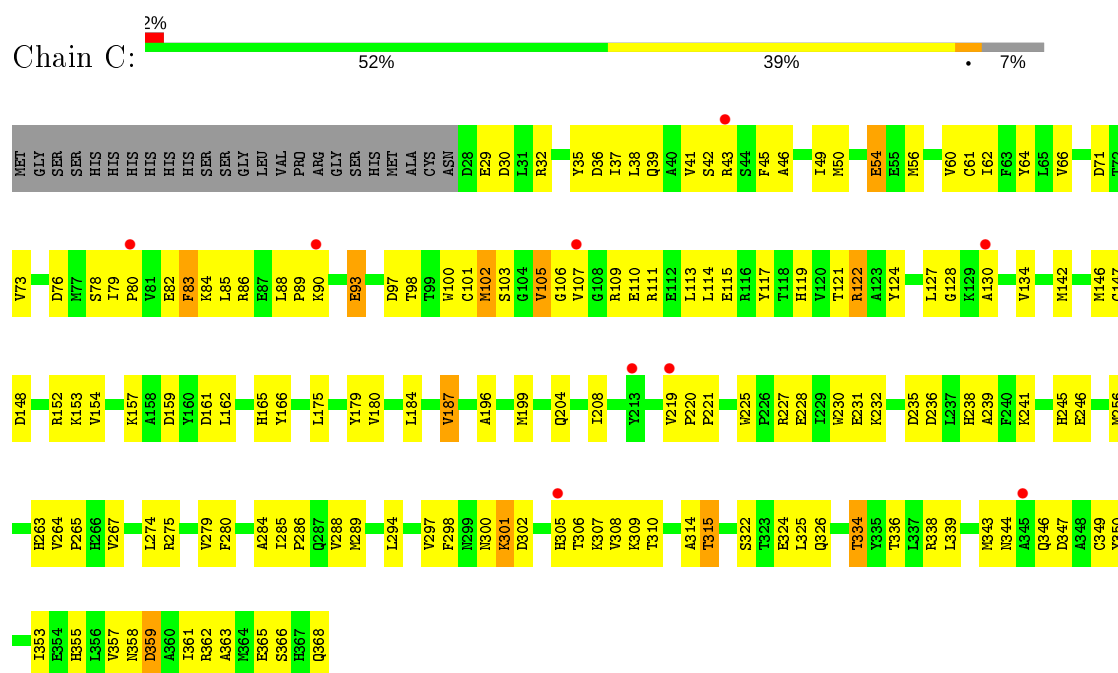


- Molecule 1: Farnesyltransferase, putative

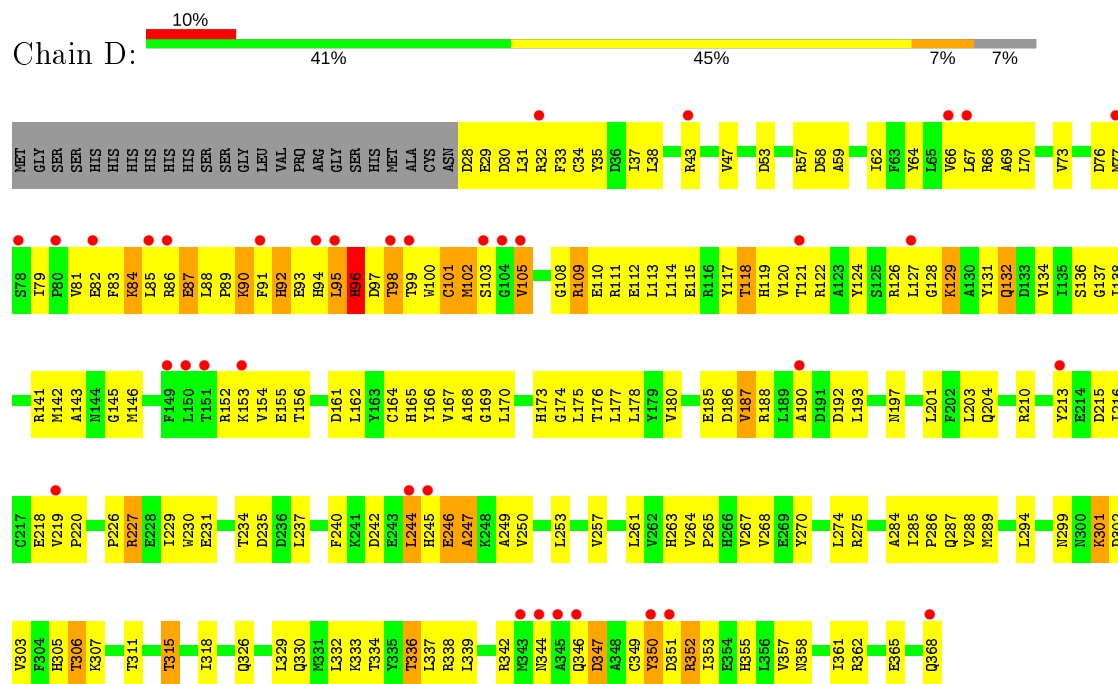


- Molecule 1: Farnesyltransferase, putative





• Molecule 1: Farnesyltransferase, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.81Å 131.42Å 142.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 24.93 – 2.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.75) 95.5 (24.93-2.74)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.76Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.213 , 0.262 0.227 , 0.276	Depositor DCC
$R_{free}$ test set	1874 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ER4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/2809	0.47	0/3806
1	B	0.25	0/2809	0.46	0/3806
1	C	0.25	0/2809	0.48	0/3806
1	D	0.26	0/2806	0.52	1/3801 (0.0%)
All	All	0.26	0/11233	0.49	1/15219 (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	D	96	HIS	N-CA-C	-6.10	94.52	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	100	0
1	B	2751	0	2698	91	0
1	C	2751	0	2698	119	0
1	D	2748	0	2694	223	0
2	A	30	0	30	2	0
2	B	30	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	30	2	0
2	D	30	0	30	6	0
3	A	99	0	0	4	0
3	B	100	0	0	0	0
3	C	78	0	0	2	0
3	D	70	0	0	1	0
All	All	11468	0	10908	531	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 24.

All (531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:O	1:D:89:PRO:HD2	1.59	1.03
1:D:29:GLU:HA	1:D:32:ARG:HE	1.24	0.99
1:D:98:THR:HA	1:D:121:THR:HG21	1.46	0.96
1:A:175:LEU:HD12	2:A:401:ER4:H21	1.49	0.94
1:D:59:ALA:HA	1:D:127:LEU:HD11	1.49	0.94
1:D:92:HIS:O	1:D:95:LEU:HG	1.67	0.92
1:B:297:VAL:HG23	1:B:303:VAL:HG21	1.52	0.91
1:D:62:ILE:HD12	1:D:127:LEU:HD12	1.55	0.87
1:A:168:ALA:HB2	1:A:204:GLN:HG3	1.57	0.86
1:C:62:ILE:HD12	1:C:127:LEU:HD11	1.56	0.86
1:C:56:MET:HE1	1:C:179:TYR:HA	1.54	0.86
1:A:366:SER:HA	1:D:108:GLY:HA2	1.57	0.85
1:D:175:LEU:HD12	2:D:401:ER4:H21	1.59	0.83
1:B:175:LEU:HD12	2:B:401:ER4:H21	1.61	0.83
1:D:88:LEU:O	1:D:91:PHE:HB2	1.78	0.82
1:D:227:ARG:HG3	1:D:230:TRP:CZ2	2.15	0.81
1:D:186:ASP:N	1:D:275:ARG:HH12	1.77	0.81
1:C:175:LEU:HD12	2:C:401:ER4:H21	1.61	0.81
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.64	0.80
1:D:153:LYS:HD2	1:D:227:ARG:CZ	2.12	0.80
1:D:98:THR:O	1:D:118:THR:HG22	1.83	0.78
1:D:127:LEU:HD23	1:D:128:GLY:N	1.99	0.78
1:D:301:LYS:HD3	1:D:301:LYS:H	1.49	0.78
1:D:344:ASN:HD21	1:D:346:GLN:HB3	1.50	0.77
1:D:103:SER:HA	1:D:115:GLU:HG2	1.67	0.77
1:D:90:LYS:HD3	1:D:93:GLU:HB2	1.67	0.77
1:A:227:ARG:HA	1:A:230:TRP:NE1	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:TYR:CZ	1:D:132:GLN:HG3	2.21	0.76
1:D:28:ASP:O	1:D:32:ARG:HG3	1.86	0.75
1:A:186:ASP:OD2	1:A:188:ARG:HB2	1.87	0.75
1:C:114:LEU:HA	1:C:117:TYR:HB2	1.68	0.75
1:C:37:ILE:HG21	1:C:113:LEU:HD13	1.69	0.74
1:D:121:THR:O	1:D:124:TYR:HB3	1.88	0.74
1:D:127:LEU:HD23	1:D:128:GLY:H	1.52	0.74
1:B:41:VAL:HG22	1:B:68:ARG:NH1	2.03	0.73
1:D:76:ASP:OD2	1:D:79:ILE:HB	1.89	0.73
1:A:344:ASN:HB3	1:A:346:GLN:HG2	1.71	0.73
1:C:80:PRO:HB2	1:C:82:GLU:HG2	1.70	0.72
1:D:117:TYR:O	1:D:120:VAL:HG12	1.90	0.71
1:D:155:GLU:HA	1:D:227:ARG:HB2	1.71	0.71
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.71	0.71
1:A:285:ILE:HB	1:A:286:PRO:HD3	1.72	0.71
1:B:62:ILE:HD12	1:B:127:LEU:HD11	1.72	0.70
1:C:43:ARG:HB2	1:C:43:ARG:NH1	2.06	0.70
1:C:358:ASN:HB3	1:C:362:ARG:NH2	2.06	0.70
1:B:297:VAL:HG23	1:B:303:VAL:CG2	2.22	0.70
1:D:152:ARG:HG2	1:D:153:LYS:H	1.56	0.69
1:D:85:LEU:HD12	1:D:89:PRO:HG2	1.74	0.69
1:D:362:ARG:HH11	1:D:362:ARG:HG3	1.58	0.69
1:A:298:PHE:O	1:A:342:ARG:NH1	2.25	0.68
1:C:83:PHE:O	1:C:86:ARG:HG2	1.93	0.67
1:C:29:GLU:O	1:C:32:ARG:HB2	1.94	0.67
1:C:46:ALA:O	1:C:50:MET:HG2	1.93	0.67
1:D:95:LEU:HD13	1:D:124:TYR:CE2	2.30	0.67
1:D:210:ARG:HD3	1:D:307:LYS:HG3	1.77	0.67
1:D:59:ALA:CA	1:D:127:LEU:HD11	2.24	0.67
1:D:311:THR:O	1:D:315:THR:HG22	1.94	0.67
1:D:180:VAL:HG21	1:D:190:ALA:HB2	1.78	0.66
1:C:106:GLY:O	1:C:111:ARG:HB2	1.96	0.65
1:C:41:VAL:HG23	1:C:42:SER:H	1.60	0.65
1:C:79:ILE:HG23	1:C:80:PRO:HD2	1.78	0.65
1:D:174:GLY:O	1:D:178:LEU:HD12	1.96	0.65
1:A:168:ALA:HB2	1:A:204:GLN:CG	2.27	0.65
1:B:293:THR:O	1:B:297:VAL:HG12	1.97	0.65
1:D:82:GLU:O	1:D:86:ARG:HD3	1.96	0.64
1:D:98:THR:HA	1:D:121:THR:CG2	2.24	0.64
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.77	0.64
1:A:330:GLN:HA	1:A:333:LYS:HZ2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:TYR:O	1:B:216:ILE:HG22	1.97	0.64
1:C:309:LYS:NZ	1:C:309:LYS:HB2	2.12	0.64
1:D:30:ASP:OD2	1:D:122:ARG:HD2	1.98	0.64
1:B:142:MET:HG3	1:B:166:TYR:O	1.97	0.64
1:D:246:GLU:O	1:D:249:ALA:N	2.31	0.63
1:D:109:ARG:NH1	1:D:109:ARG:HB3	2.13	0.63
1:D:250:VAL:O	1:D:253:LEU:HB3	1.99	0.62
1:B:214:GLU:O	1:B:218:GLU:HG3	2.00	0.62
1:B:88:LEU:HB2	1:B:89:PRO:HD3	1.81	0.62
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.82	0.62
1:C:35:TYR:O	1:C:39:GLN:HG3	1.99	0.62
1:C:42:SER:O	1:C:46:ALA:HB2	1.99	0.62
1:D:352:ARG:O	1:D:355:HIS:HB3	2.00	0.62
1:C:285:ILE:HB	1:C:286:PRO:HD3	1.82	0.62
1:C:355:HIS:O	1:C:359:ASP:HB2	2.00	0.62
1:D:154:VAL:O	1:D:227:ARG:HD3	2.00	0.62
1:D:138:ILE:CG2	1:D:170:LEU:HB3	2.30	0.61
1:D:30:ASP:HB2	1:D:126:ARG:NH1	2.14	0.61
1:C:30:ASP:CG	1:C:122:ARG:HD2	2.20	0.61
1:C:79:ILE:HD11	1:C:105:VAL:HG12	1.81	0.61
1:D:43:ARG:O	1:D:47:VAL:HG23	2.00	0.61
1:A:97:ASP:OD2	1:A:100:TRP:HB2	2.01	0.61
1:C:83:PHE:C	1:C:83:PHE:CD2	2.72	0.61
1:D:333:LYS:O	1:D:337:LEU:HD13	2.01	0.61
1:C:41:VAL:HG23	1:C:42:SER:N	2.15	0.61
1:A:67:LEU:HD22	1:A:142:MET:SD	2.41	0.61
1:C:42:SER:HB2	1:C:64:TYR:OH	2.00	0.61
1:B:243:GLU:O	1:B:246:GLU:HB2	2.01	0.60
1:D:240:PHE:HE1	1:D:249:ALA:HA	1.66	0.60
1:D:242:ASP:OD1	1:D:245:HIS:HB3	2.02	0.60
1:C:102:MET:CE	1:C:105:VAL:HG21	2.32	0.60
1:D:244:LEU:HD23	1:D:244:LEU:N	2.17	0.60
1:A:118:THR:O	1:A:122:ARG:HG2	2.02	0.59
1:A:199:MET:SD	1:A:267:VAL:HG13	2.42	0.59
1:B:33:PHE:CZ	1:B:37:ILE:HD12	2.37	0.59
1:D:186:ASP:N	1:D:275:ARG:NH1	2.49	0.59
1:B:285:ILE:HB	1:B:286:PRO:HD3	1.84	0.59
3:A:540:HOH:O	1:B:323:THR:HG21	2.01	0.59
1:A:184:LEU:HD23	1:A:276:ASP:OD2	2.02	0.59
1:B:340:ALA:HB2	1:B:357:VAL:HG21	1.84	0.59
1:A:343:MET:SD	1:A:350:TYR:HA	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:GLU:C	1:D:275:ARG:HH12	2.06	0.59
1:D:240:PHE:CE1	1:D:249:ALA:HA	2.38	0.59
1:D:117:TYR:CE1	1:D:120:VAL:HG11	2.37	0.58
1:D:68:ARG:O	1:D:68:ARG:HD3	2.03	0.58
1:B:246:GLU:OE2	1:B:301:LYS:HD2	2.03	0.58
1:D:100:TRP:O	1:D:101:CYS:HB3	2.03	0.58
1:C:227:ARG:O	1:C:231:GLU:HG2	2.02	0.58
1:A:182:SER:OG	1:A:184:LEU:HD12	2.04	0.58
1:B:264:VAL:HB	1:B:265:PRO:HD3	1.83	0.58
1:D:77:MET:HG3	1:D:220:PRO:HG2	1.86	0.58
1:D:102:MET:HE2	1:D:105:VAL:HG22	1.84	0.58
1:D:118:THR:O	1:D:121:THR:HG22	2.03	0.58
1:D:102:MET:CE	1:D:105:VAL:HG22	2.34	0.58
1:D:155:GLU:HB2	1:D:227:ARG:NH1	2.19	0.58
1:C:246:GLU:OE2	1:C:301:LYS:HE3	2.04	0.58
1:A:210:ARG:HD2	1:A:308:VAL:O	2.03	0.57
1:C:280:PHE:CZ	1:C:325:LEU:HA	2.39	0.57
1:A:142:MET:HG3	1:A:166:TYR:O	2.04	0.57
1:D:142:MET:HG2	1:D:146:MET:CE	2.34	0.57
1:D:301:LYS:HD3	1:D:301:LYS:N	2.17	0.57
1:C:310:THR:HG22	1:C:314:ALA:HB3	1.86	0.57
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.87	0.57
1:D:118:THR:HB	1:D:122:ARG:HH12	1.70	0.57
1:D:353:ILE:HG22	1:D:357:VAL:HG23	1.87	0.57
1:D:73:VAL:O	1:D:84:LYS:HE2	2.04	0.57
1:A:43:ARG:HB2	1:A:43:ARG:NH2	2.20	0.56
1:D:285:ILE:HB	1:D:286:PRO:HD3	1.86	0.56
1:D:90:LYS:NZ	1:D:93:GLU:HG2	2.20	0.56
1:D:227:ARG:O	1:D:231:GLU:HB3	2.05	0.56
1:C:142:MET:O	1:C:146:MET:HG3	2.04	0.56
1:D:43:ARG:HG3	3:D:539:HOH:O	2.05	0.56
1:C:264:VAL:HB	1:C:265:PRO:HD3	1.87	0.56
1:C:79:ILE:HD12	1:C:79:ILE:N	2.21	0.56
1:D:244:LEU:HD23	1:D:244:LEU:H	1.70	0.56
1:D:83:PHE:O	1:D:87:GLU:HB2	2.06	0.56
1:B:56:MET:HE1	1:B:179:TYR:HA	1.88	0.55
1:D:84:LYS:O	1:D:88:LEU:N	2.30	0.55
1:B:142:MET:O	1:B:146:MET:HG3	2.06	0.55
1:D:76:ASP:O	1:D:79:ILE:HG22	2.06	0.55
1:C:90:LYS:O	1:C:93:GLU:HB2	2.07	0.55
1:D:302:ASP:HA	1:D:305:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ARG:O	1:B:342:ARG:HG3	2.07	0.55
1:C:227:ARG:HA	1:C:230:TRP:NE1	2.22	0.55
1:D:173:HIS:O	1:D:177:LEU:HG	2.07	0.55
1:D:94:HIS:HD2	1:D:100:TRP:CE2	2.24	0.55
1:D:93:GLU:N	1:D:93:GLU:OE2	2.38	0.55
1:A:62:ILE:HD12	1:A:127:LEU:HD11	1.88	0.55
1:C:130:ALA:O	1:C:134:VAL:HG23	2.06	0.55
1:B:175:LEU:CD1	2:B:401:ER4:H21	2.36	0.55
1:C:324:GLU:OE1	1:C:326:GLN:HB2	2.07	0.55
1:D:109:ARG:HH11	1:D:109:ARG:HB3	1.72	0.55
1:D:213:TYR:HA	1:D:216:ILE:HG22	1.88	0.55
1:C:56:MET:O	1:C:60:VAL:HG23	2.07	0.54
1:D:142:MET:HG3	1:D:166:TYR:O	2.06	0.54
1:C:38:LEU:HD23	1:C:50:MET:HE2	1.90	0.54
1:D:339:LEU:HD23	1:D:339:LEU:O	2.07	0.54
1:C:111:ARG:O	1:C:115:GLU:HG3	2.07	0.54
1:B:102:MET:HB2	1:B:114:LEU:HB3	1.89	0.54
1:B:227:ARG:HG2	1:B:231:GLU:HB3	1.90	0.54
1:B:268:VAL:HG13	1:B:329:LEU:HD21	1.89	0.54
1:C:76:ASP:HB3	1:C:79:ILE:HD13	1.90	0.54
1:D:102:MET:HB3	1:D:105:VAL:CG2	2.38	0.54
1:D:70:LEU:HA	1:D:91:PHE:CZ	2.43	0.54
1:C:110:GLU:O	1:C:113:LEU:HB3	2.07	0.54
1:A:311:THR:O	1:A:315:THR:HG22	2.07	0.53
1:B:129:LYS:HD2	1:B:129:LYS:O	2.08	0.53
1:D:358:ASN:O	1:D:362:ARG:HG2	2.09	0.53
1:B:249:ALA:HB1	1:B:304:PHE:CE2	2.43	0.53
1:C:289:MET:CE	1:C:315:THR:HB	2.38	0.53
1:D:110:GLU:O	1:D:113:LEU:HB3	2.08	0.53
1:D:96:HIS:O	1:D:97:ASP:C	2.45	0.53
1:C:157:LYS:HG3	1:C:228:GLU:OE1	2.07	0.53
1:D:347:ASP:HB2	1:D:350:TYR:HB2	1.89	0.53
1:D:85:LEU:CD1	1:D:89:PRO:HG2	2.38	0.53
1:B:303:VAL:HG22	1:B:308:VAL:HG21	1.91	0.53
1:A:358:ASN:O	1:A:362:ARG:HB2	2.09	0.53
1:A:361:ILE:O	1:A:365:GLU:HG3	2.09	0.53
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.24	0.53
1:B:125:SER:HA	1:B:132:GLN:NE2	2.24	0.53
1:D:59:ALA:HA	1:D:127:LEU:CD1	2.31	0.53
1:A:41:VAL:HG11	1:A:68:ARG:HE	1.74	0.52
1:A:142:MET:O	1:A:146:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:O	1:D:165:HIS:HB3	2.09	0.52
1:B:314:ALA:O	1:B:318:ILE:HG13	2.10	0.52
1:B:244:LEU:O	1:B:245:HIS:HB2	2.10	0.52
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.90	0.52
1:B:244:LEU:C	1:B:246:GLU:H	2.12	0.52
1:D:237:LEU:HD12	1:D:240:PHE:CE2	2.45	0.52
1:D:250:VAL:CG2	1:D:301:LYS:HG3	2.40	0.52
1:B:242:ASP:OD2	1:B:244:LEU:HB3	2.09	0.52
1:D:180:VAL:CG1	1:D:187:VAL:HA	2.38	0.52
1:D:337:LEU:HD11	1:D:361:ILE:HD11	1.92	0.52
1:A:69:ALA:HB1	1:A:114:LEU:HD21	1.93	0.51
1:C:62:ILE:O	1:C:66:VAL:HG23	2.11	0.51
1:A:34:CYS:O	1:A:37:ILE:HG22	2.10	0.51
1:A:108:GLY:O	1:A:111:ARG:HB3	2.10	0.51
1:A:86:ARG:O	1:A:90:LYS:HE3	2.10	0.51
1:D:67:LEU:HD22	1:D:142:MET:SD	2.50	0.51
1:B:353:ILE:O	1:B:357:VAL:HG23	2.10	0.51
1:A:62:ILE:O	1:A:66:VAL:HG23	2.10	0.51
1:D:90:LYS:HZ2	1:D:93:GLU:HG2	1.75	0.51
1:D:362:ARG:NH1	1:D:362:ARG:HG3	2.25	0.51
1:D:88:LEU:CB	1:D:89:PRO:HD3	2.40	0.51
1:B:49:ILE:HG12	1:B:57:ARG:HG3	1.93	0.51
1:C:302:ASP:O	1:C:306:THR:HG22	2.11	0.51
1:D:164:CYS:HB2	1:D:201:LEU:HD22	1.93	0.51
1:C:220:PRO:HB2	1:C:221:PRO:HD2	1.93	0.51
1:C:336:THR:HG22	1:C:357:VAL:HG13	1.92	0.50
1:A:180:VAL:HG13	1:A:187:VAL:HA	1.92	0.50
1:C:274:LEU:HD13	1:C:279:VAL:HG12	1.93	0.50
1:D:137:GLY:O	1:D:141:ARG:HG3	2.11	0.50
1:D:153:LYS:HG3	1:D:227:ARG:NH1	2.27	0.50
1:D:174:GLY:C	1:D:178:LEU:HD12	2.31	0.50
1:D:284:ALA:O	1:D:288:VAL:HG23	2.11	0.50
1:D:81:VAL:C	1:D:83:PHE:H	2.13	0.50
1:D:203:LEU:HG	1:D:287:GLN:HE22	1.77	0.50
1:D:97:ASP:O	1:D:99:THR:N	2.44	0.50
1:C:236:ASP:OD2	1:C:238:HIS:HB2	2.11	0.50
1:D:210:ARG:C	1:D:210:ARG:HD2	2.32	0.50
1:C:56:MET:CE	1:C:179:TYR:HA	2.37	0.50
1:C:358:ASN:HB3	1:C:362:ARG:HH21	1.74	0.50
1:C:42:SER:HB2	1:C:64:TYR:CZ	2.47	0.50
1:D:97:ASP:C	1:D:99:THR:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:O	1:A:209:ILE:HG13	2.11	0.49
1:D:164:CYS:CB	1:D:201:LEU:HD22	2.41	0.49
1:D:250:VAL:HG21	1:D:301:LYS:HG3	1.93	0.49
1:C:196:ALA:O	1:C:199:MET:HB2	2.12	0.49
1:C:71:ASP:HB2	2:C:401:ER4:H9	1.93	0.49
1:C:45:PHE:O	1:C:49:ILE:HG13	2.12	0.49
1:C:152:ARG:HG2	1:C:153:LYS:N	2.27	0.49
1:D:117:TYR:CZ	1:D:120:VAL:HG11	2.47	0.49
1:B:102:MET:O	1:B:115:GLU:HA	2.11	0.49
1:D:185:GLU:HA	1:D:275:ARG:NH1	2.27	0.49
1:D:226:PRO:HB2	1:D:229:ILE:HG13	1.93	0.49
1:D:64:TYR:CE1	2:D:401:ER4:H12	2.47	0.49
1:A:69:ALA:HB1	1:A:114:LEU:CD2	2.43	0.49
1:B:306:THR:OG1	1:B:307:LYS:N	2.45	0.49
1:B:188:ARG:HG3	1:B:191:ASP:OD2	2.12	0.49
1:C:79:ILE:HD11	1:C:105:VAL:CG1	2.42	0.49
1:C:142:MET:HG3	1:C:166:TYR:O	2.13	0.49
1:C:38:LEU:HD22	1:C:61:CYS:SG	2.53	0.49
1:C:37:ILE:O	1:C:41:VAL:HG22	2.12	0.49
1:C:97:ASP:OD2	1:C:100:TRP:HB2	2.12	0.49
1:D:142:MET:HG2	1:D:146:MET:HE3	1.95	0.49
1:D:111:ARG:O	1:D:115:GLU:HG3	2.13	0.49
1:D:90:LYS:HD3	1:D:93:GLU:CB	2.41	0.49
1:A:197:ASN:O	1:A:201:LEU:HG	2.12	0.49
1:D:230:TRP:CG	1:D:237:LEU:HD13	2.48	0.49
1:D:344:ASN:ND2	1:D:346:GLN:HB3	2.25	0.49
1:A:298:PHE:O	1:A:342:ARG:NH2	2.46	0.49
1:A:336:THR:HG22	1:A:357:VAL:HG13	1.95	0.49
1:C:101:CYS:HB2	1:C:114:LEU:O	2.12	0.48
1:D:155:GLU:OE2	1:D:227:ARG:CZ	2.61	0.48
1:D:83:PHE:CE2	1:D:102:MET:HE3	2.47	0.48
1:D:129:LYS:HA	1:D:132:GLN:CB	2.43	0.48
1:D:85:LEU:HD12	1:D:89:PRO:CG	2.40	0.48
1:A:169:GLY:HA3	1:A:197:ASN:OD1	2.14	0.48
1:A:239:ALA:HB1	1:A:245:HIS:CD2	2.49	0.48
1:C:162:LEU:O	1:C:165:HIS:HB3	2.13	0.48
1:C:43:ARG:CB	1:C:43:ARG:HH11	2.26	0.48
1:D:185:GLU:HA	1:D:275:ARG:HH12	1.79	0.48
1:D:62:ILE:O	1:D:66:VAL:HG23	2.13	0.48
1:A:127:LEU:O	1:A:132:GLN:NE2	2.47	0.48
1:A:182:SER:CB	1:A:184:LEU:HD12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:GLN:O	1:D:330:GLN:HG3	2.14	0.48
1:C:148:ASP:OD2	1:C:152:ARG:NH2	2.46	0.48
1:A:56:MET:HE3	1:A:179:TYR:HD1	1.79	0.48
1:C:219:VAL:O	1:C:219:VAL:HG23	2.12	0.48
1:D:131:TYR:O	1:D:134:VAL:N	2.46	0.48
1:C:80:PRO:HG2	1:C:83:PHE:HB3	1.94	0.48
1:D:95:LEU:HD21	1:D:136:SER:OG	2.14	0.48
1:D:168:ALA:HB2	1:D:204:GLN:HB2	1.96	0.48
1:B:300:ASN:HD21	1:B:302:ASP:HB2	1.78	0.48
1:D:169:GLY:HA3	1:D:197:ASN:OD1	2.14	0.48
1:A:41:VAL:HG11	1:A:68:ARG:NE	2.29	0.47
1:B:219:VAL:O	1:B:219:VAL:HG13	2.13	0.47
1:C:56:MET:HE2	1:C:184:LEU:HD12	1.95	0.47
1:C:204:GLN:HE21	1:C:208:ILE:HG13	1.79	0.47
1:C:225:TRP:CG	1:C:256:MET:HE2	2.49	0.47
1:D:120:VAL:O	1:D:124:TYR:HB2	2.14	0.47
1:D:246:GLU:O	1:D:247:ALA:C	2.52	0.47
1:C:85:LEU:HD23	1:C:147:CYS:HB3	1.97	0.47
1:D:344:ASN:ND2	1:D:346:GLN:H	2.12	0.47
1:A:233:TYR:CE1	1:A:251:GLU:HG2	2.50	0.47
1:B:124:TYR:CE1	1:B:132:GLN:HA	2.50	0.47
1:B:41:VAL:HG22	1:B:68:ARG:CZ	2.44	0.47
1:C:353:ILE:O	1:C:357:VAL:HG23	2.15	0.47
1:A:146:MET:O	1:A:150:LEU:HB2	2.14	0.47
1:B:268:VAL:HG13	1:B:329:LEU:CD2	2.44	0.47
1:B:52:LEU:HD13	1:B:56:MET:HG3	1.96	0.47
1:D:263:HIS:O	1:D:267:VAL:HG23	2.14	0.47
1:D:28:ASP:OD2	1:D:32:ARG:HD3	2.15	0.47
1:D:215:ASP:HA	1:D:218:GLU:HG2	1.96	0.47
1:A:353:ILE:O	1:A:356:LEU:N	2.47	0.47
1:D:145:GLY:HA3	1:D:166:TYR:CG	2.50	0.47
1:A:49:ILE:HG12	1:A:57:ARG:HG3	1.97	0.47
1:B:168:ALA:HB2	1:B:204:GLN:HB2	1.95	0.47
1:B:345:ALA:HA	1:B:350:TYR:CG	2.49	0.47
1:C:307:LYS:HD3	1:C:309:LYS:HD3	1.97	0.47
1:C:54:GLU:H	1:C:54:GLU:CD	2.17	0.47
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.49	0.47
1:B:339:LEU:C	1:B:339:LEU:HD23	2.36	0.47
1:C:263:HIS:O	1:C:267:VAL:HG23	2.14	0.47
1:A:227:ARG:O	1:A:231:GLU:HB3	2.14	0.46
1:C:102:MET:HE2	1:C:105:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:HIS:O	1:D:306:THR:HB	2.15	0.46
1:B:79:ILE:HB	1:B:84:LYS:HE3	1.97	0.46
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.30	0.46
1:B:185:GLU:OE1	1:B:275:ARG:HG2	2.15	0.46
1:D:69:ALA:O	1:D:73:VAL:HG23	2.14	0.46
1:A:67:LEU:HD12	2:A:401:ER4:H28	1.98	0.46
1:D:219:VAL:HG13	1:D:219:VAL:O	2.16	0.46
1:D:270:TYR:CE1	1:D:274:LEU:HD21	2.51	0.46
1:B:83:PHE:CZ	1:B:87:GLU:HG3	2.51	0.46
1:A:226:PRO:HG2	1:A:229:ILE:HD12	1.98	0.46
1:B:244:LEU:C	1:B:246:GLU:N	2.68	0.46
1:A:95:LEU:HB3	1:A:124:TYR:CE2	2.50	0.46
1:C:30:ASP:OD2	1:C:122:ARG:HD2	2.16	0.46
1:C:365:GLU:HA	1:C:368:GLN:OE1	2.16	0.46
1:A:227:ARG:HA	1:A:230:TRP:CD1	2.51	0.46
1:B:210:ARG:HH11	1:B:210:ARG:HG3	1.80	0.46
1:C:285:ILE:HG12	1:C:322:SER:HB2	1.98	0.46
1:C:43:ARG:HB2	1:C:43:ARG:HH11	1.79	0.46
1:A:98:THR:HB	1:A:122:ARG:HD3	1.98	0.46
1:A:55:GLU:HG3	1:A:56:MET:N	2.31	0.46
1:C:239:ALA:O	1:C:245:HIS:HB2	2.16	0.46
1:D:29:GLU:HA	1:D:32:ARG:NE	2.09	0.45
1:D:268:VAL:HG13	1:D:329:LEU:HD21	1.98	0.45
1:B:263:HIS:O	1:B:267:VAL:HG23	2.16	0.45
1:B:341:ALA:O	1:B:342:ARG:HG2	2.16	0.45
1:B:204:GLN:HE21	1:B:208:ILE:HG13	1.82	0.45
1:C:43:ARG:NH1	1:C:43:ARG:CB	2.78	0.45
1:D:138:ILE:HD11	1:D:174:GLY:CA	2.47	0.45
1:D:152:ARG:HG2	1:D:153:LYS:N	2.26	0.45
1:D:173:HIS:CD2	1:D:193:LEU:HB3	2.51	0.45
1:B:344:ASN:C	1:B:346:GLN:H	2.19	0.45
1:A:341:ALA:C	1:A:343:MET:H	2.20	0.45
1:A:298:PHE:CZ	1:A:353:ILE:HD13	2.52	0.45
1:B:162:LEU:HG	1:B:166:TYR:CE2	2.50	0.45
1:C:78:SER:C	1:C:79:ILE:HD12	2.37	0.45
1:D:88:LEU:O	1:D:91:PHE:CB	2.59	0.45
1:C:339:LEU:HD23	1:C:339:LEU:C	2.36	0.45
1:C:154:VAL:HG13	1:C:159:ASP:HB2	1.99	0.45
1:A:68:ARG:NH2	1:A:110:GLU:OE1	2.49	0.45
1:B:357:VAL:O	1:B:361:ILE:HG13	2.16	0.45
1:C:114:LEU:HD12	1:C:114:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:GLU:CA	1:D:275:ARG:HH12	2.29	0.45
1:A:130:ALA:O	1:A:134:VAL:HG23	2.17	0.44
1:A:28:ASP:N	3:A:568:HOH:O	2.50	0.44
1:A:333:LYS:HZ2	1:A:333:LYS:HB3	1.82	0.44
1:D:94:HIS:HD2	1:D:100:TRP:NE1	2.14	0.44
1:D:138:ILE:HG23	1:D:170:LEU:HB3	1.98	0.44
1:D:142:MET:HG2	1:D:146:MET:HE2	1.99	0.44
1:B:174:GLY:O	1:B:178:LEU:HG	2.17	0.44
1:C:204:GLN:O	1:C:208:ILE:HG13	2.18	0.44
1:A:73:VAL:O	1:A:84:LYS:HE2	2.17	0.44
1:B:231:GLU:C	1:B:233:TYR:H	2.20	0.44
1:B:234:THR:HG21	1:B:240:PHE:CZ	2.52	0.44
1:D:213:TYR:O	1:D:216:ILE:HG22	2.18	0.44
1:D:98:THR:HG22	1:D:121:THR:HG23	2.00	0.44
1:B:184:LEU:HD22	1:B:276:ASP:OD2	2.17	0.44
1:C:302:ASP:HB3	1:C:306:THR:CG2	2.48	0.44
1:B:288:VAL:HA	1:B:332:LEU:CD2	2.48	0.44
1:C:121:THR:O	1:C:124:TYR:HB3	2.17	0.44
1:C:284:ALA:O	1:C:288:VAL:HG23	2.17	0.44
1:C:339:LEU:HD23	1:C:339:LEU:O	2.18	0.44
1:D:70:LEU:HD22	1:D:146:MET:CE	2.47	0.44
1:D:275:ARG:HH11	1:D:275:ARG:HG2	1.83	0.44
1:D:109:ARG:O	1:D:112:GLU:HB3	2.18	0.44
1:D:289:MET:SD	1:D:318:ILE:HD12	2.57	0.44
1:B:246:GLU:O	1:B:250:VAL:HG23	2.17	0.44
1:B:314:ALA:O	1:B:317:ARG:HG2	2.18	0.44
1:C:109:ARG:HD2	3:C:574:HOH:O	2.18	0.44
1:C:106:GLY:O	1:C:111:ARG:HD3	2.18	0.44
1:D:349:CYS:O	1:D:353:ILE:HG13	2.18	0.44
1:D:37:ILE:HG23	1:D:38:LEU:N	2.32	0.44
1:A:298:PHE:O	1:A:342:ARG:CZ	2.66	0.43
1:B:254:ASN:N	1:B:254:ASN:HD22	2.15	0.43
1:B:352:ARG:O	1:B:356:LEU:HG	2.18	0.43
1:C:308:VAL:HA	3:C:535:HOH:O	2.18	0.43
1:D:134:VAL:O	1:D:138:ILE:HG13	2.17	0.43
1:D:352:ARG:C	1:D:352:ARG:HD2	2.39	0.43
1:D:365:GLU:HA	1:D:368:GLN:OE1	2.17	0.43
1:A:330:GLN:HA	1:A:333:LYS:NZ	2.31	0.43
1:D:35:TYR:OH	1:D:57:ARG:HG2	2.18	0.43
1:B:157:LYS:HG3	1:B:228:GLU:OE1	2.17	0.43
1:D:102:MET:HB3	1:D:105:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:CD2	1:D:128:GLY:N	2.77	0.43
1:D:342:ARG:HG2	1:D:342:ARG:HH11	1.83	0.43
1:A:243:GLU:O	1:A:246:GLU:HB2	2.19	0.43
1:A:353:ILE:O	1:A:354:GLU:C	2.56	0.43
1:D:186:ASP:OD2	1:D:187:VAL:N	2.51	0.43
1:D:70:LEU:HA	1:D:91:PHE:CE1	2.53	0.43
1:B:227:ARG:HA	1:B:230:TRP:CE2	2.53	0.43
1:C:162:LEU:HG	1:C:166:TYR:CE2	2.53	0.43
1:D:33:PHE:O	1:D:37:ILE:HG22	2.17	0.43
1:D:83:PHE:CZ	1:D:102:MET:HE3	2.54	0.43
1:B:62:ILE:O	1:B:66:VAL:HG23	2.19	0.43
1:C:334:THR:O	1:C:338:ARG:HG2	2.18	0.43
1:D:143:ALA:O	1:D:146:MET:HB2	2.18	0.43
1:D:186:ASP:H	1:D:275:ARG:NH1	2.16	0.43
1:D:299:ASN:O	1:D:299:ASN:OD1	2.37	0.43
1:D:67:LEU:HD12	2:D:401:ER4:H28	2.01	0.43
1:A:307:LYS:HE2	1:A:309:LYS:HD2	2.01	0.43
1:B:343:MET:HE1	1:B:349:CYS:C	2.39	0.43
1:B:83:PHE:O	1:B:87:GLU:HG2	2.18	0.43
1:D:109:ARG:CB	1:D:109:ARG:HH11	2.30	0.43
1:D:129:LYS:HA	1:D:132:GLN:HB2	2.00	0.43
1:D:201:LEU:HD12	1:D:263:HIS:CE1	2.53	0.43
1:A:39:GLN:HE21	1:A:39:GLN:HB2	1.58	0.43
1:B:301:LYS:HG3	1:B:302:ASP:N	2.33	0.43
1:C:363:ALA:O	1:C:366:SER:HB3	2.18	0.43
1:D:332:LEU:O	1:D:336:THR:OG1	2.32	0.43
1:B:237:LEU:C	1:B:239:ALA:H	2.22	0.43
1:B:301:LYS:O	1:B:303:VAL:N	2.52	0.43
1:D:197:ASN:O	1:D:201:LEU:HG	2.19	0.43
1:D:96:HIS:HB3	1:D:97:ASP:H	1.75	0.43
1:C:102:MET:HE3	1:C:105:VAL:HG21	2.01	0.43
1:C:79:ILE:HG22	1:C:80:PRO:O	2.18	0.43
1:D:92:HIS:ND1	1:D:93:GLU:CD	2.72	0.43
1:A:281:ALA:O	1:A:285:ILE:HG13	2.18	0.42
1:B:220:PRO:HA	1:B:221:PRO:HD3	1.85	0.42
1:C:344:ASN:O	1:C:347:ASP:HB2	2.19	0.42
1:D:237:LEU:HD12	1:D:240:PHE:HE2	1.83	0.42
1:D:70:LEU:HD22	1:D:146:MET:SD	2.59	0.42
1:A:137:GLY:O	1:A:141:ARG:HG3	2.18	0.42
1:A:70:LEU:HD12	1:A:88:LEU:HD22	2.01	0.42
1:B:33:PHE:CZ	1:B:116:ARG:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LEU:HA	1:C:297:VAL:HG22	2.00	0.42
1:D:64:TYR:HA	2:D:401:ER4:H28	2.01	0.42
1:A:121:THR:O	1:A:124:TYR:HB3	2.19	0.42
1:A:253:LEU:HD21	1:A:297:VAL:O	2.20	0.42
1:A:56:MET:HE1	1:A:179:TYR:HA	2.02	0.42
1:C:30:ASP:OD2	1:C:119:HIS:HA	2.19	0.42
1:D:79:ILE:HG23	1:D:84:LYS:HE3	2.00	0.42
1:D:97:ASP:C	1:D:99:THR:N	2.73	0.42
1:C:180:VAL:HG13	1:C:187:VAL:HA	2.00	0.42
1:C:338:ARG:HE	1:C:338:ARG:HB3	1.71	0.42
1:A:173:HIS:CD2	1:A:193:LEU:HB3	2.54	0.42
1:B:195:ASN:O	1:B:198:HIS:HB2	2.20	0.42
1:B:38:LEU:HD22	1:B:61:CYS:SG	2.59	0.42
1:B:82:GLU:N	1:B:82:GLU:OE1	2.49	0.42
1:C:309:LYS:HB2	1:C:309:LYS:HZ1	1.82	0.42
1:D:68:ARG:HA	2:D:401:ER4:H9	2.01	0.42
1:A:344:ASN:O	1:A:350:TYR:HB2	2.20	0.42
1:D:210:ARG:O	1:D:210:ARG:HD2	2.19	0.42
1:A:253:LEU:CD2	1:A:300:ASN:O	2.68	0.42
1:A:346:GLN:NE2	3:A:516:HOH:O	2.51	0.42
1:B:300:ASN:O	1:B:303:VAL:HG23	2.20	0.42
1:C:204:GLN:HE21	1:C:208:ILE:CG1	2.33	0.42
1:D:30:ASP:OD2	1:D:119:HIS:HA	2.20	0.42
1:D:268:VAL:HG13	1:D:329:LEU:CD2	2.50	0.42
1:A:213:TYR:O	1:A:216:ILE:HG22	2.20	0.42
1:C:238:HIS:O	1:C:241:LYS:HG3	2.20	0.42
1:C:343:MET:SD	1:C:353:ILE:HB	2.60	0.42
1:D:301:LYS:CD	1:D:301:LYS:H	2.25	0.42
1:D:68:ARG:NE	2:D:401:ER4:H8	2.34	0.42
1:A:122:ARG:HB3	1:A:126:ARG:HH12	1.85	0.42
1:A:182:SER:HB2	1:A:184:LEU:HD12	2.01	0.42
1:A:276:ASP:HA	1:A:277:PRO:HD3	1.84	0.42
1:B:147:CYS:HA	1:B:150:LEU:HD12	2.02	0.42
1:C:43:ARG:HB2	1:C:43:ARG:CZ	2.50	0.42
1:D:167:VAL:HG23	1:D:168:ALA:N	2.35	0.42
1:D:192:ASP:C	1:D:193:LEU:HD22	2.39	0.42
1:D:347:ASP:N	1:D:347:ASP:OD2	2.52	0.42
1:D:43:ARG:H	1:D:43:ARG:HG2	1.54	0.42
1:B:145:GLY:HA3	1:B:166:TYR:CD1	2.55	0.41
1:C:349:CYS:O	1:C:350:TYR:C	2.58	0.41
1:D:138:ILE:HD11	1:D:174:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LYS:HG3	1:B:310:THR:O	2.20	0.41
1:C:357:VAL:O	1:C:361:ILE:HG12	2.20	0.41
1:D:227:ARG:HA	1:D:230:TRP:CE2	2.55	0.41
1:D:230:TRP:CD2	1:D:237:LEU:HD13	2.55	0.41
1:A:246:GLU:CD	1:A:301:LYS:HD2	2.40	0.41
1:B:118:THR:OG1	1:B:122:ARG:NH1	2.53	0.41
1:C:73:VAL:HG11	1:C:88:LEU:HD21	2.01	0.41
1:A:188:ARG:HG3	1:A:191:ASP:OD2	2.20	0.41
1:B:269:GLU:OE1	1:B:367:HIS:NE2	2.48	0.41
1:D:210:ARG:CD	1:D:307:LYS:HG3	2.46	0.41
1:B:301:LYS:C	1:B:303:VAL:H	2.24	0.41
1:A:346:GLN:HG3	1:A:347:ASP:H	1.85	0.41
1:A:276:ASP:OD1	1:A:278:SER:N	2.50	0.41
1:B:354:GLU:O	1:B:358:ASN:ND2	2.54	0.41
1:D:79:ILE:CG2	1:D:84:LYS:HE3	2.51	0.41
1:B:105:VAL:HG12	1:B:106:GLY:N	2.35	0.41
1:C:127:LEU:O	1:C:128:GLY:C	2.58	0.41
1:D:138:ILE:CD1	1:D:174:GLY:HA3	2.51	0.41
1:D:261:LEU:HA	1:D:264:VAL:HG23	2.03	0.41
1:D:334:THR:O	1:D:338:ARG:HG3	2.20	0.41
1:D:77:MET:HB3	1:D:220:PRO:HG3	2.02	0.41
1:C:83:PHE:HD2	1:C:84:LYS:N	2.19	0.41
1:D:257:VAL:HG13	1:D:294:LEU:HD11	2.03	0.41
1:A:188:ARG:HA	1:A:191:ASP:OD2	2.20	0.41
1:A:240:PHE:CE1	1:A:249:ALA:HA	2.56	0.41
1:A:43:ARG:CB	1:A:43:ARG:CZ	2.98	0.41
1:D:69:ALA:HB1	1:D:114:LEU:HD21	2.03	0.41
1:D:302:ASP:HA	1:D:305:HIS:NE2	2.36	0.41
1:D:353:ILE:O	1:D:357:VAL:HG23	2.20	0.41
1:A:312:ARG:HA	1:A:315:THR:CG2	2.50	0.40
1:A:366:SER:O	1:D:109:ARG:HD2	2.21	0.40
1:C:298:PHE:C	1:C:300:ASN:H	2.23	0.40
1:C:88:LEU:N	1:C:89:PRO:CD	2.84	0.40
1:D:70:LEU:HD21	1:D:88:LEU:HD22	2.03	0.40
1:A:324:GLU:OE1	1:A:326:GLN:HB2	2.21	0.40
1:C:239:ALA:HB1	1:C:245:HIS:CD2	2.57	0.40
1:D:186:ASP:OD1	1:D:188:ARG:HB2	2.22	0.40
1:D:97:ASP:OD1	1:D:99:THR:HG22	2.21	0.40
1:A:156:THR:HB	3:A:597:HOH:O	2.22	0.40
1:A:162:LEU:O	1:A:165:HIS:HB3	2.20	0.40
1:A:168:ALA:CB	1:A:204:GLN:HG3	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:HG2	1:A:222:ARG:CD	2.52	0.40
1:A:333:LYS:NZ	1:A:333:LYS:HB3	2.35	0.40
1:D:138:ILE:H	1:D:138:ILE:HG13	1.60	0.40
1:D:34:CYS:C	1:D:37:ILE:HG22	2.41	0.40
1:B:89:PRO:HB3	1:B:144:ASN:HD21	1.85	0.40
1:B:344:ASN:C	1:B:346:GLN:N	2.73	0.40
1:D:242:ASP:OD1	1:D:242:ASP:C	2.60	0.40
1:D:303:VAL:O	1:D:303:VAL:HG12	2.22	0.40
1:A:218:GLU:HG2	1:A:222:ARG:HD2	2.03	0.40
1:C:230:TRP:C	1:C:232:LYS:N	2.74	0.40
1:D:176:THR:O	1:D:180:VAL:HG23	2.21	0.40
1:D:245:HIS:O	1:D:246:GLU:C	2.60	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%)	314 (93%)	24 (7%)	1 (0%)	41	60
1	B	339/365 (93%)	315 (93%)	23 (7%)	1 (0%)	41	60
1	C	339/365 (93%)	312 (92%)	23 (7%)	4 (1%)	13	23
1	D	339/365 (93%)	294 (87%)	35 (10%)	10 (3%)	4	6
All	All	1356/1460 (93%)	1235 (91%)	105 (8%)	16 (1%)	13	23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	GLU
1	A	29	GLU
1	D	98	THR

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Mol	Chain	Res	Type
1	D	101	CYS
1	D	246	GLU
1	B	302	ASP
1	D	84	LYS
1	D	350	TYR
1	C	103	SER
1	D	247	ALA
1	C	305	HIS
1	D	105	VAL
1	D	132	GLN
1	D	234	THR
1	D	306	THR
1	C	107	VAL

### 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	298/318 (94%)	285 (96%)	13 (4%)	28	47
1	B	298/318 (94%)	287 (96%)	11 (4%)	34	54
1	C	298/318 (94%)	282 (95%)	16 (5%)	22	38
1	D	297/318 (93%)	273 (92%)	24 (8%)	11	21
All	All	1191/1272 (94%)	1127 (95%)	64 (5%)	22	38

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	39	GLN
1	A	82	GLU
1	A	107	VAL
1	A	161	ASP
1	A	188	ARG
1	A	204	GLN
1	A	309	LYS

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Mol	Chain	Res	Type
1	A	315	THR
1	A	333	LYS
1	A	350	TYR
1	A	352	ARG
1	A	355	HIS
1	B	37	ILE
1	B	39	GLN
1	B	118	THR
1	B	129	LYS
1	B	161	ASP
1	B	201	LEU
1	B	234	THR
1	B	235	ASP
1	B	243	GLU
1	B	310	THR
1	B	352	ARG
1	C	36	ASP
1	C	83	PHE
1	C	93	GLU
1	C	98	THR
1	C	102	MET
1	C	105	VAL
1	C	122	ARG
1	C	161	ASP
1	C	187	VAL
1	C	235	ASP
1	C	275	ARG
1	C	301	LYS
1	C	315	THR
1	C	334	THR
1	C	346	GLN
1	C	359	ASP
1	D	31	LEU
1	D	53	ASP
1	D	58	ASP
1	D	87	GLU
1	D	90	LYS
1	D	92	HIS
1	D	95	LEU
1	D	96	HIS
1	D	102	MET
1	D	109	ARG

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Mol	Chain	Res	Type
1	D	118	THR
1	D	129	LYS
1	D	156	THR
1	D	161	ASP
1	D	187	VAL
1	D	227	ARG
1	D	235	ASP
1	D	244	LEU
1	D	301	LYS
1	D	315	THR
1	D	336	THR
1	D	347	ASP
1	D	351	ASP
1	D	352	ARG

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	119	HIS
1	A	144	ASN
1	A	204	GLN
1	A	245	HIS
1	A	320	HIS
1	B	132	GLN
1	B	144	ASN
1	B	204	GLN
1	B	254	ASN
1	B	300	ASN
1	B	346	GLN
1	B	358	ASN
1	C	119	HIS
1	C	144	ASN
1	C	204	GLN
1	C	245	HIS
1	C	266	HIS
1	D	94	HIS
1	D	96	HIS
1	D	207	ASN
1	D	287	GLN
1	D	299	ASN
1	D	330	GLN

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Mol	Chain	Res	Type
1	D	344	ASN
1	D	346	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 ⓘ

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	ER4	A	401	-	31,33,33	3.03	3 (9%)	36,45,45	1.05	2 (5%)
2	ER4	B	401	-	31,33,33	3.02	3 (9%)	36,45,45	1.07	2 (5%)
2	ER4	C	401	-	31,33,33	3.03	3 (9%)	36,45,45	1.08	2 (5%)
2	ER4	D	401	-	31,33,33	3.03	3 (9%)	36,45,45	1.13	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ER4	A	401	-	-	1/14/37/37	0/5/4/4
2	ER4	B	401	-	-	1/14/37/37	0/5/4/4
2	ER4	C	401	-	-	2/14/37/37	0/5/4/4
2	ER4	D	401	-	-	0/14/37/37	0/5/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ER4	CAS-CBA	-15.93	1.39	1.51
2	A	401	ER4	CAS-CBA	-15.90	1.39	1.51
2	C	401	ER4	CAS-CBA	-15.90	1.39	1.51
2	B	401	ER4	CAS-CBA	-15.88	1.39	1.51
2	C	401	ER4	CAS-CAX	-3.96	1.39	1.52
2	A	401	ER4	CAS-CAX	-3.95	1.39	1.52
2	D	401	ER4	CAS-CAX	-3.94	1.39	1.52
2	B	401	ER4	CAS-CAX	-3.92	1.39	1.52
2	A	401	ER4	CAC-CAD	2.74	1.23	1.19
2	C	401	ER4	CAC-CAD	2.72	1.23	1.19
2	D	401	ER4	CAC-CAD	2.69	1.22	1.19
2	B	401	ER4	CAC-CAD	2.67	1.22	1.19

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	ER4	CAN-OAW-CAZ	-3.50	112.07	117.59
2	C	401	ER4	CAN-OAW-CAZ	-2.89	113.03	117.59
2	C	401	ER4	CAZ-NAU-CBA	2.87	121.75	117.64
2	A	401	ER4	CAN-OAW-CAZ	-2.84	113.12	117.59
2	A	401	ER4	CAZ-NAU-CBA	2.83	121.69	117.64
2	D	401	ER4	CAZ-NAU-CBA	2.82	121.68	117.64
2	B	401	ER4	CAZ-NAU-CBA	2.77	121.61	117.64
2	B	401	ER4	CAN-OAW-CAZ	-2.76	113.24	117.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

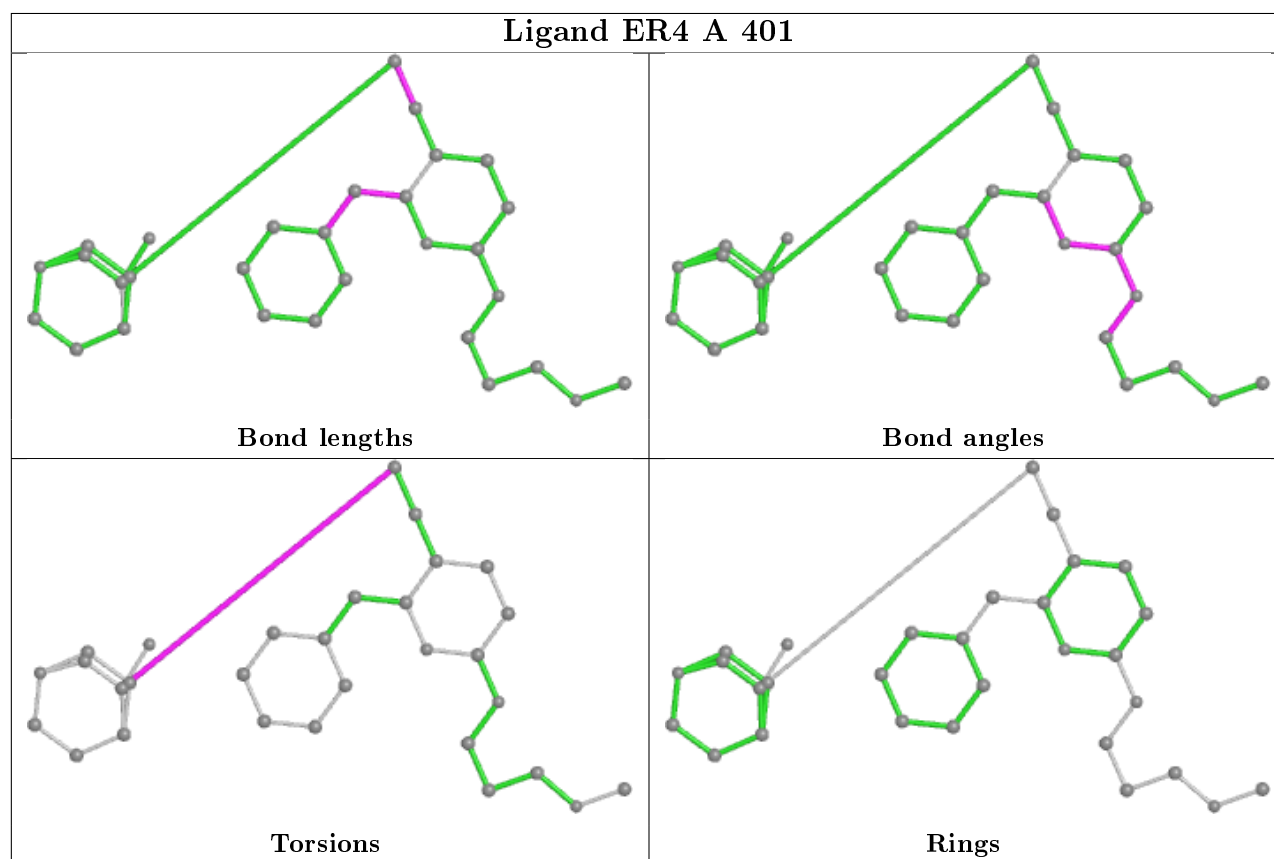
Mol	Chain	Res	Type	Atoms
2	C	401	ER4	CAX-CAS-CBA-CAY
2	A	401	ER4	CAC-CAD-CBD-CAT
2	B	401	ER4	CAC-CAD-CBD-CAT
2	C	401	ER4	CAC-CAD-CBD-CAT

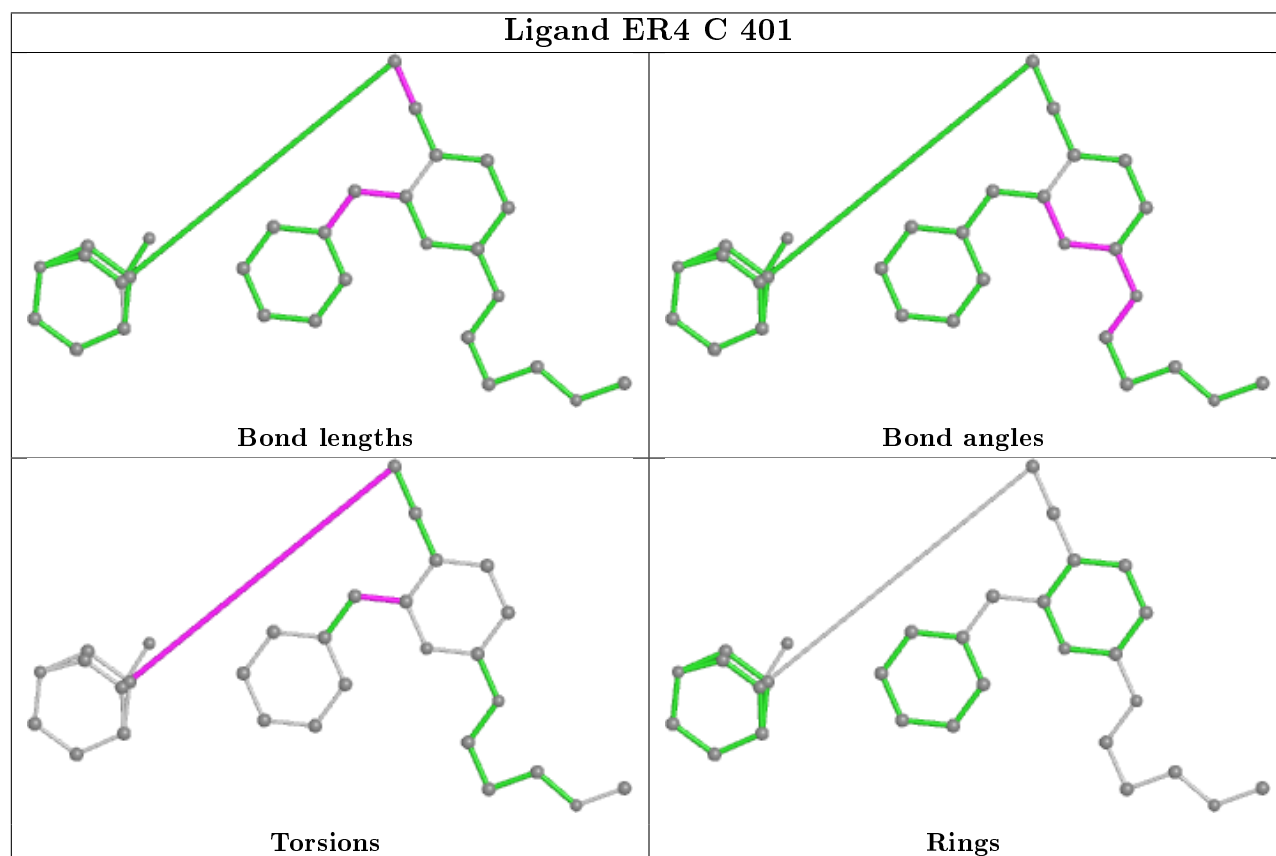
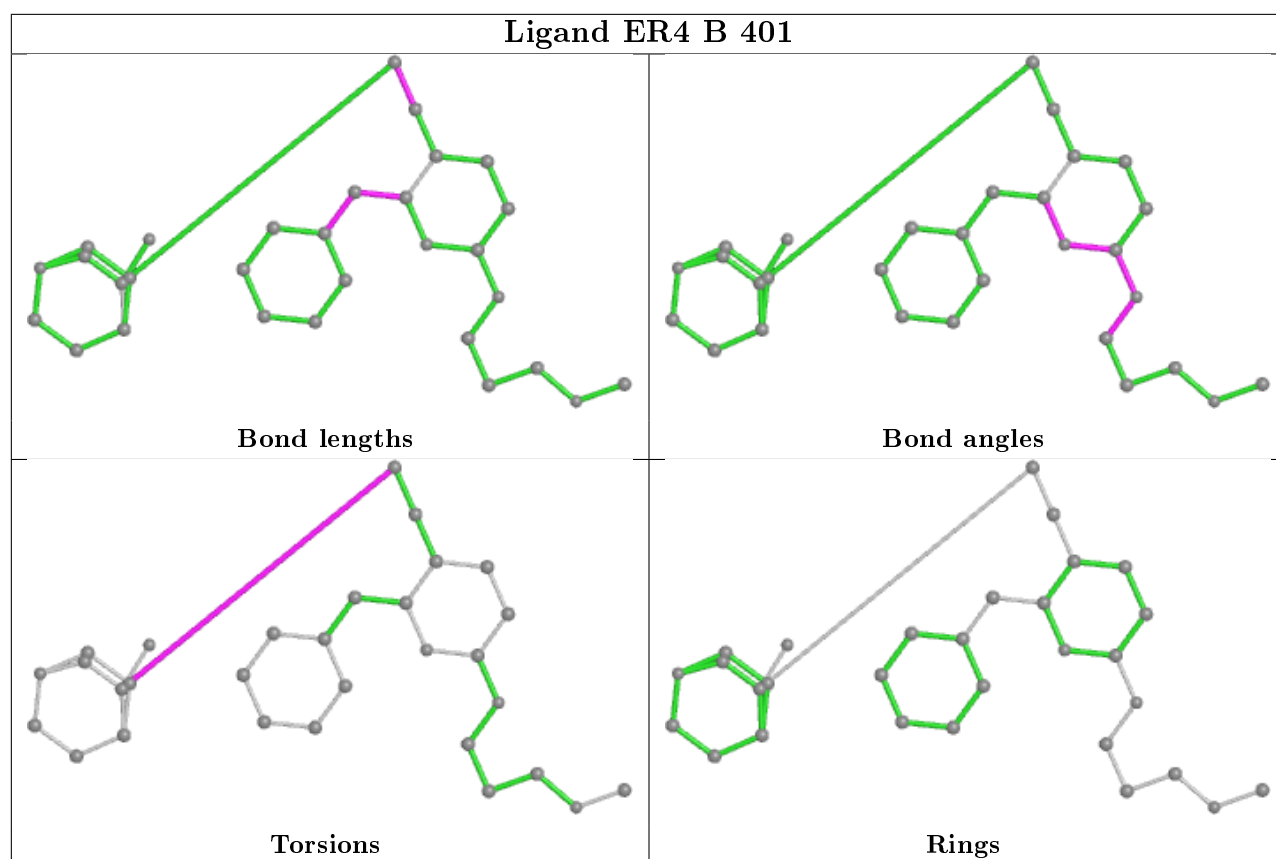
There are no ring outliers.

4 monomers are involved in 12 short contacts:

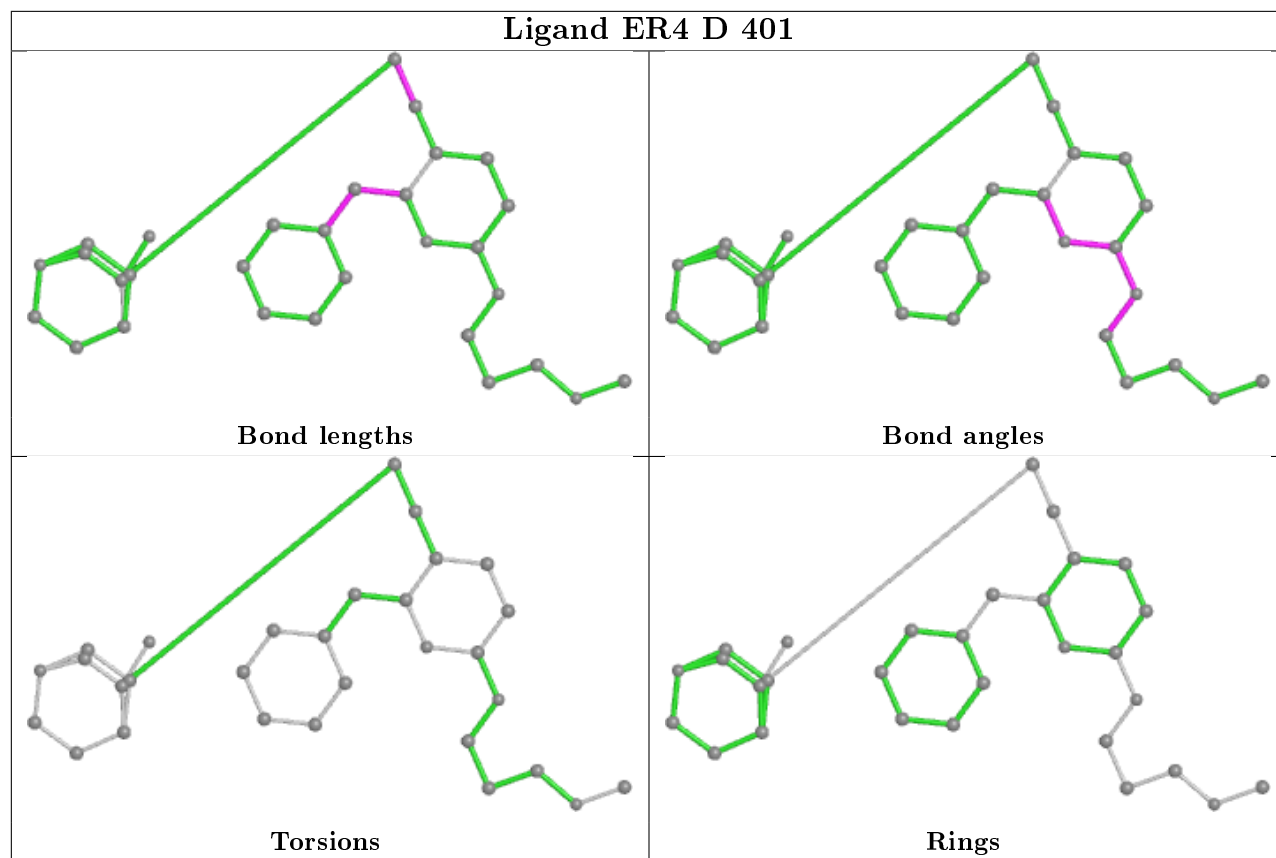
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ER4	2	0
2	B	401	ER4	2	0
2	C	401	ER4	2	0
2	D	401	ER4	6	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/365 (93%)	0.03	6 (1%) 68 76	26, 50, 75, 120	0
1	B	341/365 (93%)	0.12	11 (3%) 47 56	30, 57, 95, 107	0
1	C	341/365 (93%)	0.17	9 (2%) 56 65	26, 55, 87, 100	0
1	D	341/365 (93%)	0.58	36 (10%) 6 6	31, 76, 120, 143	0
All	All	1364/1460 (93%)	0.23	62 (4%) 33 39	26, 58, 103, 143	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	82	GLU	5.4
1	D	105	VAL	5.3
1	D	80	PRO	5.1
1	D	245	HIS	5.0
1	D	98	THR	4.7
1	D	99	THR	4.6
1	D	149	PHE	4.0
1	A	346	GLN	4.0
1	B	219	VAL	3.8
1	D	121	THR	3.6
1	D	78	SER	3.5
1	A	344	ASN	3.5
1	D	346	GLN	3.4
1	A	349	CYS	3.3
1	D	103	SER	3.3
1	D	32	ARG	3.3
1	C	213	TYR	3.2
1	C	80	PRO	3.2
1	D	127	LEU	3.2
1	C	107	VAL	3.2
1	D	91	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	43	ARG	3.1
1	D	368	GLN	2.8
1	C	219	VAL	2.8
1	D	350	TYR	2.8
1	D	190	ALA	2.8
1	B	216	ILE	2.7
1	B	345	ALA	2.7
1	B	245	HIS	2.7
1	D	343	MET	2.6
1	D	345	ALA	2.6
1	C	43	ARG	2.6
1	D	104	GLY	2.6
1	D	151	THR	2.5
1	D	95	LEU	2.5
1	B	243	GLU	2.5
1	A	43	ARG	2.5
1	D	86	ARG	2.4
1	D	344	ASN	2.4
1	B	346	GLN	2.4
1	D	94	HIS	2.4
1	C	90	LYS	2.4
1	D	77	MET	2.3
1	D	85	LEU	2.3
1	D	150	LEU	2.3
1	B	362	ARG	2.3
1	B	306	THR	2.3
1	D	219	VAL	2.3
1	D	244	LEU	2.2
1	A	348	ALA	2.2
1	D	213	TYR	2.2
1	B	241	LYS	2.2
1	D	153	LYS	2.1
1	D	66	VAL	2.1
1	D	43	ARG	2.1
1	B	217	CYS	2.1
1	A	219	VAL	2.1
1	D	67	LEU	2.0
1	C	130	ALA	2.0
1	C	345	ALA	2.0
1	C	305	HIS	2.0
1	D	351	ASP	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

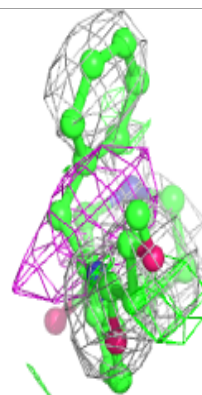
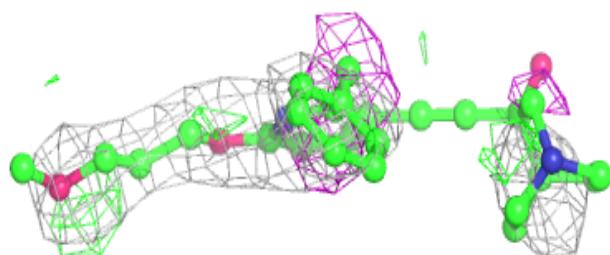
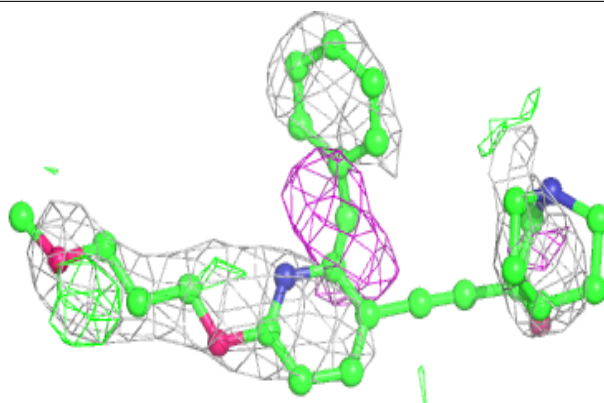
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ER4	C	401	30/30	0.67	0.50	79,92,111,112	0
2	ER4	D	401	30/30	0.67	0.46	91,102,111,111	0
2	ER4	B	401	30/30	0.78	0.34	68,74,82,83	0
2	ER4	A	401	30/30	0.80	0.38	69,86,103,103	0

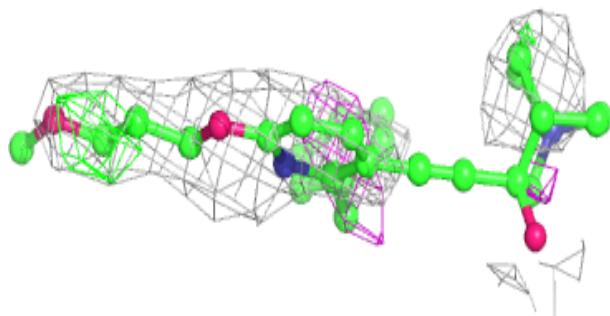
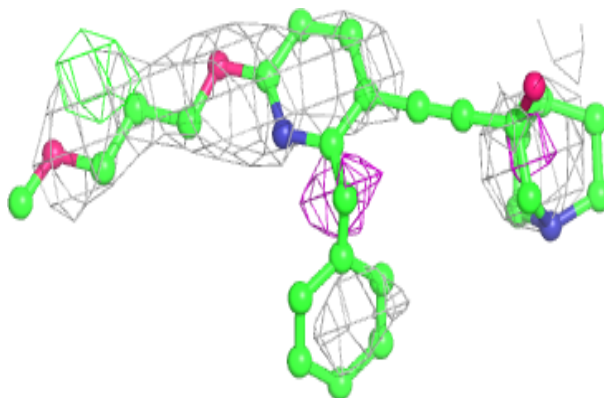
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ER4 C 401:**

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

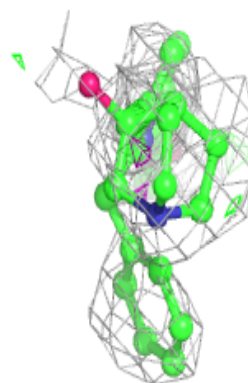
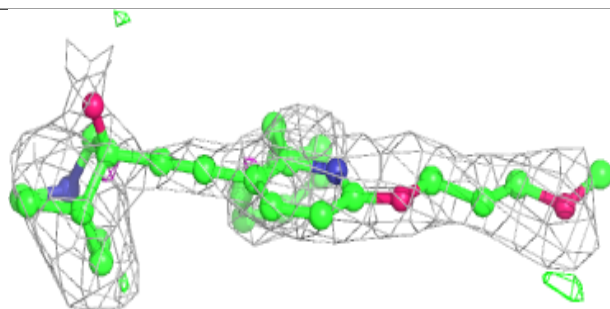
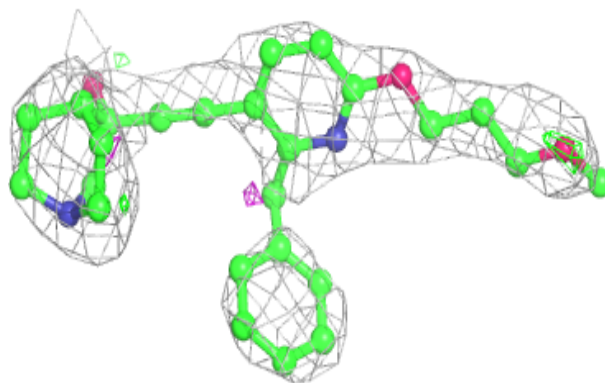
**Electron density around ER4 D 401:**

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

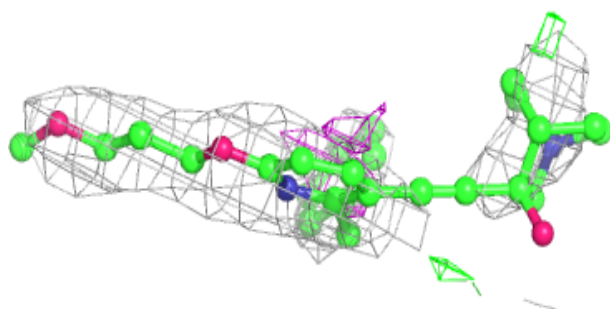
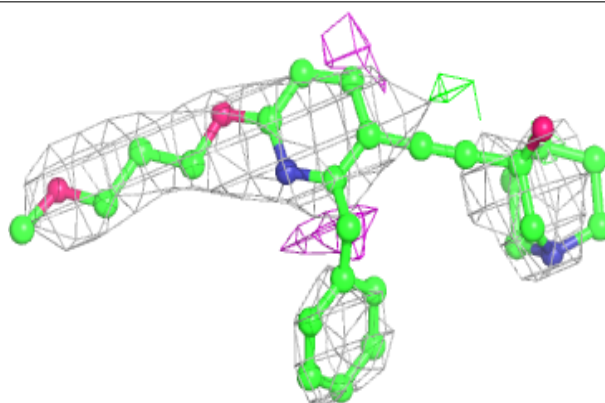


**Electron density around ER4 B 401:**

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

**Electron density around ER4 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)



## 6.5 Other polymers

There are no such residues in this entry.