



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 AM UTC

PDB ID : 1ERE / pdb_00001ere
Title : HUMAN ESTROGEN RECEPTOR LIGAND-BINDING DOMAIN IN COM-
PLEX WITH 17BETA-ESTRADIOL
Authors : Brzozowski, A.M.; Pike, A.C.W.
Deposited on : 1997-09-08
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

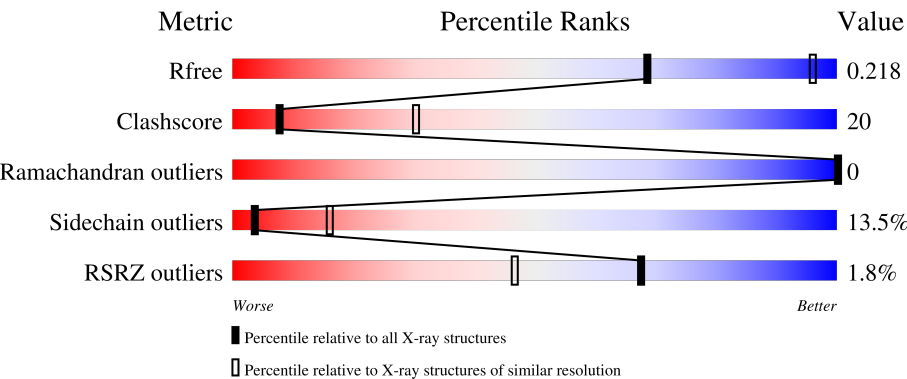
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	47%36%8%•7%
1	B	253	2% 47%36%9%•7%
1	C	253	2% 45%37%9%•7%
1	D	253	2% 47%34%9%•7%
1	E	253	2% 49%34%9%•7%

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Mol	Chain	Length	Quality of chain
1	F	253	2% 45% 38% 8% 7%

2 Entry composition [i](#)

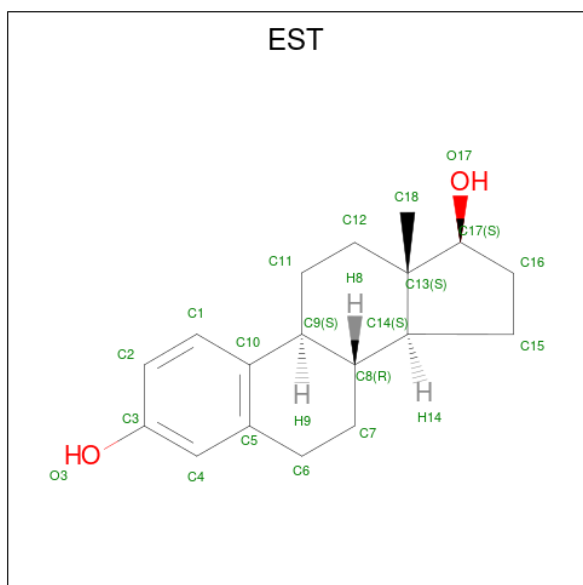
There are 3 unique types of molecules in this entry. The entry contains 11496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	B	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	C	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	D	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	E	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	F	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			

- Molecule 2 is ESTRADIOL (CCD ID: EST) (formula: C₁₈H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			20	18	2		
2	C	1	Total	C	O	0	0
			20	18	2		
2	D	1	Total	C	O	0	0
			20	18	2		
2	E	1	Total	C	O	0	0
			20	18	2		
2	F	1	Total	C	O	0	0
			20	18	2		

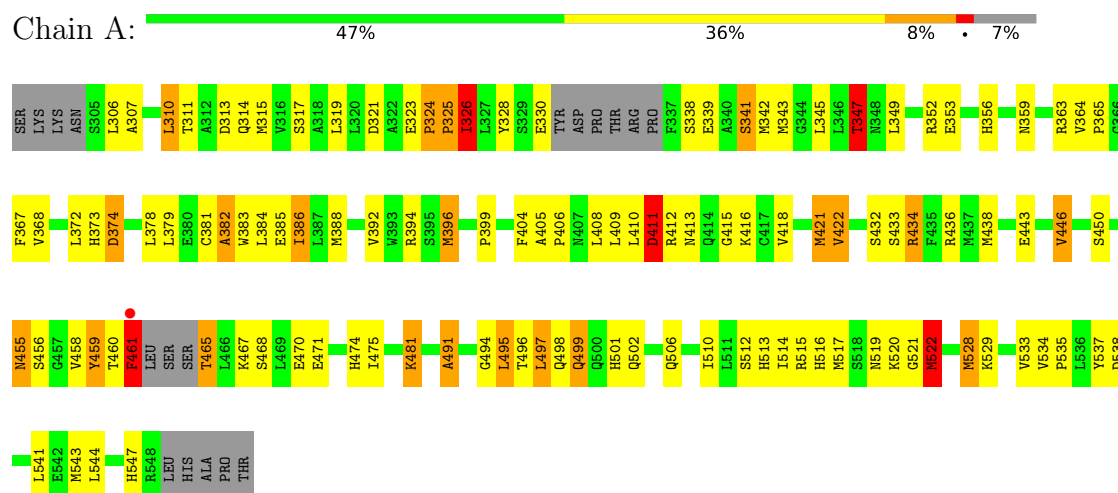
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	19	Total	O	0	0
			19	19		
3	C	20	Total	O	0	0
			20	20		
3	D	19	Total	O	0	0
			19	19		
3	E	19	Total	O	0	0
			19	19		
3	F	19	Total	O	0	0
			19	19		

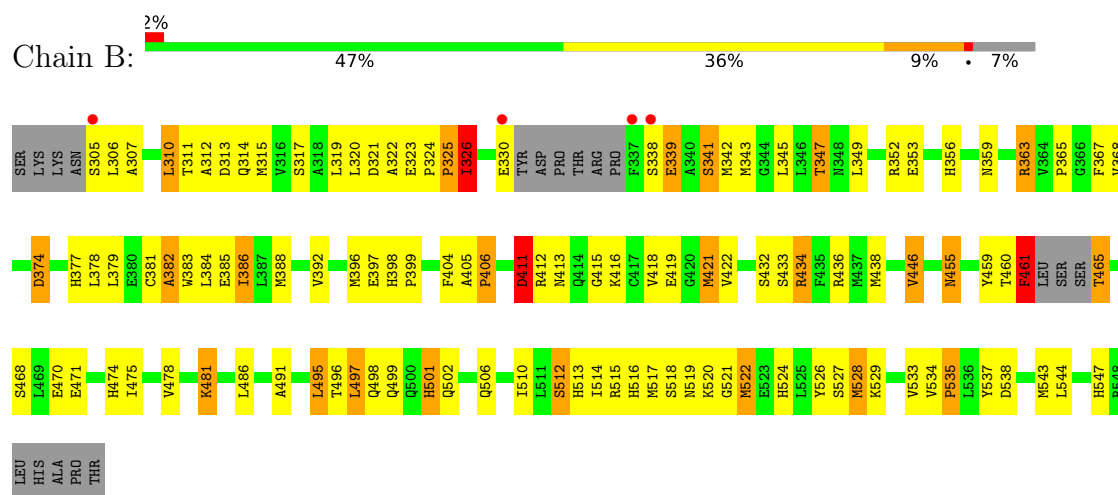
3 Residue-property plots

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

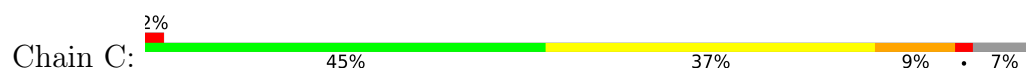
• Molecule 1: ESTROGEN RECEPTOR



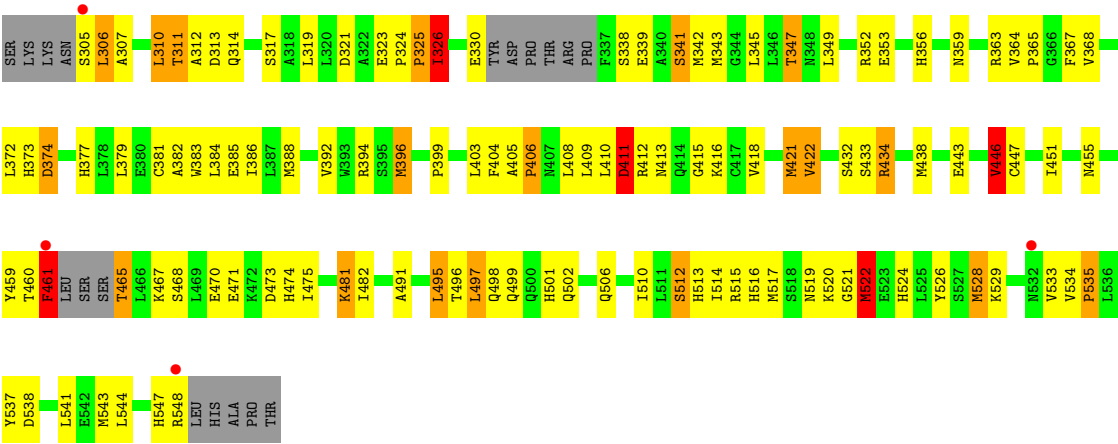
• Molecule 1: ESTROGEN RECEPTOR



• Molecule 1: ESTROGEN RECEPTOR







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.48Å 115.16Å 137.38Å 90.00° 98.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.10) 98.6 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.251 0.189 , 0.218	Depositor DCC
R_{free} test set	3398 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11496	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.74	0/1937	1.93	55/2614 (2.1%)
1	B	0.73	0/1937	1.89	51/2614 (2.0%)
1	C	0.77	0/1937	1.92	56/2614 (2.1%)
1	D	0.83	0/1937	1.97	56/2614 (2.1%)
1	E	0.77	0/1937	1.92	50/2614 (1.9%)
1	F	0.76	0/1937	1.93	61/2614 (2.3%)
All	All	0.77	0/11622	1.93	329/15684 (2.1%)

There are no bond length outliers.

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	547	HIS	CA-CB-CG	-13.89	99.91	113.80
1	D	547	HIS	CA-CB-CG	-13.46	100.34	113.80
1	E	547	HIS	CA-CB-CG	-13.39	100.41	113.80
1	F	547	HIS	CA-CB-CG	-13.06	100.74	113.80
1	B	547	HIS	CA-CB-CG	-12.81	100.99	113.80
1	A	547	HIS	CA-CB-CG	-12.06	101.74	113.80
1	E	374	ASP	CA-CB-CG	-10.25	102.35	112.60
1	F	374	ASP	CA-CB-CG	-9.88	102.72	112.60
1	D	522	MET	N-CA-CB	9.88	124.78	110.16
1	C	522	MET	N-CA-CB	9.74	124.44	110.12
1	D	356	HIS	CA-CB-CG	-9.66	104.14	113.80
1	D	352	ARG	NH1-CZ-NH2	9.57	131.74	119.30
1	A	522	MET	N-CA-CB	9.33	123.54	110.01
1	F	522	MET	N-CA-CB	9.22	123.81	110.16
1	A	374	ASP	CA-CB-CG	-8.81	103.79	112.60
1	B	374	ASP	CA-CB-CG	-8.79	103.81	112.60
1	B	522	MET	N-CA-CB	8.78	123.15	110.16
1	E	533	VAL	CA-C-O	8.78	128.02	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	ASP	CA-CB-CG	-8.75	103.85	112.60
1	F	413	ASN	CA-CB-CG	-8.73	103.87	112.60
1	B	359	ASN	CA-CB-CG	-8.69	103.91	112.60
1	E	522	MET	CA-CB-CG	8.69	131.47	114.10
1	F	533	VAL	CA-C-O	8.66	127.90	118.98
1	E	522	MET	N-CA-CB	8.63	122.94	110.16
1	A	533	VAL	CA-C-O	8.58	127.82	118.98
1	B	474	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	352	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	D	413	ASN	CA-CB-CG	-8.38	104.22	112.60
1	E	538	ASP	N-CA-C	8.28	119.93	111.07
1	A	474	HIS	CA-CB-CG	-8.21	105.59	113.80
1	A	522	MET	CA-CB-CG	8.18	130.45	114.10
1	F	367	PHE	CA-C-O	8.17	129.40	120.82
1	D	533	VAL	CA-C-O	8.15	127.38	118.98
1	A	356	HIS	CA-CB-CG	-8.02	105.78	113.80
1	A	521	GLY	CA-C-O	-8.02	112.34	121.00
1	C	516	HIS	CA-CB-CG	-8.01	105.79	113.80
1	D	521	GLY	CA-C-O	-8.01	112.35	121.00
1	A	461	PHE	CA-CB-CG	-8.01	105.80	113.80
1	B	367	PHE	CA-C-O	8.01	129.23	120.82
1	D	474	HIS	CA-CB-CG	-8.00	105.80	113.80
1	C	474	HIS	CA-CB-CG	-7.94	105.86	113.80
1	B	413	ASN	CA-CB-CG	-7.88	104.72	112.60
1	F	461	PHE	CA-CB-CG	-7.82	105.98	113.80
1	E	461	PHE	CA-CB-CG	-7.80	106.00	113.80
1	B	538	ASP	N-CA-C	7.80	119.42	111.07
1	E	367	PHE	CA-C-O	7.80	129.00	120.82
1	B	352	ARG	NE-CZ-NH2	-7.79	112.19	119.20
1	C	413	ASN	CA-CB-CG	-7.79	104.81	112.60
1	F	538	ASP	N-CA-C	7.77	119.38	111.07
1	D	367	PHE	CA-C-O	7.72	129.56	121.07
1	C	538	ASP	CA-CB-CG	-7.65	104.95	112.60
1	D	461	PHE	CA-CB-CG	-7.65	106.15	113.80
1	F	394	ARG	NE-CZ-NH1	-7.62	113.89	121.50
1	D	538	ASP	N-CA-C	7.61	119.21	111.07
1	D	522	MET	CA-CB-CG	7.59	129.28	114.10
1	A	434	ARG	NE-CZ-NH2	7.54	125.98	119.20
1	D	374	ASP	CA-CB-CG	-7.52	105.08	112.60
1	D	352	ARG	NE-CZ-NH2	-7.52	112.43	119.20
1	A	406	PRO	N-CA-CB	7.48	111.47	103.39
1	F	313	ASP	CA-CB-CG	-7.47	105.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	538	ASP	N-CA-C	7.46	119.20	111.14
1	F	404	PHE	CA-CB-CG	-7.44	106.36	113.80
1	B	356	HIS	CA-CB-CG	-7.40	106.40	113.80
1	B	522	MET	CA-CB-CG	7.38	128.86	114.10
1	A	413	ASN	CA-CB-CG	-7.37	105.23	112.60
1	F	474	HIS	CA-CB-CG	-7.32	106.48	113.80
1	A	538	ASP	N-CA-C	7.26	118.84	111.07
1	F	516	HIS	CA-CB-CG	-7.26	106.54	113.80
1	A	321	ASP	CA-CB-CG	-7.21	105.39	112.60
1	C	461	PHE	CA-CB-CG	-7.21	106.59	113.80
1	E	382	ALA	N-CA-C	7.20	122.24	113.17
1	F	521	GLY	CA-C-O	-7.20	113.23	121.00
1	C	313	ASP	CA-CB-CG	-7.19	105.41	112.60
1	B	352	ARG	NH1-CZ-NH2	7.17	128.63	119.30
1	E	326	ILE	N-CA-CB	7.16	119.58	110.99
1	A	394	ARG	NE-CZ-NH1	-7.14	114.36	121.50
1	B	325	PRO	CA-C-O	-7.12	112.97	122.08
1	C	352	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	C	406	PRO	N-CA-C	-7.07	104.10	113.65
1	F	396	MET	N-CA-C	7.05	119.57	111.11
1	E	422	VAL	CA-C-O	-7.01	113.66	120.95
1	B	461	PHE	CA-CB-CG	-7.00	106.80	113.80
1	C	386	ILE	CB-CA-C	-6.99	103.02	111.97
1	A	386	ILE	CB-CA-C	-6.98	102.94	111.88
1	B	406	PRO	N-CA-C	-6.97	104.24	113.65
1	E	356	HIS	CA-CB-CG	-6.94	106.86	113.80
1	C	455	ASN	CA-CB-CG	6.93	119.53	112.60
1	D	321	ASP	CA-CB-CG	-6.90	105.70	112.60
1	A	325	PRO	CA-C-O	-6.89	113.26	122.08
1	F	356	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	404	PHE	CA-CB-CG	-6.84	106.96	113.80
1	F	434	ARG	NE-CZ-NH2	6.84	125.35	119.20
1	A	359	ASN	CA-CB-CG	-6.83	105.77	112.60
1	E	413	ASN	CA-CB-CG	-6.83	105.77	112.60
1	B	538	ASP	CA-CB-CG	-6.82	105.78	112.60
1	A	367	PHE	CA-C-O	6.82	127.98	120.82
1	E	321	ASP	CA-CB-CG	-6.80	105.80	112.60
1	F	455	ASN	CA-CB-CG	6.79	119.39	112.60
1	D	455	ASN	CA-CB-CG	6.77	119.37	112.60
1	C	394	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	F	399	PRO	CA-C-O	-6.76	113.95	121.32
1	C	406	PRO	N-CA-CB	6.75	110.68	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	386	ILE	N-CA-CB	6.74	117.99	110.51
1	F	359	ASN	CA-CB-CG	-6.74	105.86	112.60
1	A	522	MET	CB-CA-C	-6.72	100.34	110.88
1	E	396	MET	N-CA-C	6.71	119.21	111.02
1	A	326	ILE	N-CA-CB	6.69	118.63	111.00
1	E	474	HIS	CA-CB-CG	-6.68	107.12	113.80
1	C	522	MET	CB-CA-C	-6.66	99.73	110.79
1	A	406	PRO	N-CA-C	-6.63	104.69	113.65
1	F	382	ALA	N-CA-C	6.63	121.53	113.17
1	E	352	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	F	326	ILE	N-CA-CB	6.58	118.50	111.00
1	C	526	TYR	CA-C-O	-6.57	113.92	120.82
1	C	522	MET	CA-CB-CG	6.54	127.18	114.10
1	F	522	MET	CB-CA-C	-6.49	99.81	110.85
1	F	406	PRO	N-CA-C	-6.49	104.51	113.53
1	C	352	ARG	NH1-CZ-NH2	6.49	127.74	119.30
1	C	326	ILE	N-CA-CB	6.48	118.39	111.00
1	B	512	SER	CA-CB-OG	-6.48	98.14	111.10
1	D	386	ILE	CB-CA-C	-6.47	103.68	111.97
1	B	434	ARG	NE-CZ-NH2	6.47	125.02	119.20
1	E	382	ALA	N-CA-CB	-6.47	100.92	110.49
1	C	356	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	352	ARG	NH1-CZ-NH2	6.45	127.68	119.30
1	A	516	HIS	CA-CB-CG	-6.44	107.36	113.80
1	F	422	VAL	CB-CA-C	-6.43	103.46	112.14
1	D	313	ASP	CA-CB-CG	-6.39	106.21	112.60
1	C	321	ASP	CA-CB-CG	-6.38	106.22	112.60
1	D	382	ALA	N-CA-C	6.38	121.20	113.17
1	E	352	ARG	NH1-CZ-NH2	6.38	127.59	119.30
1	D	345	LEU	CB-CA-C	-6.36	100.89	110.88
1	D	413	ASN	OD1-CG-ND2	6.35	128.95	122.60
1	F	538	ASP	CA-CB-CG	-6.35	106.25	112.60
1	D	522	MET	CB-CA-C	-6.34	100.07	110.85
1	A	433	SER	N-CA-CB	-6.32	100.84	110.01
1	E	522	MET	CB-CA-C	-6.32	100.11	110.85
1	B	313	ASP	CA-CB-CG	-6.31	106.29	112.60
1	A	455	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	433	SER	O-C-N	-6.29	115.60	122.07
1	D	326	ILE	N-CA-CB	6.28	117.57	110.72
1	C	404	PHE	CA-CB-CG	-6.27	107.53	113.80
1	E	422	VAL	O-C-N	6.25	127.93	121.87
1	D	404	PHE	CA-CB-CG	-6.24	107.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	MET	N-CA-C	6.23	118.62	111.02
1	D	446	VAL	CB-CA-C	6.23	120.55	112.14
1	B	533	VAL	CA-C-O	6.22	128.56	120.78
1	F	433	SER	N-CA-CB	-6.21	100.96	110.16
1	C	386	ILE	N-CA-CB	6.21	117.82	110.55
1	B	326	ILE	N-CA-CB	6.21	118.08	111.00
1	D	325	PRO	CA-C-O	-6.21	114.42	122.12
1	D	386	ILE	N-CA-CB	6.18	117.78	110.55
1	B	345	LEU	CB-CA-C	-6.17	101.11	110.92
1	A	382	ALA	N-CA-C	6.16	120.50	112.92
1	D	422	VAL	CB-CA-C	-6.14	103.84	112.14
1	F	501[A]	HIS	CA-CB-CG	6.13	119.93	113.80
1	F	501[B]	HIS	CA-CB-CG	6.13	119.93	113.80
1	C	521	GLY	CA-C-O	-6.10	114.41	121.00
1	E	406	PRO	N-CA-CB	6.10	110.04	103.33
1	E	386	ILE	CB-CA-C	-6.10	104.08	111.88
1	D	467	LYS	N-CA-C	-6.08	104.77	111.82
1	B	491	ALA	N-CA-C	-6.08	104.57	111.07
1	D	406	PRO	N-CA-C	-6.07	105.09	113.53
1	C	326	ILE	CB-CA-C	-6.07	103.62	110.96
1	E	422	VAL	CB-CA-C	-6.07	103.95	112.14
1	A	422	VAL	CB-CA-C	-6.06	103.96	112.14
1	F	386	ILE	CB-CA-C	-6.06	104.22	111.97
1	B	522	MET	CB-CA-C	-6.04	100.59	110.85
1	B	386	ILE	N-CA-CB	6.03	117.60	110.55
1	A	415	GLY	N-CA-C	-6.02	105.51	112.73
1	D	399	PRO	N-CA-CB	6.01	108.60	103.19
1	E	406	PRO	N-CA-C	-5.98	105.21	113.53
1	E	385	GLU	N-CA-C	-5.98	104.68	111.14
1	A	450	SER	CA-C-O	-5.98	114.08	120.42
1	E	455	ASN	CA-CB-CG	5.97	118.57	112.60
1	F	415	GLY	N-CA-C	-5.96	105.57	112.73
1	E	404	PHE	CA-CB-CG	-5.96	107.84	113.80
1	C	433	SER	N-CA-CB	-5.95	101.38	110.01
1	E	345	LEU	CB-CA-C	-5.94	101.31	110.81
1	F	433	SER	CA-C-O	5.93	126.71	120.42
1	D	491	ALA	N-CA-C	-5.93	104.74	111.14
1	D	493	ALA	CA-C-O	5.93	126.45	119.28
1	F	345	LEU	CB-CA-C	-5.91	101.86	110.96
1	E	388	MET	CA-C-O	-5.90	114.17	120.42
1	C	382	ALA	N-CA-CB	-5.89	101.97	110.56
1	F	406	PRO	N-CA-CB	5.88	109.79	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	415	GLY	N-CA-C	-5.86	105.70	112.73
1	F	326	ILE	CB-CA-C	-5.85	103.88	110.96
1	B	434	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	B	404	PHE	CA-CB-CG	-5.83	107.97	113.80
1	D	359	ASN	CA-CB-CG	-5.82	106.78	112.60
1	B	406	PRO	N-CA-CB	5.81	109.67	103.39
1	C	382	ALA	N-CA-C	5.80	120.06	112.92
1	C	394	ARG	NH1-CZ-NH2	5.80	126.85	119.30
1	B	382	ALA	N-CA-C	5.80	120.05	112.92
1	C	411	ASP	N-CA-CB	-5.78	101.60	110.85
1	B	535	PRO	CA-C-O	5.78	129.18	121.95
1	E	359	ASN	CA-CB-CG	-5.76	106.84	112.60
1	B	397	GLU	O-C-N	-5.74	114.96	122.59
1	B	516	HIS	CA-CB-CG	-5.72	108.08	113.80
1	F	467	LYS	N-CA-C	-5.72	105.19	111.82
1	D	419	GLU	O-C-N	-5.71	115.87	122.95
1	F	491	ALA	N-CA-C	-5.70	104.97	111.07
1	C	443	GLU	N-CA-CB	5.70	118.50	110.12
1	C	359	ASN	CA-CB-CG	-5.68	106.92	112.60
1	D	352	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	E	521	GLY	CA-C-O	-5.67	114.88	121.00
1	C	422	VAL	CB-CA-C	-5.67	104.49	112.14
1	B	386	ILE	CB-CA-C	-5.66	104.72	111.97
1	B	321	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	405	ALA	CA-C-N	5.65	125.49	119.28
1	A	405	ALA	C-N-CA	5.65	125.49	119.28
1	D	396	MET	N-CA-C	5.64	117.90	111.02
1	C	377[A]	HIS	CA-C-O	-5.62	115.10	121.00
1	C	377[B]	HIS	CA-C-O	-5.62	115.10	121.00
1	D	382	ALA	N-CA-CB	-5.60	102.21	110.49
1	E	313	ASP	CA-CB-CG	-5.60	107.00	112.60
1	E	434	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	499	GLN	OE1-CD-NE2	5.58	128.18	122.60
1	C	325	PRO	CA-C-O	-5.57	114.95	122.08
1	C	499	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	A	324	PRO	CA-C-N	5.56	125.54	120.03
1	A	324	PRO	C-N-CA	5.56	125.54	120.03
1	C	415	GLY	N-CA-C	-5.55	106.07	112.73
1	C	345	LEU	CB-CA-C	-5.55	102.10	110.92
1	E	451	ILE	N-CA-C	-5.54	105.10	110.42
1	F	443	GLU	N-CA-CB	5.51	118.82	110.28
1	D	451	ILE	N-CA-C	-5.51	105.00	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	382	ALA	N-CA-CB	-5.50	102.34	110.49
1	C	419	GLU	O-C-N	-5.50	116.13	122.95
1	A	443	GLU	N-CA-CB	5.49	118.29	110.16
1	E	538	ASP	CA-CB-CG	-5.49	107.11	112.60
1	E	360	TRP	O-C-N	-5.49	116.42	122.07
1	B	526	TYR	CA-C-O	-5.48	115.06	120.82
1	D	421	MET	N-CA-C	5.47	119.13	112.23
1	D	446	VAL	N-CA-CB	-5.47	103.09	110.54
1	F	522	MET	CA-CB-CG	5.47	125.05	114.10
1	A	467	LYS	N-CA-C	-5.47	105.48	111.82
1	B	326	ILE	CA-C-O	-5.46	114.26	120.65
1	F	325	PRO	CA-C-O	-5.44	115.12	122.08
1	C	491	ALA	N-CA-C	-5.44	105.25	111.07
1	A	386	ILE	N-CA-CB	5.43	116.54	110.51
1	C	434	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	A	347	THR	N-CA-CB	-5.42	102.15	110.12
1	B	495	LEU	N-CA-C	-5.41	101.35	109.95
1	F	359	ASN	CB-CG-OD1	-5.40	109.99	120.80
1	B	411	ASP	N-CA-CB	-5.40	101.84	111.08
1	F	446	VAL	CB-CA-C	5.40	120.53	112.16
1	F	526	TYR	CA-C-O	-5.39	115.14	120.70
1	C	459	TYR	CD1-CE1-CZ	5.39	129.30	119.60
1	A	495	LEU	CA-C-O	-5.39	114.92	121.28
1	E	325	PRO	CA-C-O	-5.38	115.19	122.08
1	E	386	ILE	CA-C-O	-5.38	115.68	121.27
1	F	535	PRO	N-CA-CB	5.37	109.02	103.38
1	E	467	LYS	N-CA-C	-5.37	105.60	111.82
1	B	326	ILE	CB-CA-C	-5.36	104.48	110.96
1	F	495	LEU	N-CA-C	-5.35	101.44	109.95
1	B	521	GLY	CA-C-O	-5.35	115.24	120.75
1	D	495	LEU	N-CA-C	-5.34	101.45	109.95
1	C	458	VAL	CA-C-O	-5.34	115.40	120.95
1	F	386	ILE	N-CA-CB	5.34	116.79	110.55
1	A	456	SER	N-CA-C	5.32	116.77	111.07
1	B	415	GLY	N-CA-C	-5.32	106.35	112.73
1	C	434	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	D	516	HIS	CA-CB-CG	-5.32	108.48	113.80
1	E	389	ILE	CA-C-O	5.31	126.20	120.47
1	B	419	GLU	O-C-N	-5.30	116.69	123.06
1	E	491	ALA	N-CA-C	-5.30	105.40	111.07
1	A	313	ASP	CA-CB-CG	-5.29	107.31	112.60
1	D	311	THR	CA-C-O	-5.29	115.48	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	527	SER	N-CA-C	-5.28	105.43	111.14
1	C	396	MET	N-CA-C	5.28	117.46	111.02
1	C	537	TYR	N-CA-C	-5.28	102.05	109.96
1	F	321	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	382	ALA	N-CA-CB	-5.27	102.86	110.56
1	D	411	ASP	N-CA-CB	-5.26	102.43	110.85
1	B	398	HIS	O-C-N	5.25	125.48	121.23
1	B	377[A]	HIS	CA-C-O	-5.24	115.50	121.00
1	B	377[B]	HIS	CA-C-O	-5.24	115.50	121.00
1	C	413	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	A	323	GLU	CA-C-N	5.23	125.77	120.38
1	A	323	GLU	C-N-CA	5.23	125.77	120.38
1	D	451	ILE	O-C-N	5.23	126.94	121.87
1	B	478	VAL	CA-C-O	5.23	126.39	120.95
1	F	512	SER	CA-CB-OG	-5.23	100.64	111.10
1	A	459	TYR	CD1-CE1-CZ	5.22	129.00	119.60
1	E	421	MET	N-CA-C	5.22	118.81	112.23
1	C	458	VAL	N-CA-C	5.21	115.94	110.62
1	E	527	SER	CA-C-O	-5.20	115.34	120.70
1	E	495	LEU	N-CA-C	-5.20	101.80	110.17
1	F	411	ASP	N-CA-CB	-5.19	102.55	110.85
1	C	422	VAL	O-C-N	5.18	126.90	121.87
1	D	432	SER	CA-C-O	5.18	126.05	120.55
1	E	399	PRO	N-CA-CB	5.18	108.69	103.25
1	D	433	SER	N-CA-CB	-5.17	102.51	110.01
1	C	505	ALA	O-C-N	-5.17	116.75	122.07
1	A	491	ALA	N-CA-C	-5.17	105.54	111.07
1	F	399	PRO	N-CA-CB	5.16	107.83	103.19
1	F	311	THR	CA-C-O	-5.15	115.64	121.72
1	F	306	LEU	N-CA-C	-5.14	104.75	111.02
1	D	346	LEU	CA-C-O	5.13	126.39	120.90
1	A	411	ASP	N-CA-CB	-5.09	102.38	111.08
1	D	458	VAL	N-CA-C	5.08	115.80	110.62
1	B	501[A]	HIS	CA-CB-CG	5.08	118.88	113.80
1	B	501[B]	HIS	CA-CB-CG	5.08	118.88	113.80
1	B	455	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	328	TYR	CA-C-O	-5.07	115.23	120.70
1	C	347	THR	N-CA-CB	-5.07	102.67	110.12
1	F	473	ASP	CB-CA-C	-5.07	102.93	110.88
1	E	306	LEU	N-CA-C	-5.06	104.85	111.02
1	A	458	VAL	N-CA-C	5.06	115.78	110.62
1	E	473	ASP	CB-CA-C	-5.06	102.94	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	SER	N-CA-CB	-5.05	102.69	110.01
1	E	459	TYR	CD1-CE1-CZ	5.05	128.69	119.60
1	A	345	LEU	CB-CA-C	-5.05	102.89	110.92
1	B	535	PRO	N-CA-CB	5.04	108.13	103.39
1	F	377[A]	HIS	CA-C-O	-5.04	115.71	121.00
1	F	377[B]	HIS	CA-C-O	-5.04	115.71	121.00
1	F	352	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	D	516	HIS	CA-C-N	5.02	127.01	120.28
1	D	516	HIS	C-N-CA	5.02	127.01	120.28
1	F	359	ASN	CB-CG-ND2	5.02	123.94	116.40
1	D	324	PRO	CA-C-N	5.02	125.23	120.31
1	D	324	PRO	C-N-CA	5.02	125.23	120.31
1	F	482	ILE	CA-C-O	-5.01	115.74	120.95
1	F	323	GLU	CA-C-N	5.00	125.53	120.38
1	F	323	GLU	C-N-CA	5.00	125.53	120.38
1	C	338	SER	CA-C-O	-5.00	115.75	121.40
1	C	535	PRO	N-CA-CB	5.00	108.63	103.38

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	1877	0	1890	92	0
1	B	1877	0	1890	95	0
1	C	1877	0	1890	98	0
1	D	1877	0	1890	96	0
1	E	1877	0	1890	77	0
1	F	1877	0	1890	82	0
2	A	20	0	24	0	0
2	B	20	0	24	1	0
2	C	20	0	24	2	0
2	D	20	0	24	0	0
2	E	20	0	24	1	0
2	F	20	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	18	0	0	0	0
3	B	19	0	0	0	0
3	C	20	0	0	0	0
3	D	19	0	0	0	0
3	E	19	0	0	0	0
3	F	19	0	0	0	0
All	All	11496	0	11484	457	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 20.

All (457) 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:A:513[A]:HIS:CE1	1:B:459:TYR:HE1	1.13	1.65
1:E:513[A]:HIS:CE1	1:F:459:TYR:HE1	1.11	1.62
1:E:513[A]:HIS:CE1	1:F:459:TYR:CE1	1.91	1.58
1:C:513[A]:HIS:CE1	1:D:459:TYR:HE1	1.22	1.57
1:A:513[A]:HIS:CE1	1:B:459:TYR:CE1	1.96	1.52
1:C:513[A]:HIS:CE1	1:D:459:TYR:CE1	2.07	1.43
1:A:501[B]:HIS:NE2	1:B:501[B]:HIS:HE1	1.02	1.43
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:ND1	1.79	1.42
1:A:501[B]:HIS:HE1	1:B:501[B]:HIS:NE2	1.10	1.39
1:A:501[B]:HIS:ND1	1:B:501[B]:HIS:CE1	1.89	1.36
1:C:513[A]:HIS:ND1	1:D:459:TYR:CE1	1.99	1.30
1:A:513[A]:HIS:ND1	1:B:459:TYR:CE1	2.05	1.22
1:E:513[A]:HIS:ND1	1:F:459:TYR:CE1	2.03	1.22
1:A:501[B]:HIS:ND1	1:B:501[B]:HIS:ND1	1.89	1.12
1:A:497:LEU:HD11	1:B:497:LEU:HD11	1.38	1.00
1:C:519:ASN:HD22	1:D:519:ASN:HD22	1.10	0.96
1:A:373:HIS:HD2	1:C:373:HIS:HD2	0.98	0.96
1:C:513[A]:HIS:ND1	1:D:459:TYR:HE1	1.48	0.96
1:D:496:THR:HB	1:D:499:GLN:HG3	1.49	0.95
1:A:496:THR:HB	1:A:499:GLN:HG3	1.46	0.95
1:E:513[A]:HIS:HE1	1:F:459:TYR:HE1	1.08	0.94
1:D:373:HIS:HD2	1:F:373:HIS:HD2	1.09	0.93
1:E:513[A]:HIS:CE1	1:F:459:TYR:CD1	2.57	0.93
1:E:496:THR:HB	1:E:499:GLN:HG3	1.51	0.92
1:B:496:THR:HB	1:B:499:GLN:HG3	1.51	0.92
1:F:496:THR:HB	1:F:499:GLN:HG3	1.52	0.91
1:A:513[A]:HIS:HE1	1:B:459:TYR:HE1	1.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:THR:HB	1:C:499:GLN:HG3	1.51	0.90
1:A:373:HIS:HD2	1:C:373:HIS:CD2	1.90	0.89
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:CE1	0.88	0.88
1:A:519:ASN:HD22	1:B:519:ASN:HD22	1.22	0.87
1:C:459:TYR:HE1	1:D:513[A]:HIS:CE1	1.93	0.87
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD1	2.62	0.87
1:C:497:LEU:HD11	1:D:497:LEU:HD11	1.56	0.86
1:A:501[B]:HIS:HE1	1:B:501[B]:HIS:CE1	0.49	0.86
1:A:459:TYR:HE1	1:B:513[A]:HIS:CE1	1.95	0.85
1:D:343:MET:O	1:D:347:THR:HB	1.77	0.85
1:A:373:HIS:CD2	1:C:373:HIS:HD2	1.91	0.84
1:C:459:TYR:CE1	1:D:513[A]:HIS:CE1	2.66	0.84
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:HE1	0.53	0.83
1:E:459:TYR:HE1	1:F:513[A]:HIS:CE1	1.96	0.82
1:E:459:TYR:CE1	1:F:513[A]:HIS:CE1	2.68	0.82
1:E:347:THR:HG21	1:E:535:PRO:HD2	1.60	0.82
1:D:326:ILE:HD13	1:D:326:ILE:H	1.45	0.82
1:F:343:MET:O	1:F:347:THR:HB	1.80	0.82
1:F:347:THR:HG21	1:F:535:PRO:HD2	1.62	0.82
1:A:343:MET:O	1:A:347:THR:HB	1.81	0.81
1:A:459:TYR:CE1	1:B:513[A]:HIS:CE1	2.69	0.81
1:B:343:MET:O	1:B:347:THR:HB	1.81	0.80
1:A:347:THR:HG21	1:A:535:PRO:HD2	1.63	0.80
1:E:497:LEU:HD11	1:F:497:LEU:HD11	1.62	0.80
1:C:343:MET:O	1:C:347:THR:HB	1.82	0.79
1:E:319:LEU:HB3	1:E:446:VAL:HG13	1.64	0.79
1:A:326:ILE:HD13	1:A:326:ILE:H	1.46	0.78
1:C:347:THR:HG21	1:C:535:PRO:HD2	1.64	0.78
1:E:519:ASN:HD22	1:F:519:ASN:HD22	1.32	0.78
1:B:347:THR:HG21	1:B:535:PRO:HD2	1.65	0.76
1:A:310:LEU:HB3	1:A:314:GLN:HB2	1.66	0.76
1:D:347:THR:HG21	1:D:535:PRO:HD2	1.67	0.76
1:B:311:THR:OG1	1:B:314:GLN:HG3	1.85	0.76
1:C:513[A]:HIS:CE1	1:D:459:TYR:CD1	2.72	0.76
1:D:342:MET:HE2	1:D:418:VAL:HG23	1.66	0.76
1:D:319:LEU:HB3	1:D:446:VAL:HG13	1.67	0.76
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.67	0.75
1:F:311:THR:OG1	1:F:314:GLN:HG3	1.87	0.75
1:C:342:MET:HE2	1:C:418:VAL:HG23	1.68	0.74
1:A:311:THR:OG1	1:A:314:GLN:HG3	1.88	0.74
1:C:311:THR:OG1	1:C:314:GLN:HG3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:MET:HE2	1:E:418:VAL:HG23	1.69	0.74
1:C:326:ILE:HD13	1:C:326:ILE:H	1.52	0.73
1:C:513[A]:HIS:CD2	1:D:515:ARG:HH22	2.06	0.72
1:E:326:ILE:HD13	1:E:326:ILE:H	1.54	0.72
1:F:319:LEU:HB3	1:F:446:VAL:HG13	1.70	0.72
1:D:311:THR:OG1	1:D:314:GLN:HG3	1.90	0.72
1:B:319:LEU:HB3	1:B:446:VAL:HG13	1.71	0.71
1:E:343:MET:O	1:E:347:THR:HB	1.90	0.71
1:D:373:HIS:CD2	1:F:373:HIS:HD2	2.01	0.71
1:C:310:LEU:HB3	1:C:314:GLN:HB2	1.73	0.70
1:D:373:HIS:HD2	1:F:373:HIS:CD2	2.01	0.70
1:F:326:ILE:HD13	1:F:326:ILE:H	1.56	0.70
1:A:496:THR:CB	1:A:499:GLN:HG3	2.20	0.70
1:B:326:ILE:H	1:B:326:ILE:HD13	1.55	0.70
1:F:310:LEU:HB3	1:F:314:GLN:HB2	1.74	0.70
1:F:496:THR:CB	1:F:499:GLN:HG3	2.22	0.69
1:E:496:THR:CB	1:E:499:GLN:HG3	2.23	0.69
1:A:342:MET:HE2	1:A:418:VAL:HG23	1.75	0.68
1:F:342:MET:HE2	1:F:418:VAL:HG23	1.75	0.68
1:B:310:LEU:HB3	1:B:314:GLN:HB2	1.75	0.68
1:C:319:LEU:HB3	1:C:446:VAL:HG13	1.75	0.68
1:D:496:THR:CB	1:D:499:GLN:HG3	2.23	0.68
1:E:310:LEU:HB3	1:E:314:GLN:HB2	1.74	0.68
1:D:310:LEU:HB3	1:D:314:GLN:HB2	1.75	0.67
1:B:339:GLU:HA	1:B:418:VAL:HG22	1.77	0.67
1:A:339:GLU:HA	1:A:418:VAL:HG22	1.77	0.66
1:B:496:THR:CB	1:B:499:GLN:HG3	2.23	0.66
1:D:496:THR:HG22	1:D:498:GLN:H	1.60	0.65
1:E:311:THR:OG1	1:E:314:GLN:HG3	1.97	0.65
1:D:513[B]:HIS:ND1	1:D:517:MET:HE2	2.11	0.65
1:D:383:TRP:HZ2	1:D:522:MET:HE1	1.61	0.64
1:B:342:MET:HE2	1:B:418:VAL:HG23	1.78	0.64
1:C:496:THR:CB	1:C:499:GLN:HG3	2.27	0.64
1:E:502:GLN:O	1:E:506[A]:GLN:HG3	1.98	0.64
1:A:383:TRP:HZ2	1:A:522:MET:HE1	1.62	0.64
1:B:418:VAL:HB	1:B:421:MET:HG3	1.80	0.64
1:F:418:VAL:HB	1:F:421:MET:HG3	1.79	0.64
1:A:459:TYR:CE1	1:B:513[A]:HIS:ND1	2.66	0.63
1:A:496:THR:HG22	1:A:498:GLN:H	1.63	0.63
1:C:513[A]:HIS:CG	1:D:459:TYR:CE1	2.86	0.63
1:F:339:GLU:HA	1:F:418:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:H	1:A:326:ILE:CD1	2.12	0.62
1:B:383:TRP:HZ2	1:B:522:MET:HE1	1.63	0.62
1:C:418:VAL:HB	1:C:421:MET:HG3	1.80	0.62
1:D:418:VAL:HB	1:D:421:MET:HG3	1.81	0.62
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:NE2	2.02	0.62
1:B:338:SER:O	1:B:339:GLU:C	2.43	0.62
1:C:459:TYR:CE1	1:D:513[A]:HIS:ND1	2.68	0.61
1:C:513[B]:HIS:CE1	1:C:517:MET:HE2	2.36	0.61
1:E:496:THR:HG22	1:E:498:GLN:H	1.66	0.61
1:D:326:ILE:H	1:D:326:ILE:CD1	2.14	0.60
1:A:338:SER:O	1:A:339:GLU:C	2.43	0.60
1:B:498:GLN:O	1:B:502:GLN:HG3	2.02	0.60
1:F:513[B]:HIS:ND1	1:F:517:MET:HE2	2.16	0.60
1:A:513[A]:HIS:CG	1:B:459:TYR:CE1	2.88	0.60
1:C:502:GLN:O	1:C:506[A]:GLN:HG3	2.02	0.60
1:F:338:SER:O	1:F:339:GLU:C	2.43	0.60
1:A:502:GLN:O	1:A:506[A]:GLN:HG3	2.01	0.60
1:D:495:LEU:HB3	1:D:499:GLN:HB2	1.83	0.59
1:B:513[B]:HIS:CE1	1:B:517:MET:HE2	2.37	0.59
1:C:326:ILE:H	1:C:326:ILE:CD1	2.15	0.59
1:E:339:GLU:HA	1:E:418:VAL:HG22	1.84	0.59
1:C:338:SER:O	1:C:339:GLU:C	2.44	0.59
1:E:495:LEU:HB3	1:E:499:GLN:HB2	1.84	0.59
1:C:496:THR:HG22	1:C:498:GLN:H	1.67	0.59
1:E:459:TYR:CE1	1:F:513[A]:HIS:ND1	2.70	0.59
1:D:405:ALA:HB1	1:D:406:PRO:HD2	1.84	0.59
1:A:513[B]:HIS:CE1	1:A:517:MET:HE2	2.38	0.58
1:E:418:VAL:HB	1:E:421:MET:HG3	1.85	0.58
1:E:384:LEU:O	1:E:388:MET:HG3	2.03	0.58
1:F:513[B]:HIS:CE1	1:F:517:MET:HE2	2.38	0.58
1:A:418:VAL:HB	1:A:421:MET:HG3	1.84	0.58
1:F:502:GLN:O	1:F:506[A]:GLN:HG3	2.03	0.58
1:D:513[B]:HIS:CE1	1:D:517:MET:HE2	2.39	0.58
1:F:522:MET:HE2	1:F:544:LEU:HD12	1.86	0.57
1:B:326:ILE:H	1:B:326:ILE:CD1	2.17	0.57
1:A:495:LEU:HB3	1:A:499:GLN:HB2	1.86	0.57
1:C:498:GLN:O	1:C:502:GLN:HG3	2.04	0.57
1:D:502:GLN:O	1:D:506[A]:GLN:HG3	2.05	0.57
1:E:306:LEU:O	1:E:307:ALA:C	2.46	0.57
1:C:383:TRP:HZ2	1:C:522:MET:HE1	1.69	0.57
1:D:339:GLU:HA	1:D:418:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:TRP:HZ2	1:F:522:MET:HE1	1.69	0.57
1:C:519:ASN:HD22	1:D:519:ASN:ND2	1.92	0.57
1:A:519:ASN:ND2	1:B:519:ASN:HD22	2.00	0.57
1:D:338:SER:O	1:D:339:GLU:C	2.45	0.57
1:A:513[A]:HIS:NE2	1:B:459:TYR:CD1	2.73	0.57
1:B:495:LEU:HB3	1:B:499:GLN:HB2	1.87	0.57
1:C:339:GLU:HA	1:C:418:VAL:HG22	1.86	0.56
1:E:383:TRP:HZ2	1:E:522:MET:HE1	1.70	0.56
1:E:513[B]:HIS:CE1	1:E:517:MET:HE2	2.40	0.56
1:E:338:SER:OG	1:E:341:SER:HB3	2.06	0.56
1:E:349:LEU:O	1:E:353:GLU:HG3	2.05	0.56
1:F:374:ASP:OD2	1:F:471:GLU:OE1	2.24	0.56
1:B:384:LEU:O	1:B:388:MET:HG3	2.06	0.56
1:A:501[B]:HIS:NE2	1:B:501[B]:HIS:CE1	1.95	0.55
1:E:461:PHE:HE2	1:E:475:ILE:HD12	1.72	0.55
1:A:338:SER:OG	1:A:341:SER:HB3	2.07	0.55
1:E:338:SER:O	1:E:339:GLU:C	2.49	0.55
1:F:495:LEU:HB3	1:F:499:GLN:HB2	1.88	0.55
1:A:513[A]:HIS:CD2	1:B:459:TYR:CD1	2.95	0.55
1:B:306:LEU:O	1:B:307:ALA:C	2.50	0.55
1:C:495:LEU:HB3	1:C:499:GLN:HB2	1.88	0.55
1:E:513[A]:HIS:CD2	1:F:515:ARG:HH22	2.25	0.55
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.25	0.55
1:D:306:LEU:O	1:D:307:ALA:C	2.49	0.55
1:C:513[B]:HIS:ND1	1:C:517:MET:HE2	2.22	0.54
1:D:392:VAL:HG13	1:D:432:SER:HA	1.89	0.54
1:C:497:LEU:HD21	1:D:497:LEU:HD11	1.90	0.54
1:F:384:LEU:O	1:F:388:MET:HG3	2.08	0.54
1:C:513[A]:HIS:HD2	1:D:515:ARG:HH22	1.52	0.54
1:C:513[A]:HIS:HE1	1:D:455:ASN:ND2	2.06	0.54
1:E:513[A]:HIS:ND1	1:F:459:TYR:CD1	2.72	0.54
1:F:326:ILE:H	1:F:326:ILE:CD1	2.20	0.54
1:D:328:TYR:CE1	1:D:406:PRO:HG2	2.42	0.54
1:E:383:TRP:CD1	1:E:543:MET:HB3	2.43	0.54
1:F:306:LEU:O	1:F:307:ALA:C	2.51	0.54
1:A:513[A]:HIS:CD2	1:B:515:ARG:HH22	2.24	0.53
1:F:383:TRP:CD1	1:F:543:MET:HB3	2.43	0.53
1:C:385:GLU:HG2	1:C:514:ILE:HG22	1.89	0.53
1:D:374:ASP:OD2	1:D:471:GLU:OE1	2.25	0.53
1:D:338:SER:OG	1:D:341:SER:HB3	2.09	0.53
1:F:496:THR:HG22	1:F:498:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:498:GLN:O	1:F:502:GLN:HG3	2.08	0.53
1:B:392:VAL:HG13	1:B:432:SER:HA	1.91	0.53
1:E:513[A]:HIS:NE2	1:F:459:TYR:CD1	2.77	0.53
1:F:411:ASP:O	1:F:412:ARG:C	2.52	0.53
1:A:513[A]:HIS:CG	1:B:459:TYR:CD1	2.97	0.52
1:D:311:THR:HG23	1:D:314:GLN:OE1	2.10	0.52
1:D:461:PHE:HE2	1:D:475:ILE:HD12	1.74	0.52
1:F:405:ALA:HB1	1:F:406:PRO:HD2	1.90	0.52
1:C:513[A]:HIS:ND1	1:D:459:TYR:CD1	2.71	0.52
1:F:392:VAL:HG13	1:F:432:SER:HA	1.91	0.52
1:B:383:TRP:CD1	1:B:543:MET:HB3	2.44	0.52
1:C:338:SER:OG	1:C:341:SER:HB3	2.10	0.52
1:F:349:LEU:O	1:F:353:GLU:HG3	2.10	0.52
1:C:513[A]:HIS:CG	1:D:459:TYR:CD1	2.97	0.52
1:D:498:GLN:O	1:D:502:GLN:HG3	2.10	0.52
1:E:326:ILE:H	1:E:326:ILE:CD1	2.21	0.52
1:B:461:PHE:HE2	1:B:475:ILE:HD12	1.75	0.51
1:A:306:LEU:O	1:A:307:ALA:C	2.53	0.51
1:A:311:THR:HG23	1:A:314:GLN:OE1	2.11	0.51
1:A:498:GLN:O	1:A:502:GLN:HG3	2.10	0.51
1:E:405:ALA:HB1	1:E:406:PRO:HD2	1.92	0.51
1:A:349:LEU:O	1:A:353:GLU:HG3	2.10	0.51
1:C:306:LEU:O	1:C:307:ALA:C	2.53	0.51
1:D:384:LEU:O	1:D:388:MET:HG3	2.10	0.51
1:E:374:ASP:OD2	1:E:471:GLU:OE1	2.29	0.51
1:E:513[B]:HIS:ND1	1:E:517:MET:HE2	2.25	0.51
1:A:383:TRP:CZ2	1:A:522:MET:HE1	2.44	0.50
1:A:384:LEU:O	1:A:388:MET:HG3	2.09	0.50
1:B:496:THR:HG22	1:B:498:GLN:H	1.76	0.50
1:A:496:THR:HG22	1:A:497:LEU:N	2.25	0.50
1:B:363:ARG:HG3	1:B:363:ARG:NH1	2.25	0.50
1:C:497:LEU:HD11	1:D:497:LEU:HD21	1.92	0.50
1:D:408:LEU:HD11	1:D:410:LEU:HD21	1.93	0.50
1:E:498:GLN:O	1:E:502:GLN:HG3	2.11	0.50
1:B:405:ALA:HB1	1:B:406:PRO:HD2	1.93	0.50
1:E:311:THR:HG23	1:E:314:GLN:OE1	2.12	0.50
1:B:411:ASP:O	1:B:412:ARG:C	2.53	0.50
1:C:522:MET:HE2	1:C:544:LEU:HD12	1.94	0.50
1:E:497:LEU:HD21	1:F:497:LEU:HD11	1.93	0.50
1:C:349:LEU:O	1:C:353:GLU:HG3	2.12	0.50
1:C:537:TYR:O	1:C:541:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ASP:OD2	1:B:471:GLU:OE1	2.28	0.49
1:B:496:THR:HG22	1:B:497:LEU:N	2.26	0.49
1:C:405:ALA:HB1	1:C:406:PRO:HD2	1.94	0.49
1:A:513[A]:HIS:ND1	1:B:459:TYR:CD1	2.76	0.49
1:C:515:ARG:HH22	1:D:513[A]:HIS:CD2	2.30	0.49
1:E:513[A]:HIS:CG	1:F:459:TYR:CE1	2.95	0.49
1:C:383:TRP:CD1	1:C:543:MET:HB3	2.47	0.49
1:B:383:TRP:CZ2	1:B:522:MET:HE1	2.47	0.49
1:A:461:PHE:HE2	1:A:475:ILE:HD12	1.77	0.49
1:C:315:MET:HE1	1:C:365:PRO:HB2	1.95	0.49
1:C:497:LEU:HD11	1:D:497:LEU:CD1	2.36	0.49
1:F:385:GLU:HG2	1:F:514:ILE:HG22	1.94	0.49
1:F:535:PRO:HG2	1:F:537:TYR:CE2	2.48	0.48
1:A:382:ALA:O	1:A:386:ILE:HG12	2.13	0.48
1:B:311:THR:HG23	1:B:314:GLN:OE1	2.13	0.48
1:A:491:ALA:O	1:A:494:GLY:N	2.38	0.48
1:B:502:GLN:O	1:B:506[A]:GLN:HG3	2.13	0.48
1:B:513[B]:HIS:ND1	1:B:517:MET:HE2	2.28	0.48
1:D:543:MET:HE1	1:F:372:LEU:HD12	1.94	0.48
1:B:535:PRO:HG2	1:B:537:TYR:CE2	2.48	0.48
1:D:349:LEU:O	1:D:353:GLU:HG3	2.13	0.48
1:F:405:ALA:HB1	1:F:406:PRO:CD	2.44	0.48
1:F:465:THR:O	1:F:468:SER:HB2	2.14	0.48
1:C:461:PHE:HE2	1:C:475:ILE:HD12	1.78	0.48
1:E:465:THR:O	1:E:468:SER:HB2	2.14	0.48
1:A:383:TRP:CD1	1:A:543:MET:HB3	2.49	0.48
1:D:411:ASP:O	1:D:412:ARG:C	2.56	0.48
1:A:399:PRO:HA	1:A:436:ARG:NH2	2.28	0.48
1:A:411:ASP:O	1:A:412:ARG:C	2.56	0.48
1:B:385:GLU:HG2	1:B:514:ILE:HG22	1.96	0.48
1:D:405:ALA:HB1	1:D:406:PRO:CD	2.43	0.48
1:A:385:GLU:HG2	1:A:514:ILE:HG22	1.96	0.48
1:E:342:MET:HE3	1:E:421:MET:CE	2.44	0.48
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.32	0.47
1:B:315:MET:HE1	1:B:365:PRO:HB2	1.96	0.47
1:E:315:MET:HE1	1:E:365:PRO:HB2	1.95	0.47
1:C:392:VAL:HG13	1:C:432:SER:HA	1.95	0.47
1:B:310:LEU:O	1:B:481:LYS:HE3	2.14	0.47
1:F:496:THR:HG22	1:F:497:LEU:N	2.29	0.47
1:B:305:SER:O	1:B:306:LEU:C	2.57	0.47
1:E:513[A]:HIS:CG	1:F:459:TYR:CD1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ALA:O	1:B:386:ILE:HG12	2.15	0.47
1:C:384:LEU:O	1:C:388:MET:HG3	2.13	0.47
1:D:326:ILE:HD13	1:D:326:ILE:N	2.21	0.47
1:D:383:TRP:CZ2	1:D:522:MET:HE1	2.44	0.47
1:A:515:ARG:HH22	1:B:513[A]:HIS:CD2	2.32	0.47
1:C:411:ASP:O	1:C:412:ARG:C	2.55	0.47
1:C:496:THR:HG22	1:C:497:LEU:N	2.30	0.47
1:E:496:THR:HG22	1:E:497:LEU:N	2.30	0.47
1:A:310:LEU:O	1:A:481:LYS:HE3	2.15	0.47
1:A:513[B]:HIS:ND1	1:A:517:MET:HE2	2.30	0.47
1:E:491:ALA:O	1:E:494:GLY:N	2.39	0.47
1:D:324:PRO:HB2	1:D:325:PRO:HD2	1.97	0.47
1:E:363:ARG:NH1	1:E:363:ARG:HG3	2.29	0.47
1:F:338:SER:OG	1:F:341:SER:HB3	2.15	0.47
1:F:434:ARG:O	1:F:438:MET:HG3	2.14	0.47
1:A:372:LEU:HD12	1:C:543:MET:HE1	1.96	0.46
1:D:403:LEU:CD1	1:D:409:LEU:HD22	2.45	0.46
1:F:311:THR:O	1:F:312:ALA:C	2.58	0.46
1:D:310:LEU:O	1:D:481:LYS:HE3	2.15	0.46
1:D:383:TRP:CD1	1:D:543:MET:HB3	2.50	0.46
1:E:497:LEU:HD11	1:F:497:LEU:HD21	1.97	0.46
1:E:535:PRO:HG2	1:E:537:TYR:CE2	2.50	0.46
1:F:319:LEU:CB	1:F:446:VAL:HG13	2.43	0.46
1:A:522:MET:HE2	1:A:544:LEU:HD12	1.97	0.46
1:C:363:ARG:O	1:C:365:PRO:HD3	2.16	0.46
1:A:465:THR:O	1:A:468:SER:HB2	2.15	0.46
1:C:519:ASN:ND2	1:D:519:ASN:HD22	1.93	0.46
1:E:380:GLU:HB3	1:E:546:ALA:CB	2.45	0.46
1:A:459:TYR:N	1:A:459:TYR:CD1	2.84	0.46
1:A:543:MET:HE1	1:C:372:LEU:HD12	1.96	0.46
1:C:513[A]:HIS:CE1	1:D:455:ASN:O	2.69	0.46
1:C:405:ALA:HB1	1:C:406:PRO:CD	2.46	0.46
1:C:497:LEU:CD1	1:D:497:LEU:HD11	2.36	0.46
1:D:379:LEU:HD23	1:D:379:LEU:HA	1.85	0.46
1:F:311:THR:HG23	1:F:314:GLN:OE1	2.15	0.46
1:C:408:LEU:HD11	1:C:410:LEU:HD21	1.98	0.46
1:F:408:LEU:HD11	1:F:410:LEU:HD21	1.97	0.46
1:C:434:ARG:O	1:C:438:MET:HG3	2.16	0.46
1:A:324:PRO:CB	1:A:325:PRO:HD2	2.47	0.45
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.88	0.45
1:B:349:LEU:O	1:B:353:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:MET:HB3	1:B:534:VAL:HG23	1.98	0.45
1:E:392:VAL:HG13	1:E:432:SER:HA	1.98	0.45
1:C:513[A]:HIS:NE2	1:D:455:ASN:O	2.48	0.45
1:D:535:PRO:HG2	1:D:537:TYR:CE2	2.51	0.45
1:B:465:THR:O	1:B:468:SER:HB2	2.17	0.45
1:A:363:ARG:NH1	1:A:363:ARG:HG3	2.30	0.45
1:C:383:TRP:CZ2	1:C:522:MET:HE1	2.50	0.45
1:C:459:TYR:N	1:C:459:TYR:CD1	2.85	0.45
1:A:408:LEU:HD11	1:A:410:LEU:HD21	1.97	0.45
1:C:465:THR:O	1:C:468:SER:HB2	2.16	0.45
1:D:363:ARG:HG3	1:D:363:ARG:NH1	2.32	0.45
1:C:455:ASN:ND2	1:D:513[A]:HIS:HE1	2.13	0.45
1:A:319:LEU:CB	1:A:446:VAL:HG13	2.44	0.45
1:A:537:TYR:O	1:A:541:LEU:HG	2.17	0.45
1:B:324:PRO:HB2	1:B:325:PRO:HD2	1.98	0.45
1:D:311:THR:O	1:D:312:ALA:C	2.59	0.45
1:F:363:ARG:NH1	1:F:363:ARG:HG3	2.31	0.45
1:B:324:PRO:CB	1:B:325:PRO:HD2	2.47	0.45
1:C:447:CYS:O	1:C:451:ILE:HG13	2.17	0.45
1:E:322:ALA:O	1:E:323:GLU:C	2.59	0.44
1:E:513[A]:HIS:CD2	1:F:459:TYR:CD1	3.05	0.44
1:F:324:PRO:CB	1:F:325:PRO:HD2	2.47	0.44
1:A:324:PRO:HB2	1:A:325:PRO:HD2	1.98	0.44
1:C:320:LEU:HD23	1:C:320:LEU:HA	1.79	0.44
1:C:535:PRO:HG2	1:C:537:TYR:CE2	2.53	0.44
1:E:383:TRP:CZ2	1:E:522:MET:HE1	2.50	0.44
1:E:408:LEU:HD11	1:E:410:LEU:HD21	1.99	0.44
1:E:461:PHE:CE2	1:E:475:ILE:HD12	2.51	0.44
1:F:537:TYR:O	1:F:541:LEU:HG	2.16	0.44
1:C:311:THR:O	1:C:312:ALA:C	2.61	0.44
1:E:411:ASP:O	1:E:412:ARG:C	2.60	0.44
1:E:522:MET:HE2	1:E:544:LEU:HD12	1.98	0.44
1:B:338:SER:OG	1:B:341:SER:HB3	2.17	0.44
1:D:399:PRO:HA	1:D:436:ARG:NH2	2.33	0.44
1:F:403:LEU:HD12	1:F:409:LEU:HD22	1.99	0.44
1:F:461:PHE:HE2	1:F:475:ILE:HD12	1.82	0.44
1:C:363:ARG:NH1	1:C:363:ARG:HG3	2.33	0.44
1:F:528:MET:HB3	1:F:534:VAL:HG23	1.98	0.44
1:A:535:PRO:HG2	1:A:537:TYR:CE2	2.52	0.44
1:B:522:MET:HE2	1:B:544:LEU:HD12	1.99	0.44
1:F:403:LEU:CD1	1:F:409:LEU:HD22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:THR:CG2	1:B:537:TYR:HE2	2.31	0.44
1:D:461:PHE:HD1	1:D:461:PHE:HA	1.61	0.44
1:D:522:MET:HE2	1:D:544:LEU:HD12	1.99	0.44
1:E:459:TYR:CD1	1:E:459:TYR:N	2.85	0.44
1:E:537:TYR:O	1:E:541:LEU:HG	2.17	0.44
1:B:311:THR:O	1:B:312:ALA:C	2.61	0.44
1:B:461:PHE:CE2	1:B:475:ILE:HD12	2.53	0.44
1:C:438:MET:HE2	1:C:438:MET:HB3	1.76	0.44
1:E:434:ARG:O	1:E:438:MET:HG3	2.18	0.44
1:C:403:LEU:HD12	1:C:409:LEU:HD22	2.00	0.43
1:D:324:PRO:CB	1:D:325:PRO:HD2	2.47	0.43
1:D:465:THR:O	1:D:468:SER:HB2	2.18	0.43
1:E:528:MET:HB3	1:E:534:VAL:HG23	2.01	0.43
1:F:342:MET:HE3	1:F:421:MET:CE	2.48	0.43
1:B:342:MET:HE3	1:B:421:MET:CE	2.48	0.43
1:E:405:ALA:HB1	1:E:406:PRO:CD	2.48	0.43
1:A:392:VAL:HG13	1:A:432:SER:HA	2.00	0.43
1:D:342:MET:HE3	1:D:421:MET:CE	2.48	0.43
1:D:528:MET:HB3	1:D:534:VAL:HG23	2.01	0.43
1:D:392:VAL:HG13	1:D:432:SER:CA	2.47	0.43
1:E:320:LEU:HD23	1:E:320:LEU:HA	1.71	0.43
1:A:461:PHE:CE2	1:A:475:ILE:HD12	2.53	0.43
1:B:524:HIS:CE1	1:B:528:MET:HG2	2.53	0.43
1:C:379:LEU:HD23	1:C:379:LEU:HA	1.84	0.43
1:D:447:CYS:O	1:D:451:ILE:HG13	2.19	0.43
1:E:310:LEU:O	1:E:481:LYS:HE3	2.18	0.43
1:C:342:MET:HE3	1:C:421:MET:CE	2.49	0.43
1:A:434:ARG:O	1:A:438:MET:HG3	2.18	0.43
1:B:434:ARG:O	1:B:438:MET:HG3	2.19	0.43
1:E:520:LYS:H	1:E:520:LYS:HG2	1.61	0.43
1:A:455:ASN:ND2	1:B:513[A]:HIS:HE1	2.16	0.42
1:C:364:VAL:O	1:C:365:PRO:C	2.59	0.42
1:D:491:ALA:O	1:D:494:GLY:N	2.43	0.42
1:A:315:MET:HE1	1:A:365:PRO:HB2	2.01	0.42
1:C:497:LEU:HD21	1:D:497:LEU:CD1	2.49	0.42
1:B:514:ILE:HA	1:B:517:MET:HE3	2.02	0.42
1:D:461:PHE:CE2	1:D:475:ILE:HD12	2.53	0.42
1:A:528:MET:HB3	1:A:534:VAL:HG23	2.01	0.42
1:C:452:ILE:HD11	1:C:511:LEU:HD22	2.01	0.42
1:F:379:LEU:HD23	1:F:379:LEU:HA	1.84	0.42
1:F:383:TRP:CZ2	1:F:522:MET:HE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:SER:O	1:D:528:MET:C	2.62	0.42
1:F:324:PRO:HB2	1:F:325:PRO:HD2	2.00	0.42
1:C:322:ALA:O	1:C:323:GLU:C	2.63	0.42
1:D:514:ILE:HA	1:D:517:MET:HE3	2.02	0.42
1:F:438:MET:HE2	1:F:438:MET:HB3	1.86	0.42
1:C:353:GLU:OE2	2:C:600:EST:O3	2.35	0.42
1:D:320:LEU:HA	1:D:320:LEU:HD23	1.76	0.42
1:D:385:GLU:HG2	1:D:514:ILE:HG22	2.02	0.42
1:A:364:VAL:O	1:A:365:PRO:C	2.62	0.41
1:B:399:PRO:HA	1:B:436:ARG:NH2	2.34	0.41
1:B:405:ALA:HB1	1:B:406:PRO:CD	2.49	0.41
1:C:399:PRO:HA	1:C:436:ARG:NH2	2.35	0.41
1:D:537:TYR:O	1:D:541:LEU:HG	2.20	0.41
2:E:600:EST:H152	2:E:600:EST:H181	1.85	0.41
1:C:324:PRO:CB	1:C:325:PRO:HD2	2.50	0.41
1:C:497:LEU:CD1	1:D:497:LEU:HD21	2.51	0.41
1:A:363:ARG:O	1:A:365:PRO:HD3	2.20	0.41
1:B:461:PHE:HD1	1:B:461:PHE:HA	1.64	0.41
1:C:363:ARG:H	1:C:363:ARG:HG2	1.46	0.41
1:D:397:GLU:CD	1:D:397:GLU:H	2.28	0.41
1:F:310:LEU:O	1:F:481:LYS:HE3	2.21	0.41
2:C:600:EST:H152	2:C:600:EST:H181	1.75	0.41
1:E:515:ARG:HH22	1:F:513[A]:HIS:CD2	2.37	0.41
1:B:363:ARG:H	1:B:363:ARG:HG2	1.55	0.41
1:F:305:SER:O	1:F:306:LEU:C	2.64	0.41
1:A:347:THR:CG2	1:A:537:TYR:HE2	2.34	0.41
1:C:310:LEU:O	1:C:481:LYS:HE3	2.20	0.41
1:C:347:THR:CG2	1:C:537:TYR:HE2	2.33	0.41
1:C:524:HIS:CE1	1:C:528:MET:HG2	2.56	0.41
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.74	0.41
1:B:347:THR:HG22	1:B:537:TYR:HE2	1.84	0.41
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.96	0.41
1:E:311:THR:O	1:E:312:ALA:C	2.64	0.41
1:D:328:TYR:HE1	1:D:406:PRO:HB2	1.86	0.41
1:A:513[A]:HIS:HE1	1:B:455:ASN:ND2	2.19	0.41
1:B:322:ALA:O	1:B:323:GLU:C	2.63	0.41
1:B:486:LEU:HD23	1:B:486:LEU:HA	1.93	0.41
1:D:496:THR:HG22	1:D:497:LEU:N	2.36	0.41
1:F:347:THR:HG21	1:F:535:PRO:CD	2.44	0.41
1:F:364:VAL:O	1:F:365:PRO:C	2.64	0.41
1:B:527:SER:O	1:B:528:MET:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:ARG:HG2	1:D:510:ILE:HD11	2.03	0.40
1:E:379:LEU:HD23	1:E:379:LEU:HA	1.87	0.40
1:C:403:LEU:CD1	1:C:409:LEU:HD22	2.51	0.40
1:C:461:PHE:CE2	1:C:475:ILE:HD12	2.56	0.40
1:C:527:SER:O	1:C:528:MET:C	2.64	0.40
1:E:324:PRO:HB2	1:E:325:PRO:HD2	2.02	0.40
1:F:514:ILE:HA	1:F:517:MET:HE3	2.02	0.40
1:C:377[A]:HIS:NE2	1:C:460:THR:O	2.54	0.40
2:B:600:EST:H182	2:B:600:EST:H111	1.91	0.40
1:D:534:VAL:HA	1:D:535:PRO:HD3	1.96	0.40
1:E:527:SER:O	1:E:528:MET:C	2.64	0.40
1:F:447:CYS:O	1:F:451:ILE:HG13	2.21	0.40
1:F:524:HIS:CE1	1:F:528:MET:HG2	2.55	0.40
1:A:436:ARG:HH11	1:A:436:ARG:HD2	1.75	0.40
1:B:347:THR:HG23	1:B:537:TYR:CD2	2.56	0.40
1:B:436:ARG:HH11	1:B:436:ARG:HD2	1.75	0.40
1:E:438:MET:HE2	1:E:438:MET:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/253 (92%)	223 (95%)	11 (5%)	0	100	100
1	B	234/253 (92%)	225 (96%)	9 (4%)	0	100	100
1	C	234/253 (92%)	226 (97%)	8 (3%)	0	100	100
1	D	234/253 (92%)	227 (97%)	7 (3%)	0	100	100
1	E	234/253 (92%)	225 (96%)	9 (4%)	0	100	100
1	F	234/253 (92%)	224 (96%)	10 (4%)	0	100	100
All	All	1404/1518 (92%)	1350 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	210/228 (92%)	183 (87%)	27 (13%)	4	18
1	B	210/228 (92%)	182 (87%)	28 (13%)	4	17
1	C	210/228 (92%)	181 (86%)	29 (14%)	3	15
1	D	210/228 (92%)	183 (87%)	27 (13%)	4	18
1	E	210/228 (92%)	182 (87%)	28 (13%)	4	17
1	F	210/228 (92%)	183 (87%)	27 (13%)	4	18
All	All	1260/1368 (92%)	1094 (87%)	166 (13%)	4	17

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	317	SER
1	A	326	ILE
1	A	330	GLU
1	A	341	SER
1	A	347	THR
1	A	368	VAL
1	A	381	CYS
1	A	396	MET
1	A	409	LEU
1	A	411	ASP
1	A	416	LYS
1	A	421	MET
1	A	422	VAL
1	A	446	VAL
1	A	460	THR
1	A	461	PHE
1	A	465	THR
1	A	470	GLU

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Mol	Chain	Res	Type
1	A	481	LYS
1	A	497	LEU
1	A	510	ILE
1	A	512	SER
1	A	520	LYS
1	A	522	MET
1	A	528	MET
1	A	529	LYS
1	B	310	LEU
1	B	317	SER
1	B	326	ILE
1	B	330	GLU
1	B	339	GLU
1	B	341	SER
1	B	347	THR
1	B	363	ARG
1	B	368	VAL
1	B	381	CYS
1	B	396	MET
1	B	411	ASP
1	B	416	LYS
1	B	421	MET
1	B	422	VAL
1	B	446	VAL
1	B	460	THR
1	B	461	PHE
1	B	465	THR
1	B	470	GLU
1	B	481	LYS
1	B	497	LEU
1	B	510	ILE
1	B	512	SER
1	B	518	SER
1	B	520	LYS
1	B	528	MET
1	B	529	LYS
1	C	310	LEU
1	C	317	SER
1	C	326	ILE
1	C	330	GLU
1	C	341	SER
1	C	347	THR

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Mol	Chain	Res	Type
1	C	363	ARG
1	C	368	VAL
1	C	381	CYS
1	C	396	MET
1	C	409	LEU
1	C	411	ASP
1	C	416	LYS
1	C	421	MET
1	C	422	VAL
1	C	446	VAL
1	C	460	THR
1	C	461	PHE
1	C	465	THR
1	C	470	GLU
1	C	481	LYS
1	C	497	LEU
1	C	510	ILE
1	C	512	SER
1	C	518	SER
1	C	520	LYS
1	C	522	MET
1	C	528	MET
1	C	529	LYS
1	D	310	LEU
1	D	317	SER
1	D	326	ILE
1	D	330	GLU
1	D	341	SER
1	D	347	THR
1	D	363	ARG
1	D	368	VAL
1	D	381	CYS
1	D	396	MET
1	D	411	ASP
1	D	416	LYS
1	D	422	VAL
1	D	446	VAL
1	D	460	THR
1	D	461	PHE
1	D	465	THR
1	D	470	GLU
1	D	481	LYS

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Mol	Chain	Res	Type
1	D	497	LEU
1	D	510	ILE
1	D	512	SER
1	D	518	SER
1	D	520	LYS
1	D	522	MET
1	D	528	MET
1	D	529	LYS
1	E	310	LEU
1	E	317	SER
1	E	326	ILE
1	E	330	GLU
1	E	341	SER
1	E	347	THR
1	E	363	ARG
1	E	368	VAL
1	E	381	CYS
1	E	396	MET
1	E	411	ASP
1	E	416	LYS
1	E	421	MET
1	E	422	VAL
1	E	446	VAL
1	E	460	THR
1	E	461	PHE
1	E	465	THR
1	E	470	GLU
1	E	481	LYS
1	E	497	LEU
1	E	510	ILE
1	E	512	SER
1	E	518	SER
1	E	520	LYS
1	E	522	MET
1	E	528	MET
1	E	529	LYS
1	F	310	LEU
1	F	317	SER
1	F	326	ILE
1	F	330	GLU
1	F	341	SER
1	F	347	THR

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Mol	Chain	Res	Type
1	F	368	VAL
1	F	381	CYS
1	F	396	MET
1	F	411	ASP
1	F	416	LYS
1	F	421	MET
1	F	422	VAL
1	F	446	VAL
1	F	460	THR
1	F	461	PHE
1	F	465	THR
1	F	470	GLU
1	F	481	LYS
1	F	497	LEU
1	F	510	ILE
1	F	512	SER
1	F	520	LYS
1	F	522	MET
1	F	528	MET
1	F	529	LYS
1	F	548	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	373	HIS
1	A	439	ASN
1	A	455	ASN
1	A	498	GLN
1	A	519	ASN
1	B	348	ASN
1	B	439	ASN
1	B	455	ASN
1	B	488	HIS
1	B	498	GLN
1	B	502	GLN
1	C	348	ASN
1	C	373	HIS
1	C	439	ASN
1	C	455	ASN
1	C	519	ASN

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Mol	Chain	Res	Type
1	D	348	ASN
1	D	373	HIS
1	D	439	ASN
1	D	455	ASN
1	D	498	GLN
1	E	348	ASN
1	E	439	ASN
1	E	455	ASN
1	F	348	ASN
1	F	373	HIS
1	F	439	ASN
1	F	455	ASN
1	F	502	GLN
1	F	519	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EST	B	600	-	23,23,23	1.08	1 (4%)	36,36,36	1.85	10 (27%)
2	EST	A	600	-	23,23,23	0.87	0	36,36,36	2.01	12 (33%)
2	EST	F	600	-	23,23,23	1.11	2 (8%)	36,36,36	2.02	10 (27%)
2	EST	D	600	-	23,23,23	1.16	2 (8%)	36,36,36	2.02	9 (25%)
2	EST	C	600	-	23,23,23	0.98	0	36,36,36	1.69	8 (22%)
2	EST	E	600	-	23,23,23	1.07	3 (13%)	36,36,36	1.88	10 (27%)

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	EST	B	600	-	-	-	0/4/4/4
2	EST	A	600	-	-	-	0/4/4/4
2	EST	F	600	-	-	-	0/4/4/4
2	EST	D	600	-	-	-	0/4/4/4
2	EST	C	600	-	-	-	0/4/4/4
2	EST	E	600	-	-	-	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	EST	C10-C9	-2.46	1.48	1.52
2	D	600	EST	C8-C14	-2.39	1.49	1.53
2	E	600	EST	C10-C9	-2.29	1.49	1.52
2	B	600	EST	C8-C14	-2.29	1.49	1.53
2	F	600	EST	C10-C9	-2.19	1.49	1.52
2	E	600	EST	C8-C14	-2.17	1.49	1.53
2	F	600	EST	C8-C14	-2.16	1.49	1.53
2	E	600	EST	C4-C5	2.07	1.42	1.39

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	EST	C16-C17-C13	6.29	109.48	104.52
2	C	600	EST	C15-C14-C13	-4.89	98.08	103.84
2	E	600	EST	C15-C14-C13	-4.59	98.44	103.84
2	A	600	EST	C15-C14-C13	-4.57	98.46	103.84
2	B	600	EST	C16-C17-C13	4.33	107.94	104.52
2	F	600	EST	C3-C4-C5	-4.10	116.16	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	EST	C15-C16-C17	-4.09	101.30	105.76
2	D	600	EST	C3-C4-C5	-4.08	116.18	120.77
2	F	600	EST	C16-C17-C13	4.07	107.73	104.52
2	F	600	EST	C11-C12-C13	-4.00	105.98	112.74
2	A	600	EST	C2-C3-C4	3.99	124.57	120.19
2	E	600	EST	C3-C4-C5	-3.96	116.32	120.77
2	A	600	EST	C16-C17-C13	3.95	107.63	104.52
2	B	600	EST	C11-C12-C13	-3.85	106.25	112.74
2	E	600	EST	C16-C15-C14	-3.83	97.65	105.14
2	F	600	EST	C2-C3-C4	3.78	124.33	120.19
2	A	600	EST	C11-C12-C13	-3.68	106.52	112.74
2	F	600	EST	C15-C14-C13	-3.67	99.53	103.84
2	E	600	EST	C11-C12-C13	-3.67	106.56	112.74
2	C	600	EST	C11-C12-C13	-3.65	106.58	112.74
2	D	600	EST	C2-C3-C4	3.62	124.16	120.19
2	B	600	EST	C3-C4-C5	-3.59	116.74	120.77
2	F	600	EST	C16-C15-C14	-3.52	98.25	105.14
2	A	600	EST	C15-C16-C17	-3.47	101.98	105.76
2	D	600	EST	C15-C14-C13	-3.43	99.81	103.84
2	A	600	EST	C3-C4-C5	-3.32	117.04	120.77
2	F	600	EST	C15-C16-C17	-3.24	102.22	105.76
2	B	600	EST	C15-C14-C13	-3.10	100.19	103.84
2	F	600	EST	C12-C13-C14	3.05	111.80	107.25
2	B	600	EST	C15-C16-C17	-3.02	102.47	105.76
2	C	600	EST	C12-C11-C9	-2.99	108.47	112.34
2	D	600	EST	C11-C12-C13	-2.99	107.69	112.74
2	B	600	EST	C2-C3-C4	2.98	123.46	120.19
2	B	600	EST	O17-C17-C13	2.97	121.01	114.80
2	E	600	EST	C16-C17-C13	2.74	106.68	104.52
2	E	600	EST	C2-C3-C4	2.68	123.12	120.19
2	A	600	EST	C16-C15-C14	-2.67	99.91	105.14
2	A	600	EST	C1-C2-C3	-2.66	117.07	119.88
2	A	600	EST	C12-C13-C14	2.54	111.05	107.25
2	E	600	EST	C15-C16-C17	-2.54	102.99	105.76
2	D	600	EST	C16-C15-C14	-2.49	100.27	105.14
2	A	600	EST	C13-C14-C8	-2.46	110.92	114.41
2	C	600	EST	C16-C15-C14	-2.45	100.35	105.14
2	C	600	EST	C15-C16-C17	-2.45	103.09	105.76
2	A	600	EST	C12-C11-C9	-2.39	109.25	112.34
2	D	600	EST	C6-C5-C4	-2.36	115.25	119.91
2	C	600	EST	C12-C13-C14	2.36	110.78	107.25
2	B	600	EST	C12-C11-C9	-2.31	109.36	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	EST	C12-C11-C9	-2.31	109.36	112.34
2	F	600	EST	C18-C13-C12	-2.29	107.23	110.61
2	C	600	EST	C3-C4-C5	-2.29	118.20	120.77
2	D	600	EST	O17-C17-C13	2.19	119.39	114.80
2	E	600	EST	C6-C5-C4	-2.18	115.61	119.91
2	E	600	EST	C12-C13-C14	2.12	110.41	107.25
2	F	600	EST	C6-C5-C4	-2.08	115.81	119.91
2	B	600	EST	C16-C15-C14	-2.07	101.09	105.14
2	A	600	EST	C9-C8-C14	-2.06	105.81	108.68
2	B	600	EST	C6-C5-C4	-2.06	115.85	119.91
2	C	600	EST	C2-C3-C4	2.02	122.40	120.19

There are no chirality outliers.

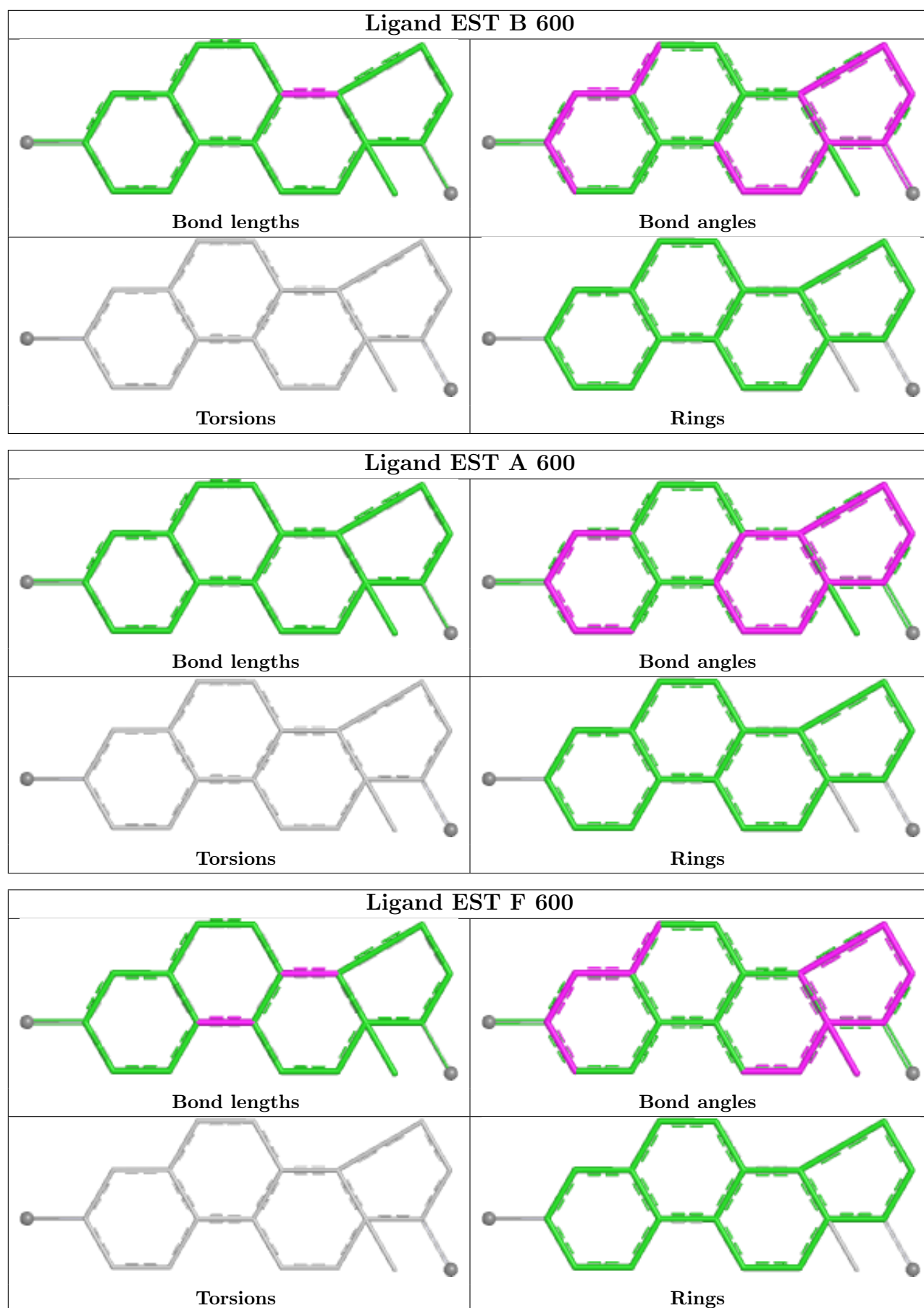
There are no torsion outliers.

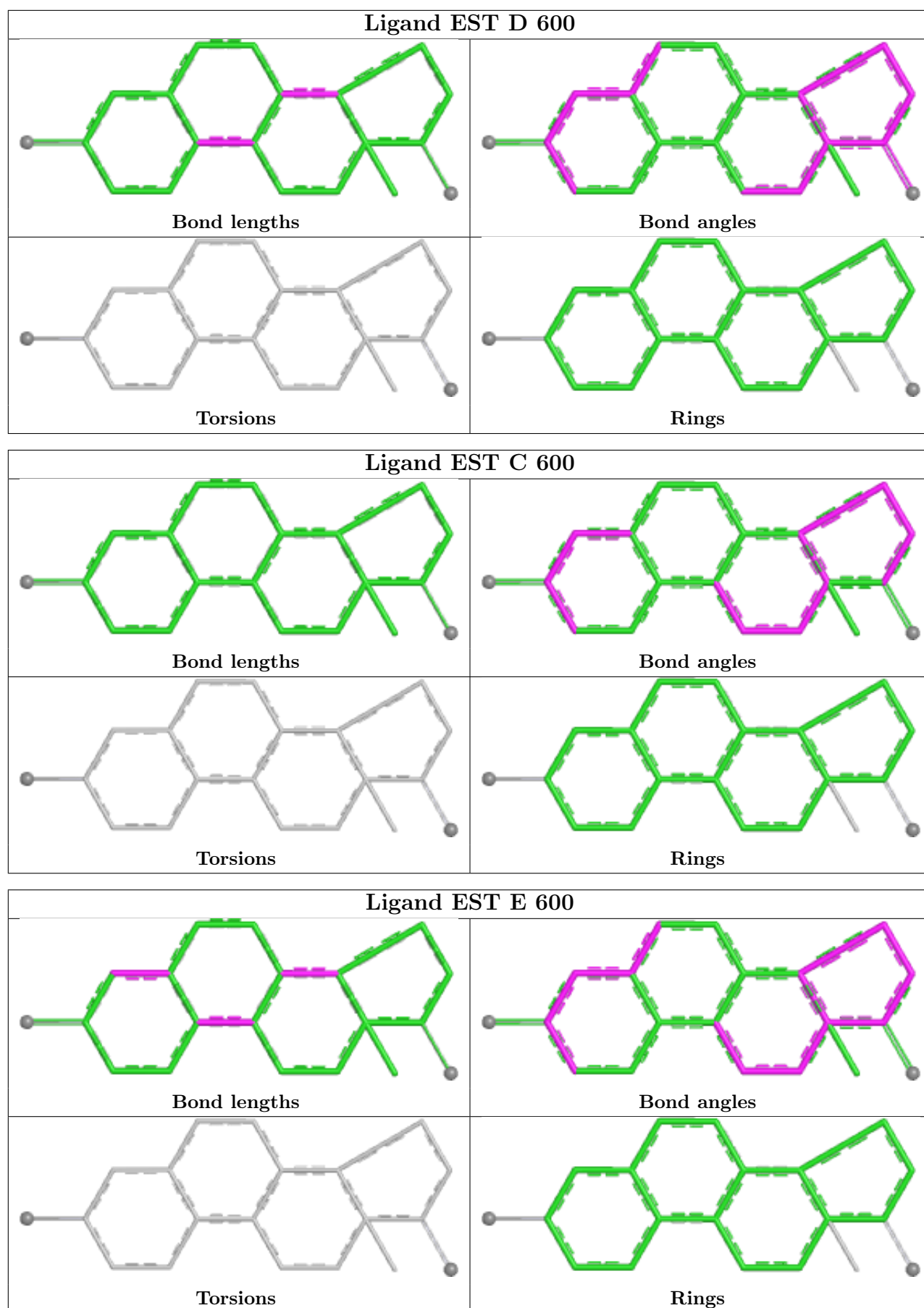
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	EST	1	0
2	C	600	EST	2	0
2	E	600	EST	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	235/253 (92%)	-0.09	1 (0%)	88 76	26, 55, 88, 128	5 (2%)
1	B	235/253 (92%)	-0.03	4 (1%)	69 48	26, 55, 88, 128	5 (2%)
1	C	235/253 (92%)	-0.12	6 (2%)	57 36	26, 55, 88, 128	5 (2%)
1	D	235/253 (92%)	-0.05	4 (1%)	69 48	25, 54, 87, 128	5 (2%)
1	E	235/253 (92%)	-0.13	6 (2%)	57 36	25, 54, 87, 128	5 (2%)
1	F	235/253 (92%)	-0.20	4 (1%)	69 48	26, 55, 87, 128	5 (2%)
All	All	1410/1518 (92%)	-0.10	25 (1%)	67 47	25, 55, 88, 128	30 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PHE	3.8
1	E	459	TYR	3.2
1	C	465	THR	3.1
1	F	305	SER	3.1
1	D	459	TYR	3.0
1	A	461	PHE	2.8
1	D	548	ARG	2.8
1	F	461	PHE	2.7
1	C	459	TYR	2.6
1	B	338	SER	2.4
1	C	330	GLU	2.4
1	C	534	VAL	2.4
1	C	494	GLY	2.3
1	C	466	LEU	2.3
1	E	461	PHE	2.3
1	F	532	ASN	2.3
1	D	535	PRO	2.3
1	B	305	SER	2.2
1	F	548	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	466	LEU	2.1
1	B	330	GLU	2.1
1	E	307	ALA	2.1
1	E	330	GLU	2.1
1	E	548	ARG	2.1
1	D	330	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

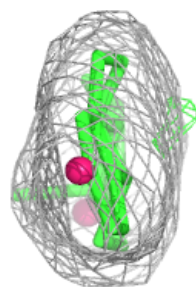
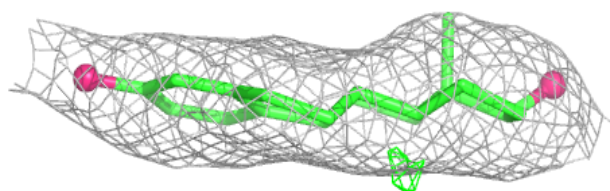
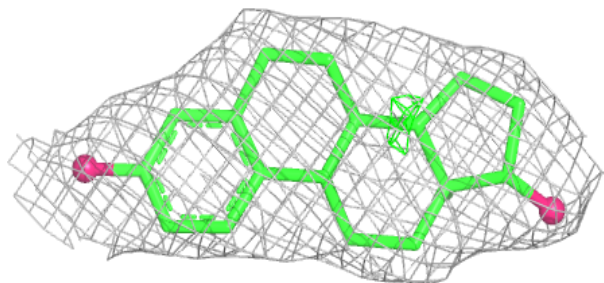
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EST	A	600	20/20	0.95	0.08	34,35,38,40	0
2	EST	B	600	20/20	0.95	0.09	33,35,39,40	0
2	EST	C	600	20/20	0.95	0.09	35,35,38,38	0
2	EST	F	600	20/20	0.95	0.10	33,35,38,40	0
2	EST	E	600	20/20	0.96	0.07	33,34,38,40	0
2	EST	D	600	20/20	0.96	0.08	32,34,38,39	0

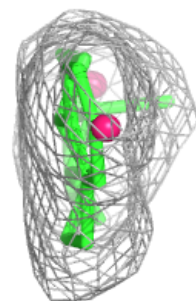
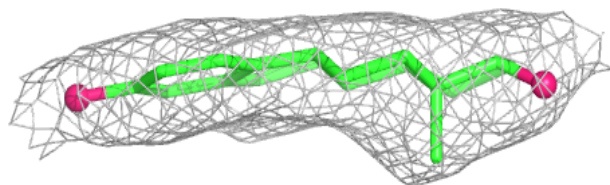
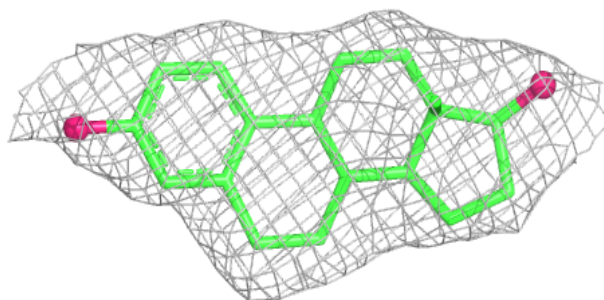
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EST A 600:

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

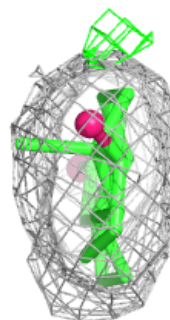
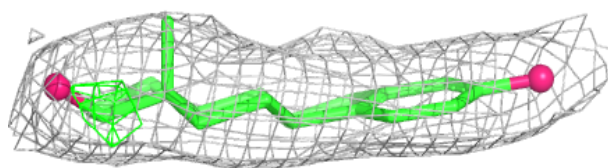
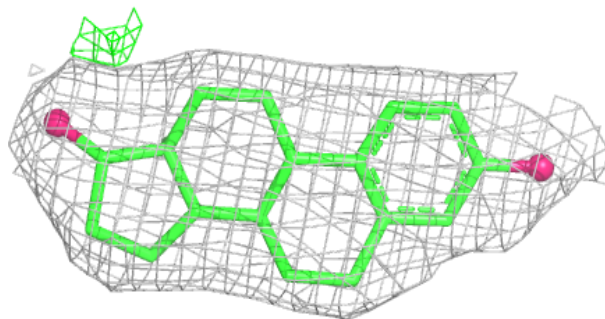
**Electron density around EST B 600:**

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

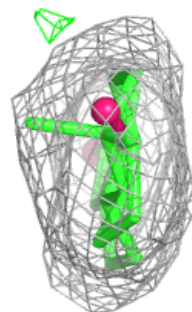
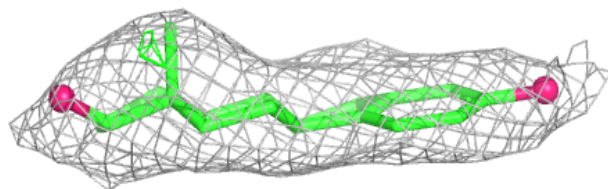
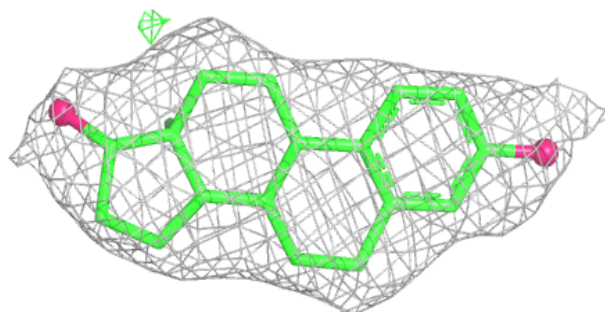


Electron density around EST C 600:

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

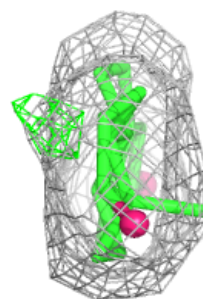
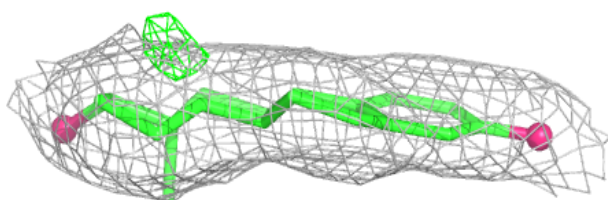
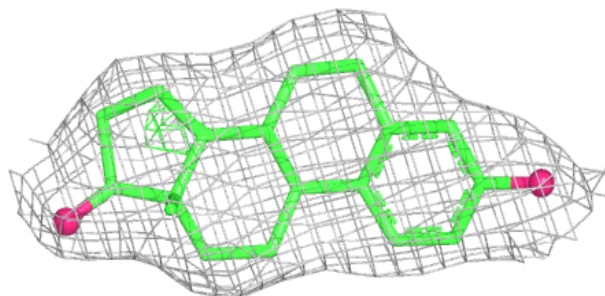
**Electron density around EST F 600:**

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

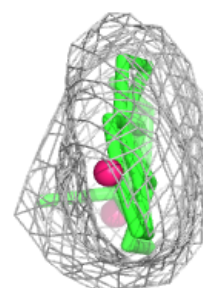
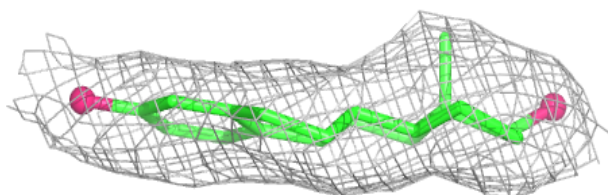
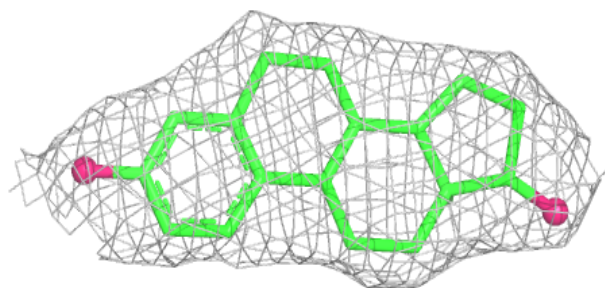


Electron density around EST E 600:

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

**Electron density around EST D 600:**

$2mF_o-DF_c$ (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.