



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:45 AM UTC

PDB ID : 1QVU / pdb_00001qvu
Title : Crystal structure of the multidrug binding transcriptional repressor QacR bound to two drugs: ethidium and proflavine
Authors : Schumacher, M.A.; Miller, M.C.; Brennan, R.G.
Deposited on : 2003-08-28
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

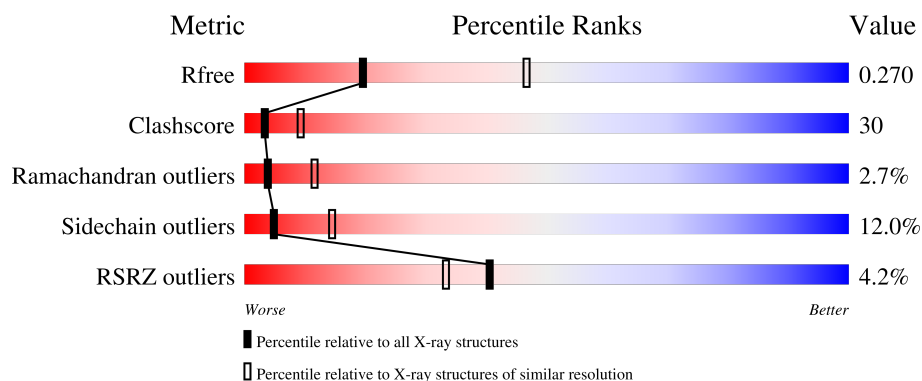
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	194	2% 51% 37% 7% • •
1	B	194	7% 28% 55% 12% • •
1	D	194	5% 45% 42% 8% • •
1	E	194	2% 48% 39% 7% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6228 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 Transcriptional regulator qacR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	D	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	A	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	E	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			

There are 28 discrepancies between the modelled and reference sequences:

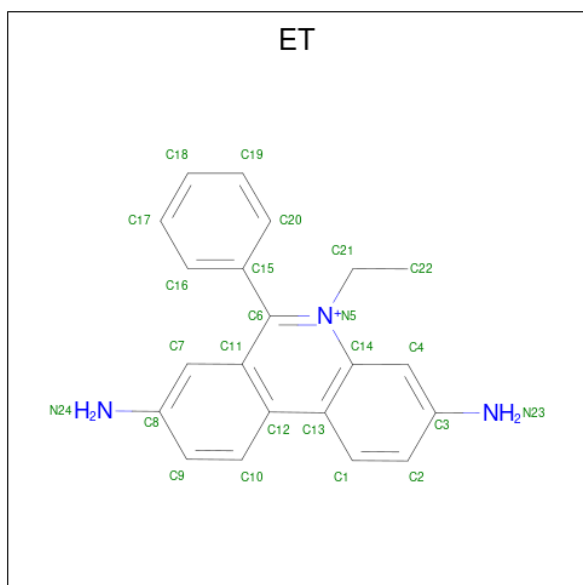
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	SER	CYS	conflict	UNP P0A0N4
B	189	HIS	-	expression tag	UNP P0A0N4
B	190	HIS	-	expression tag	UNP P0A0N4
B	191	HIS	-	expression tag	UNP P0A0N4
B	192	HIS	-	expression tag	UNP P0A0N4
B	193	HIS	-	expression tag	UNP P0A0N4
B	194	HIS	-	expression tag	UNP P0A0N4
D	141	SER	CYS	conflict	UNP P0A0N4
D	189	HIS	-	expression tag	UNP P0A0N4
D	190	HIS	-	expression tag	UNP P0A0N4
D	191	HIS	-	expression tag	UNP P0A0N4
D	192	HIS	-	expression tag	UNP P0A0N4
D	193	HIS	-	expression tag	UNP P0A0N4
D	194	HIS	-	expression tag	UNP P0A0N4
A	141	SER	CYS	conflict	UNP P0A0N4
A	189	HIS	-	expression tag	UNP P0A0N4
A	190	HIS	-	expression tag	UNP P0A0N4
A	191	HIS	-	expression tag	UNP P0A0N4
A	192	HIS	-	expression tag	UNP P0A0N4
A	193	HIS	-	expression tag	UNP P0A0N4
A	194	HIS	-	expression tag	UNP P0A0N4

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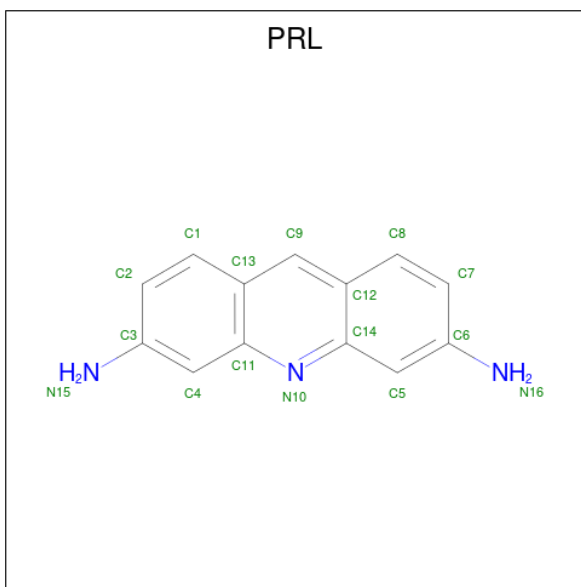
Chain	Residue	Modelled	Actual	Comment	Reference
E	141	SER	CYS	conflict	UNP P0A0N4
E	189	HIS	-	expression tag	UNP P0A0N4
E	190	HIS	-	expression tag	UNP P0A0N4
E	191	HIS	-	expression tag	UNP P0A0N4
E	192	HIS	-	expression tag	UNP P0A0N4
E	193	HIS	-	expression tag	UNP P0A0N4
E	194	HIS	-	expression tag	UNP P0A0N4

- Molecule 2 is ETHIDIUM (CCD ID: ET) (formula: $C_{21}H_{20}N_3$).

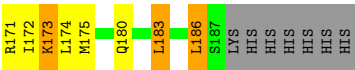


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			24	21	3		

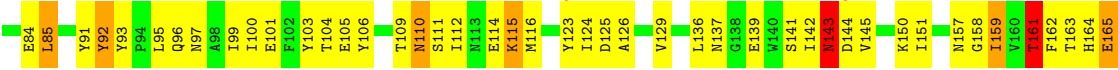
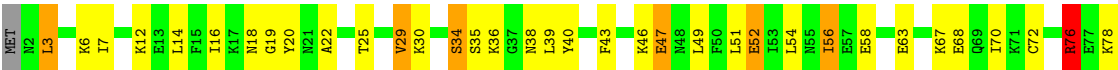
- Molecule 3 is PROFLAVIN (CCD ID: PRL) (formula: $C_{13}H_{11}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			16	13	3		



● Molecule 1: Transcriptional regulator qacR



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.80Å 171.80Å 94.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.48 – 2.96 121.48 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (121.48-2.96) 98.3 (121.48-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.273 0.220 , 0.270	Depositor DCC
R_{free} test set	1500 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6228	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: PRL, ET

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	0.86	1/1578 (0.1%)	1.12	10/2126 (0.5%)
1	B	0.70	0/1578	1.09	6/2126 (0.3%)
1	D	0.70	0/1578	1.10	14/2126 (0.7%)
1	E	0.80	0/1578	1.07	9/2126 (0.4%)
All	All	0.77	1/6312 (0.0%)	1.10	39/8504 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	ILE	CA-CB	6.11	1.61	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	GLU	N-CA-C	-8.19	101.40	112.94
1	B	161	THR	N-CA-C	8.01	119.79	111.14
1	D	91	TYR	N-CA-C	7.00	120.86	109.59
1	A	3	LEU	N-CA-C	-6.93	103.78	111.82
1	A	161	THR	N-CA-C	6.82	119.73	111.82
1	D	6	LYS	N-CA-C	-6.58	104.03	111.07
1	E	76	ARG	N-CA-C	-6.45	104.29	111.71
1	A	118	LYS	N-CA-C	-6.34	104.80	112.54
1	A	76	ARG	N-CA-C	-6.33	104.38	111.28
1	A	186	LEU	N-CA-C	-6.30	105.53	113.72
1	D	166	GLN	N-CA-C	6.14	119.88	110.36
1	A	53	ILE	N-CA-C	-6.10	103.96	110.36
1	D	186	LEU	N-CA-C	6.07	120.38	112.92
1	E	19	GLY	N-CA-C	-6.00	102.64	112.83
1	E	161	THR	N-CA-C	5.94	120.39	113.20
1	D	29	VAL	N-CA-C	5.85	115.98	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	20	TYR	N-CA-C	5.74	117.62	111.36
1	E	139	GLU	N-CA-C	-5.68	105.07	112.23
1	E	3	LEU	N-CA-C	-5.64	105.22	111.71
1	D	118	LYS	N-CA-C	-5.55	104.87	111.03
1	D	57	GLU	N-CA-C	-5.54	105.14	111.07
1	D	177	LYS	N-CA-C	-5.52	105.26	111.28
1	E	129	VAL	N-CA-C	5.51	116.24	110.62
1	A	16	ILE	CB-CA-C	-5.50	104.71	112.14
1	A	139	GLU	N-CA-C	-5.40	105.42	112.23
1	B	145	VAL	N-CA-C	5.36	115.56	110.42
1	E	49	LEU	N-CA-C	-5.25	105.47	111.14
1	D	62	GLN	N-CA-C	-5.25	106.72	113.23
1	D	160	VAL	CB-CA-C	-5.22	105.09	112.14
1	D	137	ASN	N-CA-C	-5.19	104.99	113.19
1	E	159	ILE	CB-CA-C	-5.19	105.06	112.22
1	A	168	ILE	N-CA-C	5.19	120.13	109.34
1	D	117	ASN	N-CA-C	-5.18	107.00	113.38
1	B	88	THR	N-CA-C	5.15	121.28	114.12
1	A	53	ILE	CB-CA-C	-5.14	105.30	111.88
1	B	135	ASN	N-CA-C	-5.14	105.37	111.69
1	D	76	ARG	N-CA-C	-5.13	105.81	111.71
1	D	107	TYR	N-CA-C	-5.11	106.31	112.54
1	B	10	VAL	N-CA-C	-5.01	105.66	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1547	0	1533	78	0
1	B	1547	0	1533	144	0
1	D	1547	0	1533	97	0
1	E	1547	0	1533	70	0
2	A	24	0	20	4	0
3	A	16	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6228	0	6163	375	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 30.

All (375) 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:2:ASN:ND2	1:D:3:LEU:H	1.51	1.07
1:D:97:ASN:HB2	1:E:100:ILE:HD11	1.39	1.03
1:B:107:TYR:HA	1:B:112:ILE:HG21	1.38	1.02
1:A:51:LEU:CD2	1:A:116:MET:HE3	1.88	1.02
1:E:142:ILE:HD11	1:E:186:LEU:HD13	1.36	1.00
1:E:68:GLU:HG2	1:E:85:LEU:HD21	1.42	0.98
1:B:96:GLN:HG3	1:B:157:ASN:HD21	1.27	0.96
1:B:106:TYR:O	1:B:112:ILE:HG13	1.66	0.96
1:E:111:SER:O	1:E:115:LYS:HG2	1.68	0.93
1:B:70:ILE:HD12	1:B:70:ILE:H	1.32	0.93
1:B:3:LEU:HD11	1:B:38:ASN:HD22	1.33	0.90
1:B:44:LYS:H	1:B:48:ASN:HD22	1.22	0.87
1:A:112:ILE:O	1:A:116:MET:HG3	1.73	0.87
1:E:3:LEU:O	1:E:7:ILE:HG12	1.74	0.87
1:A:142:ILE:HD11	1:A:186:LEU:HD13	1.56	0.85
1:B:16:ILE:HG12	1:B:95:LEU:HD23	1.57	0.85
1:A:51:LEU:HD21	1:A:116:MET:HE3	1.55	0.85
1:A:135:ASN:HD21	1:A:142:ILE:H	1.20	0.85
1:B:19:GLY:H	1:B:22:ALA:HB3	1.39	0.84
1:A:109:THR:O	1:A:113:ASN:HB2	1.76	0.83
1:D:39:LEU:HD21	1:D:49:LEU:HD22	1.60	0.83
1:E:163:THR:O	1:E:171:ARG:HD3	1.80	0.82
1:A:143:ASN:HD22	1:A:143:ASN:H	1.28	0.81
1:B:70:ILE:HD12	1:B:70:ILE:N	1.97	0.80
1:B:75:ASN:HB2	1:B:139:GLU:OE2	1.83	0.79
1:A:112:ILE:O	1:A:116:MET:CG	2.30	0.79
1:A:106:TYR:HB3	1:A:112:ILE:HG21	1.65	0.79
1:B:44:LYS:H	1:B:48:ASN:ND2	1.80	0.78
1:D:2:ASN:ND2	1:D:3:LEU:N	2.30	0.78
1:E:114:GLU:HB2	1:E:115:LYS:HZ3	1.48	0.77
1:D:101:GLU:HG3	1:E:97:ASN:HD21	1.49	0.77
1:A:25:THR:O	1:A:29:VAL:HG23	1.84	0.77
1:B:106:TYR:C	1:B:112:ILE:HG13	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:HG21	1:B:43:PHE:HE1	1.50	0.76
1:D:177:LYS:O	1:D:181:ILE:HG13	1.86	0.75
1:D:2:ASN:HD22	1:D:3:LEU:H	1.34	0.75
1:E:103:TYR:HD2	1:E:116:MET:HE2	1.50	0.75
1:B:47:GLU:O	1:B:51:LEU:HB2	1.87	0.74
1:A:87:LEU:HD23	1:A:172:ILE:HG12	1.70	0.74
1:B:29:VAL:HG13	1:B:34:SER:O	1.88	0.73
1:A:170:GLU:OE2	1:A:170:GLU:HA	1.87	0.72
1:D:76:ARG:HG3	1:D:183:LEU:HD13	1.72	0.72
1:B:6:LYS:O	1:B:10:VAL:HG23	1.90	0.71
1:A:143:ASN:H	1:A:143:ASN:ND2	1.85	0.71
1:D:73:LYS:HG3	1:D:74:THR:H	1.54	0.71
1:E:143:ASN:ND2	1:E:144:ASP:H	1.89	0.70
1:B:64:GLN:O	1:B:68:GLU:HG3	1.92	0.70
1:B:16:ILE:HG12	1:B:95:LEU:CD2	2.20	0.70
1:B:70:ILE:H	1:B:70:ILE:CD1	2.05	0.70
1:E:157:ASN:O	1:E:161:THR:HG23	1.92	0.70
1:A:143:ASN:HD22	1:A:143:ASN:N	1.86	0.69
1:D:55:ASN:HD21	1:D:119:LEU:HD21	1.57	0.69
1:A:106:TYR:CD1	1:A:112:ILE:HG13	2.28	0.69
1:B:39:LEU:H	1:B:39:LEU:HD22	1.57	0.69
1:E:3:LEU:HD13	1:E:38:ASN:ND2	2.07	0.68
1:E:100:ILE:O	1:E:104:THR:HG23	1.92	0.68
1:B:14:LEU:HB3	1:B:23:THR:HG21	1.75	0.68
1:B:96:GLN:NE2	1:B:157:ASN:OD1	2.27	0.68
1:D:96:GLN:NE2	1:D:157:ASN:HD21	1.92	0.68
1:E:25:THR:HG23	1:E:36:LYS:HE2	1.77	0.67
1:B:45:THR:HG23	1:B:48:ASN:HB2	1.76	0.67
1:B:100:ILE:O	1:B:104:THR:HG23	1.95	0.67
1:B:20:TYR:HH	1:B:106:TYR:HE2	1.42	0.66
1:E:105:GLU:HG2	1:E:106:TYR:CD2	2.31	0.66
1:B:15:PHE:CE1	1:B:50:PHE:HD2	2.14	0.65
1:A:163:THR:HB	1:A:171:ARG:HH11	1.62	0.65
1:B:36:LYS:H	1:B:36:LYS:HD3	1.62	0.65
1:A:79:PHE:CD2	1:A:183:LEU:HD13	2.31	0.65
1:D:2:ASN:HD22	1:D:3:LEU:N	1.93	0.65
1:D:101:GLU:HG3	1:E:97:ASN:ND2	2.12	0.64
1:A:107:TYR:H	1:A:108:LYS:HZ3	1.45	0.64
1:E:124:ILE:HD13	1:E:150:LYS:HG2	1.79	0.64
1:B:79:PHE:HD2	1:B:183:LEU:HD11	1.61	0.64
1:D:73:LYS:HG3	1:D:74:THR:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:HB3	1:A:112:ILE:HD11	1.79	0.64
1:A:3:LEU:O	1:A:7:ILE:HG13	1.97	0.64
1:B:6:LYS:HA	1:B:6:LYS:NZ	2.14	0.64
1:B:29:VAL:O	1:B:29:VAL:HG12	1.97	0.64
1:E:159:ILE:HB	1:E:175:MET:HE1	1.79	0.63
1:D:142:ILE:HD11	1:D:186:LEU:HB3	1.80	0.63
1:B:14:LEU:C	1:B:23:THR:HG21	2.23	0.63
1:A:14:LEU:HD11	1:A:31:LEU:HD12	1.81	0.63
1:B:4:LYS:HZ2	1:B:42:HIS:CG	2.17	0.63
1:B:7:ILE:HD13	1:B:32:SER:OG	1.99	0.62
1:D:43:PHE:O	1:D:44:LYS:HB2	1.98	0.62
1:A:96:GLN:O	1:A:100:ILE:HG12	2.00	0.62
1:B:39:LEU:HD22	1:B:39:LEU:N	2.14	0.62
1:B:54:LEU:HB3	1:B:119:LEU:HD11	1.81	0.62
1:B:44:LYS:N	1:B:48:ASN:HD22	1.94	0.61
1:E:76:ARG:CG	1:E:76:ARG:HH11	2.12	0.61
1:D:171:ARG:HG2	1:D:171:ARG:HH11	1.64	0.61
1:A:51:LEU:HD22	1:A:116:MET:HE3	1.78	0.61
1:D:133:GLU:O	1:D:137:ASN:HB2	2.00	0.61
1:B:116:MET:O	1:B:116:MET:HG3	2.01	0.60
1:E:114:GLU:CB	1:E:115:LYS:HZ3	2.14	0.60
1:D:64:GLN:O	1:D:68:GLU:HG3	2.02	0.60
1:D:12:LYS:HB2	1:D:53:ILE:HD12	1.83	0.60
1:E:29:VAL:HG22	1:E:34:SER:HB3	1.82	0.60
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.02	0.59
1:D:118:LYS:HD3	1:D:119:LEU:HD23	1.83	0.59
1:E:143:ASN:HD22	1:E:144:ASP:H	1.48	0.59
1:A:43:PHE:O	1:A:44:LYS:HB2	2.02	0.59
1:A:135:ASN:HD21	1:A:142:ILE:N	1.96	0.59
1:B:15:PHE:CD1	1:B:50:PHE:HD2	2.21	0.58
1:B:66:LYS:HA	1:B:69:GLN:HE21	1.67	0.58
1:B:2:ASN:O	1:B:6:LYS:HB2	2.04	0.58
1:A:87:LEU:CD2	1:A:172:ILE:HG12	2.33	0.58
1:A:91:TYR:CD1	1:A:168:ILE:HD13	2.38	0.58
1:A:68:GLU:OE1	1:A:71:LYS:HD2	2.03	0.58
1:B:118:LYS:HZ2	1:B:118:LYS:HB3	1.69	0.58
1:B:39:LEU:H	1:B:39:LEU:CD2	2.16	0.58
1:D:97:ASN:CB	1:E:100:ILE:HD11	2.24	0.57
1:B:7:ILE:HG21	1:B:43:PHE:CE1	2.37	0.57
1:B:11:ALA:HB3	1:B:53:ILE:HD11	1.85	0.57
1:D:97:ASN:HD22	1:E:100:ILE:HG12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ILE:O	1:E:172:ILE:HG13	2.05	0.57
1:B:58:GLU:HG2	1:B:92:TYR:CE2	2.39	0.57
1:B:142:ILE:HD11	1:B:186:LEU:HD13	1.87	0.57
1:A:166:GLN:NE2	1:A:170:GLU:HG3	2.20	0.56
1:E:103:TYR:CE2	1:E:116:MET:HG2	2.40	0.56
1:B:17:LYS:O	1:B:17:LYS:HG2	2.05	0.56
1:D:174:LEU:HB3	1:E:151:ILE:CD1	2.34	0.56
1:B:6:LYS:HA	1:B:6:LYS:CE	2.36	0.56
1:E:105:GLU:HG2	1:E:106:TYR:CE2	2.39	0.56
1:D:17:LYS:HG2	1:D:18:ASN:OD1	2.06	0.56
1:B:103:TYR:CE2	1:B:116:MET:HE2	2.40	0.56
1:D:134:GLY:HA3	1:D:140:TRP:CE2	2.41	0.55
1:B:45:THR:OG1	1:B:47:GLU:HG3	2.05	0.55
1:B:115:LYS:C	1:B:117:ASN:H	2.14	0.55
1:B:127:TYR:HB3	1:B:131:PHE:CE2	2.41	0.55
1:A:40:TYR:CZ	1:E:6:LYS:HD3	2.41	0.55
1:D:69:GLN:HG3	1:D:70:ILE:HD12	1.88	0.55
1:E:100:ILE:HG13	1:E:101:GLU:N	2.21	0.55
1:D:84:GLU:HG2	1:D:172:ILE:HG23	1.88	0.55
1:B:51:LEU:HD23	1:B:115:LYS:HG3	1.88	0.54
1:D:70:ILE:C	1:D:72:CYS:H	2.15	0.54
1:A:163:THR:O	1:A:171:ARG:HD3	2.07	0.54
1:D:120:GLU:HG2	1:D:120:GLU:O	2.06	0.54
1:D:45:THR:HG23	1:D:48:ASN:HB2	1.90	0.54
1:A:106:TYR:HB3	1:A:112:ILE:CG2	2.37	0.54
1:B:103:TYR:O	1:B:107:TYR:HB3	2.07	0.54
1:B:10:VAL:HG11	1:B:31:LEU:HB3	1.90	0.53
1:A:91:TYR:CE1	1:A:168:ILE:HD13	2.43	0.53
1:E:96:GLN:NE2	1:E:157:ASN:HD21	2.07	0.53
1:A:8:LEU:HD13	1:A:56:ILE:CD1	2.38	0.53
1:B:163:THR:O	1:B:171:ARG:HD3	2.08	0.53
1:D:3:LEU:O	1:D:3:LEU:HD13	2.09	0.53
1:D:76:ARG:HH11	1:D:76:ARG:HG2	1.74	0.53
1:A:135:ASN:ND2	1:A:141:SER:HA	2.23	0.53
1:E:18:ASN:HB3	1:E:22:ALA:HB3	1.91	0.53
1:A:17:LYS:HG2	1:A:18:ASN:OD1	2.09	0.53
1:D:47:GLU:OE2	1:D:112:ILE:HG13	2.09	0.52
1:E:16:ILE:HG12	1:E:95:LEU:HD23	1.91	0.52
1:B:6:LYS:HA	1:B:6:LYS:HZ1	1.72	0.52
1:B:81:LEU:O	1:B:85:LEU:HD22	2.09	0.52
1:D:73:LYS:HG3	1:D:74:THR:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HG2	1:A:160:VAL:HG13	1.91	0.52
1:A:166:GLN:HE21	1:A:170:GLU:HG3	1.74	0.52
1:B:125:ASP:O	1:B:128:HIS:N	2.42	0.52
1:B:51:LEU:HD21	1:B:115:LYS:HB2	1.91	0.52
1:D:156:VAL:O	1:D:160:VAL:HG23	2.09	0.52
1:B:114:GLU:C	1:B:114:GLU:CD	2.77	0.52
1:B:124:ILE:HD12	1:B:149:SER:HB2	1.92	0.52
1:B:164:HIS:ND1	1:B:171:ARG:NH2	2.58	0.52
1:D:96:GLN:HA	1:D:99:ILE:HD12	1.91	0.52
1:D:2:ASN:CG	1:D:3:LEU:H	2.13	0.51
1:D:83:ASN:N	1:D:83:ASN:HD22	2.06	0.51
1:B:18:ASN:HB3	1:B:22:ALA:CB	2.40	0.51
1:B:61:TRP:CZ2	1:B:82:TYR:CE1	2.98	0.51
1:A:108:LYS:H	1:A:108:LYS:HD2	1.76	0.51
1:D:76:ARG:O	1:D:80:TYR:HD2	1.94	0.51
1:D:134:GLY:HA3	1:D:140:TRP:CZ2	2.45	0.51
1:B:61:TRP:HZ2	1:B:82:TYR:CE1	2.28	0.51
1:D:97:ASN:HD22	1:E:100:ILE:CG1	2.23	0.51
1:D:103:TYR:CD2	1:D:116:MET:SD	3.03	0.51
1:D:174:LEU:HB3	1:E:151:ILE:HD11	1.93	0.51
1:B:79:PHE:CD2	1:B:183:LEU:HD11	2.43	0.51
1:B:83:ASN:O	1:B:86:SER:HB2	2.11	0.51
1:D:76:ARG:HG3	1:D:183:LEU:CD1	2.39	0.50
1:E:29:VAL:HG21	1:E:35:SER:C	2.36	0.50
1:E:180:GLN:O	1:E:181:ILE:C	2.53	0.50
1:B:6:LYS:NZ	1:B:6:LYS:CA	2.74	0.50
1:B:14:LEU:HD23	1:B:23:THR:HB	1.92	0.50
1:E:142:ILE:CD1	1:E:186:LEU:HD13	2.25	0.50
1:B:3:LEU:HD11	1:B:38:ASN:ND2	2.15	0.50
1:D:101:GLU:OE2	1:E:101:GLU:OE2	2.29	0.50
1:B:21:ASN:HD21	1:B:105:GLU:CD	2.20	0.50
1:B:18:ASN:HD22	1:B:23:THR:HG22	1.77	0.50
1:D:27:GLU:O	1:D:31:LEU:HB2	2.11	0.50
1:A:47:GLU:HG2	1:A:106:TYR:CZ	2.47	0.50
1:B:156:VAL:O	1:B:160:VAL:HG23	2.12	0.49
1:A:170:GLU:OE2	1:A:170:GLU:CA	2.56	0.49
1:B:81:LEU:HG	1:B:85:LEU:CD2	2.42	0.49
1:B:4:LYS:NZ	1:B:42:HIS:CG	2.80	0.49
1:B:38:ASN:C	1:B:40:TYR:H	2.20	0.49
1:A:107:TYR:HD2	1:A:108:LYS:NZ	2.11	0.49
1:A:161:THR:O	1:A:161:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:HD2	1:B:183:LEU:CD1	2.24	0.49
1:B:162:PHE:HB3	2:A:195:ET:H223	1.95	0.48
1:B:123:TYR:CE2	1:B:153:ALA:HB1	2.48	0.48
1:D:39:LEU:HD23	1:D:43:PHE:HD1	1.77	0.48
1:D:43:PHE:O	1:D:44:LYS:CB	2.61	0.48
1:D:93:TYR:N	1:D:94:PRO:CD	2.76	0.48
1:A:142:ILE:HD13	1:A:148:VAL:HG11	1.94	0.48
1:B:125:ASP:O	1:B:126:ALA:C	2.57	0.48
1:A:157:ASN:HD21	2:A:195:ET:H17	1.79	0.48
1:B:14:LEU:HD22	1:B:28:ILE:HD13	1.95	0.48
1:B:70:ILE:C	1:B:72:CYS:H	2.20	0.48
1:A:45:THR:HB	1:A:47:GLU:OE1	2.13	0.48
1:B:61:TRP:HE3	1:B:89:THR:HG21	1.78	0.48
1:A:107:TYR:N	1:A:108:LYS:HZ3	2.09	0.48
1:B:14:LEU:CB	1:B:23:THR:HG21	2.44	0.47
1:B:18:ASN:HB2	1:B:23:THR:HG23	1.95	0.47
1:B:48:ASN:O	1:B:52:GLU:HB2	2.13	0.47
1:E:76:ARG:HH11	1:E:76:ARG:HG3	1.78	0.47
1:A:47:GLU:HB3	1:A:112:ILE:CD1	2.43	0.47
1:D:16:ILE:HG13	1:D:95:LEU:HD23	1.96	0.47
1:A:157:ASN:ND2	2:A:195:ET:H17	2.29	0.47
1:B:114:GLU:OE2	1:B:115:LYS:HG2	2.15	0.47
1:D:81:LEU:O	1:D:85:LEU:HG	2.14	0.47
1:A:23:THR:HA	1:A:27:GLU:OE1	2.14	0.47
1:A:90:GLU:HG2	1:A:160:VAL:CG1	2.45	0.47
1:D:92:TYR:C	1:D:94:PRO:CD	2.88	0.47
1:D:177:LYS:HE3	1:D:180:GLN:OE1	2.14	0.47
1:B:29:VAL:HG22	1:B:39:LEU:HD21	1.95	0.47
1:D:55:ASN:ND2	1:D:119:LEU:HD21	2.26	0.47
1:B:3:LEU:O	1:B:7:ILE:HG12	2.15	0.46
1:B:24:THR:HG23	1:B:26:GLY:H	1.80	0.46
1:A:105:GLU:O	1:A:108:LYS:HE2	2.15	0.46
1:A:83:ASN:HB3	1:A:175:MET:SD	2.55	0.46
1:E:70:ILE:HD13	1:E:70:ILE:N	2.30	0.46
1:B:76:ARG:O	1:B:80:TYR:HD2	1.99	0.46
1:B:127:TYR:HB3	1:B:131:PHE:HE2	1.79	0.46
1:D:171:ARG:HG2	1:D:171:ARG:NH1	2.30	0.46
1:E:63:GLU:O	1:E:67:LYS:HG3	2.15	0.46
1:D:174:LEU:HB3	1:E:151:ILE:HD13	1.97	0.46
1:E:158:GLY:O	1:E:162:PHE:HD1	1.97	0.46
1:B:13:GLU:OE1	1:B:14:LEU:HD12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:HD1	1:A:96:GLN:HE21	1.64	0.46
1:D:54:LEU:HD12	1:D:54:LEU:HA	1.76	0.46
1:D:29:VAL:CG2	1:D:39:LEU:HD12	2.46	0.45
1:A:103:TYR:CZ	1:A:116:MET:SD	3.09	0.45
1:E:136:LEU:HD12	1:E:136:LEU:O	2.16	0.45
1:B:11:ALA:O	1:B:12:LYS:C	2.59	0.45
1:B:33:GLU:O	1:B:34:SER:HB2	2.17	0.45
1:B:58:GLU:HG3	1:B:119:LEU:CD2	2.46	0.45
1:B:66:LYS:HD3	1:B:69:GLN:NE2	2.31	0.45
1:B:18:ASN:HD22	1:B:23:THR:CG2	2.30	0.45
1:D:83:ASN:N	1:D:83:ASN:ND2	2.65	0.45
1:B:3:LEU:HD21	1:B:34:SER:OG	2.17	0.45
1:B:12:LYS:O	1:B:16:ILE:HG13	2.16	0.45
1:D:57:GLU:HG3	1:D:95:LEU:CD1	2.45	0.45
1:D:66:LYS:NZ	1:D:70:ILE:HD11	2.30	0.45
1:D:168:ILE:HD13	1:D:168:ILE:O	2.17	0.45
1:E:165:GLU:CD	1:E:165:GLU:H	2.25	0.45
1:B:70:ILE:C	1:B:72:CYS:N	2.72	0.45
1:D:74:THR:O	1:D:78:LYS:HG3	2.16	0.45
1:B:10:VAL:CG1	1:B:31:LEU:HD23	2.47	0.45
1:D:66:LYS:O	1:D:69:GLN:HG2	2.17	0.45
1:B:112:ILE:HG22	1:B:113:ASN:N	2.31	0.45
1:D:140:TRP:CD1	1:D:142:ILE:HG12	2.52	0.45
1:A:92:TYR:HD1	1:A:92:TYR:O	2.00	0.45
1:B:11:ALA:CB	1:B:53:ILE:HD11	2.46	0.44
1:B:95:LEU:O	1:B:99:ILE:HG13	2.18	0.44
1:D:180:GLN:HG2	1:D:184:ASN:HD21	1.81	0.44
1:A:92:TYR:O	1:A:94:PRO:HD3	2.17	0.44
1:E:72:CYS:O	1:E:78:LYS:HE2	2.17	0.44
1:D:39:LEU:HD23	1:D:43:PHE:CD1	2.52	0.44
1:A:92:TYR:O	1:A:92:TYR:CD1	2.71	0.44
1:B:45:THR:CG2	1:B:48:ASN:HB2	2.47	0.44
1:E:183:LEU:HD12	1:E:183:LEU:HA	1.69	0.44
1:A:144:ASP:OD1	1:A:144:ASP:N	2.50	0.44
1:B:18:ASN:HB3	1:B:22:ALA:HB3	2.00	0.44
1:B:118:LYS:HB3	1:B:118:LYS:NZ	2.33	0.44
1:B:177:LYS:HE3	1:B:181:ILE:HD11	2.00	0.44
1:A:142:ILE:HD11	1:A:186:LEU:CD1	2.38	0.44
1:E:12:LYS:O	1:E:16:ILE:HG13	2.17	0.44
1:E:47:GLU:CD	1:E:112:ILE:HD11	2.43	0.44
1:E:96:GLN:HG3	1:E:161:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASN:C	1:B:112:ILE:H	2.26	0.44
1:D:25:THR:OG1	1:D:36:LYS:HE2	2.18	0.44
1:A:106:TYR:CB	1:A:112:ILE:HG21	2.41	0.44
1:A:134:GLY:HA3	1:A:140:TRP:CZ2	2.52	0.43
1:D:65:TRP:CZ3	1:D:85:LEU:HD12	2.54	0.43
1:D:125:ASP:O	1:D:129:VAL:HG23	2.18	0.43
1:A:47:GLU:CB	1:A:112:ILE:HD11	2.46	0.43
1:E:34:SER:HG	1:E:38:ASN:HD22	1.65	0.43
1:E:39:LEU:HD23	1:E:39:LEU:C	2.43	0.43
1:E:163:THR:O	1:E:171:ARG:CD	2.61	0.43
1:B:34:SER:O	1:B:35:SER:C	2.61	0.43
1:B:36:LYS:HD3	1:B:36:LYS:N	2.31	0.43
1:B:176:ASN:O	1:B:180:GLN:HB2	2.18	0.43
1:B:181:ILE:HD13	1:A:186:LEU:HD23	2.00	0.43
1:D:29:VAL:HG23	1:D:39:LEU:HD12	2.00	0.43
1:B:43:PHE:HA	1:B:48:ASN:HD22	1.82	0.43
1:D:6:LYS:HG3	1:D:32:SER:HB2	2.01	0.43
1:D:57:GLU:HG3	1:D:95:LEU:HD12	1.99	0.43
1:D:135:ASN:C	1:D:137:ASN:H	2.27	0.43
1:E:56:ILE:N	1:E:56:ILE:CD1	2.81	0.43
1:A:131:PHE:CE2	1:A:148:VAL:HG12	2.53	0.43
1:A:161:THR:O	1:A:161:THR:CG2	2.67	0.43
1:B:12:LYS:CA	1:B:53:ILE:HD13	2.49	0.43
1:B:58:GLU:HG3	1:B:119:LEU:HD21	2.00	0.43
1:E:40:TYR:O	1:E:43:PHE:O	2.37	0.43
1:B:39:LEU:N	1:B:39:LEU:CD2	2.80	0.43
1:B:29:VAL:O	1:B:29:VAL:CG1	2.65	0.42
1:B:60:LYS:HD3	1:B:91:TYR:CE2	2.54	0.42
1:A:80:TYR:OH	1:A:180:GLN:HG3	2.19	0.42
1:E:91:TYR:O	1:E:93:TYR:N	2.51	0.42
1:E:177:LYS:HA	1:E:177:LYS:HD2	1.81	0.42
1:B:120:GLU:O	1:B:120:GLU:HG2	2.19	0.42
1:D:76:ARG:HG2	1:D:76:ARG:NH1	2.33	0.42
1:B:132:LYS:O	1:B:136:LEU:HD13	2.19	0.42
1:B:14:LEU:HB3	1:B:23:THR:CG2	2.44	0.42
1:D:65:TRP:CZ3	1:D:81:LEU:HD23	2.54	0.42
1:D:165:GLU:HB2	1:E:103:TYR:HE1	1.84	0.42
1:B:137:ASN:O	1:B:139:GLU:N	2.53	0.42
1:D:52:GLU:O	1:D:53:ILE:C	2.62	0.42
1:D:142:ILE:HD12	1:D:186:LEU:HD22	2.02	0.42
1:A:129:VAL:O	1:A:130:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HE2	1:A:173:LYS:HA	2.01	0.42
1:A:8:LEU:HD13	1:A:56:ILE:HD11	2.00	0.42
1:D:65:TRP:HZ3	1:D:81:LEU:HD23	1.85	0.42
1:A:13:GLU:OE1	1:A:13:GLU:HA	2.18	0.42
1:D:2:ASN:CG	1:D:3:LEU:N	2.76	0.42
1:D:50:PHE:CE1	1:D:54:LEU:HD22	2.55	0.42
1:D:118:LYS:HD3	1:D:119:LEU:CD2	2.47	0.42
1:E:178:PHE:O	1:E:179:SER:C	2.61	0.42
1:B:15:PHE:CE1	1:B:50:PHE:CD2	3.01	0.42
1:A:58:GLU:HG3	1:A:62:GLN:HE21	1.84	0.42
1:B:80:TYR:O	1:B:84:GLU:HG3	2.20	0.42
1:D:50:PHE:O	1:D:54:LEU:HB2	2.20	0.42
1:D:96:GLN:HG2	1:D:161:THR:HG21	2.01	0.42
1:A:20:TYR:N	1:A:101:GLU:OE2	2.51	0.42
1:A:135:ASN:HD22	1:A:135:ASN:HA	1.69	0.42
1:B:128:HIS:CD2	1:B:145:VAL:HG12	2.55	0.41
1:B:132:LYS:C	1:B:134:GLY:N	2.78	0.41
1:D:70:ILE:HD12	1:D:70:ILE:N	2.35	0.41
1:B:24:THR:H	1:B:27:GLU:CD	2.27	0.41
1:B:61:TRP:CE3	1:B:89:THR:HG21	2.55	0.41
1:B:62:GLN:O	1:B:66:LYS:HG2	2.20	0.41
1:E:84:GLU:HG2	1:E:172:ILE:HG23	2.01	0.41
1:D:65:TRP:O	1:D:69:GLN:HB3	2.20	0.41
1:D:70:ILE:O	1:D:72:CYS:N	2.52	0.41
1:D:120:GLU:O	1:D:124:ILE:HG13	2.20	0.41
1:D:3:LEU:O	1:D:7:ILE:HG13	2.20	0.41
1:A:67:LYS:HB3	1:A:67:LYS:HE2	1.87	0.41
1:D:36:LYS:HG2	1:D:40:TYR:CE1	2.56	0.41
1:D:92:TYR:C	1:D:94:PRO:HD2	2.45	0.41
1:D:165:GLU:HB2	1:E:103:TYR:CE1	2.55	0.41
1:E:14:LEU:HD23	1:E:14:LEU:HA	1.77	0.41
1:E:52:GLU:O	1:E:56:ILE:HD13	2.20	0.41
1:B:18:ASN:HB3	1:B:22:ALA:HB1	2.02	0.41
1:B:103:TYR:O	1:B:103:TYR:CD1	2.74	0.41
1:B:12:LYS:N	1:B:53:ILE:HD13	2.36	0.41
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.76	0.41
1:E:16:ILE:HG12	1:E:95:LEU:CD2	2.51	0.41
1:E:25:THR:CG2	1:E:36:LYS:HE2	2.47	0.41
1:B:57:GLU:O	1:B:58:GLU:C	2.64	0.41
1:B:163:THR:C	1:B:165:GLU:H	2.27	0.41
1:B:45:THR:OG1	1:B:46:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HG22	1:A:116:MET:HG3	2.03	0.41
1:B:93:TYR:N	1:B:94:PRO:CD	2.84	0.40
1:B:103:TYR:O	1:B:103:TYR:HD1	2.04	0.40
1:B:3:LEU:C	1:B:5:ASP:H	2.27	0.40
1:E:92:TYR:CD2	1:E:123:TYR:CZ	3.09	0.40
1:B:89:THR:HB	1:B:91:TYR:H	1.85	0.40
1:B:97:ASN:OD1	2:A:195:ET:H2	2.21	0.40
1:D:108:LYS:O	1:D:109:THR:C	2.65	0.40
1:E:109:THR:HB	1:E:112:ILE:HB	2.03	0.40
1:B:59:SER:O	1:B:60:LYS:C	2.65	0.40
1:D:29:VAL:HG13	1:D:34:SER:C	2.47	0.40
1:E:136:LEU:H	1:E:136:LEU:HG	1.74	0.40
1:D:108:LYS:HB3	1:D:109:THR:H	1.59	0.40
1:E:125:ASP:O	1:E:126:ALA:C	2.62	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	184/194 (95%)	168 (91%)	15 (8%)	1 (0%)	24	49
1	B	184/194 (95%)	140 (76%)	35 (19%)	9 (5%)	1	3
1	D	184/194 (95%)	159 (86%)	20 (11%)	5 (3%)	4	11
1	E	184/194 (95%)	160 (87%)	19 (10%)	5 (3%)	4	11
All	All	736/776 (95%)	627 (85%)	89 (12%)	20 (3%)	4	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	108	LYS

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Mol	Chain	Res	Type
1	B	33	GLU
1	B	138	GLY
1	D	44	LYS
1	D	71	LYS
1	A	105	GLU
1	E	110	ASN
1	E	166	GLN
1	B	39	LEU
1	B	89	THR
1	B	92	TYR
1	E	143	ASN
1	B	34	SER
1	B	116	MET
1	D	33	GLU
1	E	92	TYR
1	B	11	ALA
1	B	164	HIS
1	E	181	ILE
1	D	185	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/178 (95%)	149 (88%)	20 (12%)	5	15
1	B	169/178 (95%)	147 (87%)	22 (13%)	4	12
1	D	169/178 (95%)	154 (91%)	15 (9%)	9	24
1	E	169/178 (95%)	145 (86%)	24 (14%)	3	9
All	All	676/712 (95%)	595 (88%)	81 (12%)	5	14

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LYS
1	B	14	LEU

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Mol	Chain	Res	Type
1	B	25	THR
1	B	36	LYS
1	B	39	LEU
1	B	45	THR
1	B	47	GLU
1	B	54	LEU
1	B	58	GLU
1	B	70	ILE
1	B	85	LEU
1	B	88	THR
1	B	89	THR
1	B	112	ILE
1	B	118	LYS
1	B	119	LEU
1	B	124	ILE
1	B	143	ASN
1	B	165	GLU
1	B	166	GLN
1	B	167	ASN
1	B	181	ILE
1	D	3	LEU
1	D	24	THR
1	D	39	LEU
1	D	47	GLU
1	D	54	LEU
1	D	100	ILE
1	D	104	THR
1	D	116	MET
1	D	137	ASN
1	D	141	SER
1	D	165	GLU
1	D	168	ILE
1	D	170	GLU
1	D	173	LYS
1	D	177	LYS
1	A	30	LYS
1	A	44	LYS
1	A	48	ASN
1	A	49	LEU
1	A	52	GLU
1	A	54	LEU
1	A	63	GLU

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Mol	Chain	Res	Type
1	A	84	GLU
1	A	105	GLU
1	A	107	TYR
1	A	108	LYS
1	A	113	ASN
1	A	116	MET
1	A	117	ASN
1	A	118	LYS
1	A	135	ASN
1	A	136	LEU
1	A	143	ASN
1	A	173	LYS
1	A	183	LEU
1	E	29	VAL
1	E	30	LYS
1	E	34	SER
1	E	46	LYS
1	E	47	GLU
1	E	51	LEU
1	E	52	GLU
1	E	54	LEU
1	E	56	ILE
1	E	58	GLU
1	E	76	ARG
1	E	85	LEU
1	E	99	ILE
1	E	110	ASN
1	E	115	LYS
1	E	137	ASN
1	E	141	SER
1	E	143	ASN
1	E	145	VAL
1	E	161	THR
1	E	164	HIS
1	E	165	GLU
1	E	169	ASN
1	E	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN

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Mol	Chain	Res	Type
1	B	21	ASN
1	B	38	ASN
1	B	48	ASN
1	B	62	GLN
1	B	69	GLN
1	B	83	ASN
1	B	96	GLN
1	B	121	ASN
1	B	137	ASN
1	B	157	ASN
1	B	166	GLN
1	D	2	ASN
1	D	21	ASN
1	D	42	HIS
1	D	55	ASN
1	D	62	GLN
1	D	64	GLN
1	D	83	ASN
1	D	96	GLN
1	D	97	ASN
1	D	117	ASN
1	D	137	ASN
1	D	143	ASN
1	D	157	ASN
1	D	164	HIS
1	D	167	ASN
1	D	176	ASN
1	A	38	ASN
1	A	42	HIS
1	A	48	ASN
1	A	55	ASN
1	A	62	GLN
1	A	75	ASN
1	A	83	ASN
1	A	96	GLN
1	A	113	ASN
1	A	135	ASN
1	A	143	ASN
1	A	157	ASN
1	A	166	GLN
1	A	167	ASN
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	184	ASN
1	E	2	ASN
1	E	38	ASN
1	E	62	GLN
1	E	83	ASN
1	E	96	GLN
1	E	97	ASN
1	E	113	ASN
1	E	117	ASN
1	E	121	ASN
1	E	128	HIS
1	E	146	ASN
1	E	169	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](#)

2 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	ET	A	195	-	26,27,27	1.79	8 (30%)	35,39,39	2.05	10 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PRL	A	196	-	18,18,18	1.30	2 (11%)	26,26,26	1.01	1 (3%)

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	ET	A	195	-	-	0/6/6/6	0/4/4/4
3	PRL	A	196	-	-	-	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	195	ET	C16-C15	3.81	1.47	1.39
2	A	195	ET	C20-C15	3.05	1.45	1.39
2	A	195	ET	C15-C6	3.02	1.52	1.49
2	A	195	ET	C10-C12	2.98	1.47	1.41
2	A	195	ET	C4-C3	-2.77	1.34	1.39
2	A	195	ET	C7-C11	2.61	1.47	1.42
3	A	196	PRL	C4-C11	-2.37	1.38	1.41
2	A	195	ET	C21-N5	2.30	1.56	1.50
3	A	196	PRL	C5-C14	-2.16	1.38	1.41
2	A	195	ET	C1-C13	2.02	1.45	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	195	ET	C21-N5-C14	6.11	122.67	118.31
2	A	195	ET	C6-C11-C12	5.03	123.97	118.81
2	A	195	ET	C22-C21-N5	4.00	117.59	111.72
2	A	195	ET	C20-C15-C6	3.84	125.57	120.25
2	A	195	ET	C13-C14-N5	3.49	120.71	118.46
2	A	195	ET	C7-C11-C6	-3.21	116.70	122.66
2	A	195	ET	C21-N5-C6	-2.40	118.05	119.47
2	A	195	ET	C19-C20-C15	2.26	123.11	120.54
2	A	195	ET	C15-C6-C11	2.15	125.30	121.05
2	A	195	ET	C12-C13-C14	2.13	121.67	118.92
3	A	196	PRL	C5-C14-C12	2.12	121.42	119.20

There are no chirality outliers.

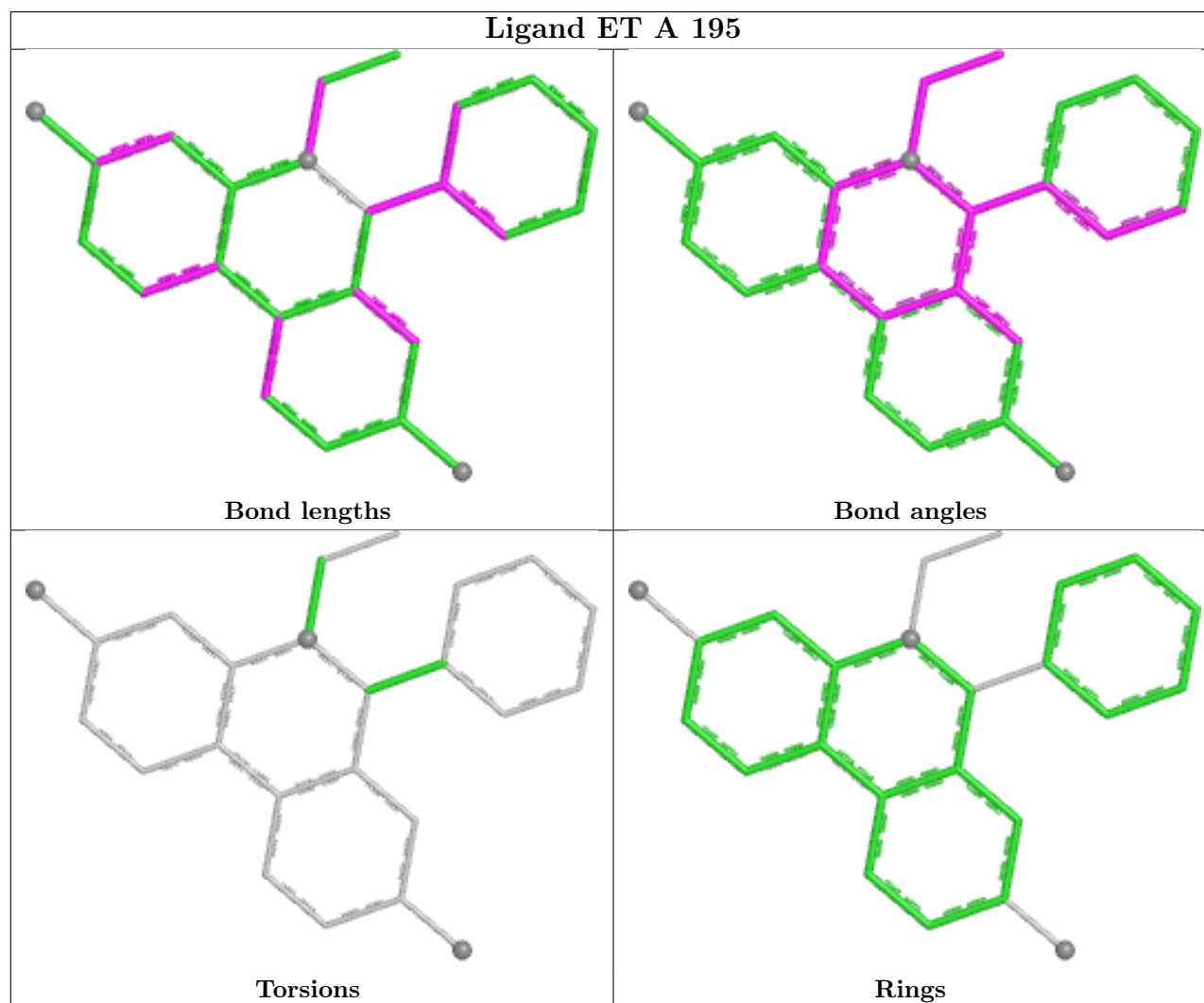
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	195	ET	4	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	186/194 (95%)	0.19	4 (2%) 62 54	46, 72, 116, 132	0
1	B	186/194 (95%)	0.58	14 (7%) 20 18	54, 97, 164, 175	0
1	D	186/194 (95%)	0.55	10 (5%) 31 26	62, 94, 128, 137	0
1	E	186/194 (95%)	0.30	3 (1%) 70 63	53, 80, 116, 129	0
All	All	744/776 (95%)	0.40	31 (4%) 40 33	46, 83, 134, 175	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	SER	4.7
1	B	45	THR	4.1
1	D	187	SER	3.9
1	E	187	SER	3.8
1	A	164	HIS	3.7
1	B	170	GLU	3.2
1	A	103	TYR	2.9
1	D	48	ASN	2.8
1	B	187	SER	2.8
1	B	109	THR	2.8
1	D	116	MET	2.8
1	B	37	GLY	2.7
1	B	169	ASN	2.7
1	D	112	ILE	2.7
1	D	165	GLU	2.5
1	B	118	LYS	2.4
1	B	103	TYR	2.4
1	E	123	TYR	2.4
1	D	111	SER	2.4
1	B	110	ASN	2.3
1	A	117	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	106	TYR	2.3
1	D	163	THR	2.2
1	D	185	GLY	2.2
1	B	3	LEU	2.2
1	D	56	ILE	2.0
1	E	144	ASP	2.0
1	A	114	GLU	2.0
1	B	41	TYR	2.0
1	B	42	HIS	2.0
1	B	29	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

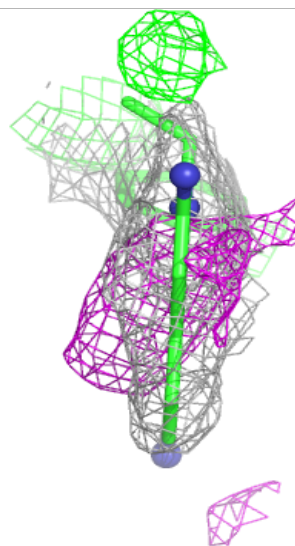
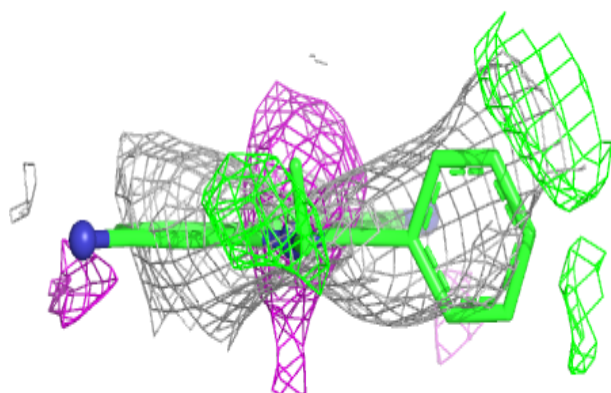
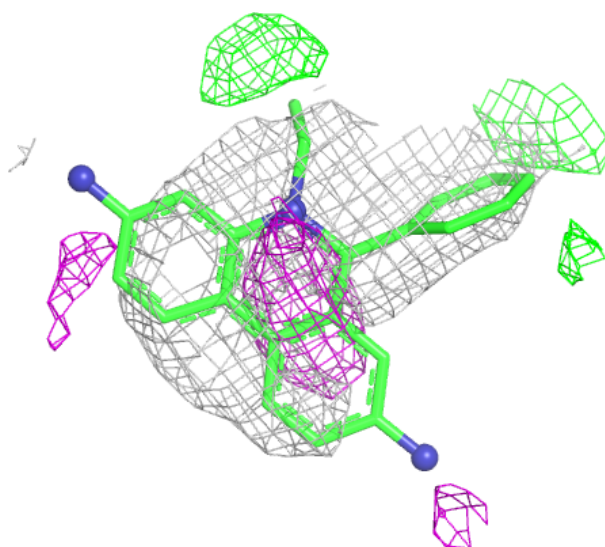
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ET	A	195	24/24	0.80	0.24	137,144,145,146	0
3	PRL	A	196	16/16	0.88	0.17	137,141,144,144	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 ET A 195:

$2mF_o-DF_c$ (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.